Solvable three boson model with attractive delta function interactions

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A one parameter solvable model for three bosons subject to delta function pair interactions in one-dimension with periodic boundary conditions is studied. The energy levels and wave functions are classified and given explicitly in terms of three momenta. In particular, eigenstates and eigenvalues are described as functions of the model parameter, $c$. Some of the states are given in terms of complex momenta and represent dimer or trimer configurations for large negative $c$. The asymptotic behaviour for small and large values of the parameter, and at thresholds between real and complex momenta is provided. The properties of the potential energy are also discussed.

I. INTRODUCTION

Quantum solvable models where the wave functions, energy eigenvalues and other quantities of physical interest can be obtained explicitly in terms of known functions or with minimum numerical effort (typically by solving a transcendental equation or by quadratures) are useful to test and refine concepts and/or numerical methods, and as first approximations to more realistic systems. Occasionally unexpected physical phenomena are revealed [1]. In this paper we shall analyze a one parameter model for three bosons subject to attractive delta function pair interactions in one-dimension with periodic boundary conditions (contrast this to three particles “on a ring”, see [2]). Our original motivation was to examine a system with attractive forces where single and compound particles may coexist. This is of particular interest when studying the kinetic theory of gases composed by particles that can form stable aggregates (such as dimers or trimers), especially when chemical reactions can occur [3]. This article deals exclusively with the model itself, which has been found to be quite complex in mathematical detail.

The literature on one-dimensional solvable models of three, and generally $N$, particles is rather extensive. These models could be primarily classified according to the type of interaction involved [1]. However, even with the same interaction but with different boundary conditions, different formal treatments are required and very different results may be found. Periodic boundary conditions are suitable for modelling a gas or a crystal lattice in the thermodynamic limit. In contrast, in the limit as the box length becomes large, information about the corresponding scattering problem of a one-dimensional system can be extracted [1-3]. Indeed these are the standard boundary conditions for actual calculations of time dependent wave function scattering [3]. The model studied here is a particular case of the “interacting bose gas” of Lieb and Liniger [3], who examined $N$ particles subject to 2-body delta function interactions and boson symmetry. Further analysis of this gas was carried out in several papers [1-3, 12], but, having different objectives and applications in mind, in none of these works was the attractive case examined, except for the appendix on the $N = 2$ case in [3]. Lieb and Liniger found some unexpected effects of the periodic confinement but did not investigate the analogous effects for $N > 2$. In a series of papers [13-16], McGuire has examined a related one-dimensional many-particle Fermion system with one particle having spin down in a sea of spin up particles, interacting via $\delta$-function potentials (both repulsive and attractive). For other models with periodic boundary conditions but different interactions, see [16-20].

If the particles are not confined in a box, the wave function obeys the standard vanishing boundary conditions (for bound states) or scattering boundary conditions, at infinite distances [21]. However, in most available models, rearrangement processes where a bound pair collides with a single particle to form a new pair are not allowed and cannot be examined. An exception is the work of McGuire on the attractive, two body, delta function interaction describing the scattering wave functions and the bound ($N$-body) states [22]. This model has been generalized, examined by means of several formalisms, or applied for different purposes [23-28]. As stated before, the attractive case for bosons has not been examined with periodic boundary conditions and the present work fills this lacuna for $N = 3$.

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II. MODEL DESCRIPTION

The stationary Schrödinger equation for three equal mass particles in 1-dimension with 2-body delta function interactions reads

\[-\frac{\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial^2 \psi}{\partial y_i^2} + 2c \sum_{i<j} \delta(y_i - y_j)\psi = \tilde{E}\psi,\]  

where \(y_i (i = 1, 2, 3)\) are the particle coordinates. If they are enclosed in a box with length \(L\) it is convenient to divide this equation by \(\frac{\hbar^2}{2mL^2}\) and use instead

\[-\frac{3}{\sum_{i=1}^{3} \frac{\partial^2 \psi}{\partial x_i^2} + 2c \sum_{i<j} \delta(x_i - x_j)\psi = E\psi,\]  

expressed in terms of the dimensionless quantities

\[x_i = y_i / L\]  

\[E = \frac{2mL^2 \tilde{E}}{\hbar^2}\]  

\[c = \frac{2m\tilde{c}L}{\hbar^2} .\]

