A SCATTERING APPROACH TO THE CLUSTER COEFFICIENTS

OF A ONE-DIMENSIONAL SYSTEM

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This thesis contains no material which has been accepted for the award of any other degree or diploma in any University, and to the best of the candidate's knowledge and belief, the thesis contains no material previously published or written by any other person, except where due reference is made in the text of the thesis.

A. M. Gibbs.
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ABSTRACT

The quantum cluster coefficients of a system are of interest because they essentially contain all the thermodynamical information about that system.

In the past, calculations have depended upon at least a partial solution of the corresponding manybody problem, severely limiting the application of the theory to only the simplest of models.

A potentially more useful approach is provided by the scattering formulation of the cluster coefficients, which seeks ultimately to relate the coefficients to physically observable parameters only. However there have been difficulties in carrying through the theory to actual models.

To investigate this approach we have chosen a simple one-dimensional system with repulsive point interactions, for which the scattering wavefunctions are known. Using the methods of formal scattering theory, we construct explicit off-shell scattering amplitudes for the two and three body systems, and verify that the amplitudes satisfy both the Faddeev and the Lippmann-Schwinger equations. The S-matrix elements we obtain from the on-shell limits of the scattering amplitudes are shown to be in agreement with the results of Yang.

The second and third cluster coefficients for the model are calculated in various ways.

In the two-body case we find that the way in which the limit to on-shell observables is taken is crucial to the validity of the result. However the delicacy of the limit is seen to arise from the rather singular nature of the model used.
For the three-body problem, we calculate the third cluster coefficient for symmetric statistics using continuum states, and verify the result, which differs from one previously published, by comparison with an independent approach.

A straight application of the S-matrix formalism yields a divergent result, and we explore these difficulties with a detailed analysis of the singularity structure of the half-off-shell scattering amplitude, using the Landau Rules on the multi scattering series.

We use a perturbation expansion to write down the leading contributions to the third cluster coefficient for distinguishable particles.

In the hardcore limit (potential strength $\to \infty$) we are able to construct the fully off-shell Green's function, and hence derive the third cluster coefficient for distinguishable particles. We calculate the third cluster coefficient for the symmetric hardcore case directly from the off-shell T-matrix.

In the light of these results we discuss the limitations of the scattering approach to the calculation of the cluster coefficients for this model.
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1.1 Background and Plan of the Thesis

In this thesis, we set out to study, within the context of a specific model, the ways in which the cluster coefficients of a system of particles can be calculated. We are particularly interested in methods based on a scattering approach, and seek to establish the extent of their applicability, and to evaluate their prospective usefulness.

With this section we outline the plan of the thesis, and briefly describe the background material and the investigations we have made of the various techniques for calculating the cluster coefficients.

Because this work entailed a large number of self-contained calculations, some of which cross-checked, we have represented the main lines of work and results in a schematic flow-chart in §1.2. This clarifies the context of each individual calculation and pinpoints the most important results achieved.

The introductory chapter concludes with a description of the model to be used, and discussion of its most important features.

In Chapter II we first review the theory of the cluster expansion, showing how it relates to the virial series, and derive some standard formulae for $b_k$, the $k$th cluster coefficient. Then in §2.2 and §2.3 we place the present work into historical perspective with a brief summary firstly of the calculations that were performed before the development of the scattering theory, and secondly, of the work that has since been done on, and within the scattering formulation. We discuss in some detail the motivation...
for the formulation, in particular the promise it holds for a relativistic generalization of statistical mechanics, and identify the difficulties that have been found.

We examine the derivation of the trace formulae, which relate the cluster coefficients to scattering operators, in §2.4, and note some assumptions about the analyticity of the scattering amplitude, which are necessary to produce an on-shell formulation. With the aid of a perturbation expansion in §2.5 we make explicit the structure of the coefficients, and relate the terms to the multi-scattering series. The forward scattering terms for \( l > 2 \) are shown to diverge and this problem is discussed in §2.6, in a qualitative way.

The Chapter concludes with an overview of the context within which the work of this thesis lies.

The first concrete example we take is the two-body problem of the model, and in Chapter III we compare the methods available to calculate \( b_2 \). It has long been known that \( b_2 \) could be computed from on-shell scattering data (phase shifts) and we are able to calculate the coefficient from either the full Green's function, or the continuum wavefunction.

However, we find that the on-shell S-matrix formula fails to produce the correct results. A careful analysis in §3.4 demonstrates that the problem is peculiar to the model being used. The scattering amplitude has a singularity at the origin in the complex energy plane and when the on-shell limit is taken before the trace operation, the residue from this pole is lost. We show that the correct \( b_2 \) is obtained by keeping the energy off-shell until the integration has been performed.
Chapter IV deals with the three-body problem. We calculate $b_3$ for symmetric particles directly from the continuum wavefunctions in §4.2, without involving box normalization, and demonstrate that a previously published calculation of this coefficient is incorrect.

In §4.3 we find that the on-shell $S$-matrix formula is impossible to apply to this model, and the problem is clearly the highly singular nature of the scattering amplitude.

To explore this more fully, we return in §4.4 to an intermediate stage in the scattering approach and take a perturbative expansion of the trace formula from which the $S$-matrix form is derived. We are able to compute the symmetric $b_3$ up to second order in potential strength, and by comparison with an expansion of the known exact coefficient, we establish that the trace formula is valid, at least to second order. However we note that it has been necessary to keep the energy off-shell.

With the same approximation method, we also find the leading contribution to $b_3$ for distinguishable particles.

In §4.5 we turn again to the scattering amplitude, and make a detailed analysis of its structure, using the Landau Rules on the terms of the multiscattering series. We find that all the singularities are contained in the first three orders of the series, but note that in the three dimensional case, the singularities only persist to second order.

In the following section we look more closely at the multiscattering series to third order, and find that in fact the full on-shell $T$-matrix is contained in the on-shell limit of the first three orders. Further, in the hardcore limit, the first three orders of the series taken on-shell, reduce exactly to the on-shell hardcore $T$.  

This suggests that it may be possible to calculate $b_3$ using only the first three orders of the multiscattering series instead of the full $T$ in the trace formula. However, we bear in mind that the trace formula requires off-shell elements of $T$, and the result we have derived holds only in the on-shell limit.

We also observe that although it is in principle simple to write down the contributions to $b_3$ from the first three orders of $T$, the integrations involved are difficult to handle, as the off-shell two-body amplitudes introduce branch points dependent on both complex energy and momentum variables. We conclude that to investigate this approach, some further simplification is needed.

The off-shell two-body form factors are simpler in the hardcore limit, so in §4.7, we look at the case of hard distinguishable particles.

We obtain an expression for the contribution to $b_3$ from the off-shell series up to third order, with two remaining integrations to perform. We are able to construct the fully off-shell Green's function and to hence calculate $b_3$ directly from the trace formula. This calculation gives us an intermediate expression which is analogous to that from the truncated multiscattering series, and we discuss the comparison.

We also compute $b_3$ from the wavefunction, verifying the result from the Green's function, and recognise it as the third cluster coefficient of a free Fermi gas.

We have the solutions of the Faddeev Equations for the problem, and note that in the case of hard classical particles, $T_2$ vanishes identically. In the light of the known singularity structure of the $T$-matrix, it is interesting to see how the singularities cancel out as $c \to \infty$. 
Taking now the case of symmetric statistics, in §4.8 we use the Low Equation to construct the fully off-shell T-matrix for bosons, and verify that it reduces to the correct on-shell hardcore $T$ in those limits.

Finally, we succeed in calculating $b_3$ for hard symmetric particles in §4.9 using the hardcore limit of the fully off-shell amplitude in the trace formula.

We use this calculation to again look at the contributions to $b_3$ from the first three orders of the multiscattering series, and draw some conclusions about the validity of the latter approach.

In Chapter V we assess the outcome of the work we have done, and discuss the value of the scattering formulation in the context of this model.
Fig. 1 systematises the work of the thesis. The main results are boxed in double lines and the section numbers refer to derivations in the text. Circled letters refer to appendices. Superscripts S,D,0 and H indicate symmetric, distinguishable and free particles, and the hardcore limit $c^{\infty}$.
1.3 The One-Dimensional Gas with Repulsive Point Interactions

The model we have chosen to work with in this thesis is a one-dimensional single species gas, interacting elastically via a two-body repulsive delta function potential of strength $2c$.

This system has been treated in a number of papers, and the n-body scattering solutions for both classical and quantum statistics are known.

Thus we have a model to which we can apply the scattering formulation of the cluster coefficients, but which is sufficiently simple for direct calculations of the coefficients to be made for comparison.

In addition, the work of Yang and Yang$^{(1,2)}$ (see Appendix G) on the thermodynamics of this model provides an independent check for our projected results.

Now in this section, we briefly summarize the development of the model by various researchers, and examine in some detail its salient features.

Choosing units such that $\hbar = 2m = 1$, the n-body hamiltonian is

$$H = - \sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i<j=1}^{n} \delta(x_i - x_j) \quad (1.1)$$

with $x_i$ being the position coordinate of the $i$th particle.

We note that the potential is local. It is also separable, being expressible as the dyad operator $\frac{c}{n} |\chi><\chi|$ where $\chi = \int |p> dp$ and $|p>$ is a two body state with relative momentum $p$. This factorization permits the formal solution of some two-body operator equations. See for example §3.4.
We also observe that an elastic interaction between two equal mass particles in one dimension can only have two possible outcomes. The particles may bounce off each other, having exchanged momenta, but with their spatial ordering preserved; or they may retain their momenta and exchange their spatial ordering. We call the latter process transmission, and the former reflection, and define the respective probability coefficients $t_{ij}$ and $r_{ij}$, where $i$ and $j$ refer to the momenta involved.

The coefficients will be functions of the relative momentum of the two particles and of the potential strength. In the hardcore limit, $c \to \infty$, we can expect the transmission coefficient to vanish and the particles will only be able to reflect. With identical particles, this situation is equivalent to the familiar free Fermi gas, so this limit provides another useful check.

In a classical Newtonian system of three or more equal mass one-dimensional bodies colliding elastically, the initial momenta can only be permuted among the bodies with the exception of the unlikely situation where all three bodies collide simultaneously. By contrast, an analogous quantum mechanical system will in general allow an infinite range of new momenta to be created by interaction, because in the intermediate states, only momentum conservation is required. Energy needs only to be conserved overall, from initial to final state, but not in intermediate processes.

However, it is a property of this model that any interaction will result only in a permutation of the original momenta and/or spatial ordering of the particles, and that in fact, no new momenta are generated.
This seemingly classical behaviour is a result of the unphysical "point" nature of the interaction, which by having zero range essentially removes the opportunity for the quantum transfer of momentum during interaction.

In the case of identical particles, the ordering can not be distinguished, so only permutation of the momentum labels need be considered.

This important feature renders the quantum n-body problem soluble, and forms the basis of Bethe's Hypothesis:

Let \( k = (k_1 \ldots k_n) \) be an ordered set of numbers corresponding to the momenta, then the total wavefunction of the system can be written:

\[
\psi_k(x) = \sum_p a(P,k)e^{iP \cdot x}
\]

where \( x = (x_1 \ldots x_n) \) and we sum over all permutations \( P \) of the \( k_i \).

The problem then reduces to determining the coefficients of the plane waves.

We note that this simplification would not be possible if the masses or interaction strengths were unequal, or if we considered the two or three dimensional problem or allowed inelastic scattering.

With distinguishable particles we would need to write an ansatz of the form of (1.2) for every distinct ordering of the particles, and there would be \((n!)^2\) coefficients to solve for. Fortunately there is a simple algorithm for computing these coefficients, due to McGuire\(^{(3)}\) who has treated the problem using an ingenious optical
analogue. The method, and the three-body solution is discussed in more detail in §4.1.

Lieb and Liniger\(^4\) have used Bethe's Hypothesis and box normalization to analyse the n-body problem with symmetric statistics.

With the aid of symmetry they showed that the potential and the periodic boundary conditions were equivalent to

\[
\psi(0, x_2, \ldots, x_n) = \psi(x_2, \ldots, x_n, L)
\]

\[
\frac{\partial}{\partial x} \psi(x_2, \ldots, x_n)_{x=0} = \frac{\partial}{\partial x} \psi(x_2, \ldots, x_n, x)_{x=L}
\]

(1.3)

in the region \(RI: 0 \leq x_1 \leq \ldots \leq x_n \leq L\), and obtained a rule for constructing the coefficients \(a(P, k)\) of the wavefunction (1.2), thus specifying the solution in \(RI\). Bose Symmetry gives the wavefunction in any other region by the simple relation

\[
\psi^S_{RI, k}(x) = \psi^S_{IK, (P^{-1}x)}
\]

where \(P\) is the permutation that takes \(RI\) to the required region, the superscript \(S\) denotes symmetric statistics and the roman subscript indicates the region in which the wavefunction is defined.

The box normalization also has the effect of quantizing the momenta, thus yielding the density of states. Some further discussion of this aspect is in Appendix C.

They derived the momentum spectrum, observing that actually the \(k_i\) are not true wave vectors since only the region \(RI\) has been considered, and went on to calculate the ground state energy
and other quantities of interest.

They also found that if the $k_i$ were not distinct, the wavefunction would vanish identically. To avoid this, we shall always require the initial momenta to be distinct. This is a reasonable condition to impose, as it rules out the rather unphysical situation where two particles remain a fixed distance apart from the initial to final state without ever interacting.

Further work was done by C.N. Yang\(^{(5,6)}\), who found the $S$-matrix for distinguishable particles, and verified its symmetry and unitarity.

The three-body problem in particular has received much attention, and some relevant results are discussed in §4.1.
II  THE THEORY OF CLUSTER COEFFICIENTS

2.1 The Cluster Expansion of the Grand Partition Function

All the thermodynamic information about a system in equilibrium is contained in its grand partition function, defined as

$$\hat{Z}(z,v,T) = \sum_{N} \frac{Q_{N}^{z}}{N!} ,$$  

(2.1)

where \( z = e^{\beta \mu} \) is the fugacity, \( \mu \) is the chemical potential, \( \beta \) is the inverse temperature \( \frac{1}{kT} \) and \( Q_{N} \) is the \( N \)-particle canonical partition function. For a quantum system of \( N \) particles with Hamiltonian \( H_{N} \),

$$Q_{N} = \text{Tr} e^{-\beta H_{N}} .$$  

(2.2)

Thermodynamic quantities such as pressure, entropy and average energy are obtained as various partial derivatives of \( \ln \hat{Z} \).

Interest therefore centres on ways of calculating \( \hat{Z} \).

For an interacting gas, the most useful approach has been the Ursell-Mayer cluster expansion which expresses \( \ln \hat{Z} \) as a power series in the fugacity

$$\ln \hat{Z}(v) = \sum_{\ell} V_{\ell} b_{\ell} z^{\ell} .$$  

(2.3)

The cluster coefficients \( b_{\ell} \) are essentially the contributions to the \( \ell \)-particle canonical partition function which are due to interacting clusters of exactly \( \ell \) particles. The classical formulation was carried over to quantum systems by Kahn and Uhlenbeck\(^{(7)}\) and in operator notation
\[ b_k = \lim_{V \to \infty} \frac{1}{V^k} \text{Tr} U_k, \quad (2.4) \]

with the \( U_k \) defined by the following

\[ W_N(1,2,\ldots,N) = e^{-\beta H_N} \quad (2.5) \]

\[ U_1(1) = W_1(1) \]
\[ U_2(1,2) = W_2(1,2) - W_1(1)W_1(2) \quad (2.6) \]
\[ U_3(1,2,3) = W_3(1,2,3) - W_1(1)W_2(2,3) - W_1(2)W_2(1,3) - W_1(3)W_2(1,2) + 2W_1(1)W_1(2)W_1(3) \]

and so on.

The effect is to isolate in \( U_k \) those processes which are truly \( \lambda \)-particle. This introduces the concept of connectedness. A system of \( \lambda \) particles may be diagrammatically represented by \( \lambda \) points. An interaction between two particles is denoted by a line joining those two points. Then a configuration is said to be connected if a continuous line can be traced between every pair of points. A configuration in general will consist of a number of connected clusters which are disconnected from each other. Free particles are simply one-clusters. (When quantum statistics are used, exchanges between pairs of identical particles connect them even if there is no other link due to interactions.)

The \( \ell \)th cluster coefficient is thus dependent only on connected clusters of \( \lambda \) particles.

Equation (2.3) leads us to the equation of state of the system in parametric form

\[ \beta P = \sum_{\ell} b_\ell z^\ell, \quad (2.7) \]
\[ \rho = \sum_{\ell} \ell b_\ell z^\ell, \]
where $P$ and $\rho$ are the equilibrium pressure and density.

The equation of state is often expressed in the virial form

$$\beta p = \sum_{l} a_{l} \rho^{l}.$$  \hspace{1cm} (2.8)

Elimination of $z$ from (2.7) and comparison with (2.8) yields the virial coefficients $a_{l}$ in terms of the cluster coefficients of order $m \leq l$. The first few are

$$a_{1} = 1$$
$$a_{2} = -b_{2} b_{1}^{-2}$$
$$a_{3} = b_{1}^{-4} (4b_{2}^{2} - 2b_{1} b_{3}) \hspace{1cm} (2.9)$$

Both the virial and cluster expansions are essentially low density and low temperature expansions. Under these conditions the probability of $\ell$ particles forming a connected cluster decreases rapidly as $\ell$ increases, so only the first few coefficients are likely to be significant.

There are some simple modifications of (2.4) which facilitate calculations. The explicit volume dependence can be removed, and in the centre of mass frame, the total kinetic energy contribution, can easily be extracted. The trace can be taken in either the position or momentum representation.

In the position representation, the volume independent form has been obtained by Lee and Yang\(^{(8)}\) by applying to (2.4) a linear transformation which centres the origin on particle 1. Since $U_{\ell}$ must be translationally invariant, we have, in one dimension

$$b_{\ell}(v) = \frac{1}{v^{\ell+1}} \int <0 x_{2}...x_{\ell} | U_{\ell} | 0 x_{2}...x_{\ell}> d^{\ell}x.$$
The $x_i$ integration then yields a factor of $V$ which cancels out. So we may write

$$b_k = \frac{1}{\ell^i \sqrt{\lambda}} \int \langle x | U_k | x \rangle \delta(x_i) d^\ell x$$

(2.10)

A similar result in the momentum representation is achieved by taking a double Fourier transform and integrating over $x$ and the momenta covered by delta functions. We find

$$b_k = \frac{1}{\ell^i 12\pi} \int \langle k | \vec{U_k} | k \rangle dk$$

(2.11)

where

$$\langle k | U_k | p \rangle = \delta(\Sigma k - \Sigma p) \langle k | \vec{U_k} | p \rangle .$$

For computational purposes, the normal $U_k$ function is used, and when the factor $\delta(\Sigma k - \Sigma p)$ becomes explicit, it is dropped.

To deal with the kinetic energy of the centre of mass, we introduce the usual generalised coordinates $q_1 \ldots q_{\ell-1}, p_1 \ldots p_{\ell-1}$ and the coordinates of the centre of mass, $R = \Sigma q_i / \ell, K = \Sigma p_i$. Taking the trace with respect to these coordinates, the centre of mass energy $e^{-\beta K^2/2\lambda m}$ where $m$ is the particle mass, factors out and the $K$ integration can immediately be performed. We find for $m=\frac{1}{2}$

$$b_k = \frac{\ell^i \beta}{\ell^i 1 (4\pi \beta)^{\frac{\ell}{2}}} \int d^{\ell-1} p \langle p | \vec{U_k}_{CM} | p \rangle$$

(2.12)

where $\vec{U_k}_{CM}$ is $\vec{U_k}$ as a function only of the $\ell-1$ independent momenta.
2.2 Approaches to the Calculation of the Cluster Coefficients

It is apparent from the defining equation (2.4) that a solution of the $l$-body problem is required to compute $b_l$. The energy spectrum or at least the density of states is needed. Only the simplest of models admit an exact solution, so even for such idealized systems as a hardcore gas, approximations are needed. Generally, the leading terms in a low temperature expansion of the coefficient are obtained.

The second cluster coefficient has been thoroughly analysed and several approaches have been fruitful. In many models, the two-body problem is soluble, so $b_2$ is easily calculable. More interestingly, Uhlenbeck and Bethe\(^{(9)}\) as long ago as 1937, were able to formulate $b_2$ in terms of the phase shifts introduced into the $\ell$th partial wave by the interaction. The phase shifts characterise the asymptotic scattering state, and as such, are on-shell physically observable quantities. This result was the first to support the intuitive notion that macroscopic (thermodynamic) properties of matter are ultimately explicable in terms of the microscopic processes between particles on a dynamical rather than statistical basis. However, extension to higher order coefficients proved too difficult. Only in 1969 was an attempt made to treat $b_3$ in the same way. Larsen and Mascheroni\(^{(10)}\), using hyperspherical harmonic wavefunctions, were able to define a unique three-body phase shift and derive an expression for $b_3$, but only for classical Boltzmann statistics and in the absence of bound states. Mascheroni\(^{(11)}\) further treated the $\ell$-body case and noted a relation between the phase shifts and diagonal elements of some scattering operators. In practice this approach yielded a low temperature expansion for $b_\ell$. 
In the meantime, most work had concentrated on developing a perturbative treatment of $b_k$ based on Lee and Yang's\(^8,12-14\) binary kernel, or on the Watson-Faddeev\(^15\) multiscattering expansion. The actual form and structure of the expansions are discussed in more detail in 52.5.

The work of Lee and Yang had achieved a number of advances for statistical mechanics. They were able to separate the statistics from the dynamics by relating the quantum cluster coefficients with either symmetric or antisymmetric statistics to the classical cluster coefficient. Using a technique analogous to the Feynman-Dyson expansion of quantum field theory, with $\beta$ playing the role of an imaginary time parameter, they developed an expansion for $U_k$ in terms of a binary kernel, which is essentially $V e^{-\beta h} (V, h = h_0 + V$ are 2-body operators). The kernel can be computed from the solution of the two-body problem. Although the expansion is still perturbative, it has an improved radius of convergence over the simple potential expansion. Even in the hardcore limit where the potential expansion diverges, the binary expansion will converge.

This expansion was utilized by Pais and Uhlenbeck\(^16\) to calculate the leading low temperature terms in $b_3$, in various channels and for different potentials, in terms of the scattering length and effective range. However their results were also dependent on a third length which could not be inferred from scattering data. Along similar lines, Larsen\(^17\) investigated the specific case of He\(^4\) with an empirically determined potential.

The multiscattering approach was first developed by Watson\(^15\). Starting with the observation by Koppe\(^18\) that a Laplace transform of $e^{-\beta H}$ led to a Green's function with hamiltonian $H$, and
using operator identities from stationary state scattering theory, Watson was able to express $T e^{-\beta H}$ in terms of weighted energy integrations over $T$-matrix elements. The expansion of $T$ in two-body $T$ matrices then yielded the multiscattering expansion of the cluster coefficients. Application of the technique to other statistical calculations was discussed in this, and later papers by Reisenfeld and Watson\(^{(19,20)}\).

Field theory diagrammatics were also used by Montroll and Ward\(^{(21)}\) to establish a graphical representation of quantum cluster integrals.

Siegert and Teramoto\(^{(22)}\) showed that the multiscattering expansion was in fact the Laplace transform of the binary collision expansion. Reiner\(^{(23)}\) also proved the equivalence of the two approaches, and went on to confirm the results of Pais and Uhlenbeck for hard bosons by use of the Watson series. Although the latter series has some computational advantages over the binary kernel series because of the symmetry of the $T$-matrix, there was no improvement in the convergence difficulties experienced in the earlier work. The formalism which Faddeev developed for the three-body problem was later exploited by Reiner\(^{(24)}\) to avoid convergence problems and provide a closed form for $b_3$. Essentially the multiscattering series is replaced by a set of coupled integral equations, the Faddeev Equations. Although they are an exact closed form, and solutions have been obtained for some local potentials, these equations cannot easily be solved for most models, so it is necessary for practical calculations to use some approximations, such as a factorizable potential.

Some further work in this direction was done by Baumgartl\(^{(25)}\) who calculated $b_3$ up to third order in the two-body scattering
amplitude elements, verifying some estimates of $b_3$ from transport theory. He also observed that some $T$-matrix elements were required off-shell.

Gibson\(^{(26)}\) working with the multiscattering series obtained the leading terms for $b_3$ for both hard spheres and bosons interacting via an arbitrary potential without bound states. Besides the leading terms previously obtained by Pais and Uhlenbeck, he verified the logarithmic term implied by the work of Adhikari and Amado\(^{(27)}\) using the more recent trace formulae. This latter approach is discussed in detail in the next section.

Gibson\(^{(28)}\) also developed an expression for $b_2$ in terms of an inverse Laplace transform of the logarithmic derivative of the Jost function and presented explicit results for some nonanalytic potentials in the limit of high temperatures.
2.3 Motivation and Development of the Scattering Theory of the Cluster Integrals

The scattering theory of the cluster integral is essentially a formulation of $b_k$ in terms of such scattering operators as the S or T matrix. It has been asserted that only on-shell elements are required. If this is the case, the formulation will be of great practical use, since on-shell scattering information can be obtained experimentally for any real physical system. This would enable the complete deduction of all the equilibrium thermodynamics of a real gas from a knowledge of the physical scattering properties of its consistent particles.

That such a programme should be possible seems intuitively clear. One does not expect macroscopic properties of a system to depend on non-physical quantities, such as the analytic continuation of scattering operators off the energy shell. However it is not so clear whether purely on-shell information is in principle sufficient or whether one needs data from within a small neighbourhood of the energy shell, such as is needed to take an energy derivative. This is a very important and fundamental question, on which a careful analysis of the scattering approach may throw some light.

Although the scattering formulation holds intrinsic interest from any point of view, its real relevance lies in the possibility of formulating the statistical mechanics of a relativistic system\(^{(29)}\). In this case, multichannel processes become significant and concepts such as the potential break down. These qualitative differences prevent a simple extrapolation of non-relativistic statistical mechanics. The only operator which is well defined in the relativistic region is the S-matrix. It can easily be made Lorentz symmetric,
and it naturally incorporates the many asymptotic states (channels) available after a high energy collision. Particle production and annihilation are taken care of by using a second quantized representation in the appropriate Hilbert Space. It is evident therefore that a formulation of the cluster coefficients in terms of the $S$-matrix will readily lend itself to a relativistic generalization. The fact that the formulation is not perturbative is another useful feature in the relativistic limit where the interaction will generally be strong and there will not necessarily be a one to one correspondence between ideal gas states and the states of the fully interacting system.

It is valid to question whether in fact, the cluster expansion itself is meaningful at relativistic energies. Being a perturbative expansion, it does break down at high densities or with strong interactions; however convergence is best at high temperatures. Since an energetic relativistic system such as a plasma will generally be at a very high temperature, the cluster approach will be valid at least as a first approximation in the small region of local equilibrium after a collision.

Historically, the development of the scattering approach dates from 1937 when Uhlenbeck and Bethe\(^9\) published their phase shift formulae for $b_2$. The phase shifts are of course simply related to the on-shell $S$-matrix elements. Goldberger\(^{30}\) in 1959 rederived the formulae for $b_2$ using the $S$-matrix directly, and suggested a general $S$-matrix formulation of the cluster coefficients.

The 1956 work of Watson\(^{15}\) in which he expresses diagonal elements of $e^{-\beta H}$ in terms of $T$-matrix elements is equivalent to
the later trace formulae of Dashen Ma and Bernstein\(^{(31)}\) and others, needing only the application of some well known operator identities from scattering theory. (This was pointed out by Swenson\(^{(32)}\) in 1971). Off-shell information was explicitly required.

Some important work was done by Smith\(^{(33,34)}\) in 1962-3, in terms of a "collision lifetime" operator, \(\mathcal{Q}\). This operator is also called "time delay", and contains all the physical information about the collision process; in fact, as Smith noted, \(\mathcal{Q} = i\hbar \frac{dS^+}{dE}\). His main result was a cluster expansion of the partition function involving terms like \(\int e^{-\beta E} \text{Tr}\mathcal{Q}(E)dE\). These results are essentially identical to the present S-matrix formulae, but their significance was overlooked until Dashen Ma and Bernstein\(^{(31)}\) independently obtained them in 1969.

In the meantime, the so-called trace formulae, which relate \(\text{Tr} e^{-\beta H}\) to scattering operators, were studied by Buslaev\(^{(35)}\) and Berezin\(^{(36)}\), for three particles in the first instance, and then for the general case with both elastic and arbitrary scattering, but with the restriction of single channel processes. The extension to multichannel scattering for three particles was made by Buslaev and Merkurev\(^{(37)}\). With these trace formulae they essentially had the S-matrix formulation of the cluster coefficients. However closer investigation by Berezin\(^{(38,39)}\) revealed serious singularities corresponding to forward scattering which were not easily removable. He concluded that the formulae contained additional terms which would regularize the trace and conjectured that they depended on the logarithm of the two body S-matrix. This suggestion was developed in 1970 in the three dimensional case by Buslaev and Merkurev\(^{(40)}\),
resulting in some unwieldy correction terms which arose from the explicit treatment of the singular two-body contributions.

Dashen, Ma and Bernstein\(^{(31)}\) noted the existence of the forward singularities in their own scattering formulation. They recognised that these terms were due to three body processes in which the first and second collisions were distant in time and space, and asserted that all such terms would cancel when combined and that the divergences were therefore spurious. Mathematically, the singularities arose because of the infinite extension of the plane wave momentum eigenstates used, and they suggested an alternative basis such as angular momentum eigenstates or wave packets would avoid the problem.