Note that \(c\) is the only parameter of the model, and that, according to (3), the effect of enlargening the box or making the interaction stronger are equivalent. This work addresses the attractive case in particular, corresponding to \(c \leq 0\). But the repulsive case \((c \geq 0)\) is also covered since the nature of the solutions for the repulsive case are the same as one class of solutions for the attractive case. Of particular interest is how the wavenumbers associated with a wavefunction change, as the potential parameter \(c\) varies continuously from repulsion to attraction.

The delta function potential produces a jump in the derivatives of the wave function where two particles meet. This jump is proportional to \(c\) and to the wave function at that point,

\[\left( \frac{\partial \psi}{\partial x_j} - \frac{\partial \psi}{\partial x_k} \right)_{x_j = x_k^+} - \left( \frac{\partial \psi}{\partial x_j} - \frac{\partial \psi}{\partial x_k} \right)_{x_j = x_k^-} = 2c \psi|_{x_j = x_k} .\]

Since the delta function interaction allows the particles to cross each other, all orderings are possible, each ordering corresponding to a particular “region” of coordinate space and one of the permutations of the three particles. On the basis that the particles are bosons, it is sufficient to study the wave function in only one of these regions, specifically the “primary” region

\[R_{123} : 0 \leq x_1 \leq x_2 \leq x_3 \leq 1.\]

The wave function in any other region \(R_{ijk}\) of coordinate space is then simply obtained from the wave function in \(R_{123}\) by interchanging the particle labels. In region \(R_{123}\), the equations (2) and (3) can be written as

\[-\frac{3}{\sum_{i=1}^{3} \frac{\partial^2 \psi}{\partial x_i^2} = E\psi,\]  

for \(x_1 \neq x_2 \neq x_3 \neq x_1\), and the jump conditions

\[\left. \left( \frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} \right) \psi \right|_{x_{j+1} = x_j} = c\psi|_{x_{j+1} = x_j} .\]

If periodic boundary conditions are also imposed, a displacement of 1 in any of the coordinates \(x_j\) leaves the function unchanged. In particular, in \(R_{123}\) this means that the wave function obeys

\[\psi(0, x_2, x_3) = \psi(x_2, x_3, 1) .\]

Similarly, the derivatives satisfy

\[\frac{\partial}{\partial x} \psi(x, x_2, x_3)|_{x=0} = \frac{\partial}{\partial x} \psi(x_2, x_3, x)|_{x=1} .\]
In a two-body collision between particles of equal mass, the delta function interaction can only interchange the momenta of the incident particles or leave them unchanged. In other words, there is no diffraction, that is, no “new” momenta, different from the initial ones, are created. For three equal mass particles with delta two-body interactions, the eigenstates can thus be written in terms of only three plane waves with (dimensionless) “momenta” \( \{k_j\} \),

\[
\psi(x_1 \leq x_2 \leq x_3) = \sum_P a(P) P \exp \left( i \sum_{j=1}^{3} k_j x_j \right),
\]

where the sum is over all permutations \( P \) of the \( \{k_j\} \), and \( a(P) \) are coefficients to be fixed by the boundary conditions determined by the periodicity, Eqs. (10) and (11), and by the delta function interaction, Eq. (9). This wave function form is known as the “Bethe ansatz” and it was first applied to spin chains [29]. In the context of the Bose gas, Yang and Yang [12] used a continuity argument to show that for positive \( c \) all states are given by (12) with real \( k \)’s, a result which was later established rigorously by Dorlas [30]. In the present work it is shown that all states for \( c \geq 0 \) are continuously connected to \( c \leq 0 \) states in \( k \) space so we are confident that the eigenstates discussed later form in fact a complete set. An important difference with the repulsive case is that for \( c < 0 \) the \( k \)’s may become complex.

From (8) and (12) the energy is simply obtained as

\[
E = \sum_{j=1}^{3} k_j^2,
\]

but this should not be interpreted as purely kinetic energy since there is generally a potential energy contribution to \( E \). Note that Eq. (8) is the Schrödinger equation only when the positions of the particles are all different. The true kinetic energy has to take into account the jumps in the wave function derivative at the region boundaries. The calculation of the potential energy is however somewhat involved and is discussed in the Appendix.

The structure of the coefficients \( a(P) \) is imposed by the jump boundary condition (8) as explained, e.g., in [8]: The amplitudes for two permutations differing by a transposition of two particles are related by a factor \( -e^{i\theta_{j\ell}} \),

\[
a(123) = 1 \\
a(213) = -e^{i\theta_{21}} \\
a(132) = -e^{i\theta_{32}} \\
a(321) = -e^{i(\theta_{21}+\theta_{31}+\theta_{32})} \\
a(312) = e^{i(\theta_{31}+\theta_{32})} \\
a(231) = e^{i(\theta_{21}+\theta_{31})}
\]

where

\[
e^{i\theta_{j\ell}} = \frac{c - i(k_j - k_{\ell})}{c + i(k_j - k_{\ell})}.
\]

By substituting (12) and (14) into the periodicity conditions (10) and (11), the following set of coupled transcendental equations is found

\[
e^{-ik_j} = \exp \left[ i \sum_{s=1}^{3} \frac{\theta_{sj}}{3} \sum_{s=1}^{3} \theta_{sj} \right], \quad j = 1, 2, 3,
\]

where, by convention, \( \theta_{jj} = 0 \). Solving Eq. (17) for the \( k_j \) gives

\[
k_1 = 2\pi m_1 - \theta_{21} - \theta_{31} \\
k_2 = 2\pi m_2 - \theta_{12} - \theta_{32} \\
k_3 = 2\pi m_3 - \theta_{23} - \theta_{13},
\]

for some set of integers \( \{m_j\} \), while the \( \theta_{j\ell} \) are given in terms of the \( k_j \) by

\[
\theta_{j\ell} = i \ln \left[ \frac{c + i(k_j - k_{\ell})}{c - i(k_j - k_{\ell})} \right] = -2 \arctan \left( \frac{k_j - k_{\ell}}{c} \right).
\]
While it may appear to be natural to choose the principal branch of the logarithm and the arctangent, another choice is more appropriate. Since a state is uniquely defined by the set of numbers \( \{ k_j \} \), irrespective of the order, because the particles are bosons, it is convenient to order the \( \{ k_j \} \), when they are real, according to

\[
k_1 \leq k_2 \leq k_3.
\]

(20)

Consistent with this, the ranges of \( \theta_{21}, \theta_{32} \) and \( \theta_{31} \) are chosen to satisfy

\[
-2\pi < \Re(\theta_{j\ell}) \leq 0,
\]

(21)
on the basis that the corresponding \( k_j - k_1 \) are positive. In this way, solving for the set of \( \{ k_j \} \) is equivalent to solving for the set of \( \theta_{j\ell} \) and it is noted that, for the above choice for the range of \( \theta_{j\ell} \), the \( \theta_{j\ell} \)'s vary continuously over their allowed ranges. This is also true if some of the \( k_j \)'s and/or \( \theta_{j\ell} \)'s become complex, as discussed in latter sections. Thus the \( m_j \) provide a unique classification of the energy levels, and for a given set of \( m_j \), the energy eigenvalue (and eigenvector) can be followed continuously as a function of \( c \), as \( c \) varies from \( \infty \) to \(-\infty\).