They also claimed that only on-shell elements of the S-matrix were required in a practical evaluation, but the proof of this depends on the smoothness of the T-matrix. This will be discussed in §2.5.

In two subsequent papers, Dashen and Ma\(^{(41,42)}\) showed that the divergent terms could indeed be avoided in the angular momentum representation. Summation over the angular momentum \(\ell\) effectively smeared out the forward singularities. They proved that this summation converged and showed that the same result could be obtained by keeping the energy off shell until the last step. In this case the forward terms were not singular since the resolvent for the intermediate state (between the first and second scattering) was not forced to blow up by an energy conserving delta function. Finally, they showed that a correct result could also be obtained with on-shell elements if a small rotation about some arbitrary third axis is introduced. After the integrations have been performed, the limit of zero rotation is taken.

These modifications, while preserving the intent of the
formulation in principle, severely restrict its potential usefulness. The formulation has been used to calculate leading low energy terms for $b_3$ by Adhikari and Amado, who also rewrote the formulae in terms of the K-matrix. Osborn and Tsang, using the equivalent time delay formulation calculated the second and third virial coefficients for distinguishable particles, and in 1976 Osborn developed a very interesting extension to systems consisting of two species of particles, one of which was a bound pair of the other. The only approximation required was the use of Boltzmann statistics for the freely propagating states. The bound states were properly symmetrized. By using a two fugacity expansion, he was able to express all cluster coefficients in terms of on-shell time delay operators.

The time delay approach was also used by Bolle and Smeesters to obtain a high temperature perturbation expansion of $b_2$ for analytic potentials, and again by Osborn and Tsang to develop generalized expressions for the higher cluster coefficients of a quantum gas, consisting of distinguishable particles interacting via arbitrary short range (falling off faster than coulomb) potentials, which may be attractive enough to have bound states. The theory explicitly accounts for multichannel scattering, and by short circuiting any connection to S or T matrices, avoids completely the problem of forward singularities. However the disadvantage is that the time delay, though an observable in principle, is not a useful one in practice, because the width of a resonance in an experimental scattering amplitude will be related to the time delay only in the hypothetical case of an incident beam which is a very short wavepacket. This point has been discussed by Dodd and McCarthy.
2.4 The Scattering Formalism for $b_k$

Equation (2.4) defines the $\chi$th cluster coefficient

$$b_k = \lim_{V \to \infty} \frac{1}{L^4 V} \text{Tr}(e^{-\beta H})_c$$

(2.13)

where the suffix $c$ denotes that the trace is taken over the connected part of the operator only, as described by equations (2.6).

When the interaction is removed, (2.13) defines $b_k^0$, which will be finite for systems obeying quantum statistics, because the symmetry acts effectively as an "exchange interaction", linking otherwise free particles.

For identical particles, practical calculations are generally made of

$$b_k - b_k^0 = \lim_{V \to \infty} \frac{1}{L^4 V} \text{Tr}[\Lambda(e^{-\beta H} - e^{-\beta H_0})]_c$$

(2.14)

where $H_0$ is the free $\ell$-particle hamiltonian, and $\Lambda$ is the symmetrization operator

$$\Lambda = \sum_P (\pm) \delta_P P$$

(2.15)

summing over all the permutations $P$ of the particle labels, $\delta_P$ being the order of $P$, and the upper sign applying to bosons, the lower to fermions. The effect of this operator is to ensure that the trace is taken with respect to properly symmetrized states, and we now retain those terms which are connected by exchanges as well as those connected by interactions.
From an examination of equation (2.6) it is apparent that the trace in (2.14) can be written as a sum of terms of the form

\[ \text{Tr}(e^{-\beta H'} - e^{-\beta H_0}) \]

where \( H' \) is a Hamiltonian of the system partly or fully interacting. For example

\[
\frac{h_3 - h_0}{3! V} \lim_{V \to \infty} \frac{1}{3! V} \left[ \text{Tr}(e^{-\beta H} - e^{-\beta H_0}) - \sum a \text{Tr}(e^{-\beta H_a} - e^{-\beta H_0}) \right] = 0
\]

(2.16)

where \( H_a = H_0 + V_a, \ a \in \{(12), (13), (23)\}, \) and the third particle in each case is propagating freely.

So to proceed with developing the scattering formalism, we need only consider the basic expression \( \text{Tr}(e^{-\beta H} - e^{-\beta H_0}) \).

In the absence of bound states, the spectra of both \( H \) and \( H_0 \) fall on the positive real axis. We denote the eigenvalues by \( \{E_i\} \) and \( \{E_i^0\} \) respectively. When the system is in a finite volume, these are discrete sets. They approach a continuum as \( V \to \infty \), at which point it is valid to interpret the trace as an integration rather than a sum over states.

Now by Cauchy's Integral Theorem, we can write

\[
\text{Tr}(e^{-\beta H} - e^{-\beta H_0}) = -\frac{1}{2\pi i} \oint_C \frac{dZ}{Z-H} \text{Tr} \left( \frac{1}{Z-H} - \frac{1}{Z-H_0} \right)
\]

(2.17)

where the clockwise contour \( C \) encloses the origin and the spectra of \( H \) and \( H_0 \) in the complex energy \( Z \) plane. Recognising the resolvent operators in the integrand, we have

\[
\text{Tr}(e^{-\beta H} - e^{-\beta H_0}) = -\frac{1}{2\pi i} \oint_C \frac{dZ}{Z} e^{-\beta Z} \text{Tr}(G_0)
\]

(2.18)

which, with the aid of a well known scattering identity, leads directly
to Watson's T-matrix form

$$\text{Tr}(e^{-\beta H} - e^{-\beta H_0}) = - \frac{1}{2\pi i} \int_C dZ \ e^{-\beta Z} \text{Tr}(G_0 T G_0). \quad (2.19)$$

We observe that because the trace is taken with respect to eigenstates of the free Green's function, only diagonal elements of $T$ are required. However, the elements are also functions of $Z$ and therefore are off-shell. The most useful development of (2.19) has been through the expansion of $T$ into the multiscattering series. We explore this in the following section and utilize the approach for practical calculations in §4.5-§4.7 and §4.9. We have also in §4.9 applied (2.19) directly to compute the cluster coefficient of a system for which we have found the fully off-shell T-matrix.

To arrive at the S-matrix formulation, we take equation (2.17) and compress the contour to within $\pm i\epsilon$ of the real axis. Then

$$\text{Tr}(e^{-\beta H} - e^{-\beta H_0}) = - \frac{1}{2\pi i} \int_0^\infty dE \ e^{-\beta E} \text{Tr} \left[ \frac{1}{E-H+i\epsilon} - \frac{1}{E-H_0+i\epsilon} - \frac{1}{E-H-i\epsilon} + \frac{1}{E-H_0-i\epsilon} \right]$$

$$= - \frac{1}{2\pi i} \int_0^\infty dE \ e^{-\beta E} \text{Tr} \left[ \frac{d}{dE} \ln \left( \frac{E-H+i\epsilon}{E-H_0+i\epsilon} \right) - \ln \left( \frac{E-H+i\epsilon}{E-H_0+i\epsilon} \right) + \ln \left( \frac{E-H_{-i\epsilon}}{E-H_0-i\epsilon} \right) \right]$$

which becomes, with the aid of a result proved in Appendix B,

$$\text{Tr}(e^{-\beta H} - e^{-\beta H_0}) = - \frac{1}{2\pi i} \int_0^\infty dE \ e^{-\beta E} \text{Tr} \left[ \frac{d}{dE} \ln \left( \frac{E-H+i\epsilon}{E-H_0-i\epsilon} \right) \right]. \quad (2.20)$$

Consider now the unitary operator

$$0 \equiv \frac{E-H-i\epsilon}{E-H_0+i\epsilon} \frac{E-H_0+i\epsilon}{E-H+i\epsilon}$$

$$= (I - 2i\epsilon G^+) (I + 2i\epsilon G^0_0)$$
where $I$ is the identity operator. Replacing $G^+$ by $G_0^+G_0^+ T G_0^+$ and simplifying, we find

$$0 = I - 2i\varepsilon G_0^+ \left( G_0^- G_0^- \right) T G_0^-$$

where we have inserted the identity $I = G_0^- G_0^-$. In the limit $\varepsilon \to 0$, we obtain

$$0 = I - 2\pi i \delta(E-H_0)(E-H_0) T \frac{1}{E-H_0}$$

$$= I - 2\pi i \delta(E-H_0) T$$  \hspace{1cm} (2.21)

since $H_0$ and $T$ commute. This is the usual definition of the $S$-matrix.

Substituting back into (2.20), we have

$$\text{Tr}(e^{\beta H} - e^{\beta H_0}) = -\frac{1}{2\pi i} \int_0^\infty dE \ e^{\beta E} \text{Tr} \left( \frac{d}{dE} \ln S^{-1} \right)$$

$$= \frac{1}{2\pi i} \int_0^\infty dE \ e^{\beta E} \text{Tr} \left( S^{-1} \frac{dS}{dE} \right)$$  \hspace{1cm} (2.22)

Equation (2.22) forms the crux of the scattering formulation of the cluster coefficients, as developed by Dashen, Ma and Bernstein\(^{(31)}\).

A clean separation of the dynamical and statistical factors has been achieved, the exponential carrying only the temperature, and the $S$-matrix term containing all the necessary interaction data. This represents a clear improvement on the left hand side of (2.22), in which the exponential carries mixed information via $\beta$ and the full spectra of the hamiltonians of the system.

We note however, that the derivation of (2.22) has not been rigorous. In particular, we need to look more carefully at the way
in which the various limits are taken. The relevant processes are the infinite volume limit and the real energy \((\epsilon \to 0)\) limit.

The interdependence of these two limits is a well known result of scattering theory\(^{(48)}\). The parameter \(\epsilon\) essentially describes the length of the wave packets in the finite volume \(V\). In the limit \(\epsilon \to 0\), the wave packets become plane waves of infinite extent. Obviously this limit makes no sense in a box of finite size, so it is necessary to take the limit \(V \to \infty\) before, or at least simultaneously with, the limit \(\epsilon \to 0\), and in such a way that \(1/\epsilon\) is always much less than the time required for the system to traverse the box.

The volume enters into equations (2.17) to (2.22) by way of the states used to evaluate the trace and by the volume dependence of the operators. While the system is in a finite box, the energy eigenstates are quantized and the trace needs to be performed as a sum over the complete set of discrete states. The spectrum becomes continuous in the infinite volume limit and the sum can then be replaced by an integration over the momenta, plus a sum over discrete bound states if any. So it seems that provided the trace in (2.22) is interpreted as an integral, the formula will be correct.

However, there is a complication, in that the volume dependence of the operators also depends on their connectedness. Returning to equation (2.14), it is only the overall connected part of the trace that is proportional to \(V\), cancelling the factor \(V^{-1}\). A disconnected term is proportional to \(V^m\), where \(m\) is the number of separate internally connected components of the term. Thus the infinite volume limit is only defined after the disconnected contributions are subtracted.
So when the Hamiltonian on the left hand side of equation (2.22) involves more than one interacting pair, the system should be taken to be still in a finite volume. In this case, one cannot use the conventional S-matrix as defined by (2.21), because it implies that the limit $\varepsilon \to 0$ has already been taken. To be rigorous, one can define

$$S(V,E+i\varepsilon) = I - 2i\varepsilon G^+_0 T G^-_0$$

(2.23)

Then

$$\text{Tr}_V(e^{-\beta H} - e^{-\beta H_0}) = \frac{1}{2\pi i} \int_0^\infty dE \ e^{-\beta E} \text{Tr}_V(S^{-1} \frac{d}{dE} S)$$

(2.24)

and

$$\lim_{V \to \infty} \lim_{\varepsilon \to 0} S(V,E+i\varepsilon) = S(E)$$

(2.25)

and $\text{Tr}_V$ indicates that the trace is taken with respect to discrete states in the volume $V$.

One could then construct the connected part of (2.24) and in the end take the simultaneous limits of (2.25). This procedure, while clumsy, would be strictly correct.

However, what we would like to do is to take the connected part of (2.22) using the S-matrix defined in the infinite domain, since these are more likely to be available for most models. The necessary assumption is that the limit of the connected pair is equivalent to the connected part of $\lim_{V \to \infty} \lim_{\varepsilon \to 0} \text{Tr}(S^{-1} \frac{dS}{dE})$. Although this step is not rigorous mathematically, since we are taking differences of singular terms, it is justifiable in the sense that similar manipulations
are frequently and usefully performed in scattering theory.

So we henceforth take it that equation (2.22) holds in the real energy and infinite volume limit and that the connected parts of both sides may be formed by the subtraction of the appropriate disconnected terms.

A more significant problem arises out of the assertion\(^{31}\) that only on-shell S-matrix elements enter into equation (2.22). Naturally if this were so, it would render the formula of great practical value, so we now examine the argument in its support.

Since we are considering real on-shell energies, we must take the trace with respect to the continuum states, for the reason discussed earlier. We label the states by their energy and suppress the remaining parameters which are irrelevant to the present discussion.

\[
\text{Tr}(S^{-1} \frac{d}{dE} S) = \text{Tr}[(I+2\pi i \delta(E-H_0)T^+(E)) \frac{d}{dE}(I-2\pi i \delta(E-H_0)T(E))]
\]

\[
= (-2\pi i) \int dE' dE'' \left\{ [\delta(E'-E'') + 2\pi i \delta(E-E')] T^+_{E',E''}(E) \right\} \frac{\partial}{\partial E} \delta(E-E'') T_{E''E'}(E),
\]

(2.26)

where the \( T \) matrix elements are characterized by three energy parameters thus

\[
\langle E' | T(E) | E'' \rangle = T_{E',E''}(E).
\]

When all three labels match, \( T_{EE}(E) \), the element is termed on-shell.

Performing some integrations in (2.26), we obtain

\[
\text{Tr}(S^{-1} \frac{d}{dE} S) = -2\pi i \frac{\partial}{\partial E} T_{EE}(E) - (2\pi i)^2 \int dE' \delta(E-E') \left[ \int dE'' T^+_{E',E''}(E) \frac{\partial}{\partial E} \delta(E-E'') T_{E''E'}(E) \right]
\]

(2.27)
of which the first term is already on-shell.

The expression in square brackets can be written as

\[
\frac{\partial}{\partial E} \int dE' T_{E'E'}(E) \delta(E-E') T_{E'E'}(E) - \int dE' \left( \frac{\partial}{\partial E} T_{E'E'}(E) \right) \delta(E-E') T_{E'E'}(E) = \frac{\partial}{\partial E} \left( T_{EE}(E) - T_{EE}(E) \right) + R
\]  

(2.28)

It can be shown with the aid of the unitarity property

\[
T^+(G_0 - G_0^+) T = T(G_0 - G_0^+) T^+
\]  

(2.29)

that \( R \) vanishes. When the remaining term on the RHS of (2.28) is substituted back into (2.27), it also becomes on-shell after the final energy integration. Thus

\[
\text{Tr} \left( S \frac{-1 dS}{dE} \right) = -2\pi i \frac{\partial}{\partial E} T_{EE}(E) - (2\pi i)^2 \frac{\partial}{\partial E} \left( T_{EE}(E) T_{EE}(E) \right)
\]  

(2.30)

which depends only on on-shell elements of the scattering amplitude.

However we note that to arrive at this result, we have several times used the delta function property

\[
\int dE' \delta(E-E') T_{E'E'}(E) = T_{EE}(E)
\]

which is only valid provided \( T_{E'E'}(E) \) is continuous at \( E' = E \).

We see that the question of on-shell information being sufficient to calculate the cluster coefficients depends critically on the singularity structure of the scattering amplitude. We return to this problem in §2.6, and several sections of Chapter IV deal with it in the context of the model described in §1.3.
There are some alternate forms of the scattering approach, such as that due to Smith (33, 34) involving the lifetime collision operator \( Q \), which is defined as \( \hbar S \frac{dS^+}{dE} \). Although the two forms are equivalent, the question of whether on-shell elements only are needed may be easier to analyse in the S-matrix form. Also the Q-matrix elements are not directly observable. Recall our earlier comment at the end of §2.3.

Another form, due to Adhikari and Amado (27), involves the K-matrix

\[
K = (I - V P G_0)^{-1} V
\]  

(2.28)

where \( P \) means the principal part.

Applying (2.27) with the aid of the identity

\[
G_0^+ = P \left( \frac{1}{E-H_0} \right)^+ i\pi \delta(E-H_0)
\]

(2.29)

to (2.20), it is not difficult to show that

\[
\text{Tr}(e^{\beta H} - e^{-\beta H_0}) = -\frac{1}{2\pi i} \text{Tr} \int_0^\infty e^{\beta E} \frac{d}{dE} \tan^{-1}(i\pi \delta(E-H_0)K) dE
\]

(2.30)

This form is particularly amenable to low temperature approximations, since for small \( E \), we can use \( \tan^{-1} x \approx x \).

One feature common to all the forms given is that they readily lend themselves to perturbative expansions. This is a very useful tool for studying behaviour near troublesome singularities, and further clarifies the structure of the partition function, facilitating the identification and removal of disconnected contributions. We look at this in the following section.

It also enables some approximate calculations to be made (see for example §4.4).
2.5 The Structure of the Cluster Coefficients

We seek now to establish in more detail the structure of the cluster coefficients, following on the development of the previous section.

Combining equations (2.14) and (2.18), we have

$$b_k - b_k^0 = -\frac{1}{2\pi i} \lim_{\nu \to \infty} \frac{1}{\nu_1 V} \int_C dz \ e^{\nu z} \ Tr[A \ (G-G_0)]_e \quad (2.31)$$

The connected part of the trace is formally obtained in a manner analogous to the construction of the $U_q$ functions by

Combining equations (2.14) and (2.18), we have

The connected part of the trace is formally obtained in a manner analogous to the construction of the $U_q$ functions by equations (2.6). If the total system potential is a sum of two body potentials, $V = \sum_a V_a$, then all terms of the form $A'(G'-G_0)$ must be subtracted from $A(G-G_0)$, where $G'$ is the propagator of the system with one or more of the pair potentials switched off, and $A'$ is the symmetrization operator defined by (2.15), but acting only on the interacting particles.

To make explicit the way in which these disconnected terms subtract from the full propagator, we can use either a potential expansion by iteration of the identity

$$G = G_0 + G_0 \ V \ G \quad (2.32)$$

or the multiscattering expansion of the T-matrix, noting that

$$G - G_0 = G_0 \ T \ G_0 \quad (2.33)$$

We examine first the perturbation series generated by (2.32). It is evident that the terms arising out of the disconnected partly interacting operators $A'(G'-G_0)$ will be subsets of the expansion
of the fully interacting $A(G-G_0)$, so subtraction becomes simply a matter of cancellation.

A diagrammatic representation of the terms makes this clear.

Represent the $\ell$ particles by $\ell$ vertical lines, joined by a dotted line at every interaction. The symmetrization operators introduce permutations of the particles in the final state. These are factorized into interchanges which are represented by crossed particle lines, and the overall diagram has the sign appropriate to the statistics of the particles and the order of the permutation. The diagrams are read downwards to give the corresponding term from left to right, with a free particle propagator $G_0$ at the beginning and one after every interaction.

For example, in Fig. 2, (i) is the diagram of a fourth order term in the third cluster coefficient, and its contribution to the trace is $\text{Tr}(G_0 V_2 G_0 V_1 G_0 V_1 G_0 V_3 G_0)$.

![Diagrams](image)

(i) (ii) (iii) (iv)

**Figure 2.**

To determine the connectedness of a particular term both interactions and exchanges must be taken into account. Thus (i) and (ii) are connected while (iii) and (iv) are not.
It is apparent that the disconnected diagrams are the ones that are cancelled off when the connected part of the trace is taken.

This leads to a direct way of evaluating (2.31), by simply taking contributions from connected diagrams only. As an approximation method, terms up to a given order in potential strength (number of interactions) can be calculated. See for example §4.4. Alternately, we need to look at a way of at least partially summing the series.

Such an approach is provided by the multiscattering expansion

\[ T = \sum_{a} t_{a} + \sum_{a \neq \beta} t_{a} G_{\beta} t_{\beta} + \sum_{a \neq \beta} \sum_{\beta \neq \gamma} t_{a} G_{\beta} G_{\gamma} t_{\gamma} + \ldots \]  

(2.34)

where the two-body t-matrices satisfy

\[ t_a = V_a + V_a G_0 t_a \]  

(2.35)

Iterating (2.35) it is clear that each \( t_a \) represents the sum of all repeated interactions between the same pair of particles. Diagramatically we have

\[ \text{Figure 3.} \]

where the circle denotes the two-body t operator.
Expanding the $T$ in (2.33) and comparing the resultant series to the perturbation expansion generated by (2.32), we see that each term of the multiscattering series is the sum of an infinite subseries of the potential expansion.

From (2.30) we have now

$$b_y - b_y^0 = \frac{1}{2\pi i} \lim_{V \to \infty} \frac{1}{V} \int_C dz e^{-\beta z} \text{Tr}[\Lambda(G_0 \sum_a t_a G_0 + G_0 \sum_{a\beta} t_a G_0 t_\beta G_0 + \ldots)]_c$$

(2.36)

The diagrammatic representation of the terms of the integrand is exactly analogous to that of the potential series, but the partial summation greatly simplifies the overall structure by eliminating all diagrams with consecutive repeated interactions between the same pair of particles.

As before, the connected part of the trace is obtained by retaining only those terms corresponding to connected diagrams, taking account of symmetrization as well.

We note that the multiscattering series is not perturbative since each $t_a$ contains the potential to all orders.

In the preceding section, we saw that the analyticity of the scattering amplitude in the neighbourhood of the energy shell was critical in determining whether the on-shell S-matrix formulation would be valid. The virtue of the expansion form (2.35) is that it makes this problem more accessible by expressing the half-off-shell scattering amplitude in terms of the simpler two-body off-shell amplitudes.

We shall use this approach in §4.5 to determine the analytic structure of the scattering amplitude for our model and to identify
explicitly the source of the troublesome forward singularities mentioned in §2.3.

For the present, we restrict ourselves to some qualitative comments in the following section on the nature and significance of these divergent terms.
2.6 Forward Divergences and Other Singularities in the Scattering Formalism

When the trace in (2.36) is taken with respect to energy eigenstates in the momentum representation, it is found that certain terms diverge in the on-shell limit. These have been called forward divergences because they arise from terms in the multiscattering series which correspond to forward scattering diagrams.

To illustrate this we take an arbitrary off-shell second order term of the three-particle amplitude

\[
\langle p | t_i (z) G_0 (z) t_j (z) | p' \rangle = \int dp'' \frac{\delta (\Sigma p - \Sigma p'') \delta (p_i - p'') \chi (q_i, q'', p_i, z) \delta (\Sigma p'' - \Sigma p') \delta (p'' - q') \chi (q'', q', p', z)}{z - p''^2}
\]

where the momentum vectors \( p, p', p'' \) are an abbreviation for the full state vectors \( p_1, p_2, p_3 \) etc, and the \( \chi 's \) are the two body amplitudes with the momentum conserving delta functions extracted.

Forward scattering corresponds to the situation \( p = p ' \). In this case the delta functions completely determine the intermediate momenta, forcing energy conservation throughout. If we now put \( z \) on-shell, the propagator of course diverges.

We note that the matrix elements required for the trace in (2.36) are precisely these forward scattering elements and that we do aim to use the formulation on-shell, so these divergences are a problem.

This is not to say that the singularities in \( T \) will cause divergences in the cluster coefficients. Naturally the cluster
coefficients must be well-defined, and indeed no problems arise if the formalism is kept off-shell until the last step, or as will be seen later, if different basis states are used. But although we know that the divergences are spurious and must cancel, they are troublesome in that they render the calculations difficult.

We also observe that this behaviour is completely independent of the form of $\chi$ and therefore of the nature of the interaction, provided that it is a local two-body one. In fact these are the well-known potential independent rescattering singularities of the on-shell multiparticle amplitude.

Mathematically they arise from the use of plane wave states as a basis, which are of infinite extent and result in the delta functions that force energy conservation.

Physically they correspond to processes where a particle may travel between two scattering events over a distance large compared with the range of the force. Such processes, also termed double scattering, are evidently not true three-body interactions, but rather two two-body interactions, linked by the long range exchange of a real particle.

A more realistic approach would be to replace plane waves with wave packet states. In this case, there would not be a unique momentum associated with each particle and the highly singular delta functions would not appear. The physical effect is to limit the range of overlap of the wavefunctions by localising the particles. However any calculations in this representation would be difficult because wave packet states are not eigenstates of the
Hamiltonians.

One alternative suggested by Dashen, Ma and Bernstein\(^{(31)}\) is to work in an angular momentum representation. Because the angular momentum \(l\) is a conserved quantity, the basic identity (2.22) can be derived for each \(l\), with an ultimate summation over \(l\). The forward amplitudes then do not appear at all.

Two other approaches, keeping the energy off-shell and using a rotation operator, have been discussed in §2.3. Although they are formally valid\(^{(41,42)}\) they do to some degree defeat the purpose of the original on-shell formulation. We shall use the off-shell approach later for specific calculations on our model, but because the model is one-dimensional, both the angular momentum representation and the rotation technique are inapplicable to our work.

In fact, the forward singularities are more difficult to handle in one-dimensional systems not only because the choice of base states is more restricted, but also because the singularities persist to a higher order than in three-dimensional models.

Taking three-particle systems specifically, it has been found that in three-dimensional models only the second order terms are divergent. Stelbovics\(^{(49)}\) has shown that third and higher order terms are analytic for arbitrary separable two-body potentials. The model we use is directly comparable, being a one-dimensional analogue with point vertex functions, and we have found (see §4.5) with an analysis similar to that of Stelbovics, that both second and third order forward scattering terms are singular, while fourth and higher order terms are analytic.

The singularities persisting to a higher order in one dimension than in three can be understood in terms of the reduced phase space...
for intermediate integrations to remove singularities.

Other possible sources of singularities include bound states, poles in the amplitudes and anomalous threshold scattering.

Bound states have been explicitly dealt with by several of the authors cited, and since our model is repulsive, we shall not consider them further.

The poles arising out of the amplitudes of our model are well off-shell and not troublesome. Possibly for some potentials they may need to be considered.

The question of anomalous thresholds in three-particle amplitudes has not been fully explored. Rubin, Sugar and Tiktopoulous have derived mass constraints for three dimensional anomalous thresholds by Landau analysis. These conditions may preclude anomalous threshold scattering for three equal mass one-dimensional particles.

Forward scattering singularities persist to higher orders for systems of four or more particles. Examples may be found in the papers of Dashen et al. (**1, **41, **42)
2.7 Conclusions

In this chapter we have seen how the cluster coefficients are defined and their relation to the thermodynamics of the system they describe.

Because of their significance to statistical mechanics, much work has been devoted to establishing computational methods that can be applied to models of interest.

A brief examination of these developments has revealed that, apart from the second cluster coefficient which is essentially simpler, most of the techniques evolved yield only low energy approximations for $b_3$, and that extension to any higher coefficients appears very difficult.

The exception is the on-shell S-matrix formulation, which promises direct calculation of any coefficient from experimental data, and further, is readily generalized for a relativistic system.

However, we have also seen that there are serious difficulties with this formulation associated with the regularity of the scattering amplitude.

It is our aim in this thesis to explore the scattering approach and to gain an understanding of the problems in its application. We do this by selecting a model which is simple enough to solve directly, and examine the outcome of applying the various techniques at our disposal. The model, which we have described in §1.3, has several features which make it suitable for our purpose.

Its cluster coefficients are already known, thanks to the work of Yang and Yang, providing ready checks for other methods.

Besides having the $\lambda$-particle eigenfunctions both in a box and in the continuum limit, and the S-matrix, we are also able to
construct the three body scattering amplitude and thus study directly the source of the troublesome singularities.

Finally, there are several useful limits built into the model. Letting \( c \to 0 \) for symmetric statistics yields the free Bose gas, but if \( c \to \infty \) the system behaves like a free Fermi gas. For some calculations, it will be convenient to consider distinguishable particles, but generally we use symmetric statistics.

We turn now, in the following two chapters to examine first the two body problem, and then the three body case of the model, and to investigate how far the scattering formulation can be taken in the context of these systems.
3.1 Description of the System

We take now the two-body case of the model described in §1.3, and establish some of its properties, so that we may investigate in the following sections, various ways of calculating the second cluster coefficient, and in particular, the approach developed in §2.5.

The system consists of two particles in one dimension, with position coordinates \( x_1 \) and \( x_2 \), interacting via a repulsive delta function potential \( v \) such that

\[
\langle x_1 x_2 | v | x_1' x_2' \rangle = 2c \delta(x_1 - x_1') \delta(x_2 - x_2') \delta(x_1' - x_2')
\]

The hamiltonian is

\[
h = h_0 + v = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} + 2c \delta(x_1 - x_2)
\]

or in centre of mass coordinates, \( r = x_1 - x_2 \), \( p = \frac{1}{2}(k_1 - k_2) \), where \( k_1 \) and \( k_2 \) are the initial momenta of the particles,

\[
h | r p \rangle = (2p^2 + 2c \delta(r)) | r p \rangle
\]

and \( K = k_1 + k_2 = 0 \) defines the frame.

The initial state of the system must have no interactions in its past, so if \( x_1 < x_2 \), and particle 1 has momentum \( k_1 \) originally, then \( k_1 > k_2 > 0 \). We note that the momentum labels serve to distinguish between the actual two values of momentum, and do not refer to particle labels. After interaction, either particle may have either momentum.

Footnote: We shall use lower case letters to denote two-body operators as distinct from the analogous many-body operators. Statistics will be indicated throughout the thesis by the suffixes D, S or A for distinguishable, symmetric or antisymmetric.
The most direct method of obtaining the wavefunction is to take an initial state and consider the effect of interaction, which can result only in reflection or transmission. So we can write

\[
\psi_k^D(x) = \frac{1}{2\pi} \begin{cases} 
    e^{i k \cdot x} + r_{12} e^{i(k_1 x_2 + k_2 x_1)} & x_1 > x_2 \\
    t_{12} e^{-i k \cdot x} & x_1 < x_2 
\end{cases} \tag{3.1}
\]

where \( k \) and \( x \) are \((k_1, k_2)\) and \((x_1, x_2)\) and \( r_{12} \) and \( t_{12} \) are the reflection and transmission coefficients respectively.

The boundary conditions

\[
1 + r_{12} = t_{12} \text{ at } x_1 = x_2 \tag{3.2}
\]

\[
-\frac{\partial \psi}{\partial x} \bigg|_{-\epsilon}^{\epsilon} + c \psi(0) = 0 \tag{3.3}
\]

determine the coefficients. Equation (3.3) is obtained by integrating the Schrödinger Equation from \( r = -\epsilon \) to \( +\epsilon \).

It is not difficult to show that

\[
t_{12} = \frac{2|p|}{2|p|+ic} \tag{3.4}
\]

\[
r_{12} = \frac{-ic}{2|p|+ic}
\]

The wavefunction for two bosons can be obtained by symmetrizing (3.1)

\[
\psi_k^S(x) = \frac{1}{2^k} \frac{1}{2\pi} \begin{cases} 
    Z_{12} e^{i k \cdot x} + e^{i(k_1 x_2 + k_2 x_1)} & x_1 > x_2 \\
    e^{i k \cdot x} + Z_{12} e^{i(k_1 x_2 + k_2 x_1)} & x_1 < x_2
\end{cases} \tag{3.5}
\]
where we define \( Z_{12} = r_{12} + t_{12} = \frac{2|p|-ic}{2|p|+ic} \) \( (3.6) \)

The bose wavefunction can also be obtained by use of Bethe's hypothesis and periodic boundary conditions, as outlined in §1.3, and this method yields the more symmetric result

\[
\psi^S_k(x) = \frac{1}{2\pi} \frac{1}{2\pi} (e^{i\theta_{12}} e^{ik.x} + e^{i\theta_{12}} e^{i(k_1x_2+k_2x_1)}) x_1 < x_2 \quad (3.7)
\]

where \( \theta_{12} = 2 \tan^{-1} \frac{c}{k_1-k_2} \). The symmetry requirement

\[
\psi^S_k(x_1 x_2) = \psi^S_k(x_2 x_1)
\]

gives the wavefunction for \( x_1 > x_2 \). The forms (3.5) and (3.7) are equivalent, differing only by the phase factor \( e^{i\theta_{12}} \).

It is a simple matter to show that the wavefunctions satisfy the Lippmann-Schwinger equation

\[
|\psi_k> = |\psi_k> + g^+_0 v|\psi_k>
\]

where \( |\psi_k> \) is the free particle state and \( g^+_0 \) the free particle propagator. This indicates that the wavefunction is a proper representation of the asymptotic scattering state and is correctly normalized in the infinite domain.

Conversely, equation (3.8) may also be used to construct the wavefunctions. The off-shell t-matrices are obtained from either of the identities

\[
t(z) = v + v g_0(z) t(z) \quad (3.9)
\]

\[
t(z) = v + v g(z) v \quad (3.10)
\]
where $z$ is an arbitrary energy parameter, and $g$ the propagator
\[
\frac{1}{z-h}, \quad \text{and the half off-shell } t \text{ from }
\]
\[
\langle pK|t|p'K'\rangle = \langle pK|\psi_p\psi_{p'K'}\rangle
\]

We find
\[
\langle pK|t^D(z)|p'K'\rangle = \frac{D}{z} \delta(K-K') \frac{\sqrt{2z-K^2}}{\sqrt{z-K^2+i\epsilon}}
\]
\[
\langle pK|t^S(z)|p'K'\rangle = \frac{2}{z} \frac{D}{z} \delta(K-K') \frac{\sqrt{2z-K^2}}{\sqrt{z-K^2+i\epsilon}}
\]

On-shell these become
\[
\langle pK|t^D|p'K'\rangle = \frac{D}{z} \delta(K-K') \frac{2|p'|}{2|p'|+i\epsilon}
\]

and
\[
\langle pK|t^S|p'K'\rangle = \frac{2}{z} \frac{D}{z} \delta(K-K') \frac{2|p'|}{2|p'|+i\epsilon}
\]

The on-shell $S$-matrices are now derived from the defining equation
\[
S(E) = I - 2\pi i \delta(E-h_0)t(E)
\]

which yields, with $E = 2p^2 + \frac{1}{2}K^2$.
\[
\langle pK|S^D|p'K'\rangle = \delta(K-K') \left[ \delta(p-p') \frac{2|p|}{2|p|+i\epsilon} + \delta(p+p') \frac{-i\epsilon}{2|p|+i\epsilon} \right]
\]

and
\[
\langle pK|S^S|p'K'\rangle = \delta(K-K') \left[ \delta(p-p') + \delta(p+p') \right] \frac{2|p|-i\epsilon}{2|p|+i\epsilon}
\]

which can also be written
\[
\langle k_1 k_2 |S^S|k_1' k_2'\rangle = \left[ \delta(k_1-k_1') \delta(k_2-k_2') + \delta(k_1-k_2') \delta(k_2-k_1') \right] Z_{12}
\]
3.2 Direct Calculation of the Second Cluster Coefficients in the Position Representation

Knowledge of the wavefunction enables a direct calculation of the second cluster coefficients from equation (2.10). Taking the case of symmetric statistics first, we write

\[
\frac{b_2^s-b_2^0}{2} = \frac{1}{2} \int_{-\infty}^{\infty} \langle x_1 x_2 | U_2^0 | x_1 x_2 \rangle \delta(x_1) dx_1 dx_2
\]

\[
= \frac{1}{2} \int_{-\infty}^{\infty} dx \, dk \, e^{-\beta k^2} \left[ \psi_k^S(x) \psi_k^S(x) - \psi_k^S(x) \psi_k^S(x) \right] \delta(x_1)
\]

where the free particle wavefunctions \( \psi_k^S(x) \) are properly symmetrized for bosons. We use equation (3.7), and by algebraic manipulation obtain

\[
\frac{b_2^s-b_2^0}{2} = \frac{1}{2} \int_{-\infty}^{\infty} dx \, dk \, \delta(x_1) e^{-\beta (k_1^2 + k_2^2)} e^{i(k_1 \cdot k_2)(x_1 \cdot x_2)} e^{i\theta_{12} - 1}
\]

\[
\quad \text{for } x_1 < x_2
\]

Now

\[
e^{i\theta_{12} - 1} = e^{2i (k_1 \cdot k_2)} e^{i\theta_{12} - 1} = \frac{2ic}{k_1 - k_2 - ic} = -2c \int_{0}^{\infty} e^{i(k_1 + ic)s} ds
\]

This integral representation of a pole is a very useful technique which will frequently be used in the calculations of this and the next chapter. Completing the squares in \( k_1 \) and \( k_2 \) in the exponent we have

\[
\frac{b_2^s-b_2^0}{2} = -\frac{c}{4\pi^2} \int_{0}^{\infty} ds \int_{-\infty}^{\infty} dx dk \delta(x_1) e^{-\beta (k_1 \cdot k_2)^2/2\beta} e^{-\beta(x_1^2 + x_2^2)/2\beta} e^{i\theta_{12} - 1}
\]

\[
= -\frac{c}{4\pi^2} \left( \frac{\pi}{\beta} \right)^2 \int_{-\infty}^{\infty} dx \int_{0}^{\infty} ds \, e^{-\beta(x_1^2 + x_2^2)/2\beta c^2} \delta(x_1) \quad \text{for } x_1 < x_2
\]
We now perform the $x_1$ integration, relabel $s + x_2$ as $s$, and noting that this form is only valid for $x_2 > 0$, divide $\int_{-\infty}^{\infty} dx_2$ into $\int_{-\infty}^{0} dx_2$ and $\int_{0}^{\infty} dx_2$. The appropriate form for $x_2 < 0$ is obtained by exchanging $x_1$ and $x_2$ in the wavefunction and following through the same process. By taking $x = x_2$ in one integral and $x = -x_2$ in the other, we can combine the terms, resulting in

$$-\frac{c}{2\pi \beta} \int_{0}^{\infty} dx \int_{x}^{\infty} ds \ e^{(s^2/2\beta) - cs} e^{cx}$$

To evaluate this expression further, we integrate by parts with respect to $x$, using the formula

$$\int_{0}^{\infty} dx \ u(x) \int_{x}^{\infty} dy \ v(y) = [U(x) \int_{x}^{\infty} dy \ v(y)] \bigg|_{x=0}^{x=\infty} - \int_{0}^{\infty} dx \ U(x) \frac{d}{dx} [V(\infty) - V(x)]$$

$$= -U(0) \int_{0}^{\infty} dy \ v(y) + \int_{0}^{\infty} dx \ U(x) \ v(x) \quad (3.17)$$

where $\frac{dU(x)}{dx} = u(x)$ and $\frac{dV(x)}{dx} = v(x)$. We find

$$b_2^S b_2^S = -\frac{c}{2\pi \beta} \left[ -\frac{1}{c} \int_{0}^{\infty} ds \ e^{(s^2/2\beta) - cs} + \int_{0}^{\infty} dx \ e^{cx} e^{(s^2/2\beta) - cx} \right]$$

$$= \frac{1}{2\pi \beta} \int_{0}^{\infty} ds \ e^{-s^2/2\beta} (e^{-cs} - 1) \quad (3.18)$$

We have published this result\(^{(51)}\) and it has also been obtained by Servadio\(^{(52)}\).

For distinguishable particles, we use the wavefunction (3.4), and with a similar method, arrive at
\[ b_2^D = \frac{1}{4\pi \beta} \int_0^\infty ds \ e^{-s^2/2\beta} (e^{-cs} - 1) \quad (3.19) \]

We observe the interesting relation

\[ b_2^S - b_2^{S0} = 2b_2^D \quad (3.20) \]

which is a result of the symmetrization procedure.
3.3 Calculation of $b_2^S - b_2^S_0$ from the S-matrix

We are now in a position to test the validity of the on-shell S-matrix prescription for the second cluster coefficient.

Since it is convenient to work in the centre of mass frame, we combine equations (2.12) and (2.23) to write

$$b_2^S - b_2^S_0 = \frac{1}{21} \frac{1}{(4\pi\beta)^{\frac{3}{2}}} \frac{1}{2\pi i} \int_0^\infty dE \ e^{-\beta E} \ Tr(S^S_\text{CM} \ dE \ S^S_\text{CM})$$  \ (3.21)

where we have added a factor of $\frac{1}{2}$ to compensate for double symmetrization of this integrand (see Appendix A) and where

$$\langle p \mid S^S_\text{CM} \mid p' \rangle = (\delta(p-p') + \delta(p+p')) \ \frac{2|p|-ic}{2|p|+ic}$$

from equation (3.14a). Then the trace of (3.21) becomes

$$\int_0^\infty dE \ e^{-\beta E} \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' \ \langle p \mid S^S_\text{CM} \mid p' \rangle \ \frac{d}{dE} \ \langle p' \mid S^S_\text{CM} \mid p \rangle$$  \ (3.22)

If we wish to use the on-shell formulation, we have the condition $E = 2p^2 = 2p'^2$ and the energy differentiation can be expressed as a momentum derivative. However there is already a problem, since the diagonal elements required for the trace contain products of delta functions like $\delta^2(p+p')$ and $\delta(p+p')\delta(p-p')$.

One possible, though non-rigorous, way to proceed would be to ignore either the first or second set of delta functions. We show in §4.3 that if we keep the second set of delta functions, the energy differentiation of them yields a term which cancels all the dynamical information, leaving only a constant.
On the other hand, keeping the first set of delta functions only, yields

\[ \int_{-\infty}^{\infty} dE \ e^{-\beta E} \int_{-\infty}^{\infty} dp' \left( \delta(p-p') + \delta(p+p') \right) \frac{2|p|+ic}{2|p|} dE \frac{2|p'|-ic}{2|p'|} \]

which with \( E = 2p^2 \) becomes

\[ 2 \int_{-\infty}^{\infty} dp \ e^{2\beta p^2} \frac{4ic}{4p^2+c^2} = 4 \int_{-\infty}^{\infty} dp \ e^{2\beta p^2} \left( \frac{1}{2p-ic} - \frac{1}{2p+ic} \right) \quad (3.23) \]

Relabelling \( p \) as \(-p\) in the second term, combining and using the integral representation (3.16) for the pole, we obtain

\[ 8i \int_{-\infty}^{\infty} dp \int_{0}^{\infty} ds \ e^{-2\beta p^2} \cdot 2ip \cdot cs \]

We complete the square in \( p \), perform the \( p \) integration and returning to equation (3.21), find

\[ b_2^{S} - b_2^{S_0} = \frac{1}{2\pi i} \int_{0}^{\infty} ds \ e^{s^2/2\beta \cdot cs} \quad (3.24) \]

which is only part of the complete \( b_2^{S} - b_2^{S_0} \) given by (3.18).

Although the procedure used to arrive at this result has not been strictly rigorous, we have found that the origin of the discrepancy lies in the actual derivation of the on-shell formalism. Returning to equation (2.18), we observe that as an off-shell operator identity it is strictly valid provided the contour \( C \)
remains off the real axis. After the trace has been performed, it is permissible to take the on-shell limit, \( \epsilon \rightarrow 0 \). However in arriving at (2.23), this limit has been taken before the trace, in the step

\[
\lim_{\epsilon \rightarrow 0} 2i\epsilon \ G_0^+ G_0^- = 2\pi i \delta(E-H_0)
\]

If the T-matrix which this expression multiplies is analytic in the region of the propagator poles, there is no difficulty. If however the on-shell T-matrix contains singularities on the real axis, great care must be taken in the way the contour \( C \) is compressed, so that no residues are lost. This is in fact what has happened in the above calculation, as will be seen in the next section.

We observe also, that the correct result can be obtained from (3.24) by subtracting the free particle limit \( (c \rightarrow 0) \), so that what we have actually got from the S-matrix formula, is \( b_2^s \).
3.4 Calculation of $b^D_2$ from $g$

The delicacy of the on-shell limit can perhaps best be illustrated by the case of distinguishable particles, where we are able to calculate $\text{Tr}(g-q_0)$ directly. This means we can go back to the stage of equation (2.18), and examine precisely what happens when $\eta \to 0$.

If we define the ket $|x\rangle = \int |p\rangle dp$, the potential can be written as the dyad

$$\nu = \frac{c}{\pi} |x\rangle \langle x|$$

and we can write

$$<x|g = <x|q_0 + <x|q_0 \frac{c}{\pi} |x\rangle \langle x|g$$

which gives us

$$<x|g = \frac{<x|q_0}{1 - \frac{c}{\pi} <x|q_0 |x\rangle}$$

So

$$\text{Tr}(g-q_0) = \text{Tr} q_0 \nu \ n g$$

$$= \frac{c}{\pi} \int \frac{<x|q_0 |x\rangle <x|q_0 |x\rangle}{1 - \frac{c}{\pi} <x|q_0 |x\rangle} \ dk$$

$$= \frac{c}{\pi} \ln(1 - \frac{c}{\pi} <x|q_0 |x\rangle)$$

Now the matrix element $<x|q_0 |x\rangle$ can be computed by contour integration in the upper half of the complex - $p$ plane, and we find
\[ <\chi|q_0|\chi> = \begin{cases} -\frac{\pi i}{\sqrt{2z}} & \text{for } \text{Im}z > 0 \\ \frac{\pi i}{\sqrt{2z}} & \text{for } \text{Im}z < 0 \end{cases} \]

and so

\[ \text{Tr}(g-g_0) = \begin{cases} \frac{-ic}{2z(ic+\sqrt{2z})} & \text{for } \text{Im}z > 0 \\ \frac{-ic}{2z(ic-\sqrt{2z})} & \text{for } \text{Im}z < 0 \end{cases} \] (3.25)

Now from equations (2.12) and (2.18) we have

\[ b_2 = \frac{\sqrt{2}}{2\eta} \frac{1}{(4\pi^2)^{\frac{1}{2}}} \frac{-1}{2\pi i} \int_{C} e^{\beta Z} \text{Tr}(g-g_0) dz \] (3.26)

\[ = -\frac{-1}{(2\pi \beta)^{\frac{1}{2}} 2\pi i} \int_{C} e^{\beta Z} \frac{-ic}{2z(iz+\sqrt{2z})} dz \] (3.27)

where the sign in the denominator is determined as in (3.25). We observe that the integrand has a pole at the origin \( Z = 0 \). If we take the limit \( \eta \to 0 \) at this stage, the contour \( C \) which encloses the origin, collapses to the positive real axis and we lose the contribution of the residue at \( Z = 0 \).

\[ \lim_{\eta \to 0} \int_{C} e^{\beta Z} \frac{-ic}{2z(iz+\sqrt{2z})} dz = -ic \int_{0}^{\infty} e^{\beta E} \frac{1}{2E(ic+\sqrt{2E})} - \frac{1}{2E(ic-\sqrt{2E})} dE \]

\[ = 2ic \int_{0}^{\infty} \frac{e^{\beta E}}{\sqrt{2E(2E+C^2)}} dE \] (3.28)

Letting \( E = 2p^2 \), we note that the resulting integral
\[
4ie \int_0^{\infty} dp \frac{e^{-2\beta p^2}}{4p^2 + e^2}
\]

has the same form as (3.23) obtained via the S-matrix, and so leads to the incorrect result.

If on the other hand we keep the energy off-shell, we must take the residue of (3.27) at \( Z = 0 \), which is

\[
\left( \frac{-1}{(2\pi)^{1/2}} \right) \frac{1}{4\pi i} (-2\pi i) \left( -\frac{1}{2} \right) = \frac{-1}{4(2\pi\beta)^{1/2}}
\]

\[
= \frac{-1}{4\pi\beta} \int_0^{\infty} e^{-z^{2}/2\beta} \, ds \quad (3.29)
\]

which is just the term we need to render the correct result, (3.19).
4.1 Description of the System

In this chapter we deal with the three-body case of the model described in §1.3.

The hamiltonian of the system is given by (1.1), with \( n = 3 \), and its wavefunctions have the form of Bethe’s ansatz (1.2),

\[
\psi_k(x) = \sum_{P} a(P, k) e^{ipk \cdot x}
\]

(4.1)

where \( x = (x_1, x_2, x_3) \) are the position coordinates, \( k = (k_1, k_2, k_3) \) are the initial momenta of the particles such that \( k_1 > k_2 > k_3 \) and we sum over the six permutations \( P \) of \( k \).

Lieb and Liniger’s \(^4\) analysis of the three boson case, outlined in §1.3, yielded the symmetric wavefunction in region \( RI : 0 < x_1 < x_2 < x_3 < L \), and hence by symmetry in all other regions.

In \( RI \), the coefficients \( a(P, k) \) are given by the following rule. Let \( P \) be decomposed into a series of transpositions of adjacent \( k_i \) only. For each transposition write down the factor \(-e^{i \theta_{s,t}}\) where \( k_s \) was to the left of \( k_t \) before the operation. Then \( a(P, k) \) is the resultant product of these factors and the normalization factor \( 6^{-\frac{1}{2}}(2\pi)^{-3/2} \), with

\[
\theta_{s,t} = \theta(k_s - k_t) = -2 \tan^{-1} \frac{k_s - k_t}{c}.
\]

(4.2)

Turning to distinguishable particles, we remove the symmetry which rendered the box normalized system soluble. However, McGuire\(^3\) has developed an alternative treatment which does not depend on symmetric statistics, but uses the analogy of the
propagation of electromagnetic waves through wedges of conducting material. This permits the application of a simple ray tracing procedure to obtain the total wavefunction.

The evolution of the system is represented by a trajectory in a two dimensional position space which is divided into six regions, as in Fig. 4. Collisions between particles occur on the boundaries \( x_1 = x_2 \) etc.

An incoming wave is one which has no collisions in its past. If the initial particle ordering is \( x_1 < x_2 < x_3 \), this condition leads to the requirement \( k_1 > k_2 > k_3 \), and the incoming ray is in region I.

![Figure 4.](image)

It is important to note that although the \( j \)th particle has momentum \( k_j \) in the initial state, the subscripts on the momenta do not refer to the particles assuming those momenta, but merely
serve to distinguish between the three values. On the other hand, the position coordinates do carry the particle labels.

Thus the reflection and transmission coefficients, defined for the two-body problem in equations (3.4), are now labelled by the momenta involved in the interaction

\[
t_{ij} = \frac{|k_i - k_j|}{|k_i - k_j| + ic} \quad (4.3)
\]

\[
r_{ij} = \frac{-ic}{|k_i - k_j| + ic}
\]

and again

\[
z_{ij} = r_{ij} + t_{ij} = \frac{|k_i - k_j| - ic}{|k_i - k_j| + ic} \quad (4.4)
\]

The total wavefunction is found by tracing both rays \( \alpha \) and \( \beta \) through the diagram in Fig. 4, until they become outgoing waves, i.e. having no possible further collisions. This corresponds to the particles being in ascending order of both position and momentum. It turns out that on any path from incoming to outgoing state, there are exactly three interactions, each contributing the appropriate coefficient to the wave amplitude.

This again points up the classical-like features of the model, in that there are no repeated interactions, or new momenta generated. We made this observation in §1.3, noting that this property was peculiar to the particular model, and that it depended upon the masses and interaction strengths being equal. In the optical analogue, it appears as the absence of diffraction.

However the treatment is not entirely classical-like, because to obtain the full solution we add the contributions from both rays
These correspond to the two possibilities, particle 2 may first interact with either particle 1 or particle 3.

If we use the notation

$$[ijk] = \frac{1}{(2\pi)^3} e^{i(k_1x_1 + k_jx_2 + k_1x_3)}$$ (4.5)

we can express the total wavefunction in tabular form:

<table>
<thead>
<tr>
<th>Region</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
<th>VI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Wave Type</td>
<td>123</td>
<td>r_{12}r_{13}</td>
<td>r_{23}r_{12}r_{13}</td>
<td>t_{12}</td>
<td>t_{23}</td>
<td>t_{12}t_{13}</td>
</tr>
<tr>
<td></td>
<td>[231]</td>
<td>-</td>
<td></td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>[312]</td>
<td>-</td>
<td>r_{13}r_{23}</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>[213]</td>
<td>r_{12}</td>
<td>-</td>
<td>r_{12}t_{13}</td>
<td>-</td>
<td>t_{13}t_{23}r_{12}</td>
</tr>
<tr>
<td></td>
<td>[132]</td>
<td>r_{23}</td>
<td>-</td>
<td></td>
<td>t_{12}t_{13}r_{23}</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>[321]</td>
<td>r_{12}r_{13}r_{23}</td>
<td>r_{13}t_{12}</td>
<td>r_{12}t_{23}</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 1.

Symmetrization in the usual way yields the corresponding wavefunction for bosons

$$(31)_{\psi}^{S}_{ik}(x) = [123] + Z_{12}[213] + Z_{23}[132] + Z_{12}Z_{13}Z_{23}[321] + Z_{12}Z_{13}[231] + Z_{23}Z_{13}[312].$$ (4.6)

The suffix I denotes that this holds for that region only. Any other region can be written as a permutation of I, and the
wavefunction there will be

\[ \psi^S_{PIk}(x) = \psi^S_{Ik}(P^{-1}x) \]

(4.7)

Gaudin has shown that the set of such wavefunctions satisfies a closure relation in region I, and is orthonormal.

A more convenient form of the coefficients of equation (4.1) for some calculations will be

\[ a(P,k) = e^{-i \sum_{i<j} \arctan \left( \frac{c}{k_{Pi} - k_{Pj}} \right)} \]

(4.8)

We have shown that all these forms of the wavefunction are equivalent within a constant phase factor, \( e^{-i(\theta_{12} + \theta_{23} + \theta_{13})} \).

We have also established in Appendix D, that the wavefunctions satisfy the Lippmann-Schwinger Equations. This is an important result because it confirms that the wavefunctions are indeed full scattering solutions valid in the infinite domain, which renders the \( L \rightarrow \infty \) limit to be taken in some calculations valid.

We now calculate the T-matrices from these wavefunctions, using

\[ \langle P | T | k \rangle = \langle P | V | \psi_k \rangle \]

(4.9)

which is an expression of the operator identity \( T = V \). In the position representation this becomes

\[ \langle P | T | k \rangle = \frac{2c}{(2\pi)^{3/2}} \int e^{iP \cdot x} \left( \delta(x_1 - x_2) + \delta(x_1 - x_3) + \delta(x_2 - x_3) \right) \psi_k(x) d^3x \]  

(4.10)
For distinguishable particles the wavefunction tabulated in Table 1 applies and we divide the region of integration into the six segments I through VI. The potential delta functions have the effect of constraining the integration to the boundaries between the regions. Because the wavefunction is necessarily continuous across each boundary, the coefficients in the regions on either side may be used to find the limiting values on the actual boundaries. To simplify the calculations, we take regions II, III and VI and perform the remaining investigations along both boundaries of each. All terms are of the type

$$\frac{2C}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} t_{12} e^{i(k_1 + k_2 \cdot P_1 \cdot P_2) x + i(k_3 \cdot P_3) x_3} dx dx_3$$

The $x_3$ integration yields a denominator with a small positive imaginary part inserted to ensure that the integral vanishes at the upper limit. The final $x$ integration results in an overall momentum conserving delta function. However there is no requirement of energy conservation from the initial $|p>$ to the final $|k>$ state. Thus what we have is the half-off-shell $T$ matrix for distinguishable particles

$$<p|T^p|k> = \frac{2ic}{(2\pi)^2} \delta (E_k - E_p) \left[ \frac{t_{12} t_{13} t_{23}}{k_1 - P_1 + i\eta} - \frac{t_{23}}{k_1 - P_1 - i\eta} + \frac{t_{12} t_{13} t_{23}}{k_1 - P_2 + i\eta} \right]$$

$$+ \frac{t_{12} t_{23}}{k_1 - P_3 + i\eta} - \frac{t_{13}}{k_2 - P_2 + i\eta} - \frac{t_{12} t_{13}}{k_2 - P_2 - i\eta} + \frac{t_{23}}{k_2 - P_1 + i\eta} + \frac{t_{12} t_{13} t_{23}}{k_2 - P_3 + i\eta}$$

$$+ \frac{t_{12} t_{13} t_{23}}{k_3 - P_3 + i\eta} - \frac{t_{12} t_{13} t_{23}}{k_3 - P_3 - i\eta} - \frac{t_{12} t_{23}}{k_3 - P_1 - i\eta} + \frac{t_{23}}{k_3 - P_2 + i\eta} + \frac{t_{12} t_{13} t_{23}}{k_3 - P_2 - i\eta}$$

$$+ \frac{t_{12} x_{13} t_{23}}{k_1 - P_1 + i\eta} - \frac{t_{13} t_{23}}{k_1 - P_1 - i\eta} + \frac{t_{12} t_{13} t_{23}}{k_1 - P_2 + i\eta} + \frac{t_{23}}{k_1 - P_2 - i\eta} + \frac{t_{12} t_{13} t_{23}}{k_1 - P_3 + i\eta}$$

$$+ \frac{t_{13} t_{23}}{k_1 - P_3 + i\eta} - \frac{t_{12} t_{13} t_{23}}{k_2 - P_2 + i\eta} - \frac{t_{23}}{k_2 - P_2 - i\eta} + \frac{t_{13} t_{23}}{k_2 - P_1 + i\eta} + \frac{t_{12} t_{13} t_{23}}{k_2 - P_3 + i\eta}$$

$$+ \frac{t_{23}}{k_2 - P_3 + i\eta} - \frac{t_{13} t_{23}}{k_2 - P_3 - i\eta} + \frac{t_{12} t_{13} t_{23}}{k_2 - P_1 + i\eta} + \frac{t_{23}}{k_2 - P_1 - i\eta} + \frac{t_{12} t_{13} t_{23}}{k_2 - P_3 + i\eta}$$

When bosons are considered we use the wavefunction (4.6) in a similar way and find
\[
<\Psi|T^0|\kappa> = \frac{2ie}{(2\pi)^2} \delta(E\kappa-E\mu) \sum_{j=1}^{3} \left[ \frac{1+Z_{12}}{k_3-P_j + i\eta} + \frac{Z_{23}(1+Z_{13})}{k_2-P_j + i\eta} + \frac{Z_{12}Z_{13}(1+Z_{23})}{k_1-P_j + i\eta} \right. \\
- \left. \frac{1+Z_{23}}{k_1-P_j + i\eta} - \frac{Z_{12}(1+Z_{13})}{k_2-P_j + i\eta} - \frac{Z_{13}Z_{23}(1+Z_{12})}{k_3-P_j - i\eta} \right]
\]

(4.12)

Symmetrizing (4.11) yields the same result.

The fully off-shell \( T \) matrices, which also contain an explicit dependence on an intermediate energy \( Z \) not equal to either the initial or final energies, are in principle obtainable from the Low equation. This is considerably more difficult to evaluate and is treated in §4.8.