On taking the product of the three equations of the form of Eq. (17), it follows that the total momentum \( p \) is quantized,

\[
p \equiv \sum_j k_j = 2\pi(m_1 + m_2 + m_3) = 2\pi n_p.
\]

(22)

This is the eigenvalue of the corresponding total momentum operator, which commutes with the hamiltonian \( H \). It is clear that \( p \) is an invariant to the “motion” of an eigenvalue as \( c \) varies continuously from \( \infty \) to \(-\infty\). For each solution set \( \{ k_j \} \) there is another set \( \{ k'_j \} \) that also solves (17) and is related to the former by

\[
k'_j = k_j + 2\pi n_0.
\]

(23)

The transformation \( \{ k_j \} \rightarrow \{ k'_j \} \) amounts to shifting the total momentum by \( 6\pi n_0 \). This means that any state can be mapped to another state in the central momentum strip \(-3\pi < p \leq 3\pi\), and vice versa, by such a transformation. Thus we shall limit ourselves to study only those states having total momentum in this strip, namely, \( n_p = -1, 0, 1 \).

A convenient set of variables, especially when the three \( k \)'s are real, that uniquely define the state is \( p, \delta_1 \) and \( \delta_2 \), where \( \delta_1 \) and \( \delta_2 \) are, respectively, the relative momenta between particles 12 and 23, namely

\[
\delta_1 \equiv k_2 - k_1, \quad \delta_2 \equiv k_3 - k_2.
\]

(24)

(25)

Note that, when real, the order assumed for the \( k_j \), Eq.(17), implies that \( \delta_j \geq 0 \). The \( k \)'s are given in terms of these variables by

\[
k_1 = \frac{1}{3}(p - 2\delta_1 - \delta_2), \quad k_2 = \frac{1}{3}(p + \delta_1 - \delta_2), \quad k_3 = \frac{1}{3}(p + \delta_1 + 2\delta_2).
\]

(26)

(27)

(28)

and the energy takes the form

\[
E = \frac{1}{3}[p^2 + 2(\delta_1^2 + \delta_2^2 + \delta_1\delta_2)].
\]

(29)

Combinations of Eqs. (18) and (19) give the two coupled equations for \( \delta_1 \) and \( \delta_2 \),

\[
\delta_1 = i \ln \left[ \frac{\left( \frac{c + i\delta_1}{c - i\delta_1} \right)^2 - c - i\delta_2}{c + i\delta_2} \right] + 2\pi n_1
\]

(30)

\[
\delta_2 = i \ln \left[ \frac{\left( \frac{c + i\delta_2}{c - i\delta_2} \right)^2 - c - i\delta_1}{c + i\delta_1} \right] + 2\pi n_2.
\]

(31)
where, on the basis that the principal part of the logarithm is taken, \( n_1 \) is not necessarily equal to \( m_2 - m_1 \), nor is \( n_2 \) necessarily equal to \( m_3 - m_2 \). In fact, unlike the \( m_j \), the \( n_j \) do not have to remain constant as a given “root” of the coupled equations \( \{ \delta_1(c), \delta_2(c) \} \) changes continuously with a variation of \( c \). That is why we shall not classify the roots according to “local” values \( \{ n_1(c), n_2(c) \} \), but according to their values \( \{ n_0^1, n_0^2 \} \) for no interaction, namely for \( c = 0 \). These are unambiguously related to the set of quantum numbers \( m_j \), see Eqs. (30,31) and (32) below. If, as \( c \) changes, the argument of one of the logarithms, say \( z_j \), crosses the negative real axis (which is the branch cut for the principal part of the logarithm), its phase changes abruptly by \( \pm 2\pi \) and the corresponding \( n_j \) has to jump up or down by one unit in order to follow the root continuously. Of course, these discontinuities have no physical consequence and merely reflect the choice made for the branch of the logarithm. For several formal manipulations and in particular for the object of obtaining asymptotic expressions, it is useful to avoid the discontinuities by continuing analytically the logarithm across the branch cut, i.e., by passing to the contiguous Riemann sheet when the argument \( z_j \) crosses the real, negative axis. This will be discussed further in Sec. IV to clarify the trajectories of the \( k_j \) as \( c \) changes smoothly.