For the present we are more interested in the on-shell scattering operators so that we can examine equation (2.22) in the on-shell limit. The \( T \)-matrices (4.11) and (4.12) can be placed on-shell by applying the energy conserving delta function \( \delta(E\kappa-E\mu) \). It is convenient at this point to take the limit \( \eta \to 0 \) as this generates a delta function from each pole

\[
\lim_{\eta \to 0} \frac{1}{k_i - P_j + i\eta} = \frac{1}{k_i - P_j} + i\pi \delta(k_i - P_j)
\]

(4.13)

We have shown that all the principal part terms vanish on-shell, (proof is given in Appendix F), leaving after some algebra

\[
\delta(E\kappa-E\mu) <\Psi|T^0|\kappa> = -\frac{1}{2\pi i} \left[ \delta_{11} \delta_{22} \delta_{33} (t_{12} t_{13} t_{23} - 1) + \delta_{12} \delta_{23} \delta_{31} x_{12} t_{13} t_{23} \\
+ \delta_{13} \delta_{23} \delta_{31} (r_{12} r_{13} r_{23} + r_{13} t_{12} t_{23}) + \delta_{11} \delta_{23} \delta_{32} x_{12} t_{13} t_{23} \\
+ \delta_{12} \delta_{23} \delta_{31} t_{12} r_{23} + \delta_{13} \delta_{21} \delta_{32} t_{13} r_{12} r_{23} \right]
\]

(4.14)

where \( \delta_{ij} = \delta(k_i - P_j) \) and we have used the identity

\[
\delta(E\kappa-E\mu) \delta(E\kappa-E\mu) \delta(k_i - P_j) = \frac{\delta(k_i - P_j)}{2 |k_j - k_k|} \left( \delta(k_j - P_i) \delta(k_k - P_j) + \delta(k_j - P_p) \delta(k_k - P_i) \right)
\]

(4.15)
with \((ijk)\) being any permutation of \((123)\).

Similarly we find

\[
\delta(e_k^2 - e_p^2) \langle k^\prime | T^S | k \rangle = \frac{c}{4\pi} \sum_p \delta(k-p) \left\{ \frac{(1+Z_{123})(1+Z_{12})}{k_1-k_2} + \frac{(1+Z_{13})(1+Z_{12}+Z_{23})}{k_1-k_3} + \frac{(1+Z_{23})(1+Z_{12}Z_{13})}{k_2-k_3} \right\} \tag{4.16}
\]

We are now in a position to write down the fully on-shell matrix elements of \(S\), which are given by

\[
\langle k^\prime | S(E=e_k^2-e_p^2) | k \rangle = \langle k^\prime | (1-2\pi i \delta(e_p^2-k^2) T) | k \rangle \tag{4.17}
\]

So we have

\[
\langle k^\prime | S^D | k \rangle = \delta_{11} \delta_{22} \delta_{33} t_{12} t_{13} t_{23} + \delta_{12} \delta_{21} \delta_{33} t_{12} t_{13} t_{23}
\]

\[
+ \delta_{13} \delta_{22} \delta_{31} (t_{12} t_{13} t_{23} + t_{13} t_{12} t_{23}) + \delta_{11} \delta_{23} \delta_{32} t_{23} t_{12} t_{13}
\]

\[
+ \delta_{12} \delta_{23} \delta_{31} t_{13} t_{12} t_{23} + \delta_{13} \delta_{21} \delta_{32} t_{13} t_{12} t_{23} \tag{4.18}
\]

and

\[
\langle k^\prime | S^S | k \rangle = \sum_p \delta(k-p) Z_{12} Z_{13} Z_{23} \tag{4.19}
\]

It can easily be verified that (4.19) can be obtained from (4.18) by symmetrization.

The \(S\)-matrix (4.18) has been obtained by McGuire\(^3\) and also by C.N. Yang\(^5,6\) who used group methods and a generalized form of Bethe's Hypothesis to treat the \(N\)-body problem with either repulsive or attractive delta function potentials.
Thacker$^{(54,55)}$ has also studied the three particle system using field theoretic methods and has calculated the scattering amplitude by summing the perturbation series and hence constructed the wavefunction, without recourse to Bethe's Hypothesis.
4.2 Direct Calculation of $b_3^S - b_3^S$ in the Position Representation

Although the wavefunctions (4.6) can be obtained by imposing box normalization, once the limit $L \rightarrow \infty$ has been taken they are essentially fully scattering solutions in the infinite domain, as indicated by the fact that they satisfy the Lippmann-Schwinger Equations. (See Appendix D).

In this section, we present some published work (51) (reprint at end of thesis), in which we have been able to compute the exact third cluster coefficient for symmetric particles directly from the continuum wavefunctions. As a first step towards a scattering formulation of the cluster coefficients, this is an important result.

Subtracting the ideal gas term from equation (2.10) we have

$$b_3^S - b_3^S = \frac{1}{3!} \int_{-\infty}^{\infty} <0x_2x_3 | U_3 - U_3^0 | 0x_2x_3> dx_2 dx_3. \quad (4.20)$$

We use the symmetric wavefunctions with coefficients in the form (4.8). The limits of the regions of configuration space I through VI are now extended to $\pm \infty$, for example

RII : $-\infty < x_2 < x_1 < x_3 < \infty$.

We can then use (4.7) to rewrite (4.20) in the more symmetric and useful form

$$b_3^S - b_3^S = \frac{2}{3!} \int_I <x_1x_2x_3 | U_3 - U_3^0 | x_1x_2x_3> (\delta(x_1) + \delta(x_2) + \delta(x_3)) d^3x. \quad (4.21)$$

We consider first the term $<x | U_3 - U_3^0 | x>$, and using $H_I$ to denote the three particle operator $H_0 + V_I$, we write
\[ \langle x | U_{3} - U_{3}^{0} | x \rangle = \frac{1}{(2\pi)^{3}} \int_{-\infty}^{\infty} \, \, \, dk e^{-\frac{\beta k^{2}}{2}} \left[ \frac{1}{L^{3}} \sum_{p} \left( e^{i (k_{j} x_{j} + k_{k} x_{k})} + e^{-i (k_{j} x_{j} + k_{k} x_{k})} \right) \right] \]

where \( \frac{\beta}{L^{3}} \) is the free particle energy and \( \alpha \) is the symmetric free wavefunction for three and two particles respectively. Continuing, we write

\[ \langle x | U_{3} - U_{3}^{0} | x \rangle = \frac{1}{(2\pi)^{3}} \int_{-\infty}^{\infty} \, \, \, dk e^{-\frac{\beta k^{2}}{2}} \left[ \frac{1}{L^{3}} \sum_{p} \left( e^{i (\theta_{j} k \cdot \theta_{k})} - e^{-i (\theta_{k} \cdot \theta_{j})} \right) \right] \]

where \( \theta_{ij} = \tan^{-1} c / k_{j} - k_{i} \).

This expression is considerably simplified by observing that the thirty six terms in the first summation contain only six distinct terms, each repeated six times. We also relabel the dummy variables \( k_{j} \) and \( k_{k} \) in the second term of the second summation, and obtain

\[ \langle x | U_{3} - U_{3}^{0} | x \rangle = \frac{1}{(2\pi)^{3}} \int_{-\infty}^{\infty} \, \, \, dk e^{-\frac{\beta k^{2}}{2}} \left[ \frac{1}{L^{3}} \sum_{p} \left( e^{i (\theta_{j} k \cdot \theta_{k})} - e^{-i (\theta_{k} \cdot \theta_{j})} \right) \right] \]
Several cancellations are now made, which remove the disconnected terms corresponding to no interactions \((P = I)\), and to particles 1 \((P = (23))\) and 3 \((P = (12))\) propagating freely. We note however that the terms involving scattering between particles 1 and 3 only do not cancel. This is because the restriction to one dimension prevents particles 1 and 3 from interacting without also scattering from particle 2 which is between them in region I.

The remaining terms are

\[
\langle x|U_3-U_3^0|x\rangle = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \frac{k^2}{\beta} \left[ (e^{2i(\theta_{12}+\theta_{13}+\theta_{23})} - e^{2i\theta_{13}}) e^{i(k_1+k_3)(x_1-x_3)} 
+ (e^{2i(\theta_{12}+\theta_{13})} - 1) e^{i(k_1+k_2)x_1+(k_2+k_3)x_2+(k_3+k_1)x_3} \right. 
+ (e^{2i(\theta_{13}+\theta_{23})} - 1) e^{i(k_1+k_3)x_1+(k_2+k_1)x_2+(k_3+k_2)x_3} \bigg]\]

(4.23)

where we have used \(\theta_{ij} = -\theta_{ji}\).

To perform the \(k\) integration we need to simplify the coefficients further.

\[
(e^{2i\theta_{ij}-1}) = \frac{2ic}{k_i-k_j-i\epsilon} 
= -2c \int_0^\infty e^{-i(k_i-k_j-c)s} ds \]

(4.24)

and

\[
(e^{2i(\theta_{12}+\theta_{13})}-1) = (e^{2i\theta_{12}}-1)(e^{2i\theta_{13}}-1)+(e^{2i\theta_{12}}-1)+(e^{2i\theta_{13}}-1) \]

(4.25)

We also need the non-trivial identity

\[
e^{2i\theta_{13}}(e^{2i(\theta_{12}+\theta_{23})}-1)
= [(e^{2i\theta_{12}}-1)+(e^{2i\theta_{23}}-1)][1-(e^{2i\theta_{13}}-1)+\frac{3}{2} \frac{4ic}{k_i-k_j-2i\epsilon}] \]

(4.26)
which can be proved by substitution.

Now with (4.25) and (4.26) all the terms of (4.24) can be expressed as exponentials. Integration proceeds over the $k$ parameters first, by completion of squares. We are left with a sum of terms like

$$\frac{1}{(2\pi)^3} \left( \frac{\pi}{\beta} \right)^{3/2} 4c^2 \int_0^\infty ds \, dt \, e^{-\frac{1}{4\beta} \left[ (x_1 \cdot x_2 \cdot s)^2 + (x_2 \cdot x_3 + s \cdot t)^2 + (x_3 \cdot x_1 + t)^2 \right] / 4\beta \cdot cs \cdot ct}$$

and

$$\frac{1}{(2\pi)^3} \left( \frac{\pi}{\beta} \right)^{3/2} 2c \int_0^\infty ds \, e^{-\frac{1}{4\beta} \left[ (x_1 \cdot x_2 \cdot s)^2 + (x_2 \cdot x_3 + s \cdot t)^2 + (x_3 \cdot x_1)^2 \right] 4\beta \cdot cs}$$

which are then to be substituted back into (4.22) and integrated over the $x$ parameters. Because of the restriction to the region $-\infty < x_1 < x_2 < x_3 < \infty$, the parameters will also appear as limits of integration, such as in the term

$$\frac{1}{3} \left( \frac{1}{2\pi} \right)^{3/2} 4c^2 \int_0^\infty ds \int_0^\infty dx \int_{-\infty}^{+\infty} dx_3 \int_0^\infty e^{-\frac{1}{4\beta} \left[ (s + x_2)^2 + (x_2 \cdot x_3 + s \cdot t)^2 + (x_3 + t)^2 \right] / 4\beta \cdot cs \cdot ct}$$

These are integrable by parts using the formula (3.17), and after lengthy but straightforward algebra, we are left with

$$b^S_3 - b^S_3 = -\frac{6}{(2\pi)^3} \left( \frac{\pi}{\beta} \right)^{3/2} \int_0^\infty ds \int_0^\infty dt \, e^{-\frac{1}{2 \beta} (s^2 + t^2 + s \cdot t)} \frac{e^c s \cdot ct}{e^c s \cdot ct - 1}. \quad (4.27)$$

Our result (24) differs from that obtained with a similar approach by Servadio (52) who found only part of $\langle x | U_3 - U_3 | x \rangle$. Fortunately, the work of Yang and Yang (1,2) provides a check which verifies our formula (4.27). Their work, based on the $n$-body eigenstates with periodic boundary conditions, is discussed in Appendix G, where it is also shown that our cluster coefficient
(4.27) is in agreement with their results.

We observe that the essential feature which renders this calculation possible is the symmetry of the Bose-Einstein wavefunction, which enables the six regions of integration in (4.21) to be reduced to one. For distinguishable particles, the wavefunction in each region bears no relation to that in the others, and no such simplification is available. N. White\textsuperscript{53} has investigated this case and concluded that the necessary integrations are too difficult to perform.

In conclusion then, we have calculated \( S, S' \) by direct integration in configuration space using asymptotic states rather than the more usual box normalized wavefunctions. Although the asymptotic eigenfunctions carry more information than the on-shell scattering operators, the success of this calculation does represent a partial achievement of the aim of deriving cluster coefficients from purely physical scattering parameters.

Further, we have demonstrated that the previously published result of Servadio\textsuperscript{52}, who attempted the same calculation, is incorrect, and that our result is in agreement with the work of Yang and Yang.
4.3 The S-Matrix Formulation of $b_3^S - b_3^{S_0}$

We now examine what happens when the S-matrix formula (2.22) is directly applied to this model.

The symmetric on-shell three body and two body S-matrices are given by (4.19) and (3.14) respectively.

Taking the connected part of (2.22) we have

$$\text{Tr}(e^{-\beta H} - e^{-\beta H_0}) = \frac{1}{2\pi i} \int_0^\infty dE \int dk dk'$$

$$\times \left\{ \delta (k-pk') \sum P \delta (k-k') \frac{d}{dE} \left( \sum Q \delta (k'-ok) \right) \right\}$$

$$- \sum_{i<j} \left( \delta_{ kk}' \left( \delta_{ i i } \delta_{ j j } + \delta_{ i j } \delta_{ j i } \right) \right) \frac{d}{dE} \left( \sum_{ij}' \delta_{ kk}' \left( \delta_{ i i } \delta_{ j j } + \delta_{ i j } \delta_{ j i } \right) \right)$$

(4.28)

where we have used the notation $\delta_{ ij } = \delta (k_i - k_j)$ and

$$Z_{ij}' = |k_i' - k_j'|^{-ic}$$

$$|k_i' - k_j'|^{+ic}$$

An attempt to evaluate this expression immediately runs into a problem of interpretation. Because the S-matrix is on-shell, the energy does not enter explicitly into its elements. In fact the energy and momentum variables are not all independent and the energy derivative could be expressed in terms of partial momentum derivatives. Similarly the energy integration could be transformed into a momentum integration. Whichever way the energy integration is performed, the trace operation will have to be interpreted as being over the remaining parameters only.

A more serious difficulty however is the divergence of products of delta functions whenever their arguments match. This renders
the expression (4.28) as it stands completely meaningless, since every term is non-integrable.

This same problem was encountered in §3.3 with the two-body case. We found there however, that a result, albeit an incorrect one, could be obtained by ignoring one set of delta functions, and that it differed from the correct result only by the free particle limit.

It is a simple task to demonstrate that this approach is not useful in the three-body case.

Let

$$f(k) = Z_{12}Z_{13}Z_{23}$$

and consider the expression

$$\int \int \frac{dk}{dE} \frac{dk'}{dE} f^*(k') \sum_p \delta(k-pk') \frac{d}{dE} [f(k) \sum_q \delta(k'-qk)] \quad (4.29)$$

which is contained in the RHS of (4.28).

If we choose to ignore the first set of delta functions, and write

$$\frac{d}{dE} = 2k_1 \frac{d}{dk_1} + 2k_2 \frac{d}{dk_2} + 2k_3 \frac{d}{dk_3}$$

then (4.29) becomes

$$\sum_p \int \frac{dk}{dE} \left[ f^*(pk) \left( 2k_1 \frac{d}{dk_1} + 2k_2 \frac{d}{dk_2} + 2k_3 \frac{d}{dk_3} \right) f(k) - 6f^*(k) f(pk) \right]$$

$$- f^*(k) \left( 2k_1 \frac{d}{dk_1} + 2k_2 \frac{d}{dk_2} + 2k_3 \frac{d}{dk_3} \right) f(pk) \right) .$$
Because of the symmetry and reality of $f(k)$, the first and last terms cancel and the remaining term reduces to a constant.

Obviously this is not a satisfactory approach as we have lost all dynamical information, and the trace integration must now diverge. We note also that the delta functions are the direct cause of the problem, because the effect of differentiating them is to transfer the differentiation to the rest of the integrand with a change of sign, which cancels the direct derivative term.

The alternative line, of ignoring the second set of delta functions in (4.29) is no more fruitful. The $k'$ integrations and the energy differentiation can be immediately performed, yielding terms which also diverge when the remaining energy and $k$ integrations are carried out.

We conclude that the present model is too highly singular to permit fully on-shell calculations. In terms of the analysis of §2.5 the real energy limit has been taken too early.

To investigate further, we return to equation (2.18) and examine in the following several sections, how far one can go with the scattering formalism for this model.
4.4 Perturbative Approximations to \( b_3^S - b_3^S_0 \) and \( b_3^D \)

One step back from the S-matrix formulation of \( b_3^S - b_3^S_0 \) is the form (2.18) in terms of the Green's function. We are able to compute this expression directly in the limit \( c \to \infty \) for distinguishable particles (see §4.6), but for finite strength interactions this is too difficult and we must resort to one of the series expansions developed in §2.5. The multiscattering expansion is not perturbative and we shall examine it in §4.6.

The potential expansion on the other hand is perturbative, and since we can also expand our exact result (4.27) in powers of \( c \), we are able to carry out a direct check of the validity of the scattering approach at least up to the stage of equation (2.18), to a given order in \( c \).

We take the case of bosons, and write out terms up to second order in \( c \)

\[
\text{Tr}(e^{\beta H} - e^{\beta H_0}) \approx \frac{-1}{2\hbar^2} \text{Tr} \int_C d\gamma e^{\beta \gamma} [(I+P_{12}+P_{13}+P_{23}+P_{123}+P_{132}) (G_0(V_1+V_2+V_3)G_0

+ G_0(V_1+V_2+V_3)G_0(V_1+V_2+V_3)G_0)

- (I+P_{12}) (G_0V_3G_0+G_0V_3G_0V_3G_0)

- (I+P_{13}) (G_0V_2G_0+G_0V_2G_0V_2G_0)

- (I+P_{23}) (G_0V_1G_0+G_0V_1G_0V_1G_0)]
\]

where \( P_{ij} \) denotes the interchange \( (ij) \) and \( P_{ijk} \) denotes the
cycle (ijk).

After all possible cancellations are performed we are left with

\[
\text{Tr} (e^{\beta H - e^{\beta H_0}}) = \frac{-1}{2\pi i} \text{Tr} \int_C dZ \ e^{\beta Z} \left\{ \left( (P_{12} + P_{13} + P_{123} + P_{132}) G_0 V_1 G_0 + (P_{12} + P_{13} + P_{123} + P_{132}) G_0 V_3 G_0 \right) + \left( (P_{12} + P_{13} + P_{123} + P_{132}) G_0 V_1 G_0 V_1 G_0 + (P_{12} + P_{13} + P_{123} + P_{132}) G_0 V_2 G_0 V_2 G_0 + (P_{13} + P_{23} + P_{123} + P_{132}) G_0 V_3 G_0 V_3 G_0 + (I + P_{12} + P_{13} + P_{123} + P_{132}) \sum_{i \neq j} G_0 V_i G_0 V_j G_0 \right) \right. \\
+ \left. \sum_{i \neq j} G_0 V_i G_0 V_j G_0 \right\}.
\]

The first square bracket contains all first order terms, while the second contains all second order terms. We observe that since the momentum variables will be integrated over when the trace is taken, they are dummy parameters, and we can relabel them in terms of similar form to give the same contributions.

So to first order

\[
\text{Tr} (e^{\beta H - e^{\beta H_0}}) = -12 \cdot \frac{c}{\pi} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_C dZ \ e^{\beta Z} <k|P_{12} G_0 V_1 G_0 |k> \\
= -6 \cdot \frac{c}{\pi^2} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_C dZ \ e^{\beta Z} \frac{\delta(k_1 - k_3)}{(Z - k)^2} \quad (4.32)
\]
where we have used

$$<\mathcal{P}|V_1|k> = \frac{e}{\pi} \delta(<\Sigma p-\Sigma k>) \delta(p_1-k_1)$$

and dropped the momentum conserving delta function for the reason explained in §2.2. Expressing $\frac{1}{(Z-k^2)^2}$ as $-\frac{d}{dz} \frac{1}{Z-k^2}$ and integrating by parts with respect to $Z$, we find

$$\text{Tr}(e^{\beta H_1} e^{\beta H_0}) = -\frac{6e}{\pi^2} \int_{-\infty}^{\infty} dk \delta(k_1-k_3) \left[ -\frac{e^{\beta Z}}{Z-k^2} \right]_{Z=\infty-i\epsilon}^{Z=\omega+i\epsilon} + \beta C Z Z-k^2$$

The first term vanishes at both limits, and the second yields the residue

$$-\frac{12e}{\pi} \int_{-\infty}^{\infty} dk \delta(k_1-k_3) e^{\beta k^2} = \frac{-12e}{\sqrt{2}}$$

(4.33)

From equation (2.11), the first order contribution to $b_3^S - b_3^S$ is $-\frac{C}{\sqrt{2}\pi}$. Second order contributions are of three types, and we calculate one term of each.

$$-\frac{1}{2\pi i} \left( \frac{e}{\pi} \right)^2 \int_C d\zeta \int dp e^{\beta Z} \frac{1}{Z-k^2} \delta(\Sigma p-\Sigma k) \delta(k_3-p_1) \frac{1}{Z-k^2} \delta(p_1-k_1) \frac{1}{Z-k^2}$$

$$= -\frac{1}{2\pi i} \left( \frac{e}{\pi} \right)^2 \int_C d\zeta \int dp \frac{e^{\beta Z}}{(Z-2k_1^2-(k_2+k_3-k_1)^2)^2(Z-k^2)}$$

(4.34)

is the contribution from each of the twelve terms of form $P G_0 V_i G_0 V_i G_0$, with $P \neq I$ or $P_{j,k}$. There are also twelve terms of form $P G_0 V_i G_0 V_j G_0$ with $i \neq j$ and $P = P_{i,j,k}$ or $P_{i,j}$. These give the contribution
The third type of term, of which there are 24, also has the form
\[ P G_i V_i G_j V_j G_l \] with \( i \neq j \), but now \( P \neq P_{ijk} \) or \( P_{ij} \) and the contribution is

\[ -\frac{1}{4\pi^2} \left( \frac{c}{\pi} \right)^2 \int_C dz \int_\beta \frac{e^{-\beta z}}{(z-k)^2} \delta(z-k) \delta(z-p) \frac{1}{z-p} \delta(z-p_2) \frac{1}{z-p_3} \]

\[ = -\frac{1}{4\pi^2} \left( \frac{c}{\pi} \right)^2 \int_C dz \int dk \frac{e^{-\beta z}}{(z-k)^2} \delta(z-k) \frac{1}{z-k} \delta(z-p_2) \frac{1}{z-p_3} \]

\[ = -\frac{1}{4\pi^2} \left( \frac{c}{\pi} \right)^2 \int_C dz \int dk \frac{e^{-\beta z}}{(z-k)^2} \delta(z-k) \frac{1}{z-k} \delta(z-p_2) \frac{1}{z-p_3} \]

Combining all second order terms we have

\[ -12 \cdot \frac{1}{4\pi^2} \left( \frac{c}{\pi} \right)^2 \int_C dz e^{-\beta z} \int dk \left[ \frac{d^2}{dz^2} \left( \frac{1}{z-k} \right) + \frac{d^2}{dz^2} \frac{1}{z-k} \right] \]

We integrate by parts with respect to \( Z \), once in the first term, and twice in the second, observing that the terms evaluated at the limits \( (Z = \infty) \) vanish.

The result

\[ -12 \cdot \frac{1}{4\pi^2} \left( \frac{c}{\pi} \right)^2 \int_C dz \int dk e^{-\beta z} \left[ \frac{-\beta}{(z-k)^2} + \frac{\beta^2}{z-k^2} \right] \]

can be integrated around the clockwise contour \( C \) by use of Cauchy's Residue Theorem yielding
\begin{align*}
12 \left( \frac{c}{n} \right)^2 \beta \int dk \left[ \frac{\text{e}^{-\beta (\frac{k^2}{2} + (k_2 + k_3 + k_1)^2)} - \frac{\text{e}^{-\beta k^2}}{k^2 - 2k_1^2 - (k_2 + k_3 - k_1)^2}} + \beta \text{e}^{-\beta k^2} \right]
\end{align*}

To evaluate further we utilize the unitary linear transformation

\begin{align*}
P_1 &= \frac{1}{\sqrt{3}} (k_1 + k_2 + k_3) \\
P_2 &= \frac{1}{\sqrt{2}} (k_2 - k_3) \\
P_3 &= \frac{1}{\sqrt{6}} (k_2 + k_3 - 2k_1)
\end{align*}

which diagonalises the exponents and factorises the denominator

\begin{align*}
12 \left( \frac{c}{n} \right)^2 \beta \int dp \left[ \frac{\text{e}^{-\beta (p_1^2 + p_3^2)}}{(\sqrt{3}p_3 + p_2)(\sqrt{3}p_3 - p_2)} + \frac{\text{e}^{-\beta p_2^2}}{(\sqrt{3}p_3 + p_2)(\sqrt{3}p_3 - p_2)} + \beta \text{e}^{-\beta p_2^2} \right] (4.39)
\end{align*}

The first term is evaluated by contour integration with respect to \( p_2 \), the resulting pole is then expressed as an integral by use of

\begin{align*}
\frac{1}{x + i\eta} = -i \int_0^\infty e^{i(x + i\eta)s} \, ds
\end{align*}

(4.40)

and the remaining integrations are immediately performed by completing the squares in the exponents. The two poles of the second term are treated in a similar way and the third term is directly integrable. We obtain

\begin{align*}
12 \left( \frac{c}{n} \right)^2 \pi (\pi \beta)^{1/2} \left[ \frac{\pi}{\sqrt{3}} - \int_0^\infty ds \int_0^\infty dt \text{e}^{(s^2 + t^2 + st)} + 1 \right]
\end{align*}

Now to evaluate the double integral, we observe that the substitution of \( s-t \) for \( s \) leads to
If we consider the cartesian $s-t$ plane, it is clear that the second term on the right is integrated over exactly half the first quadrant, that between the $s$-axis and the $s=t$ diagonal. Since the integrand is symmetric in $s$ and $t$, this term is just half of the integral over the whole first quadrant, so we have

$$
\int_0^\infty \int_0^\infty e^{-(s^2+t^2+st)} \, ds \, dt = \frac{1}{2} \int_0^\infty \int_0^\infty e^{-(s^2+t^2-st)} \, ds \, dt
$$

and therefore

$$
\int_0^\infty \int_0^\infty e^{-(s^2+t^2+st)} \, ds \, dt = \frac{1}{3} \left[ \int_0^\infty \int_0^\infty e^{-(s^2+t^2+st)} \, ds \, dt + \int_0^\infty \int_0^\infty e^{-(s^2+t^2-st)} \, ds \, dt \right]
$$

Relabelling $s$ as $-s$ in the second term of the RHS and combining with the first we obtain

$$
\int_0^\infty ds \int_0^\infty dt \, e^{-(s^2+t^2+st)} = \frac{1}{3} \int_0^\infty ds \int_0^\infty dt \, e^{-(s^2+t^2+st)}
$$

$$
= \frac{\pi^2}{3} \int_0^\infty dt \, e^{-3t^2/4}
$$

$$
= \frac{\pi}{3\sqrt{3}}
$$

So from (4.40) and (2.11) the total second order contribution to $b_3 - b'_3$ is

$$
\left( \frac{C}{\pi} \right)^2 (\beta \pi)^\frac{b^2}{2} [1 + 2 \frac{\pi}{3\sqrt{3}}]
$$

(4.43)
For comparison we now recall the exact form of $b_3^S - b_3^{S_0}$ from equation (4.27)

$$b_3^S - b_3^{S_0} = \frac{6}{(2\pi)^3} \pi \int_0^\infty ds \int_0^\infty dt \ e^{-(s^2 + t^2 + st)/2\beta} (e^{-2cs - ct} - e^{-cs})$$

(4.44)

which with the help of (4.42) checks exactly with the second order perturbation calculation (4.43).

We have thus verified the validity of equation (2.18) up to second order in potential strength, but only in an off-shell approach. Had we attempted to take the energy on-shell, say at the stage of equation (4.38) the propagators would have diverged, once again the forward singularities of §2.6.

Although we do not have an exact solution for the third cluster coefficient for distinguishable particles, we can compute the low order terms in the same way as we have done for bosons. The
calculation is simpler because there are no exchange effects to take account of, and the requirement of connectedness eliminates all first order terms. This immediately indicates that the statistics make an important qualitative difference to the thermodynamics of the system, and we do not expect a linear relationship between $b_3^D$ and $b_3^S - b_3^S_0$, as equation (3.20) might have suggested.

\[
\text{Tr}(e^{\beta H}) = -\frac{1}{2\pi i} \text{Tr} \int_C dz \frac{e^{\beta Z}}{z^{1/2}} \left( \sum_{i \neq j} G_i G_j V_i V_j G_0 + \text{third \& higher order terms} \right)
\]

(4.46)

The leading contribution to $b_3^D$ therefore arises from the six terms of the form

\[
-\frac{1}{2\pi i} \left( \frac{e^{\beta Z}}{z^{1/2}} \right) \int_C \int dk \int dp \frac{e^{\beta Z} \delta(p_i - k_j) \delta(k_i - k_j)}{(z - p_i^2)^{1/2}(z - k_j^2)^{1/2}}
\]

which is the same as (4.36), and gives

\[
b_3^D = \frac{1}{2} \left( \frac{e^{\beta Z}}{z^{1/2}} \right) \frac{(\beta \pi)^{1/2}}{2} 
\]

(4.47)

It is in principle a simple matter to write down the higher order terms for either statistics, although evaluation will become progressively more laborious. It is equally clear, from the expansion of the exact cluster coefficient (4.27) in powers of $\zeta$, that there will be a finite contribution from every order of the potential expansion. This is not necessarily so with the multiscattering series, of which each term is already an infinite partial sum of the potential series.
4.5 The Singularity Structure of the Scattering Amplitude

The multiscattering expansion of $T$ provides the best approach for studying the singularity structure of $T$.

We shall examine the first three orders of the series explicitly. Terms of higher order are most readily expressed as integrals, and to analyse these we use the technique of the Landau Rules. For completeness, a brief discussion of this method is given in Appendix H.

The multiscattering expansion of an arbitrary off-shell matrix element of $T$ can be written

$$<p | T(Z) | k> = \sum_i <p | t_i(Z) | k> + \sum_{i \neq j} <p | t_i(Z) G_0(Z) t_j(Z) | k>$$

$$+ \sum_{i \neq j \neq k} <p | t_i(Z) G_0(Z) t_j(Z) G_0(Z) t_k(Z) | k> + ... \ (4.48)$$

The centre of mass frame, $\Sigma p = \Sigma k = 0$ will be used throughout.

The off-shell $t$ elements in three body phase space can be constructed from (3.12) by adding a delta function to conserve the momentum of the non-interacting particle and adjusting the energy term to give the correct on-shell limit by subtracting the kinetic energy of the free particle. Thus

$$<p | t_i(Z) | k> = \frac{c}{\pi} \delta (p_i - k_i) \delta (\Sigma p - \Sigma k) \delta \left( \frac{2z - 3k_i}{\sqrt{2z - 3k_i^2 + 4ic}} \right)$$

$$= \frac{c}{\pi} \delta (p_i - k_i) \delta (\Sigma p - \Sigma k) \chi (k_i) \quad (4.49)$$
which defines the functions \( \chi(k_1) = \chi(k_1, z) \)

For the present, we neglect the poles and cuts arising out of the \( \chi \)'s, and return at the end of the section to comment on their significance.

Similarly, we ignore the effects of symmetrization for identical particles. It will later be evident from inspection that symmetrization does not alter the analytic character of the scattering amplitude.

The aim of this analysis is to determine the relevance of the singularity structure of \( T \) to the calculation of the cluster coefficients via equation (2.19), and in particular to observe the effect of putting the energy on-shell. Accordingly we are ultimately interested in the forward elements of (4.48), that is when \( p = k \), since only these enter into the trace, and in the on-shell limit, \( E = k^2 \).

First order terms are given by (4.49), and are singular by virtue of the delta function. However we note that only those first order terms which are connected by an exchange involving the free particle, will contribute to the connected part of (2.19). In this case the delta function will become \( \delta(p_i - p_j) \) and the integral will be defined.

Momentum conservation determines the intermediate state momenta in all second order terms, as illustrated by Fig. 5.

\[ \begin{array}{c}
\text{Figure 5.}
\end{array} \]
The contribution from this diagram is

\[
\left< \mathbf{p} | t_i \, G_0 \, t_j | \mathbf{k} \right> = \left( \frac{e}{\pi} \right)^2 \frac{\chi(p_i) \chi(k_j)}{Z - 2(p_i^2 + k_j^2 + p_i k_j)} \quad (4.50)
\]

where we have dropped the momentum conserving delta function for the reason explained in the derivation of (2.11).

When a diagonal element is taken and the energy is put on-shell, the propagator diverges because the denominator vanishes. These terms are the second order forward singularities discussed in §2.6.

Third order terms involve one integration, over the intermediate momentum \( q \), as shown in Fig. 6,

\[
\begin{array}{c}
\text{Figure 6.} \\
\end{array}
\]

and the associated term is

\[
\left< \mathbf{p} | t_i \, G_0 \, t_j \, G_0 \, t_k | \mathbf{k} \right> = \left( \frac{e}{\pi} \right)^3 \int dq \, \frac{\chi(p_i) \chi(q) \chi(k_j)}{(Z - 2(p_i^2 + q^2 + p_i q))(Z - 2(q^2 + k_j^2 + q k_j))} \quad (4.51)
\]

where \((ijk)\) and \((\ell mn)\) are both permutations of \((123)\), and \(j \neq \ell\).
To examine the behaviour of the propagator in the on-shell limit of the forward elements of (4.51), we let \( Z + p^2 + i\eta = k^2 + i\eta \).

For \( p_j > p_k \) and \( k_m > k_n \), the denominator factorizes thus:

\[
\frac{1}{(-2)^2(q-p_j - i\eta)(q-p_k - i\eta)(q-k_m - i\eta)(q-k_n - i\eta)}
\]

(4.52)

Since \( j \neq l \), \( p_j \) must match either \( k_m \) or \( k_n \). If \( p_j = k_n \), we have a pinch singularity in (4.51) at \( q = p_j \) and the integral diverges.

The terms in which this happens are the third order forward singularities which are peculiar to one-dimensional models. These are also discussed in §2.6.

A general \( n \)th order term has the form

\[
\left(\frac{c}{n}\right)^{n-1} dq_1 \ldots dq_{n-2} \chi(p_i) \chi(q_1) \ldots \chi(q_{n-2}) \chi(k_n) \frac{(Z-2(p^2 + q^2 + p_i q_i)) \ldots (Z-2(q_j^2 + q_{j+1}^2 + q_j q_{j+1}^2)) \ldots (Z-2(q_{n-2}^2 + k_n^2 + k_n q_{n-2}^2))}{(Z-2(p^2 + q^2 + p_i q_i)) \ldots (Z-2(q_j^2 + q_{j+1}^2 + q_j q_{j+1}^2)) \ldots (Z-2(q_{n-2}^2 + k_n^2 + k_n q_{n-2}^2))}
\]

(4.53)

To determine whether there are any pinches between propagator poles we write the Feynmanised denominator (see Appendix H),

\[
D = \alpha_1 (Z-2p_1^2 - 2q_1^2 - 2p_1 q_1) + \ldots + \alpha_{n-1} (Z-2k_{n-2}^2 - 2k_{n-2} q_{n-2}).
\]

The integral (4.53) will be singular when all of the following are satisfied:

\[
\alpha_1 = 0 \text{ or } Z-2p_1^2 - 2q_1^2 - 2p_1 q_1 = 0 \\
\vdots \\
\alpha_{n-1} = 0 \text{ or } Z-2k_{n-2}^2 - 2k_{n-2} q_{n-2} = 0
\]

(4.54)
and
\[ \frac{\partial \beta}{\partial q_1} = -2(\alpha_1(p_1 + 2q_1) + \alpha_2(q_2 + 2q_1)) = 0 \]

\[ \frac{\partial \beta}{\partial q_j} = -2(\alpha_j(q_{j-1} + 2q_j) + \alpha_{j+1}(q_{j+1} + 2q_j)) = 0 \quad (4.55) \]

\[ \frac{\partial \beta}{\partial q_{n-2}} = -2(\alpha_{n-2}(q_{n-3} + 2q_{n-2}) + \alpha_{n-1}(k_3 + 2q_{n-2})) = 0 \]

Taking differences of successive equations of (4.54), and defining \( \lambda_j = \frac{q_j}{q_j + q_{j+1}} \in [0,1] \) in equations (4.55) we have

\( (p_1 - q_2)(p_1 + q_1 + q_2) = 0 \) or \( \alpha_1 = 0 \) or \( \alpha_2 = 0 \) or both

\[ \frac{\partial \beta_{(q_j - q_{j+1})}(q_{j-1} + q_j + q_{j+1})}{\partial q_j} = 0 \) or \( \alpha_j = 0 \) or \( \alpha_{j+1} = 0 \) or both

\[ \frac{\partial \beta_{(q_{n-3} - k_3)}(q_{n-3} + q_{n-2} + k_3)}{\partial q_{n-2}} = 0 \) or \( \alpha_{n-2} = 0 \) or \( \alpha_{n-1} = 0 \) or both

\( \lambda_1 p_1 + 2q_1 + (1 - \lambda_1)q_2 = 0 \)

\[ \frac{\partial \beta_{q_{j-1} + 2q_j + (1 - \lambda_j)q_{j+1}}}{\partial q_j} = 0 \quad (4.57) \]

\[ \frac{\partial \beta_{q_{n-2} q_{n-3} + 2q_{n-2} + (1 - \lambda_{n-2})k_3}}{\partial q_{n-2}} = 0 \]

Taking two pairs of equations, the \( j \)th and \( j+1 \)th of (4.56) and (4.57).
(q_{j-1}-q_{j+1})(q_{j-1}+q_j+q_{j+1}) = 0 \text{ or } q_j = 0 \text{ or } q_{j+1} = 0 \text{ or both}

\lambda_j q_{j-1} + 2q_j + (1-\lambda_j)q_{j+1} = 0 \tag{4.58}

(q_j-q_{j+2})(q_j+q_{j+1}+q_{j+2}) = 0 \text{ or } q_{j+1} = 0 \text{ or } q_{j+2} = 0 \text{ or both}

\lambda_{j+1} q_j + 2q_{j+1} + (1-\lambda_{j+1})q_{j+2} = 0 \tag{4.59}

we now consider all the possibilities, excluding the trivial solution \( q_i = 0 \) \( i=1, \ldots, n-1 \):

(i) \( q_j \neq 0, q_{j+1} \neq 0, q_{j+2} \neq 0, q_{j-1} \neq q_{j+1}, q_j \neq q_{j+2} \)

Then \( \lambda_j, \lambda_{j+1} \in (0,1) \) and we can eliminate \( q_{j-1} \) from (4.58) and \( q_{j+2} \) from (4.59) obtaining

\[
\frac{q_j}{q_{j+1}} = \frac{2\lambda_j - 1}{2 - \lambda_j} \quad \text{and} \quad \frac{q_j}{q_{j+1}} = \frac{1 + \lambda_{j+1}}{1 - 2\lambda_{j+1}}
\]

which implies

\[
\lambda_j = \frac{1}{1 - \lambda_{j+1}}.
\]

This result is inconsistent with the ranges of \( \lambda_j \) and \( \lambda_{j+1} \).

(ii) \( q_j \neq 0, q_{j+1} \neq 0, q_{j+2} \neq 0, q_{j-1} = q_{j+1}, q_j \neq q_{j+2} \)

gives the inconsistent result

\[
\frac{1 + \lambda_{j+1}}{1 - 2\lambda_{j+1}} = \frac{1}{2}
\]

(iii) \( q_j \neq 0, q_{j+1} \neq 0, q_{j+2} \neq 0, q_{j-1} \neq q_{j+1}, q_j = q_{j+2} \)

gives the inconsistent result

\[
\frac{2\lambda_j - 1}{2 - \lambda_j} = -2
\]
(iv) $\alpha_j \neq 0, \alpha_{j+1} \neq 0, \alpha_{j+2} \neq 0, \alpha_{j-1} = \alpha_{j+1}, \alpha_j = \alpha_{j+2}$
gives the inconsistent result

$$\frac{q_j}{q_{j+1}} = -2, \frac{q_j}{q_{j+1}} = -\frac{1}{2}$$

(v) $\alpha_j = 0, \alpha_{j+1} \neq 0, \alpha_{j+2} \neq 0$
implies $\lambda_j = 0$ which gives the inconsistent result $\frac{1}{2} = \frac{1+\lambda_{j+1}}{1-2\lambda_{j+1}}$
irrespective of values of $\alpha_i$ for $i < j$

(vi) $\alpha_j = 0, \alpha_{j+1} \neq 0, \alpha_{j+2} = 0$
implies $\lambda_j = 0$ and $\lambda_{j+1} = 1$ which gives the inconsistent
results $2q_j = -q_{j+1}$ and $q_j = -2q_{j+1}$ (unless $q_j = q_{j+1} = z = 0$)

(vii) $\alpha_j \neq 0, \alpha_{j+1} \neq 0, \alpha_{j+2} = 0$
implies $\lambda_{j+1} = 1$ so $q_j = -2q_{j+1}$ which is inconsistent with (4.58)
unless $q_{j-1} = q_j = q_{j+1} = z = 0$

(viii) $\alpha_j \neq 0, \alpha_{j+1} = 0, \alpha_{j+2} = 0$
yields only the relation $q_{j-1} = -2q_j$ which is inconclusive. If $j > 1$ then cases (vi) or (vii) will apply. If $j=1$, the first
of equations (4.54) determines $Z = \frac{3}{2}p_i^2$ and we have to look to the
remaining equations to establish consistency or otherwise. If all
the higher $\alpha$'s are also zero, the Landau Rules are all satisfied.
However this singularity only exists off-shell in our model, since
the on-shell energy in the centre of mass frame is $\frac{3}{2}p_i^2 + \frac{1}{2}(p_j - p_k)^2$
and we require the momenta to be distinct.

It can easily be verified that if any of the higher $\alpha$'s are non-
zero, cases (v) to (vii) will cover all possibilities except the
following:

(ix) $\alpha_1 \neq 0, \alpha_{n-1} \neq 0$ all other $\alpha_i = 0$
The first and the last of equations (4.54) determine $Z$ as $\frac{3}{2}p_i^2$ and
\[ \frac{3}{2}k^2 \] respectively, so that \( p_i = k_i \). This again is an off-shell singularity which we can discard on-shell in our model. Lastly we have

\( (x) \quad \alpha_j = 0, \quad \alpha_{j+1} = 0, \quad \alpha_{j+2} \neq 0 \)

which we treat in a similar way to (viii).

We note that the singularity structure determined by this analysis arises only from the behaviour of the propagators in the multiscattering series. By ignoring the structure of the amplitude functions \( \chi(k_i) \), we implicitly assume that any singularities they may have are well off the real axis and do not interfere with the propagator poles.

It can be verified from (4.49) that this is valid for the present model.

The more general case of three dimensional systems interacting via a superposition of Yukawa potentials has been studied by Rubin, Sugar and Tiktopoulos \(^{50}\) and they have found the corresponding assumption to be valid for that class of potentials also.

To summarise, we have found that the on-shell singularities of the scattering amplitude of a one-dimensional system with a two body potential, are contained in the first three orders of the multiscattering series, and arise out of divergent propagators.

The significant terms are the second and third order on-shell forward scattering elements.

Fourth and higher order terms are all regular apart from a pole at \( z = p_i = k_i = q_i = 0 \) in all orders. We can justifiably neglect this point which corresponds to the unphysical situation of all the particles being stationary with zero energy. We also
reject solutions with non-distinct momenta. Not only does the wavefunction vanish in this case, but such a configuration would also clearly be highly singular as the particles carrying the same momenta would always be a fixed distance apart and never collide.
4.6 The On-Shell Limit of the Multiscattering Series

Since all the forward singularities of the scattering amplitude are contained in the first three orders of the multiscattering series, we shall now examine these terms in the on-shell limit.

Consider the expression

\[ -2\pi i \langle p | \delta(E-H_0) \left[ \sum_{i} t_i + \sum_{i \neq j} t_i G_0^+ t_j + \sum_{i \neq j \neq k} t_i G_0^+ t_j G_0^+ t_k \right] | k \rangle \]  \hspace{1cm} (4.60)

The first order terms can be immediately written down from (4.49) with \( Z = k^2 \), and simplified with the aid of the identity (4.15) and the definition of the reflection coefficients (4.3), to

\[ (r_{12} + r_{13} + r_{23}) \delta_{11} \delta_{22} \delta_{33} + r_{12} \delta_{12} \delta_{21} \delta_{33} + r_{13} \delta_{13} \delta_{22} \delta_{31} + r_{23} \delta_{11} \delta_{23} \delta_{32} \]  \hspace{1cm} (4.61)

where we use the notation \( \delta_{ij} = \delta(k_i - p_j) \).

The scattering diagram in Figure 7 depicts a typical second order term with contribution

\[ -2\pi i \langle p | \delta(E-H_0) t_i G_0^+ t_j | k \rangle \]

\[ = -2\pi i \frac{(S^2 \delta(k_i^2 - p_i^2) \delta(Ek - Ep)}{2k_j - p_j - p_k} \frac{|k_i - k_k|}{|k_i - k_k| + ic} \frac{1}{-2(p_i - k_i + in) (p_j - k_j + in)} \]  \hspace{1cm} (4.62)

where the upper signs apply for \( k_i > k_k \) and the lower for \( k_i < k_k \).

Expressing the denominator as a difference of the poles and using
\[
\frac{1}{x+i\eta} = p \frac{1}{x} + i\pi \delta(x)
\]

and the identity (4.15) again, the RHS of (4.62) becomes

\[
\frac{1}{2} [r_{jk} r_{ik} (\delta_{ii} \delta_{jj} \delta_{kk} + \delta_{ii} \delta_{jj} \delta_{ki} + \delta_{ij} \delta_{kj} \delta_{li})] + r_{ij} r_{ik} (\delta_{ii} \delta_{jj} \delta_{kk} + \delta_{ij} \delta_{kj} \delta_{li})
\]

+ principal part terms \quad (4.63)

It has been shown in Appendix F that the sum of principal part terms of the on-shell T-matrix vanish, so we drop these, and taking the sum \( \sum_{i \neq j} \) explicitly, we obtain the total second order contribution to (4.60):

\[
(r_{12r_{23}+r_{12r_{13}+r_{13r_{23}}} \delta_{11} \delta_{22} \delta_{33}} + (r_{12r_{23}+r_{13r_{23}}} \delta_{11} \delta_{22} \delta_{33})
\]

\[+(r_{12r_{13}+r_{12r_{23}}} \delta_{12} \delta_{21} \delta_{33} + (r_{12r_{13}+r_{13r_{23}}} \delta_{13} \delta_{22} \delta_{33})
\]

\[+\frac{1}{2}(r_{12r_{13}+r_{12r_{23}+r_{13r_{23}}} \delta_{12} \delta_{23} \delta_{31} + (r_{13r_{23}+r_{13r_{23}}} \delta_{13} \delta_{21} \delta_{32}) \quad (4.64)
\]

Third order contributions involve integration over one intermediate momentum variable, as can be seen from the typical diagram in Figure 8. The corresponding term is

\[
-2\pi i <p|\delta(E-H_0)t_i G_0^+ t_j G_0^+ t_k|k>
\]

\[
= -2\pi i \left( \frac{3}{4} \delta(k^2-p^2) \delta(E-k_p) \right) \frac{|k_i-k_j|}{|k_i-k_j|} \int_{-\infty}^{\infty} dq \frac{|p_j+p_k-2q|}{|p_j+p_k-2q|+ic} \frac{|k_i+k_j-q-k_k|}{|k_i+k_j-q-k_k|+ic}
\]

Figure 8.
where the signs in the denominator are determined as follows:

In the first two factors, the upper signs apply when $p_k > p_j$ and the lower when $p_k < p_j$, while in the last two factors, the upper signs apply when $k_l < k_j$ and the lower when $k_l > k_j$.

The integral may be evaluated by contour integration in the upper half of the complex $q$ plane, where there will always be two simple poles from the propagators, whatever the relative values of the $p$'s and $k$'s. There may also be one or two poles from the amplitude factors depending on the sign of their arguments. These will also contribute residues to the total third order term.

Proceeding then with the $q$-integration, we obtain from the propagator poles a sum of terms of the form

$$\frac{1}{(q-p_j + i\eta)(q-p_k + i\eta)(q-k_l + i\eta)(q-k_j + i\eta)}$$

(4.65)

subject to $p_k < p_j$, $k_l < k_j$. Since $k_l$ and $k_j$ are necessarily distinct, we can drop the imaginary infinitesimal in the factor $\frac{1}{k_l - k_j + i\eta}$. The last factor yields a principal part, which again will vanish on-shell, and a delta function. Applying the delta function to the amplitude factors, and with the help of (4.15), (4.66) becomes
\[
\frac{1}{2} \frac{-ic}{|k_j - k_i| + ic} \frac{-ic}{|p_j - p_k| + ic} \frac{-ic}{|k_j - k_k| + ic} (\delta(k_i - p_k) \delta(k_j - p_i) \delta(k_k - p_j)) + \delta(k_i - p_k) \delta(k_j - p_i) \delta(k_k - p_j))
\]

It is evident that the restrictions \( p_k < p_j \) and \( k_j < k_i \) will preclude the second term from ever contributing, so we are left with

\[
\frac{1}{2} r_{ij} r_{ik} r_{jk} \delta_{ik} \delta_{ji} \delta_{kj} (p_k < p_j, k_j < k_i)
\]

All the other terms arising from (4.66) can similarly be evaluated. We also have to include all the third order terms of the form

\[
-2\pi i \langle P | \delta(E - H_0) t_i G_0^+ t_j G_0^+ t_i | k \rangle
\]

Finally the summations over \( i, j, k \) are performed explicitly, bearing in mind the inequality restrictions associated with each term, and the initial condition \( k_1 > k_2 > k_3 \). We find the third order contribution

\[
\frac{1}{2} r_{12} r_{13} r_{23} \left[ 2 \delta_{11} \delta_{22} \delta_{33} + 2 \delta_{11} \delta_{22} \delta_{32} + 4 \delta_{11} \delta_{22} \delta_{31} + 2 \delta_{12} \delta_{21} \delta_{33} + 3 \delta_{12} \delta_{23} \delta_{31} + 3 \delta_{13} \delta_{21} \delta_{32} \right] (4.67)
\]

In addition there are contributions from the amplitude factor residues arising out of (4.65).

For comparison we now take the full on-shell T-matrix, as given by (4.14), rewriting the coefficients in terms of reflection coefficients only with the aid of the relation \( t_{ij} = 1 + r_{ij} \), and collecting terms we find
\[-2\pi i \langle q | \delta(E - \epsilon_0) T^D | k \rangle = \delta_{11} \delta_{22} \delta_{33} [r_{12} r_{13} r_{23} + r_{12} r_{13} + r_{12} r_{23} + r_{13} r_{23} + r_{12} + r_{13} + r_{23}] + \delta_{12} \delta_{21} \delta_{33} [r_{12} + r_{12} r_{13} + r_{12} r_{23} + r_{12} r_{13} r_{23}] + \delta_{13} \delta_{22} \delta_{31} [r_{13} + r_{13} r_{23} + r_{12} r_{13} + 2 r_{12} r_{13} r_{23}] + \delta_{11} \delta_{23} \delta_{32} [r_{23} + r_{12} r_{23} + r_{13} r_{23} + r_{12} r_{13} r_{23}] + \delta_{12} \delta_{23} \delta_{31} [r_{12} r_{23} + r_{12} r_{13} r_{23}] + \delta_{13} \delta_{21} \delta_{32} [r_{12} r_{23} + r_{12} r_{13} r_{23}] \quad (4.68)\]

Adding (4.61), (4.64) and (4.67), we obtain the RHS of (4.68) with the aid of the identity

\[r_{12} r_{13} + r_{12} r_{23} + r_{13} r_{23} = 2 r_{12} r_{23} - r_{12} r_{13} r_{23}.\]

What we have shown is that the full on-shell T-matrix is contained in the first three orders of the multiscattering series when taken on-shell. It follows that the sum of the amplitude factor residues from the third order terms and the full contributions of the fourth and all higher orders of the multiscattering series vanishes on-shell.

We also know from §4.5 that all the troublesome on-shell singularities of the scattering amplitude are contained in the first three orders.

This suggests a natural partitioning of the T matrix thus

\[T = T' + T_{\text{sing}} \quad , \quad (4.69)\]
where $T_{\text{sing}}$ is the sum of the first three orders and $T'$ is then non-singular on-shell. The corresponding $S$-matrices can be calculated through the usual identity

$$S = (S' + S_{\text{sing}}) = I - 2\pi i \delta(E-H_0)(T' + T_{\text{sing}}),$$

and then substituted into the $S$-matrix formula (2.22). The contributions from the singular part will have to be calculated explicitly off-shell, but the remaining non-singular part $S'$ should give no problem in (2.22).

However the results of this section indicate that there may be no contribution at all from $S'$, depending on the significance of the third-order amplitude factor residues.

The situation is even clearer in the hardcore limit, where the amplitude factors become $\frac{|k_i - k_j|}{i\pi}$, and the only singularities are those of the propagators. In this case, the first three orders of the multiscattering series on-shell actually reduce exactly to the full on-shell $T$-matrix. Then $S'$ vanishes and only the singular terms arising out of the first three orders contribute to the on-shell $S$-matrix.

One wonders therefore whether it may be possible to construct $b_3$ from just the first three orders of the scattering amplitude in Watson's $T$-matrix formula (2.19). However, as we have already observed, off-shell elements of $T$ are required in this expression, and it may be that contributions from higher orders will then be significant, and that the first three orders will yield only part of the full $b_3$. 
Taking the case of distinguishable hardcore particles, for which we can calculate the third cluster coefficient exactly, we examine this suggestion in the following section.
4.7 Some Results for Distinguishable Particles in the Limit $c \to \infty$

In a sense this system is the simplest non-trivial case we can take. The limit $c \to \infty$ simplifies the amplitudes from

$$\frac{1}{n} \sqrt{2\pi} \frac{1}{\sqrt{3}} \left( \sqrt{2\pi} \frac{1}{\sqrt{3}} + ic \right)^{-1},$$

to just $\frac{1}{n} \sqrt{2\pi} \frac{1}{\sqrt{3}}$, and since the particles are distinguishable, we need not worry about exchange effects.

These features permit us to carry through some calculations which have proved too difficult in the case of finite strength interactions. In particular we are able to calculate $b_3$ directly, not only from the continuum wave-functions, but also from the full Green's function.

To begin, we take the $c \to \infty$ limit explicitly in (4.3), Table 1, (4.11), (4.14) and (4.18) to obtain a description of the system:

$$\lim_{c \to \infty} r_{ij} = -1$$

$$\lim_{c \to \infty} t_{ij} = 0$$

$$\lim_{c \to \infty} \psi^D_k(x) = \psi^{HD}_k(x)$$

$$\begin{cases}
[x]_{[123]+[231]+[312]-[213]-[132]-[321]} & x \in \text{RI} \\
0 & x \not\in \text{RI}
\end{cases}$$

$$\langle p | T^{HD} | k \rangle = \frac{\delta(\Sigma k - p)}{2\pi^2} \left[ \frac{k_2-k_3}{k_1-p_3+i\eta} + \frac{k_1-k_3}{k_2-p_1+i\eta} + \frac{k_1-k_2}{k_3-p_2+i\eta} - \frac{k_2-k_3}{k_1-p_1+i\eta} \right]$$

$$- \frac{k_1-k_3}{k_2-p_3+i\eta} - \frac{k_1-k_2}{k_3-p_1-i\eta}$$

$\dagger$ We use the superscript $H$ to denote that the hardcore limit $c \to \infty$ has been taken.
\[ \delta(\Sigma p^2 - \Sigma k^2) < \mathcal{P} | T^{\text{HD}} | k > = \frac{1}{2\pi i} \left( \delta_{11} \delta_{22} \delta_{33} + \delta_{13} \delta_{22} \delta_{31} \right) \] (4.74)

and finally

\[ < \mathcal{P} | S^{\text{HD}} | k > = \delta_{13} \delta_{22} \delta_{31} \] (4.75)

We observe that since the particles may only reflect, their spatial ordering is always preserved and the wavefunction is therefore confined to the region RI. Further, the only possible final state is that with the middle particle having its original momentum, the other two particles having exchanged momenta.

Now to calculate \( b_3^{\text{HD}} \) directly, we need the wavefunctions in momentum space. Taking the Fourier Transform of (4.72) we have

\[ < \mathcal{P} | \psi > = \frac{1}{(2\pi)^2} \delta(\Sigma k - \Sigma p) \sum_{p} \frac{(-)^{\delta_P}}{(p_1 - k_1 + i\eta)(p_3 - k_3 - i\eta)} \] (4.76)

where \( \delta_P \) is the order of the permutation \( P \).

Similarly we find the free wavefunction

\[ < \mathcal{P} | \phi > = \frac{1}{(2\pi)^2} \delta(\Sigma k - \Sigma p) \sum_{p} \frac{1}{(P_{p_1} - k_{p_1} + i\eta)(P_{p_3} - k_{p_3} - i\eta)} \] (4.77)

and the two-particle wavefunctions in three-particle space

\[ < \mathcal{P} | \psi_k >^i = \frac{1}{(2\pi)^2} \delta(\Sigma k - \Sigma p) \sum_{p=1, (j k)} \frac{(-)^{\delta_P}}{(p_1 - k_{p_1} + i\eta)(p_3 - k_{p_3} - i\eta)} \] (4.78)

where here we sum only over the identity and single interchange permutations.
The trace of the connected part of the Green's function in the
centre of mass frame can now be computed in a straightforward
manner.

\[
\text{Tr } G = \int \frac{d^3 p d^3 k}{E - k^2} \left[ |\langle p | \psi_k^* \rangle|^2 - |\langle p | \phi_k^* \rangle|^2 \right] \sum_{i=1}^3 \left( |\langle p | \psi_k \rangle|^2 - |\langle p | \phi_k \rangle|^2 \right) \quad (4.79)
\]

One \( p \) integration is immediately removed by the momentum
conserving delta function, and the remaining two are performed by
taking residues in the upper half plane. After some combinatorics
we find

\[
\text{Tr } G = \frac{1}{\pi^2} \Im \int \frac{dk}{E - k^2} \left[ \frac{1}{(k_3 - k_1 + i\eta)(k_3 - k_2 + i\eta)} + \frac{1}{(k_2 - k_3 + i\eta)(k_2 - k_1 + i\eta)} \right. \\
\left. + \frac{1}{(k_1 - k_3 + i\eta)(k_1 - k_2 + i\eta)} \right]
\]

\[
= - \frac{3}{\pi^2} \Im \int \frac{dk}{E - k^2} \frac{1}{(k_3 - k_1 + i\eta)(k_3 - k_2 + i\eta)} \quad (4.80)
\]

It follows from (2.5), (2.6), (2.18) and (4.80) that

\[
\text{Tr}(U_3)_{\text{CM}} = - \frac{3}{\pi^2} \Im \int \frac{dk}{(k_3 - k_1 + i\eta)(k_3 - k_2 + i\eta)} e^{-\frac{\beta k^2}{2}} \quad (4.81)
\]

To evaluate, we express the poles as integrals by use of
(4.40), then complete the squares in each \( k_i \) in the combined
exponent. The \( k \) integration then yields a factor of \( (\frac{\pi}{B})^{3/2} \) and
we are left with
\[
\text{Tr}(U_3)_{CM} = \left(\frac{\pi}{\beta}\right)^{3/2} \frac{3}{\pi^2} \int_0^\infty ds dt \ e^{-(s^2+t^2+s_1 t)/\beta} = 2\left(\frac{\pi}{3\beta}\right)^4
\]

with the aid of the result (4.42).