There are certain symmetries of the parameterization \( \delta_1, \delta_2 \) and \( p \) which can lead to energy degeneracies. The interchange \( \delta_1 \leftrightarrow \delta_2 \) together with the change in sign of \( p \) are equivalent to the changes \( k_1 \leftrightarrow -k_3 \) and \( k_2 \leftrightarrow -k_2 \), which, for real \( k \)'s, inverts the order of Eq. \( \{ 21 \} \) to \( -k_1 > -k_2 > -k_3 \). This is also equivalent to taking the complex conjugate of the wavefunction. Thus, if \( k_1 \neq -k_3 \) and/or \( k_2 \neq 0 \), these are two different states with the same energy, a two-fold degeneracy. On the other hand, if \( k_1 = -k_3 \) and \( k_2 = 0 \), which is the special case that \( \delta_1 = \delta_2 \) and \( p = 0 \), then this symmetry reproduces the same state, the wavefunction is real, and the state is nondegenerate. In terms of the classification of the states of the central momentum strip by the \( n_0^j \), it follows that interchanging \( n_1^0 \) and \( n_2^0 \), \( (n_1^0 \neq n_2^0) \), amounts to the interchange of \( \delta_1 \) and \( \delta_2 \), and, see Eq. \( \{ 27 \} \) below, to change the sign of \( p \), so that all signs of the \( k \)'s are changed and the complex conjugate state is obtained. But for the “diagonal” case, \( n_1^0 = n_2^0 \), there is no degeneracy. These states are real and even under the parity transformation \( x_j \rightarrow -x_j \).

A second symmetry of the parameterization \( \delta_1, \delta_2, p \) is the interchange \( \delta_1 \leftrightarrow -\delta_2 \) while \( p \) remains unchanged. This is equivalent to the changes \( k_1 \leftrightarrow k_3 \) and \( k_2 \leftrightarrow k_2 \), which inverts the order of Eq. \( \{ 21 \} \) to \( k_1 > k_2 > k_3 \) but does not change the momenta themselves. But since the order of the \( k \)'s is immaterial, this is just another way of labeling the same state. In terms of the \( n_0^j \) this means that \( (n_1^0, n_2^0) \) and \( (-n_2^0, -n_1^0) \) are actually the same state.

Because of the stated symmetry relations and the fact that any eigenstate can be translated by the total momentum shift \( \{ 23 \} \) to the central momentum strip, an exhaustive analysis of all possible states is achieved by examining the cases \( n_2^0 \geq n_1^0 \geq 0 \), since any other case is either equivalent to one of them or obtained by a simple transformation. An understanding of the behaviour of the roots and their limiting properties for different ranges of \( c \) requires a detailed analysis of how to carry out the analytical continuation of the logarithms in Eqs. \( \{ 28,31 \} \) as \( c \) varies. This is provided in the following sections. To keep track of the global picture a handy summary of the results is provided in the final Section, and a set of figures illustrate the essential aspects.

**III. THE REFERENCE CASE OF “NO INTERACTION”**

For \( c = 0 \) there is no interaction and the particles move freely. In this case

\[
e^{i\theta_{j\ell}} = -1 ,
\]

and with the present choice for the range of the \( \theta_{j\ell} \),

\[
\theta_{21} = \theta_{32} = \theta_{31} = -\pi.
\]

It follows that

\[
a(ijk) = 1
\]

\[
\delta_1 = 2\pi n_1^0 = 2\pi(m_2 - m_1 - 1)
\]

\[
\delta_2 = 2\pi n_2^0 = 2\pi(m_3 - m_2 - 1).
\]

Equivalently, the \( k_j \) are all real multiples of \( 2\pi \). Due to the conventional order \( \{ 21 \} \), only the case where \( n_j^0 \geq 0 \) needs to be considered in order to account for all the states of the system.