The third cluster coefficient can now be written down by use of formula (2.11)

\[
b^3_{\text{HD}} = \frac{1}{3^{3/2} (4\pi \beta)^{1/2}} \tag{4.82}
\]

We recognise this as the third cluster coefficient for a non-interacting Fermi gas \(^{(56)}\). This interesting, though not unexpected, result indicates that the system behaves like three free fermions, the effect of the interaction being simply to preclude two particles from being in the same state, and thus altering the statistics from classical to antisymmetric.

An alternate approach is provided by the Green's function

\[
\langle x | G^+ (E) | x' \rangle = \int \frac{dk}{E-k^2+i\epsilon} \frac{\langle x | \Psi_k > \langle \Psi_k | x' >}{E-k^2+i\epsilon} \]

\[
= \left(\frac{1}{2\pi}\right)^3 \int_{k_1 > k_2 > k_3} dk \frac{1}{E-k^2+i\epsilon} \int_{P,Q} (-)^{P+Q} e^{i(k_p \cdot x - k_Q \cdot x' - k_3 \cdot x')} \tag{4.83}
\]

The momenta restrictions arise from the wavefunction (4.72).

If we take \( x \in I \) (\( x_1 < x_2 < x_3 \)), then \( \Psi_k (x) = 0 \) unless \( k_1 > k_2 > k_3 \), and this further implies \( x' \in I \), otherwise \( \Psi_k (x') \) will vanish.
Relabelling variables and combining the resulting regions of integration, we obtain

$$\frac{1}{2\pi} \int_{k} \frac{1}{E-k^2+i\varepsilon} \sum_{p} (-)^{p} e^{ik \cdot (x_p' - x')} \quad (4.84)$$

At this stage it is convenient to transform to polar coordinates. Let the scalar $k$ be the radius, $w = \cos \theta$ and put $E = u^2$. The $\varphi$ integration yields the factor $2\pi$, so we have

$$\frac{1}{2\pi} \int_{0}^{\infty} \int_{-1}^{1} dw \frac{k^2}{u^2-k^2+i\varepsilon} \sum_{p} (-)^{p} e^{ik \cdot (x_p' - x')} w$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \frac{k}{u^2-k^2+i\varepsilon} \sum_{p} (-)^{p} e^{ik \cdot (x_p' - x')} \quad (4.85)$$

Contour integration in the upper half plane yields

$$\langle x \mid G^+(E=u^2) \mid x' \rangle = \left\{ \begin{array}{ll}
\frac{1}{4\pi} \sum_{p} (-)^{p} e^{iu \cdot (x_p' - x')} & \text{if } x, x' \in \text{RI} \\
0 & \text{otherwise.}
\end{array} \right.$$  

Similarly we find

$$\langle x \mid G_0^+(E=u^2) \mid x' \rangle = -\frac{1}{4\pi} e^{iu \cdot (x-x')} \quad \forall x, x'$$

and

$$\langle x \mid G_1^+(E=u^2) \mid x' \rangle = -\frac{1}{4\pi} \sum_{p=1}^{\infty} (-)^{p} e^{iu \cdot (x_p' - x')} \quad \forall x, x'$$
So the connected part of the full Green's function is

$$\langle x | G_+^e(u^2) | x' \rangle = - \frac{1}{4\pi} \left[ \frac{e^{iL(x(123)\cdot x')}}{|x(123) - x'|} + \frac{e^{iL(x(132)\cdot x')}}{|x(132) - x'|} \right]$$ (4.86)

where the subscripts on the coordinates are the permutation cycles to be applied to those coordinates.

In the same way we calculate

$$\langle x | G^-_e(u^2) | x' \rangle = - \frac{1}{4\pi} \left[ \frac{e^{-iL(x(123)\cdot x')}}{|x(123) - x'|} + \frac{e^{-iL(x(132)\cdot x')}}{|x(132) - x'|} \right]$$ (4.87)

Hence

$$\text{Tr}(G_+^e(u^2) - G^-_e(u^2)) = - \frac{1}{2\pi} \int_{-\infty}^{\infty} \int ds \, dt \, e^{i \sqrt{2s^2 + 2t^2 + 2st}}$$

$$\left(1 - e^{-i \sqrt{2s^2 + 2t^2 + 2st}}\right)$$ (4.88)

where $s = x_1 - x_2$, $t = x_2 - x_3$. Now diagonalizing the quadratic by the change of variable

$$x = s + \frac{1}{2}t, \quad y = \frac{\sqrt{3}}{2}t$$

we can then transform to polar coordinates $r = \sqrt{x^2 + y^2}$, $\theta$, and

(4.88) becomes

$$\text{Tr}(G_+^e(u^2) - G^-_e(u^2)) = - \frac{1}{2\pi} \int_0^{2\pi} d\theta \int_0^{\infty} r \, dr \, \frac{e^{i \sqrt{2ur}} - e^{-i \sqrt{2ur}}}{\sqrt{2}r}$$

$$= - \frac{2i}{\sqrt{3}u}$$ (4.89)
Substituting back into equations (2.10) and (2.18), and performing the simple energy integration, we obtain the third cluster coefficient

\[ b_3^{HD} = \frac{1}{3^{3/2}(4\pi)^{1/2}} \]  

(4.90)

in agreement with our previous result (4.82).

We now turn to examining the approach suggested at the end of the previous section and compare the contributions to \( \text{Tr}(G_0\Gamma G_0)_c \) from the first three orders of the multiscattering series to the exact expression (4.80) for \( \text{Tr}G_c \).

Since there is no exchange, first order terms are all disconnected. Higher order terms are all connected.

There are six second order terms, all of the form

\[
\left\{ G_0 t_j G_0 t_k G_0 | \mathcal{P} > | \mathcal{P} \right\} \text{dP} = \left( \frac{1}{i\pi} \right)^2 \int \text{dP} \frac{\delta(E_P)\sqrt{22-3P_i^2}\sqrt{22-3P_j^2}}{\left( Z-P^2 \right)^2 \left( Z-2P_i^2-2P_j^2-2P_i P_j \right)}
\]

(4.91)

where we have used the hardcore limit of (4.49),

\[
\left\langle \mathcal{P} | t_j^{\text{II}}(z) | k \right\rangle = \frac{1}{i\pi} \delta(p_i-k_i)\delta(E_p-E_k)\sqrt{22-3k}^2
\]

(4.92)

and performed some of the integrations covered by delta functions.

Third order terms fall into two classes of six terms each

\[
\left\{ G_0 t_j G_0 t_j G_0 t_k G_0 | \mathcal{P} > | \mathcal{P} \right\} \text{dP} = \left( \frac{1}{i\pi} \right)^3 \int \text{dPdQ} \frac{\delta(E_P)\sqrt{22-3P_i^2}\sqrt{22-3Q_i^2}\sqrt{22-3P_j^2}}{\left( Z-P^2 \right)^2 \left( Z-2P_i^2-2Q_i^2-2P_i Q_i \right) \left( Z-2P_k^2-2Q^2-2P_k Q \right)}
\]

(4.93)
where \( i \neq k \), and

\[
\langle \mathbf{p} | G_0 t_i G_0 t_j G_0 | \mathbf{p} \rangle = (\frac{1}{11})^3 \int \frac{dp dq}{(z_p^2)^2} \frac{\delta(E_p)(2Z-3p_1^2)^{\frac{\sqrt{2Z-3q^2}}{2}}}{(z_p^2-2q_1^2-2p_1^2 q)^2} (4.94)
\]

Adding all second and third order terms we have

\[
- \frac{6}{\pi^2} \int \frac{dp}{(z_p^2)^2} \frac{\delta(E_p)(2Z-3p_1^2)^{\frac{\sqrt{2Z-3q^2}}{2}}}{(z_p^2-2p_1^2 p_2^2-2p_1 p_2)} + \frac{1}{i\pi} \int \frac{dq}{(z_p^2-2q_1^2-2q p_1)(z_p^2-2q^2-2q p_2)} (4.95)
\]

We compare this expression to the exact \( \text{Tr} G_c \), (4.80), which can be rewritten as

\[
\text{Tr} G_c = - \frac{6}{\pi^2} \int \frac{dp}{(z_p^2)^2} \frac{\delta(E_p)}{4(p_3-p_1+i\eta)(p_3-p_2+i\eta)} + \frac{1}{(p_3-p_1-i\eta)(p_3-p_2-i\eta)} (4.96)
\]

To establish whether (4.95) is equivalent to the RHS of (4.96), we need to place the energy parameter \( Z \) on-shell, to remove the square root terms. However, the propagators then diverge. If the energy is left off-shell, there seems to be no way of relating (4.95) to the RHS of (4.96), even if the straightforward \( q \)-integration is performed. It is possible that the two expressions will yield the same result after both the trace and energy integrations, however the presence of the square roots make these integrations very unwieldy.
For the moment the question of the sufficiency of the first three orders of the multiscattering series remains open. We will return to it in §4.9 where we look at hard symmetric particles. The advantage there is that we have the fully off-shell T-matrix (§4.8) so that we can make a comparison between the exact off-shell expression and the contributions from the first three orders.

Before we leave this section we look at another interesting feature of the hard distinguishable case.

Examination of the solutions to the Faddeev Equations (see Appendix E), reveals that in the hardcore limit $T_2$ vanishes identically. This is another effect of the impenetrability of the particles in this limit. In the light of the known analytic structure of the scattering amplitude it may be instructive to see how the divergent terms in $T_2$ cancel out.

By taking the contributions to $T_2$ from the multiscattering series up to third order explicitly we are able to demonstrate that the singular terms do in fact cancel.

Applying the limit $c \rightarrow \infty$ to the Faddeev Equation (E.2) we have

$$
\langle p | T_1^{HD} | k \rangle = \left( \frac{1}{2\pi} \right)^2 \delta(\Sigma_k - \Sigma_p) \left[ \frac{k_2 - k_3}{k_2 - p_1 + i\eta} - \frac{k_1 - k_2}{k_3 - p_1 + i\eta} - \frac{k_2 - k_3}{k_1 - p_1 + i\eta} \right]
$$

$$
\langle p | T_2^{HD} | k \rangle = 0
$$

$$
\langle p | T_3^{HD} | k \rangle = \left( \frac{1}{2\pi} \right)^2 \delta(\Sigma_k - \Sigma_p) \left[ \frac{k_2 - k_3}{k_1 - p_3 + i\eta} + \frac{k_1 - k_2}{k_3 - p_3 + i\eta} - \frac{k_1 - k_3}{k_2 - p_3 + i\eta} \right] (4.97)
$$

where as can easily be checked
\[<p| [T_1^{HD} + T_2^{HD} + T_3^{HD}] | k> = <p| T^{HD} | k>\]

and the \( T_i \) satisfy the Faddeev Equations

\[ T_i = t_i + t_i G^i_0 (T_j + T_k) \quad i \in [1,2,3]\]

which can be iterated to give three subseries of the multiscattering expansion.

We know from our earlier analysis of this expansion that the first three orders of the series contains singular terms, yet \( T_2^D \) is identically zero, implying that the divergent terms cancel out in the limit \( c \to \infty \). We now examine how this happens.

The first order matrix element can be immediately written down in the half-off-shell case, from (3.12)

\[ <p| t_2 | k> = \delta(Ep-Ek)\delta(p_2-k_2)\tau_{13}(E-\frac{3}{2}p_2^2) \quad (4.98)\]

where \( (E - \frac{3}{2}p_2^2) \) is the energy of particles 1 and 3 in the centre of mass frame.

The second order matrix elements involve integration over one set of intermediate states, which can be immediately performed, to give

\[ <p| [t_2G^t_0 t_1 + t_2G^t_0 t_3] | k> = \delta(Ep-Ek)\tau_{13}(E-\frac{3}{2}p_2^2)\]

\[ \left[ \frac{1}{E-p_2^2-k_1^2-(p_2+k_1)^2+i\eta} \frac{k_2-k_3}{\pi i} + \frac{1}{E-p_2^2-k_3^2-(p_2+k_3)^2+i\eta} \frac{k_1-k_2}{\pi i} \right] \]

in the half-off-shell case with \( E = k^2 \). The propagators can be factorized using the fact that \( \Sigma k_i = 0 \), and then separated by
partial fractions, giving the total second order contribution to $T_2^D$

$$- \frac{1}{2\pi i} \delta(\Sigma_p - \Sigma_k) T_{13}(E - \frac{3}{2}p_2^2) \left[ \frac{1}{p_2 - k_2 - i\eta} - \frac{1}{p_2 - k_3 + i\eta} + \frac{1}{p_2 - k_1 - i\eta} - \frac{1}{p_2 - k_2 + i\eta} \right]$$

The first and last terms in the square brackets combine to give a delta function term which exactly cancels the first order term (4.98), leaving only

$$\frac{1}{2\pi i} \delta(\Sigma_p - \Sigma_k) T_{13}(E - \frac{3}{2}p_2^2) \left( \frac{1}{p_2 - k_2 - i\eta} - \frac{1}{p_2 - k_2 + i\eta} \right) \quad (4.99)$$

which is singular.

There are four third order terms and the use of diagrams allows their contributions to be immediately written down with only one remaining integration.

Figure 9.
\[
\delta(\Xi_p - \Xi_k) \tau_{13}(E - \frac{3}{2}p_2^2) \int dq \frac{1}{E - 2(q^2 + p_2^2 + qk_2) + i\eta} \\
= \delta(\Xi_p - \Xi_k) \tau_{13}(E - \frac{3}{2}p_2^2) \int dq \frac{\sqrt{2E - 3q^2}}{E - 2(q^2 + p_2^2 + qk_2) + i\eta} \\
\left[ \frac{2(k_1 - k_3)}{E - 2(q^2 + k_2^2 + qk_2) + i\eta} + \frac{k_1 - k_2}{E - 2(q^2 + k_3^2 + qk_3) + i\eta} + \frac{k_2 - k_3}{E - 2(q^2 + k_1^2 + qk_1 + i\eta)} \right]
\]

As before, we take \( E = k^2 \), factorize the propagators in the square bracket and separate by partial fractions. Completing the square in \( q \) in the first propagator, we obtain

\[
\delta(\Xi_p - \Xi_k) \tau_{13}(E - \frac{3}{2}p_2^2) \int dq \frac{\sqrt{2E - 3q^2}}{(E \frac{3}{2}p_2^2) - (q^2 + p_2^2)^2 + i\eta} \left[ \frac{1}{2\pi i(k_1 - q + i\eta)} + \frac{3}{q - k_3 + i\eta} \right] + \delta(q - k_2)
\]

of which the last part can be immediately simplified to

\[
- \frac{1}{2\pi i} \delta(\Xi_p - \Xi_k) \tau_{13}(E - \frac{3}{2}p_2^2) \left( \frac{1}{p_2 - k_3 + i\eta} - \frac{1}{p_2 - k_1 - i\eta} \right)
\]

cancelling (4.99) exactly. So the remaining term from the first three orders is
\[
\frac{3}{(2\pi i)^2} \delta(\Sigma k \cdot p) \tau_{13}(E - \frac{3}{2}p^2) \left[ \frac{dq\sqrt{2E - 3q^2}}{(\frac{E}{2} - \frac{3}{4}p^2) - (q + \frac{E}{2})^2 + i\eta} \right] \left( \frac{1}{k_1 - q + i\eta} + \frac{1}{q - k_3 + i\eta} \right)
\]

(4.101)

We now analyse the structure of this integral to verify that all the divergent terms have cancelled, and that the remainder term contains no on-shell singularities.

Considering the integrand in the complex \( q \) plane, the singularity structure is illustrated in Figure 10.

There is a pair of branch points at \( q = \pm \sqrt{\frac{2E}{3}} + i\epsilon \) arising from the square root. Cuts may be made parallel to the real axis and away from the origin. The propagator has simple poles at \( q_1, q_2 = -\frac{D_2}{2} \pm \frac{1}{2} (\sqrt{2E - 3p^2} - i\eta) \). The bracketed term yields a simple pole at \( q_3 = k_1 + i\eta \) or \( q_4 = k_3 - i\eta \).

The integral becomes singular if any pair of poles pinches the real axis from above and below, that is, take the forms \( x + i\eta, x - i\eta \).
It appears that the propagator poles do this when $\sqrt{2E-3p_2^2} = 0$. However this is not an on-shell singularity because in the centre of mass frame

$$E = p^2 = \frac{3}{2} p_2^2 + \frac{1}{2} (p_1 - p_3)^2,$$

so this case would correspond to the situation $p_1 = p_3$, contravening the requirement that the momenta be distinct, which also precludes a pinch between $q_3$ and $q_4$.

Other possible pinches can be ruled out by consideration of the ranges of the real part of the poles.

The restrictions $\Sigma k_1 = 0$ and $k_1 > k_2 > k_3$ imply that $k_1 > 0$, $k_3 < 0$ and on-shell when $E = k_2^2$, we find that

$$0 < \frac{1}{2} \sqrt{\frac{2E}{3}} < k_1 < \frac{1}{2} \sqrt{\frac{2E}{3}}$$

and

$$-\frac{1}{2} \sqrt{\frac{2E}{3}} < k_3 < -\frac{1}{2} \sqrt{\frac{2E}{3}} < 0$$

The propagator poles are only likely to be troublesome when they are near the real axis, so we need only consider the domain $|p_2| < \sqrt{\frac{2E}{3}}$ where the square root remains real.

In this domain, it is not difficult to show that

$$-\frac{1}{2} \sqrt{\frac{2E}{3}} \leq \Re(q_1) \leq \frac{1}{2} \sqrt{\frac{2E}{3}}$$

and

$$-\frac{1}{2} \sqrt{\frac{2E}{3}} \leq \Re(q_2) \leq \frac{1}{2} \sqrt{\frac{2E}{3}}$$

We see that there is no overlap in the ranges of the real parts of $q_1$ and $q_4$, or in the ranges of $q_2$ and $q_3$, and
therefore no pinches are possible. So the remainder term (4.101) is analytic on-shell, as expected.
4.8 The Fully Off-Shell $T$-Matrix

The fully off-shell $T$-matrix is in principle constructible from the half-off-shell amplitudes by means of the Low Equation, $T = V + VGV$, thus,

$$<p|T(z)|k> = <p|V|k> + \int <p|V|\psi_k', \frac{1}{Z-k'}Z \psi_k'| V|k'> dk'$$  \hspace{1cm} (4.102)

$$= <p|V|k> + \int \frac{<p|T|k'><k|T'|* dk'}{Z-k'}$$  \hspace{1cm} (4.103)

where we have taken a spectral representation of the Green's function on the basis of the complete set $\{|\psi_k'>\}$ of asymptotic scattering states, and then used the relation $V|\psi_k'> = T|k'>$.

The matrix elements appearing in the integrand of (4.103) are now half-off-shell amplitudes, as given by (4.11) and (4.12) for distinguishable and symmetric particles respectively.

Evidently from the form of these amplitudes, the evaluation of each contributing term is straightforward, but the resulting expression will be very unwieldy.

Fortunately, in the case of symmetric statistics, we have been able to simplify the overall expression considerably.

Recalling the half-off-shell amplitude (4.12), we observe that it can be written in the more symmetric form

$$<p|z^S|k> = \frac{-2ie}{(2\pi)Z} \frac{\delta(Ek-Ep)}{(k_1-k_2+ic)(k_1-k_3+ic)(k_2-k_3+ic)}$$

$$\times 2i \text{ Im} \sum_{\text{cyclic}} \sum_{j=1}^{3} \frac{2(k_{p_1}-k_{p_2})(k_{p_3}-k_{p_1}-ic)(k_{p_2}-k_{p_3}+ic)}{k_{p_3}-p_j+i\pi}$$  \hspace{1cm} (4.104)
where we sum only over cyclic permutations \( P \) of (123).

Substituting into equation (4.103), the integral term becomes

\[
- \frac{c^2}{\pi} \int \frac{dk'}{[k'_1-k'_2]^2+c^2} \left( \frac{\delta(S\nu-Ek') \delta(\epsilon k-Ek')}{[(k'_1-k'_2)^2+c^2][(k'_1-k'_3)^2+c^2]} \right) \text{Re} \sum_{k=1}^{2} \sum_{m=1}^{3} \sum_{cyclic \ P} \sum_{cyclic \ Q} 2(k'_1-k'_2)(k'_1-k'_3+ic)(k'_2-k'_3+ic)
\]

\[
\times \frac{2(k'_1-k'_2)(k'_1-k'_3+ic)(k'_2-k'_3+ic)}{k'_1-k'_2+i\eta} \frac{2(k'_{Q_1}-k'_{Q_2})(k'_{Q_1}-k'_{Q_3}-ic)(k'_{Q_2}-k'_{Q_3}+ic)}{k'_{Q_3}-k'_{m}+i\eta}
\]

\[
= - \frac{2}{k'_{Q_3}-k'_{m}-i\eta}
\]

(4.105)

where we have used the identity

\[(\text{Im } z_1)(\text{Im } z_2) = -2\text{Re}(z_1(z_2-z^*_2))\]

To fully exploit the high degree of symmetry possessed by (4.105), and to reduce the number of parameters by integrating over the total momentum, we define the coordinates

\[
q_1 = k'_3
\]

\[
q_2 = k'_{P_1} - k'_{P_2}
\]

\[
q_3 = k'_{P_1} + k'_{P_2} + k'_{P_3}
\]

The Jacobian of this transformation is \( \frac{1}{2} \), and the \( q_3 \) integration can immediately be performed, leaving

\[
- \frac{12c^2}{\pi} \delta(S\nu-Ek) \int dq_1 dq_2
\]

(4.106)
where we have replaced the summation over cyclic $P$ by a factor of 3, since each $P$ will give the same contribution after integration, and where we have dealt explicitly with the cyclic permutations $Q$ by defining

$$A_1(k_m) = \frac{q_2(3q_1-q_2-2ic)-3q_1-q_2+2ic}{q_1-k_m+in}$$

$$A_2(k_m) = \frac{(-q_2-3q_1)(q_2-ic)(3q_1-q_2+2ic)}{\frac{1}{2}q_2-\frac{1}{2}q_1-k_m+in} \quad (4.107)$$

$$A_3(k_m) = \frac{(3q_1-q_2)(-q_2-3q_1-2ic)(q_2+ic)}{-\frac{1}{2}q_2-\frac{1}{2}q_1-k_m+in}$$

As a useful consistency check and also as an interesting exercise, we now show that this fully off-shell amplitude reduces to the correct half-on-shell T-matrix in the hardcore limit.

Taking the sums over the cyclic permutations $P$ and $Q$ explicitly, and multiplying out and collecting terms, we have for the integral term (4.105) in the centre of mass frame

$$-\frac{4}{3(2\pi)^3} \delta(E_k-E_p) \sum_{k_{m,n}} \int \frac{dE_k'}{2c'} \left[ \frac{k_{31}^2 c^2}{k_{31}^2 + c^2} \left( \frac{1}{(k_{2m}^2-k_m+in)(k_{2m}^2-p_y+in)} \right) 
+ \frac{k_{31}^2 c^2}{k_{31}^2 + c^2} \left( \frac{k_{2m}^4 c^2}{k_{2m}^4 + c^2} \left( \frac{k_{12}^4 c^2}{k_{12}^4 + c^2} - 1 \right) \left( \frac{1}{(k_{2m}^2-k_m+in)(k_{2m}^2-p_y+in)} \right) 
+ \frac{2k_{2m}^4 k_{12}^4 c^2}{(k_{2m}^4 - ic)(k_{12}^4 + ic)} \left( \frac{1}{(k_{1m}^4-k_m+in)(k_{1m}^4-p_y+in)} \right) 
- \frac{2k_{2m}^4 k_{12}^4 c^2}{(k_{2m}^4 + ic)(k_{12}^4 + ic)(k_{31}^4 - ic)} \left( \frac{1}{(k_{1m}^4-k_m-in)(k_{1m}^4-p_y+in)} \right) 
\right) 
\right.$$

+ complex conjugates]

$$\right)$$

(4.108)
We label the four main terms within the square brackets together with their complex conjugates, A, B, C and D respectively, and treat each in turn.

Term A is readily factorizable, yielding a product of delta functions:

\[
- \frac{4}{3(2\pi)^2} \delta(\Sigma k - \Sigma p) \sum_{k, m} \delta(k_m - p_{\parallel}) \int \frac{dk'}{2\pi} \frac{\delta(\Sigma k')}{2Z-k'^2} \frac{k'^2 + c^2}{k'^2 + c^2} \delta(k'_2 - k_m) \\
= \frac{4}{3(2\pi)^2} \delta(\Sigma k - \Sigma p) \sum_{k, m} \delta(k_m - p_{\parallel}) \left[ -\frac{\pi c^3}{2Z-3k^2 + c^2} + \frac{\pi c^2 \sqrt{2Z-3k^2} c}{m} \right]
\]

(4.109)

where we have used contour integration in the upper half plane to perform the third \(k'\) integration, the first two being covered by delta functions.

In the limit \(c \rightarrow \infty\), the first term of (4.109) is cancelled by the Born term from (4.103)

\[
\langle p|V|k \rangle = \frac{4c}{2\pi \delta} \delta(\Sigma k - \Sigma p) \sum_{k, m} \delta(k_m - p_{\parallel})
\]

where we have adjusted the normalization, as explained in Appendix A.

The remaining term becomes in the half-on-shell \((Z=k^2)\) hardcore limit

\[
- \frac{1}{3\pi} \delta(\Sigma k - \Sigma p) \sum_{k} \left[ k_2 \delta(k_1 - p_{\parallel}) - k_3 \delta(k_2 - p_{\parallel}) + k_1 \delta(k_3 - p_{\parallel}) \right]
\]

(4.110)

We now look at term B, and define \(x = k'_1\), \(y = k'_2\). Changing variables in the integral we simplify the expression to
$$-\frac{4}{3} \frac{24}{(2\pi)^2} \frac{1}{2} \delta(\Sigma k-\Sigma p) \sum_{\ell_m} \int \frac{dx \, dy}{Z^{1/2} x^2 - \frac{3}{2} y^2} \frac{x^2 e^3}{x^2 + c^2}$$

(4.111)

$$\left[ \frac{i y}{(3y-x+2ic)(3y+x+2ic)} \left( y-k_m + i\eta \right) \left( y-p_{\ell} + i\eta \right) + \text{c.c.} \right]$$

Taking the first term in brackets, we combine the first two factors and separate the second two by partial fractions, and do the same with the second complex conjugate term. The simple pole terms may be expressed as a principal part and a delta function by use of

$$\frac{1}{x+i\eta} = \text{p} \frac{1}{x} + i\pi \delta(x) \quad (4.112)$$

The principal parts cancel, and the total square bracket term reduces to

$$\frac{\pi}{k_m - p_{\ell}} \left( \frac{2}{4c^2 + x^2} \left( k_m \delta(y-k_m) - p_{\ell} \delta(y-p_{\ell}) \right) \right) \quad (4.113)$$

in the limit $c \to \infty$. We substitute this back into term $B$ (4.111), integrate over $y$ directly with the aid of the delta functions, and over $x$ by contour integration, taking only those residues of highest order in $c$, and obtain

$$\frac{8}{\pi^2} \delta(\Sigma k-\Sigma p) \sum_{\ell_m} \frac{1}{k_m - p_{\ell}} \left[ - \frac{c^2}{6} \left( \frac{k_m}{2Z+c^2-3k^2_m} - \frac{p_{\ell}}{2Z+c^2-3p^2_{\ell}} \right) \right.$$  

$$\left. + \frac{c^2}{3} \left( \frac{k_m}{2Z+4c^2-3k^2_m} - \frac{p_{\ell}}{2Z+4c^2-3p^2_{\ell}} \right) \right]$$

Finally, taking the hardcore limit in this expression, we are left with
as the total contribution for term B.

We treat terms C and D together, and first take the limit \( c \to \infty \), which after some straightforward algebra, becomes

\[
2 \ k_1^2 \ k_1^2 \ (2\pi i)^2 \ \delta(k_1^2 - p_\ell) \ \delta(k_2^2 - k_m^2)
\]

The contribution to the off-shell hardcore \( T \) is readily calculated:

\[
- \frac{2}{3} \ \frac{1}{\pi^2} \ \delta(\Sigma_k - \Sigma p) \ \sum_{\ell, m} \ \frac{(p_\ell + 2k_m) (p_m + 2p_\ell)}{Z - 2k^2 - 2p_\ell^2 - 2k^2 p_\ell} \ (4.115)
\]

and we now place this half-on-shell, \( z = k^2 \), factorize the denominators and obtain

\[
\frac{4}{3} \ \frac{1}{\pi^2} \ \delta(\Sigma_k - \Sigma p) \ \left[ \frac{p_\ell + 2k_1}{p_\ell - k_2 - i\eta} + \frac{p_\ell + 2k_1}{p_\ell - k_3 + i\eta} \right] + \frac{p_\ell + 2k_2}{p_\ell - k_1 - i\eta} + \frac{p_\ell + 2k_2}{p_\ell - k_3 + i\eta} + \frac{p_\ell + 2k_3}{p_\ell - k_1 - i\eta} \nonumber
\]

Applying (4.112) to each pole, we find, after some algebra, that the principal part terms give a contribution

\[
\frac{6}{\pi} \ \delta(\Sigma_k - \Sigma p) \ \ (4.116)
\]

and the delta function terms yield

\[
\frac{2i}{3\pi} \ \delta(\Sigma_k - \Sigma p) \ \sum_{\ell} k_{13} \ \delta(p_\ell - k_2) \ \ (4.117)
\]
We can now combine (4.110), (4.114), (4.116) and (4.117) to obtain the half-on-shell hardcore T-matrix, with an extra symmetrization factor of $6^\frac{1}{2}$ (see Appendix A),

$$6^\frac{1}{2}<\hat{p}|T^\text{HS}(k^2)|k> = \frac{-2i}{\pi} \delta(\Sigma k - \Sigma p) \{k_{12}\delta(k_3 - p_k) + k_{23}\delta(k_1 - p_k) + k_{31}\delta(k_2 - p_k)\}$$

(4.118)

It can be readily verified that this expression is in agreement with the $c \rightarrow \infty$ limit of (4.16).

Although we have reduced the fully off-shell symmetric amplitude to a relatively compact form in (4.106), its structure is still complex enough to make manipulations difficult. The $q$ integrations in (4.106) (or the $k'$ integrations in (4.105),) can be performed by contour integration in the complex planes, but because there are several poles and branch points in each term, this process generates extremely long and cumbersome expressions.

We are particularly interested in finding a partitioning of the amplitude which isolates the on-shell forward scattering singularities, and leaves a manageable non-singular remainder which could be taken on-shell through the trace formula. Such a partitioning was discussed in §4.6, where it appeared that the first three orders of the multiscattering series could be a reasonable guess for the singular component to be subtracted.

For this approach to be useful, we would like to identify these singular terms within the full amplitude, so that they cancel by subtraction, and the remaining terms are tractable. The singular terms would then be treated explicitly off-shell to find their contribution.

However in spite of the simplifications resulting from the
symmetry of the particles, we have not been able to carry this program through because of the sheer complexity of the expressions involved.

The only further simplification left to us is to take the hardcore limit in the three symmetric particle system.
4.9 The Hardcore Limit with Symmetric Statistics

The wavefunction for this system is simply obtained from

\[(4.6)\]

\[
\lim_{c \to \infty} \Psi_{1k}^S(x) = \Psi_{1k}^{HS}(x) = \frac{1}{6^3} \left[ [123]+[231]+[312]-[213]-[132]-[321] \right] (4.119)
\]

and

\[
\Psi_{1k}^{HS}(x) = \Psi_{1k}^{HS} \left( P^{-1} x \right)
\]

We note by comparison with (4.72) that the effect of taking symmetric rather than distinguishable particles is to extend the wavefunction to the entire available space. Although the transmission coefficient is still zero, the identicality of the particles allows exchange at each interaction.

The half-off-shell and on-shell T matrices, and the on-shell S-matrix can also be easily found by applying the \( c \to \infty \) limit to (4.12), (4.16) and (4.19) respectively.

We are now interested in the third cluster coefficient of this system.

If we take the hardcore limit in \( b_3^S - b_3^{S0} \) (4.27), we find that this expression vanishes identically,

\[
\lim_{c \to \infty} (b_3^S - b_3^{S0}) = b_3^{HS} - b_3^{S0} = 0 . \quad (4.120)
\]

So

\[
b_3^{HS} = b_3^{S0} .
\]

It is also a well-known result that

\[
b_n^{S0} = (-)^{n+1} b_n^{A0} \quad (4.121)
\]
where $b_n^{A_0}$ is the nth cluster coefficient of a non-interacting one-dimensional gas of antisymmetric particles.

From (4.82), we recall that the third cluster coefficient of the system of hard distinguishable particles was also equal to $b_3^{A_0}$, so we have the interesting relations

$$b_3^{HS} = b_3^{S_0} = b_3^{A_0} = b_3^{HD} = \frac{1}{6\sqrt{3}\pi\beta}$$

(4.122)

It is a simple matter to check the third coefficient for the free symmetric and free antisymmetric gases by summing the contributions from the connected free particle diagrams

$$\text{Tr}(e^{-\beta H_0}) = \int \frac{dk}{(2\pi)^3} \sum_{P \neq I} \sum_{P_{ij} = 1 \neq j} e^{-\beta H_0}$$

(4.123)

$$= 2 \int \frac{dk}{(2\pi)^3} \delta(Ek) \delta(k_1 - k_2) \delta(k_2 - k_3) e^{-\beta k^2}$$

$$= \frac{2}{3}$$

So from (2.12)

$$b_3^{S_0} = \frac{1}{6\sqrt{3}\pi\beta}$$

in agreement with (4.122). If antisymmetric statistics were considered each permutation in (4.123) would have a factor $(-)^{S_0}$. The same cancellations would occur and since the only two remaining permutations, the cycles (123) and (132), are both even, the same value for the trace would be obtained. Hence we verify the equality of $b_3^{S_0}$ and $b_3^{A_0}$.

We turn now to the fully off-shell T-matrix derived in the last section. The hardcore limit has already been found in the
process of arriving at (4.118), so from (4.109), (4.114) and (4.115) and the Born term we have

\[
\langle p | T^{HS} (Z) | k \rangle = - \frac{2}{\pi^2} \delta (\Sigma k - E p) \left[ \frac{\pi i}{6} \sum_{k_m} \delta (k_m - p_{k_m}) \sqrt{2Z - 3k_m^2} + 3 \right] + \frac{1}{3} \sum_{k_m} \frac{(p_{k_m} + 2k_m) (k_m + 2p_{k_m})}{(Z - 2k_m^2 - 2p_{k_m}^2 - 2k_{m_{\perp}}^2)} \right] \tag{4.124}
\]

As a test of the trace formula (2.19), we would like to use this off-shell T-matrix to calculate \( \text{Tr}(e^{-\beta H} e^{-\beta H_0}) \), which we know already from (4.120), should vanish.

First we construct the connected part of the off-shell \( T \) by subtracting the disconnected terms

\[
\langle p | \sum_{k} (1 + P_{nm}) T^H (Z) | k \rangle = - \frac{2}{\pi^2} \delta (E p - \Sigma k) \left[ \frac{\pi i}{6} \delta (k_{\mu} - p_{k_{\mu}}) \sqrt{2Z - 3k_{\mu}^2} \right] \tag{4.125}
\]

from \( \langle p | \sum_p T^{HS} | k \rangle \). Since (4.124) is already symmetric in the momenta, the effect of the sum over permutations is to multiply the expression by 6. So (4.125) cancels the terms with \( m = \perp \) in the first summation of (4.124), and

\[
\text{Tr}(G_0 T^{HS} (Z) G_0) = - \frac{12}{\pi^2} \left[ \frac{dp \delta (\Sigma p)}{(Z - p^2)^2} \left\{ \pi i \delta (p_1 - p_2) \sqrt{2Z - 3p_1^2} + \frac{2(p_1 + 2p_2)(2p_1 + p_2)}{Z - 2p_1^2 - 2p_2^2 - 2p_1 p_2} \right. \\
+ \left. \frac{9p_1^2}{Z - 6p_1^2} + 3 \right\} \right] \tag{4.126}
\]

Performing the integrations covered by delta functions and relabelling parameters, we have
The trace of the Hamiltonian operator for (Z) is given by:

\[ \text{Tr}(G_0 T \text{HS} (Z) G_0) = -\frac{12\pi^2}{i^2} \int \frac{dx \sqrt{2Z-3x^2}}{(Z-6x^2)^2} + \int \frac{dx dy 2(2x+y)(x+2y)}{(Z-2x^2-2y^2-2xy)^3} \]

\[ + 9 \int \frac{dx dy x^2}{(Z-6x^2)(Z-2x^2-2y^2-2xy)^2} + 3 \int \frac{dx dy}{(Z-2x^2-2y^2-2xy)^2} \]  

(4.127)

we treat each integral in turn

\[ \frac{dx \sqrt{2Z-3x^2}}{(Z-6x^2)^2} = \frac{2i\pi}{3E} \int \frac{dt}{(1-t^2+i\eta)^{3/2}} = \frac{3\pi}{3E} \int \frac{dt}{(1-t^2+i\eta)^{3/2}} \]

\[ + \frac{i\pi}{3E} \int \frac{dt}{(1-t^2+i\eta)^{3/2}} \]  

(4.128)

\[ \int \frac{dx dy 2(2x+y)(x+2y)}{(Z-2x^2-2y^2-2xy)^3} = \frac{1}{2} \int du \frac{u(u+3z)}{(u^2-u_0^2)^3} = \frac{2i\pi}{3E} \int \frac{dt}{(1-t^2+i\eta)^{3/2}} \]  

(4.129)

where \( u = y+\frac{x}{2} \), \( u_0 = \frac{Z}{2} - \frac{3}{4} x^2 \), and we have performed the \( u \) integration by contour integration, and then applied the transformation \( t = \frac{3}{2E} \) \( x \).

The \( y \) integration in the third integral can be immediately performed by completing the square in \( y \) and then by residues, finally transforming to \( t \) again.

\[ 9 \int \frac{dx dy x^2}{(Z-6x^2)(Z-2x^2-2y^2-2xy)^2} = -\frac{3\pi i}{E} \int \frac{t^2 dt}{(1-t^2+i\eta)(1-t^2+i\eta)^{3/2}} \]

\[ = \frac{3\pi i}{4E} \int \frac{dt}{(1-t^2+i\eta)^{3/2}} \]  

(4.130)

Lastly

\[ 3 \int \frac{dx dy}{(Z-2x^2-2y^2-2xy)^2} = -\frac{3\pi i}{2E} \int \frac{dt}{(1-t^2+i\eta)^{3/2}} \]  

(4.131)
We observe that there are three basic integrals appearing in (4.128) - (4.131). These are evaluated in Appendix I. There is also another integral in (4.130) which we now express in terms of the basic ones, by integration by parts

\[
\int \frac{dt}{(1-4t^2+i\eta)(1-t^2+i\eta)^{3/2}} = \left[ \frac{1}{(1-4t^2+i\eta)(1-t^2+i\eta)^{3/2}} \right]_{-\infty}^{\infty} - \int \frac{8t^2 dt}{(1-4t^2+i\eta)^2(1-t^2+i\eta)^5}
\]

\[
= 2\int \frac{dt}{(1-4t^2+i\eta)(1-t^2+i\eta)^{3/2}} - 2\int \frac{dt}{(1-4t^2+i\eta)^2(1-t^2+i\eta)^5} \quad (4.132)
\]

Now combining (4.128) - (4.131) and (I.1), (I.2), (I.3) we have

\[
\text{Tr}(G_0T^{HS}(z)G_0) = -\frac{3\hbar}{4\pi} [-2I_1-4I_2+12I_3] = 0 \quad (4.133)
\]

verifying (4.120).

Thus we have successfully and directly tested the scattering trace formula (2.19), in an off-shell form.

Finally, we look again at the hypothesis that the third cluster coefficient of this model is calculable from just the first three orders of the multiscattering series.

We wish to formulate the expression

\[
\text{Tr}\left[P G_0 \left( \sum_i t_i G_0 t_i + \sum_{i \neq j} t_i G_0 t_j G_0 t_k \right) G_0 \right]_{\text{CM}} \quad (4.134)
\]

and to compare it to

\[
\text{Tr}\left[P G_0 T^{HS}(z) G_0 \right]_{\text{CM}}
\]

which we have at (4.127).
The connected first order terms of (4.134) are those of the form

$$\left< p \left| P \right| G_0 \right| \left. G_0 \right| P \right>_{CM} \frac{dp}{\pi} = \frac{1}{1!} \int \frac{dp/2Z-3p^2}{(Z-6p^2)^2} \tag{4.135}$$

where the permutation $P$ is such that $P_i \neq i$. There are twelve of these terms.

Second order terms are all connected, and they fall into two categories, twenty four terms for which $P_i \neq j$, and twelve terms for which $P_i = j$, giving a total contribution to (4.134) of

$$24 \left( \frac{1}{\pi} \right)^2 \int \frac{dp_1 dp_2 \sqrt{2Z-3p_1^2} \sqrt{2Z-3p_2^2}}{(Z-2p_1^2-2p_2^2-2p_1 p_2)^3} + 12 \left( \frac{1}{\pi} \right)^2 \int \frac{dp_1 dp_2(2Z-3p_1^2)}{(Z-2p_1^2-2p_2^2-2p_1 p_2)^3(Z-6p_1^2)} \tag{4.136}$$

There are also two classes of third order terms, depending on whether $P_i = i$ or $P_i \neq i$, and their total contribution to (4.134) is

$$48 \left( \frac{1}{\pi} \right)^3 \int \frac{dp \sqrt{2Z-3p_1^2} \sqrt{2Z-3p_2^2} \sqrt{2Z-3p_3^2}}{(Z-2p_1^2-2p_2^2-2p_1 p_2)^2(Z-2p_1^2-2p_2^2-2p_1 p_3)^2(Z-2p_2^2-2p_1 p_3)^2} + 24 \left( \frac{1}{\pi} \right)^3 \int \frac{dp(2Z-3p_1^2) \sqrt{2Z-3p_2^2}}{(Z-2p_1^2-2p_2^2-2p_1 p_2)^2(Z-2p_1^2-2p_2^2-2p_1 p_3)^2(Z-6p_1^2)} \tag{4.137}$$

Adding (4.135), (4.136) and (4.137) we find for (4.134)

$$- \frac{12}{\pi^2} \int \frac{dp/2Z-3p^2}{(Z-6p^2)^2} + 2 \int \frac{dp_1 dp_2 \sqrt{2Z-3p_1^2} \sqrt{2Z-3p_2^2}}{(Z-2p_1^2-2p_2^2-2p_1 p_2)^3} + \int \frac{dp_1 dp_2(2Z-3p_1^2)}{(Z-2p_1^2-2p_2^2-2p_1 p_2)^3(Z-6p_1^2)}$$
Now comparing (4.138) and (4.127) we notice that the first terms of each are exactly equal and that there are marked similarities in the structure of the remaining terms.

Considering the second term of (4.138), if we were to put $Z = p^2$ in the square root factors only and then apply $\delta(\Sigma p)$, we would obtain the second term of (4.127) exactly. To transform the third term of (4.138) into the third term of (4.127) we would need to apply $Z = p^2$ and then $\delta(\Sigma p)\delta(p_1-p_2)$ to the numerator.

Although there is of course no justification for any of these procedures, it is remarkable that they yield the exact terms of (4.127) with the correct numerical coefficients.

The last two terms of (4.138) are not so clearly related to the last term of (4.127). One integration needs to be performed and the resulting terms need to be combined in some simplifying way. We have not yet established that this can be done, nor fully evaluated (4.138). If our hypothesis is correct, (4.138) should vanish overall, but a rigorous evaluation is hampered by the presence of so many poles and branch cuts.
The aim of this work has been to investigate the scattering approach to the calculation of cluster coefficients, within the context of a particular model.

We have been interested in exploring the areas of applicability of the various scattering methods, with particular reference to the effects of the forward singularities in the on-shell amplitudes.

The one-dimensional model we have used was selected because its wavefunctions and S-matrix were known, and we were also able to construct the half-off-shell amplitudes, offering several avenues for testing out the scattering formalism. In addition the cluster coefficients were deducible from the work of Yang and Yang\(^{(1,2)}\) which was based on an independent approach and thus provided an excellent check.

These advantages have been partly offset by some inherent features of one-dimensional models.

Whereas in three-dimensional models, forward singularities only occur in the first two orders of the multiscattering series for the three particle amplitude, we found in §4.5 that these forward singularities persisted to third order for all one-dimensional systems. The divergent terms were seen to arise from pinches in the propagators forced by energy conservation through the intermediate states. Mathematically the divergences can be understood in terms of the reduced phase space available in one-dimensional models as compared to analogous three-dimensional systems, for smoothing integrations to remove the delta functions of momentum conservation.

A physical picture of the scattering processes also support this argument. It is apparent that the reduction in the degrees
of freedom of particles confined to one dimension will be very significant since it precludes the interaction of non-adjacent particles except by also interacting with the particles in between. There is no such restriction in two or three-dimensional systems.

Not only do one-dimensional models have a higher degree of singularity, but the ways of handling these divergent terms are also more restricted.

We saw in §2.3 and in §2.6 that two of the techniques suggested, the use of angular momentum eigenstates as a basis, and the use of a rotation operator, were obviously inapplicable to one-dimensional systems.

This leaves just two approaches for dealing with the singularities. One is to keep the formulation off-shell altogether, and the other is to find some partitioning of the amplitude which isolates the singular terms and leaves a tractable analytic remainder. In the latter case we expect to treat the singular terms explicitly off-shell, and to be able to apply the trace formula to the regularised remainder on-shell.

We have examined both of these approaches in depth as they apply to our model.

Although we have been able to formulate all the singular terms explicitly, as the first three orders of the multiscattering series, the partitioning approach has not been useful for this model. We saw in §4.6 that the full on-shell T-matrix is contained in the first three orders on-shell, and the difficulties in subtracting the singular terms from the full T even in the hardcore case, were discussed at the end of §4.8. Were such a subtraction possible, it appears likely that the regularized remainder would not contribute significantly, if at all, to the
cluster integrals.

Thus we have been forced to resort largely to off-shell calculations, and in this direction we have had more success.

In calculating the second and third cluster coefficients by direct integration in coordinate space (§3.2 and §4.2), we established that these coefficients were obtainable from off-shell scattering information, since the wavefunctions we used were asymptotic and independent of box normalization.

In §4.7 and §4.9 we used trace formulae with off-shell scattering operators to calculate \( b^\text{HD}_3 \) and \( b^\text{HS}_3 \). These results represent the most direct test of the trace formulation we have achieved and indicate that the scattering approach is valid at least in the off-shell form.

But the important question of the validity of the on-shell trace formulae cannot be determined by investigation of this model. It is clear from the discussion of §2.4 that the argument used to arrive at an on-shell formulation depends on the analyticity of the on-shell amplitude, and the highly singular nature of our T-matrices has been amply demonstrated.

However the same features which render this model so singular have also enabled us to perform some interesting off-shell calculations, which for most models would be impossible, and in the process of investigating difficulties such as the delicacy of the limiting processes, we have learnt a great deal about the structure of the model.
A. A Note on Symmetrization

The symmetrization of an arbitrary n-particle state $|\chi\rangle$ is effected by the straightforward application of the operator

$$A = (n!)^{-\frac{1}{2}} \sum_P (\pm)^{\delta_P} P$$

(A.1)

where we sum over all the permutations $P$ of the $n$ particle labels, $\delta_P$ being the order of the permutation, and the sign appropriate to the statistics of the particles. The normalization constant $(n!)^{-\frac{1}{2}}$ ensures that if $|\chi\rangle$ is a properly normalized state, then $A|\chi\rangle$ will be a properly normalized and symmetrized state.

To take properly symmetrized matrix elements of an operator $O$, it is sufficient to use symmetrized states for either the "in" or "out" state, rather than both, provided care is taken to adjust the overall normalization of the matrix element.

Formally, an arbitrary symmetrized matrix element will be

$$\langle \chi | A^\dagger O A | \chi' \rangle = \langle \chi | A^\dagger O | \chi' \rangle$$

(A.2)

since $[O,A] = 0$.

Now

$$A^\dagger A = (n!)^{-1} \sum_{PQ} (\pm)^{\delta_{PQ}} P Q$$

$$= \sum_{P'} (\pm)^{\delta_{P'}} P'$$

by well-known properties of permutations.

So we find
\[ \langle \chi | A^+ 0 | \chi' \rangle = (\pi !)^{\hbar Results \} \langle \chi | A^+ 0 | \chi' \rangle \\
\]

\[ = (\pi !)^{\hbar Results \} \langle \chi_{\text{symm}} | 0 | \chi' \rangle \quad \text{(A.3)} \]

where \( |\chi_{\text{symm}}\rangle = A |\chi\rangle \).
Proof that $\text{Tr ln AB} = \text{Tr ln A} + \text{Tr ln B}$

Let $A$ and $B$ be two non-singular $n \times n$ matrices which do not necessarily commute.

Then

$$\det(AB) = \det A \det B$$

(B.1)

and the well-known identity

$$\det A = e^{\text{Tr ln A}}$$

can be used to rewrite (B.1) as

$$e^{\text{Tr ln(AB)}} = e^{\text{Tr ln A}} e^{\text{Tr ln B}}$$

from which the required result is proved by comparison of exponents.
C Density of States Approach to the Cluster Coefficients

We observed in §1.3 that since imposing box normalization conditions onto a system would quantize the momenta, one should be able to deduce the density of states, \( N(k, L) \) where \( L \) is the length of the box.

If it were possible to take the limit \( L \rightarrow \infty \), these functions could be used to transform the trace in (2.14) from a formal sum over states to integrals over the momenta.

For example with three particles

\[
\text{Tr} U_3 = \sum_{n_1 n_2 n_3} \langle n_1 n_2 n_3 | \left[ \left( e^{-\beta H} - e^{-\beta H_0} \right) - \sum_a \left( e^{-\beta H_a} - e^{-\beta H_0} \right) \right] n_1 n_2 n_3 \rangle \quad (C.1)
\]

where we have labelled the states by the quantum numbers \( n_1, n_2, n_3 \).

If we now took the limit \( L \rightarrow \infty \) in each term, we could replace the sum by the integral

\[
\int dk \, e^{-\beta k^2} \left[ \left( \frac{dn}{dk} \right)^2 - \left( \frac{dn^0}{dk} \right)^2 - \sum_a \left( \frac{dn^a}{dk} \right)^2 - \left( \frac{dn^0}{dk} \right)^2 \right] \quad (C.2)
\]

where \( \frac{dn}{dk} \) is the determinant of a 3x3 matrix whose \( i,j \)th element is \( \frac{\partial n_i}{\partial k_j} \), and the superscripts 0 and \( a \) indicate the free particle limit and the case with only pair \( a \) interacting, respectively.

Essentially \( \frac{dn}{dk} \) is the Jacobian of the transformation from \( n \) to \( k \) variables.

We note from the discussion of limits in §2.4 that only the overall connected part of the summand in (C.1) is defined in the
limit \( L^{*\infty} \), so (C.2) is not rigorous.

However if the resulting expression (C.2) were a correct representation of \( \text{Tr}U_3 \), it would be quite useful.

In particular, for our model, the work of Lieb and Liniger\(^{(4)}\) gives the density of states functions directly from the momentum quantization condition,

\[
k_{\perp} = n_{\perp} \frac{2\pi}{L} + \frac{1}{L} \sum_{j \neq i} \theta_{ij}
\]

where \( \theta_{ij} \) is defined by (4.2), and \( n_{\perp} \) is any integer. All the \( \frac{\partial n_{\perp}}{\partial k_{\perp}} \) can now be obtained by differentiation, and the Jacobian determinant constructed. It turns out that the subtraction of the disconnected terms in (C.2) results in the systematic cancellation of certain types of terms from the full \( \frac{dn_{\perp}}{dk_{\perp}} \) and in fact we are able to formulate \( \frac{dn_{\perp}}{dk_{\perp}} \) for the general \( \ell \)-body case of our model as

\[
\ell \frac{L}{2\pi} \sum_{i} C_{ij} \ldots C_{pq}
\]

where we sum over all the distinct products of \( \ell-1 \) factors, which are connected (in the sense that each factor \( C_{\ell m} \) "connects" particles \( \ell \) and \( m \)), and where

\[
C_{ij} = \frac{c}{\pi} \frac{1}{k_{ij}^2 + c^2} - \delta(k_i - k_j)
\]

Thus this approach gives a relatively simple prescription for calculating the \( \ell \)th cluster coefficient of the model with symmetric statistics.
However, we have found that this approach is incorrect.

Comparison of (C.5) and (G.9) shows that in the case $l=3$, the density of states method includes an extra delta function in one term of the correct integrand.

One effect of this is to render the integrand more symmetric than it should be. It is a feature of one-dimensional models that there is a certain asymmetry built-in by virtue of the fact that non-adjacent particles can only interact by also interacting with the particle(s) between them. Thus the particles though symmetric, are not equivalent, and this asymmetry has shown up, for example in the wavefunction (4.6) where the coefficient of the wave type [321] with particles 1 and 3 interchanged, is $Z_{12}Z_{13}Z_{23}$ and not just $Z_{13}$ as might have been expected. Similar observations can be made about the form of the T-matrices.

The source of the error is most likely in the process from (C.1) to (C.2). Not only are the individual disconnected terms not defined in the $L^\infty$ limit, but there is also the question of interchanging $\lim_{c\to 0}$ and $\lim_{L^\to \infty}$ in constructing $\left| \frac{dn^0}{dk} \right|$, and as Lieb and Liniger have pointed out, the $c\to 0$ limit is pathological.
D The Lippmann-Schwinger Equation

Scattering wavefunctions with the correct asymptotic form must satisfy the integral equation

\[ |\psi> = |\phi> + G^+_0 V |\psi> , \]  \hspace{1cm} (D.1)

known as the Lippmann-Schwinger equation.

We can verify that our wavefunctions do satisfy (D.1), and present here an outline of the proof.

In momentum space, (D.1) becomes

\[ <p|\psi_k> = <p|\phi_k> + <p|G^+_0 V |\psi_k> \]

or

\[ <p|\psi_k> - <p|\phi_k> = <p|T|k> \]

\[ \frac{1}{k^2 - p^2 + i\epsilon} \]  \hspace{1cm} (D.2)

Taking the most general case of distinguishable particles, we have the half-off-shell T-matrix at (4.11), and the wavefunction given by Table 1, which is transformed into momentum space by the usual Fourier Transform. The free particle wavefunction is similarly treated and we obtain on the LHS of (D.2) a sum of terms of the form

\[ \frac{1}{(2\pi)^2 \delta(\Sigma_k - \Sigma_p)} \frac{f(P,k)}{(k_i - p_{p1} + i\eta)(k_j - p_{p3} - i\eta)} \]  \hspace{1cm} (D.3)

where the coefficients \( f(P,k) \) are some combinations of reflection and transmission coefficients.

On the RHS we have a sum of terms of the form

\[ \frac{2i\epsilon}{(2\pi)^2 \delta(\Sigma_k - \Sigma_p)} \frac{1}{k^2 - p^2 + i\epsilon} \frac{q(k)}{k_i - p_{p1} + i\eta} \]  \hspace{1cm} (D.4)
where the coefficients $g(k)$ are also combinations of reflection and transmission coefficients.

Taking a term which has a positive imaginary part in the pole, we write the pole as

$$\frac{1}{k_i - p_j + i\eta} = \frac{1}{k_i - p_j} - i\pi\delta(k_i - p_j) \quad (D.5)$$

and (D.4) becomes

$$\frac{2ie}{(2\pi)^2}(-i\eta)\delta(\Sigma k - \Sigma p) g(k) \delta(k_i - p_j) - \frac{P.P. \text{ term}}{-2(k_j - p_i - i\epsilon)(k_i - p_j + i\epsilon)} + P.P. \text{ term} \quad (D.6)$$

where we have factorized the propagator with the aid of the two delta functions, and the signs of $i\epsilon$ are interchanged if $k_j < k_i$.

Now using (D.5) in reverse, (D.6) becomes

$$\frac{2ie}{(2\pi)^2} \frac{i\pi}{2} \delta(\Sigma k - \Sigma p) g(k) \frac{1}{(k_j - p_i - i\epsilon)(k_i - p_j + i\epsilon)} \left[ \frac{1}{k_i - p_j - i\eta} - \frac{1}{k_i - p_j + i\eta} \right] + P.P. \text{ terms} \quad (D.7)$$

$$= \frac{1}{(2\pi)^2} \delta(\Sigma k - \Sigma p) g(k) \frac{ie}{k_j - k_i} \left[ \frac{1}{(k_j - p_i + i\epsilon)(k_i - p_j + i\epsilon)} - \frac{1}{(k_j - p_i - i\epsilon)(k_i - p_j + i\epsilon)} \right]$$

$$+ P.P. \text{ terms} \quad (D.8)$$

where we have separated the overall denominator into partial fractions.

It can be shown by a proof similar to that in Appendix F, that the sum of all the principal part terms vanish on-shell, and the remaining terms are of the form of the terms on the LHS, (D.3).

The proof is completed by collecting terms, absorbing the factors $\frac{ie}{k_j - k_i}$ into the $g(k)$, and verifying that the resulting coefficients match those on the LHS.
The Faddeev T-matrices $T_i$ satisfy the coupled integral equations

$$<p|T_i|k> = <p|t_i|k> + <p|t_iG_0(T_j + T_k)|k> \quad i=1,2,3 \quad (E.1)$$

Each of these Faddeev Equations generates a subseries of the full multiscattering expansion (2.34), and from these it is easy to verify that

$$<p|\sum_{i=1}^{3} T_i|k> = <p|T|k> \quad (E.2)$$

We observe that each term in the series for $<p|T_i|k>$ will begin with an element

$$<p|t_i|k'> = \frac{c}{\pi} \delta(\Sigma \kappa' - \Sigma p) \delta(k'_i - p_i) \frac{|k'_j - k'_k|}{|k'_j - k'_k| + i\epsilon}, \quad (E.3)$$

and that apart from the overall momentum conserving delta function, the only $p$ dependence of $<p|T_i|k>$ will be on $p_i$. This suggests a quick way of obtaining the Faddeev T matrices from the full T.

Taking the case of distinguishable particles half-off-shell, the T-matrix is given by (4.11), and we postulate that

$$<p|T_1^D|k> = \frac{2ic}{(2\pi)^2} \delta(\Sigma \kappa - \Sigma p) \left[ \frac{t_{123}}{p_1-k_1+i\epsilon} + \frac{r_{12}r_{23}t_{123} + t_{12}r_{13}}{p_1-k_2+i\epsilon} + \frac{r_{12}r_{13}}{p_1-k_2+i\epsilon} \right]$$

$$<p|T_2^D|k> = \frac{2ic}{(2\pi)^2} \delta(\Sigma \kappa - \Sigma p) \left[ \frac{t_{123}}{p_2-k_2+i\epsilon} + \frac{t_{12}r_{13}r_{23}}{p_2-k_3+i\epsilon} - \frac{t_{13}r_{23}}{p_2-k_2+i\epsilon} - \frac{r_{12}t_{13}r_{23}}{p_2-k_1+i\epsilon} \right]$$
To prove this, we use (E.4) to substitute back into (E.1), and evaluating the resulting integrals on the RHS, verify that we obtain the appropriate \( T_1 \) of (E.4).

For example, taking \( i=1 \)

\[
\begin{align*}
\langle p | T_1 | k \rangle &= \frac{-2 i c}{(2 \pi)^2} \delta(\Sigma p - \Sigma p') \left[ \frac{t_{12} t_{13} t_{23}}{p_2 - k_2 + i \eta} - \frac{r_{23} t_{13}}{p_3 - k_2 + i \eta} - \frac{r_{12} r_{23} t_{13} + r_{13} t_{12}}{p_3 - k_1 + i \eta} \right] \\
&= \frac{-i c^2}{4 \pi^3} \frac{x}{x + ic} \delta(\Sigma p - \Sigma k) \left[ \frac{1}{-2 \left( (p + p_1^2 / 2, x^2 / 2) \right)} \left[ t_{12} t_{13} + \ldots + t_{12} t_{13} t_{23} + \ldots \right] \right] (E.6)
\end{align*}
\]

where \( x = \sqrt{Z - 3 p_1^2} \).

The \( p \) integration is then performed by contour integration, and after much lengthy algebra, we regain \( T_1 \) as given by (E.4) minus the Born term (E.3).
Proof that the Principal Parts of $T$ Vanish on-shell

Application of the identity (4.13) to (4.12) placed on-shell gives

$$\delta(\Sigma k^2 - \Sigma p^2) \langle \mathcal{P} | T | k \rangle = \delta(\Sigma k^2 - \Sigma p^2) \left\{ \frac{C}{2\pi i} \delta(\Sigma k - \Sigma p) \sum_{j=1}^{3} (1+Z_{12}) \delta(k_j - p_j) \right.$$  

$$+ Z_{23} (1+Z_{13}) \delta(k_j - p_j)$$  

$$+ Z_{12} Z_{13} (1+Z_{23}) \delta(k_j - p_j) + (1+Z_{23}) \delta(k_j - p_j) + Z_{12} (1+Z_{13}) \delta(k_j - p_j)$$  

$$+ Z_{13} Z_{23} (1+Z_{12}) \delta(k_j - p_j) \right\} \ (F.1)$$

We shall show that the second square bracket, the principal part term, vanishes identically in this on-shell limit.

Algebraic manipulation of the coefficients of the poles in the principal part term reduces it to

$$\frac{2ic\delta(\Sigma k - \Sigma p) \delta(\Sigma k^2 - \Sigma p^2)}{6^5 (2\pi)^2} \frac{24}{d(ic)^2} \sum_{j=1}^{3} \left[ \frac{n_{312} m_{12}}{k_3 - p_j} - \frac{n_{313} m_{13}}{k_2 - p_j} + \frac{n_{323} m_{23}}{k_1 - p_j} \right] \ (F.2)$$

where we define

$$d = \frac{(k_{12} + ic)(k_{13} + ic)(k_{23} + ic)}{(ic)^3}$$

$$m_{ij} = \frac{1}{2} (k_i - k_j)$$

$$n_k = \frac{1}{3} (k_i + k_j - 2k_k) = -k_k \text{ in the centre of mass frame of reference.}$$
The summand further simplifies to

\[
\frac{p_j^2 (n_3 m_{12} + n_2 m_{13} + n_1 m_{23}) + p_k (n_3^2 m_{12} + n_2^2 m_{13} + n_1^2 m_{23})}{(p_j - n_3) (p_j - n_2) (p_j - n_1)}
\]

and the first bracket of the numerator vanishes by simple substitution.

Taking the sum over \( j \) explicitly, the remaining term after some algebra becomes

\[
\frac{(\alpha - \alpha') (\beta' \alpha' - 3 \alpha \beta' - 2 \alpha' \beta)}{(n_3^3 + \alpha n_1^3 + \beta) (n_2^3 + \alpha n_2^3 + \beta) (n_1^3 + \alpha n_1^3 + \beta)}
\]

(F.3)

where we define

\[
p_j = -n_j', \\
\alpha = n_1 n_2 + n_1 n_3 + n_2 n_3, \\
\alpha' = n_1' n_2' + n_1' n_3' + n_2' n_3', \\
\beta = -n_1 n_2 n_3, \\
\beta' = -n_1' n_2' n_3'
\]

Now we observe that in the centre of mass frame of reference, \( \alpha \) and \( \alpha' \) are proportional to the initial and final energies respectively, so that the expression (F.3), being linearly dependent on the difference \( (\alpha - \alpha') \), must vanish in the on-shell limit.

Thus the principal part term (F.2) of the on-shell T-matrix vanishes identically and the assertion is proved.
G Yang and Yang's Formulation of $b_k$ for this model

Taking Lieb and Liniger's $\lambda$-particle wavefunction\(^{(4)}\) (of which (4.1, 4.2) is the three-body form) as a starting point, Yang and Yang\(^{(1,2)}\) arrive at an equation of state in the form of an integral equation for the pressure at temperature $T$:

$$P = \frac{1}{2\pi\beta} \int_{-\infty}^{\infty} dk \ln \left(1 + e^{-\beta \varepsilon(k)}\right)$$

with

$$\varepsilon(k) = -\mu + k^2 - \frac{1}{\pi\beta} \int_{-\infty}^{\infty} \frac{dq}{c^2 + (k-q)^2} \ln \left(1 + e^{-\beta \varepsilon(q)}\right)$$

The Lagrange multiplier $\mu$ arises from a variation to maximize entropy, and is shown to be the chemical potential, enabling the introduction of the fugacity

$$z = e^{-\beta \mu}$$

and the formulation of the fugacity expansion

$$e^{-\beta \varepsilon(k)} = \sum_{n=0}^{\infty} a_n(k,\beta) z^n$$

The coefficients $a_n(k,\beta)$ are obtained by taking the exponential of (G.1)

$$e^{-\beta \varepsilon(k)} = z e^{-\beta k^2 \mathcal{O} \ln(1 + e^{-\beta \varepsilon(q)})}$$

where the operator $\mathcal{O}$ is defined by

$$\mathcal{O} = \frac{c}{\pi} \int_{-\infty}^{\infty} dq \frac{1}{c^2 + (k-q)^2}$$
and then expanding first the logarithm and then the exponential in (G.3). (We note that the operators 0 and λn do not commute).

Equating coefficients with the expansion (G.2) yields

\[ a_0 = 0 \]
\[ a_1 = e^{-8k^2} \]
\[ a_2 = a_10a_1 \]
\[ a_3 = a_1[0a_2 - \frac{1}{2}0a_1^2 + \frac{1}{2}(0a_1)^2] \]
\[ a_4 = a_1[0a_3 - 0(a_1a_2) + 0a_10a_2 - \frac{1}{2}0a_10a_1^2 + \frac{1}{3}0a_1^3 + \frac{1}{6}(0a_1)^3] \]

etc.

The pressure can then also be written as a fugacity expansion

\[ p = \frac{1}{2\pi\beta} \int_{-\infty}^{\infty} dk. [a_1z+(a_2-\frac{1}{2}a_1^2)z^2+(a_3-a_1a_2+\frac{1}{3}a_1^3)z^3+...] \] (G.5)

which is essentially the cluster expansion (2.7).

A direct comparison of coefficients yields

\[ b_\lambda = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk A_\lambda \] (G.6)

with

\[ A_1 = a_1 \]
\[ A_2 = a_2-\frac{1}{2}a_1^2 \]
\[ A_3 = a_3-a_1a_2+\frac{1}{3}a_1^3 \] (G.7)

etc.

Thus the symmetric cluster coefficients to any order can be computed by a series of quadratures.
In particular, we evaluate the third coefficient for comparison with (4.27).

\[ b_3^s - b_3^0 = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left( A_3 - A_3^0 \right) \]

\[ = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left( a_3 - a_1 a_2 \right) \]  

(G.8)

Since the free-particle limit of the operator \( \hat{0} \) is just \( \delta(k-q) \).

Direct calculation yields

\[ b_3^s - b_3^0 = \frac{3}{4\pi} \int \frac{dk}{2\pi} e^{-\beta k^2} \left[ \frac{1}{\pi} \frac{1}{c^2 + (k_1 - k_2)^2} \right] \left[ \frac{1}{\pi} \frac{1}{c^2 + (k_2 - k_3)^2} \right] - \delta(k_2 - k_3) \]  

(G.9)

We now show this expression to be equivalent to our result (4.27).

Factorizing the denominators, separating them into partial fractions and expressing the resultant terms as integrals of exponentials, as was done in (3.16), the RHS of (G.9) becomes

\[ \frac{3}{4\pi} \left( \frac{1}{2\pi} \right)^2 \int \frac{dk}{\pi} e^{-\beta k^2} \int ds dt \]

\[ \int ds \int ds \left[ e^{i(k_1 - k_2)^s} + e^{i(k_1 - k_2)^s} \right] \]

\[ e^{-i(k_1 - k_2)^s} \]

\[ + e^{-i(k_1 - k_2)^s} \]

\[ e^{i(k_1 - k_2)^s} \]

\[ + e^{i(k_1 - k_2)^s} \]

\[ \left( e^{-c_s - c_t} - e^{-c_s} \right) \]  

(G.10)

where we have also expressed the delta function in (G.9) as an integral of an exponential.

We proceed now to perform the \( k \) integration by completion of squares in the exponents, and obtain
Finally we use the relation

$$
\int_0^{\infty} ds dt e^{-(s^2+t^2-st)/2\beta} f(s,t) = 2 \int_0^{\infty} ds dt e^{-(s^2+t^2+st)/2\beta} f(s+t,t) \quad (G.12)
$$

and symmetry of the integrand to transform (G.11) into (4.27), thus demonstrating agreement between our result for \( b_3^s - b_3^0 \), and the work of Yang and Yang.

The relation (G.12) can itself be easily proved by a change of variable, \( s \to s+t \), in the LHS, and use of the \( s,t \) symmetry of the integrand.
The Landau Rules provide a useful technique for determining the analytic structure of functions with a certain integral representation. In the following we briefly summarize the rules, referring to Eden et al.\(^{58}\) for a fuller discussion.

If a function \( F(z) \) can be expressed in the form

\[
F(z) = \int_{\mathbb{R}^n} dx_1...dx_n \frac{f(z,x_1)}{S_1(z,x_1)...S_m(z,x_1)} \tag{H.1}
\]

where \( f(z,x_1) \) is regular and the \( S_i \) may vanish for some values of \( z \), then we can use Feynman's identity to write

\[
F(z) = (m-1) \int_{\mathbb{R}^n} dx_1...dx_n \int_0^1 d\alpha_1...d\alpha_m \frac{\delta(\sum \alpha_i - 1) f(z,x_1)}{(\alpha_i S_i)^m} \tag{H.2}
\]

The integrand now contains the singularity surface

\[ D = \sum \alpha_i s_i = 0 \quad \text{in a space of} \quad n+m \quad \text{parameters, which gives rise to a singularity in} \quad F(z) \quad \text{when} \]

\[
D = 0 \tag{H.3}
\]

\[
\frac{\partial D}{\partial \alpha_i} = 0, \quad \text{i.e.} \quad \alpha_i = 0 \quad \text{or} \quad s_i = 0 \quad \text{i} \in [1,m] \tag{H.3}
\]

\[
\frac{\partial D}{\partial x_j} = 0 \quad \text{j} \in [1,n]
\]

all hold. These conditions constitute the Landau Rules.
Some Useful Integrals

\[ \int_{-\infty}^{\infty} \frac{dt}{(1-t^2+i\eta)^{1/2}} = \left. \frac{t}{(1-t^2+i\eta)^{1/2}} \right|_{-\infty}^{\infty} = \frac{2}{i} \quad (I.1) \]

\[ \int_{-\infty}^{\infty} \frac{dt}{(4t^2-a^2-i\eta)(1-t^2+i\eta)^{1/2}} = \frac{\pi i}{2a\sqrt{1-a^2/4}} - \frac{i \arcsin a/2}{a\sqrt{1-a^2/4}} \quad (I.2) \]

Proof

In the complex-\( t \) plane the integrand has simple poles at \( \pm \left( \frac{a}{2} + i\eta \right) \), and branch points at \( t = \pm (1-i\eta) \).

To complete the contour in the upper half plane we make a branch cut above the positive real axis from \( 1 + i\eta \) to \( \infty + i\eta \) and deform the contour around it.

The integral is now given by the residue at the upper pole plus the branch cut integral.

Residue at \( t = \frac{a}{2} + i\eta = \lim_{t \to a/2} \frac{2\pi i}{2(2t+a+i\eta)(1-t^2+i\eta)^{1/2}} = \frac{\pi i}{2a\sqrt{1-a^2/4}} \)

Branch cut integral = \(-2i\int_{1}^{\infty} \frac{dt}{(4t^2-a^2)(t^2-1)^{1/2}} \)

\[ = -\frac{i}{2a} \int_{1}^{\infty} \left[ \frac{1}{t^2-a^2} - \frac{1}{t^2+a^2} \right] \frac{1}{(t^2-1)^{1/2}} \ dt \]

\[ = -\frac{i}{2a} \frac{1}{\sqrt{1-a^2/4}} \left[ \arcsin \frac{a}{t} \bigg|_{t=a/2}^{t=\infty} + \arcsin \frac{a}{t} \bigg|_{t=1}^{t=1} \right] \]

\[ = \frac{i \arcsin a/2}{a \sqrt{1-a^2/4}} \].
Hence we obtain (I.2) above.

For the case $a=1$, we find

\[
\int_{-\infty}^{\infty} \frac{dt}{(4t^2-1-i\eta)(1-t^2+i\eta)^{1/2}} = \frac{2\pi i}{3\sqrt{3}} .
\]

I.3 \[
\int_{-\infty}^{\infty} \frac{dt}{(4t^2-1-i\eta)^2(1-t^2+i\eta)^{1/2}} = -\frac{i}{3}(1 + \frac{2\pi}{3\sqrt{7}})
\]

Proof

\[
\int_{-\infty}^{\infty} \frac{dt}{(4t^2-a^2-i\eta)^2(1-t^2+i\eta)^{1/2}} = \frac{1}{2a} \frac{\partial}{\partial a} \int_{-\infty}^{\infty} \frac{dt}{(4t^2-a^2-i\eta)(1-t^2+i\eta)^{1/2}}
\]

\[
= \frac{i}{2a} \frac{\partial}{\partial a} \left[ \frac{\pi}{a/4-a^2} - \frac{2 \arcsin \frac{a}{2}}{a/4-a^2} \right]
\]

from (I.2).

Evaluating the derivative and then taking $a=1$ yields the required result.
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Cluster coefficients for the one-dimensional Bose gas with point interactions

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Exact expressions for the cluster coefficients $b_1$ and $b_3$ for the one-dimensional Bose gas with repulsive $\delta$-function interactions are found. The calculation depends only on scattering information in the form of two- and three-body scattering wavefunctions. Although not in agreement with a previous calculation by Servadio, our results are shown to be consistent with the work of Yang and Yang which involves the use of periodic rather than scattering boundary conditions.

I. INTRODUCTION

Both the thermodynamic properties$^{1-3}$ and the $S$ matrix$^{4,5}$ are known for a system of bosons moving in one dimension and interacting through repulsive $\delta$-function potentials. It is interesting to ask whether the statistical mechanics of this system can be deduced from the $S$-matrix along the lines suggested by the general theory of Dashen, Ma, and Bernstein.$^6$ In such an approach the solutions of the $n$-body problem in a finite domain are not needed; only scattering information is used to construct the partition function. In addition to providing a specific illustration of the relationship between the $S$ matrix and statistical mechanics, this type of calculation could be of practical use in finding new results for other one-dimensional gases where the $S$-matrix or scattering solutions are known$^{4,5}$ but where the solutions satisfying periodic boundary conditions are not available.

In this paper an exact expression for the third virial coefficient for the one-dimensional Bose gas with repulsive point interactions is found. The calculation uses scattering information in the form of the two- and three-body scattering wavefunctions. The question of whether on-shell information alone is sufficient to determine the equilibrium thermodynamic properties of the gas is not answered, since our starting point is not the $S$ matrix, but the cluster operator of Lee and Yang.$^7$ It is not clear whether the cluster coefficients may be expressed in terms of $S$-matrix elements since the formal limiting processes used in Ref. 3 are not valid for the singular amplitudes of this system. We hope to return to this question later. However, we are able to demonstrate that the third virial coefficient may be calculated from the solutions of the scattering problem without invoking box normalization.

Servadio$^8$ has also applied the cluster formulation to the one-dimensional Bose gas with point interactions. Although our expression for the second cluster coefficient $b_2$ agrees with the result stated in Ref. 8, the results for the matrix elements of the third cluster operator $U_3$ disagree.

An independent check is provided by the work of Yang and Yang$^{2,3}$ where the equation of state is found by a different method employing periodic boundary conditions. In the Appendix the results of this paper are shown to be consistent with the theory of Yang and Yang. In view of this agreement we believe that the expression given in Ref. 8 for the third cluster operator is incorrect.

II. DEFINITIONS AND BACKGROUND RESULTS

We consider a system of $n$ bosons interacting through two-body repulsive $\delta$-function potentials of strength $c$. The scattering wavefunction $\phi_{1,n}(x)$ associated with incoming momenta $k_1 \cdots k_n$ is a linear combination of all possible plane-wave types$^{4,9}$:

$$\phi_{1,n}(x) = \left[ \frac{n!}{(2\pi)^n} \right]^{1/2} \sum_P a(P) \exp(i \sum_{k=1}^n k_x x_k).$$

The sum runs over all permutations $P$ of order $n$ and the coefficients $a(P)$ are determined in terms of the momenta $k_1 \cdots k_n$ and the strength $c$ of the interaction by

$$a(P) = \exp \left( \frac{i}{2} \sum_{k=1}^n k_x x_k \right),$$

with

$$\psi_{ij} = 2 \tan^{-1} \left( \frac{c}{k_i - k_j} \right).$$

The wavefunction (1) is only valid in the region $-\infty < x_1 < x_2 < x_3 \cdots < x_n < \infty$, but the wavefunction in all other regions may be obtained from (1) by symmetry considerations.

Gaudin$^9$ has shown that the scattering wavefunctions (1) satisfy the closure relation

$$\int \cdots \int \phi_{1,n}(x) \phi_{1,n}(y) = \delta^n(x - y).$$

We recall that the equilibrium pressure $\rho$ and density $n$ are determined in terms of the cluster coefficients $b_n$, the fugacity $z$, and the inverse temperature $\beta$ by

$$\rho = \beta^{-1} \sum_{n=1}^{\infty} b_n z^n,$$

$$\rho = \sum_{n=1}^{\infty} nb_n z^n.$$ 

In the coordinate representation and in the infinite volume limit the coefficients $b_n$ may be calculated from the expression

$$b_n = \frac{1}{n!} \int (x_1, x_2, x_3, \ldots, x_n) \left| U_n \right| 0, x_2, \ldots, x_n \rangle dx_2 \ldots dx_n.$$  

The cluster operator $U_n$ is the connected part of the operator $W_n = e^{-\beta H_n}$, where $H_n$ is the $n$-particle Hamiltonian. Explicitly,

$$\langle x_1 | U_n | x_1 \rangle = \langle x_1 | W_n | x_1 \rangle,$$

$$\langle x_1 x_2 | U_n | x_1 x_2 \rangle = \langle x_1 x_2 | W_n | x_1 x_2 \rangle,$$

$$\langle x_1 x_2 x_3 | U_n | x_1 x_2 x_3 \rangle = \langle x_1 x_2 x_3 | W_n | x_1 x_2 x_3 \rangle.$$
With the help of the complete set of scattering states of Eq. (4), the matrix elements of $W_o$ may be expressed as

$$\langle x' | W_o | x \rangle = \int dk_1 \ldots dk_n v_i^{*}(k_i) \exp[-\beta (k_1^2 + k_2^2 + \ldots + k_n^2) + \phi(k)](x).$$

Our aim is to calculate the coefficients $b_0$ and $b_2$ directly from Eqs. (7) using Eq. (8). The third virial coefficient is then given by

$$a_3 = (4b_2^2 - 2b_0)/b_2^2.$$

III. THE CLUSTER COEFFICIENT $b_0$

The calculation of $b_0$ from Eq. (7b) is quite straightforward but we include here some of the details which are repeated in the more complex calculation of $b_3$ in Sec. IV. The calculation is simplified by considering the difference between the coefficient $b_0$ and its value $b_0^B = (4\pi\beta)^{-1/2} 2^{-3/2}$ in the ideal Bose limit, where the interaction strength $\epsilon \to 0$. In this limit the coefficients $a(P)$ of the plane waves in Eq. (1) are unity.

Using Eq. (8) we have

$$\langle x_1 x_2 | e^{-ib\phi} - e^{-ib\phi^B} \rangle = \frac{1}{2\pi} \int dk \int dk_2 e^{i(kx_1 - k_2x_2)} e^{i(kx_1 - k_2x_2)(a(P)a^*(Q) - 1)}.$$

We note that the disconnected parts, i.e., the terms which are independent of $x_1$ and $x_2$, cancel. From Eq. (3) the factor

$$[21] = e^{i\epsilon a} - 1$$

in Eq. (9) is a simple pole which may be written as

$$[21] = 2ic(k_1 - k_2 - \epsilon c)^{-1} = -2c \int_0^\infty e^{-i(x_1 - x_2 - \epsilon c)} dx.$$

With the help of this representation, the integrations over the momenta in Eq. (9) may be performed yielding

$$\langle x_1 x_2 | U_2 - U_0 | x_1 x_2 \rangle = -2c \left( \frac{\pi}{2\beta} \right) e^{\epsilon(x_1 - x_2)} \int_0^\infty \epsilon^{s-1/2} e^{-\epsilon s} ds.$$

The expression (11) is only valid for $x_1 < x_2$. However, it is easy to see from their definition that the matrix elements of $U$ are symmetric in the coordinates, so that in order to calculate $b_2$ from Eq. (6), we take

$$b_2 = \frac{1}{2\beta} \int_0^\infty (x_2 - x_1) dx_2 x_2 \langle x_2 | U_2 - U_0 | x_1 \rangle dx_1.$$

From Eqs. (11) and (12), we find, on integrating by parts,

$$b_2 = \frac{4c}{(2\pi)^2} \int_0^\infty ds e^{-s/2\beta} \int_0^\infty ds e^{-s/2\beta} ds.$$

The results (11) and (13) have already been obtained by Servadio.

IV. THE CLUSTER COEFFICIENT $b_2$

Again consider the difference between $b_2$ and its value $b_0^B = (4\pi\beta)^{-1/2} 2^{-3/2}$ in the ideal Bose limit. From Eq. (7c),

$$\langle x_1 x_2 x_3 | U_3 - U_0^B | x_1 x_2 x_3 \rangle = \langle x_1 x_2 x_3 | e^{-ib\phi} - e^{-ib\phi^B} \rangle \langle x_1 x_2 | e^{-ib\phi} - e^{-ib\phi^B} \rangle \langle x_1 x_2 x_3 | e^{-ib\phi} - e^{-ib\phi^B} \rangle.$$

After using Eq. (8) and exploiting the symmetry in the momentum variables, the right-hand side of Eq. (14) becomes

$$\int d\epsilon d\epsilon^2 \langle [213] | [213] + [132] + [321] \rangle + \langle [321] | [321] + [213] + [312] \rangle - \langle [321] | [321] \rangle,$$

where we have introduced the notation

$$[ijk] = e^{i(\epsilon_1 - \epsilon_2 + \epsilon_3) x_1} e^{i(\epsilon_2 - \epsilon_3) x_2} e^{i(\epsilon_3 - \epsilon_1) x_3},$$

$$[ijk] = e^{i/2k(x_2 + x_3 - x_3 - x_2)} - 1,$$

and

$$\int d\epsilon d\epsilon^2 = \frac{1}{(2\pi)^2} \int_0^\infty d\epsilon_1 d\epsilon_2 d\epsilon_3 e^{-\epsilon_1^2 - \epsilon_2^2 - \epsilon_3^2}.$$

First we note that the coefficient $[213] - [321]$ of the plane wave [213] which represents the scattering of particles 1 and 2 with particle 3 propagating freely, vanishes. Similarly the disconnected part [132] of the cluster integral, which results from the scattering of particle 2 and 3 while particle 1 propagates freely, vanishes due to the cancellation of the three-body term [132] and the two-body term [32]. On the other hand [321] and [31] are not equal, so that a term involving [321] which is independent of $x_2$ survives. The different treatment of the scattering of particles 1 and 3 results from the definite ordering of the particles in the initial state. In order for particles 1 and 3 to interchange momenta in three-body processes, they must also scatter from particle 2. It should also be remarked that although the term [321] is independent of $x_2$, there is no difficulty with convergence when integrating over $x_2$ in the process of forming the coefficient $b_2$. Since $x_3$ is limited by the condition $x_1 < x_2 < x_3$, the $x_1$ and $x_3$ dependence is sufficient to produce convergence.

By taking the above cancellations into account and by suitable relabeling of variables, the expression (15) becomes

$$\int d\epsilon d\epsilon^2 (2[231][213] + [321][321] - [321]).$$

In terms of the integral representation of the plane-wave coefficients of Eq. (10),

$$[231] = [21][31] + [31] + [21]$$

and

$$[321] - [31] = (1 + [31])([21] + [32] + [21] + [32]) = (1 - [31] + \frac{3}{2} [31])([21] + [32]),$$

where

$$[31] = \frac{4c}{k_0 - \beta}.$$

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APPENDIX

In the theory of Yang and Yang the third cluster coefficient is determined by

\[
\frac{b_3}{b_3} = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\theta (a_3 - a_1 a_2),
\]

(A1)

where

\[
a_1 = e^{-\alpha s^2}, \quad a_2 = e^{-\alpha t^2} O a_1
\]

\[
a_3 = e^{-\alpha s^2} \frac{6}{7\alpha} a_1^2 - \frac{6\alpha}{7} a_2^2 + O a_2,
\]

and \(O\) is the integral operator

\[
\frac{c_1}{c_2} \int_{-\infty}^{\infty} dq - \frac{1}{(k - q)^2}.
\]

After some simplification, we obtain

\[
\frac{b_3}{b_3} = \frac{3}{4\pi} \int_{-\infty}^{\infty} d\theta \int_{-\infty}^{\infty} d\phi \int_{-\infty}^{\infty} d\eta \int_{-\infty}^{\infty} d\xi \frac{1}{\pi \sqrt{(k_1 - k_2)^2 + c^2}}
\]

\[
\times \left[ 1 \right] \left( k_2 - k_3 \right)^2 + c^2 - 0(k_2 - k_3) \right].
\]

(A2)

When the pole terms are expressed as integrals as in Eq. (10) and the integrations over the momenta performed, the right-hand side of Eq. (A2) becomes

\[
\frac{3}{(2\pi)^2} \frac{\pi^{3/2}}{\beta} \int_{-\infty}^{\infty} d\sigma \int_{-\infty}^{\infty} d\rho \int_{-\infty}^{\infty} d\omega \left[ e^{-1/2(\sigma^2 + \rho^2 + \omega^2)} + e^{-1/2(\sigma^2 + \rho^2 + \omega^2) \omega} (e^{-c\sigma} - 1) \right].
\]

(A3)

Now, if \(f(s, t)\) is symmetric in \(s\) and \(t\), then

\[
\int_{0}^{\infty} ds \int_{0}^{\infty} dt e^{-1/2(s^2 + t^2)} f(s, t)
\]

\[
= 2 \int_{0}^{\infty} ds \int_{0}^{\infty} dt e^{-1/2(s^2 + t^2)} f(s, t).
\]

(A4)

Using the identity (A4) to simplify (A3), we obtain the desired result, Eq. (10).