The total momentum in the central momentum strip for a state \( (n_1^0, n_2^0) \) is determined by noticing, from \( \{ 27 \} \), that if \( k_2 \) is to be a multiple of \( 2\pi \), then \( \delta_1 - \delta_2 \) has to be a multiple of \( 6\pi \). For any pair \( n_1^0, n_2^0 \), and \( p = 2\pi n_p \) \( (n_p = 0, \pm 1) \), there is only one possible solution for \( n_p \), namely

\[
n_p = \begin{cases} 
0 & \text{if } n_0^1 - n_0^2 = 3n \\
-1 & \text{if } n_0^1 - n_0^2 = 3n + 1 \\
1 & \text{if } n_0^1 - n_0^2 = 3n + 2 
\end{cases} \quad n = 0, \pm 1, \pm 2, \ldots
\]
For the states where one of the \( n_i^0 \) is zero, two \( k \)'s are equal. The equality of two \( k \)'s can occur only at \( c = 0 \) and at certain critical \( c \) values discussed in Sec. V. (In general, for \( c \neq 0 \), the wave function vanishes if two \( k_j \) are equal.) For the ground state, \( n_i^0 = n_i^0 = 0 \), the three \( k_j \) are equal and the wave function is a constant.

The classification scheme used in the remainder of this paper, for the energy eigenvalues and states, is based on following \( \delta_1 \) and \( \delta_2 \) as continuous functions of \( c \) from the reference non-interacting system. A symbol such as \((1, 2)\) gives the values of the quantum numbers \( n_1^0 \) and \( n_2^0 \) and identifies a given “root” \( \{ \delta_1(c), \delta_2(c) \} \) of the transcendental equations and the corresponding eigenstate (within the central strip of total momentum) irrespective of the value of \( c \). Note that the three “quantum numbers” \( n_1^0, n_2^0, n_p \) are equivalent to the set of quantum numbers \( \{ m_j \} \). The total momentum given in (37) is independent of the value of \( c \).

IV. REAL \( k \) SOLUTIONS

On the assumption that the \( k_j \) all remain finite (and real), it follows that

\[
\begin{align*}
\theta_{21} \\
\theta_{32} \\
\theta_{31}
\end{align*}
\rightarrow \begin{cases}
0 & \text{if } c \to \infty; \\
-2\pi & \text{if } c \to -\infty,
\end{cases}
\]

(38)

with the consequence, see Eq. (38), that

\[
\begin{align*}
-\infty & \leftrightarrow c \to \infty \\
2\pi(m_1 + 2) & \leftrightarrow k_1 \to 2\pi m_1 \\
2\pi m_2 & \leftrightarrow k_2 \to 2\pi m_2 \\
2\pi(m_3 - 2) & \leftrightarrow k_3 \to 2\pi m_3.
\end{align*}
\]

(39)

Bounds on the \( k \) differences can be narrowed by examining separately, the detailed properties of the \( \theta \)'s for positive and negative \( c \), by the following reasoning: On the basis of the chosen order for the \( k_j \), Eq. (20), it follows that

\[
k_3 - k_1 \geq k_2 - k_1, \quad k_3 - k_2.
\]

(40)

As a consequence, for \( c > 0 \) and \(-\pi \leq \theta_{j\ell} \leq 0 \) for \( (j > \ell) \),

\[
\tan\left(\frac{\theta_{31}}{2}\right) \leq \tan\left(\frac{\theta_{21}}{2}\right), \quad \tan\left(\frac{\theta_{32}}{2}\right)
\]

(41)

and

\[
\theta_{31} \leq \theta_{21}, \quad \theta_{32},
\]

(42)

so that

\[
-\pi \leq \theta_{31} - \theta_{32} \leq 0
\]

(43)

and

\[
2\pi n_1^0 - \pi \leq 2\pi(m_2 - m_1) - \pi + 2\theta_{21} \leq \delta_1 = k_2 - k_1 = 2\pi(m_2 - m_1) + 2\theta_{21} + \theta_{31} - \theta_{32} \leq 2\pi(m_2 - m_1) + 2\theta_{21} \leq 2\pi(n_1^0 + 1).
\]

(44)

An analogous argument for \( c < 0 \) leads to

\[
2\pi(n_1^0 - 1) < \delta_1 = k_2 - k_1 \leq 2\pi n_1^0 + \pi,
\]

(45)

with the lower bound approached according to Eq. (39). Bounds for \( \delta_2 \) involving \( n_2^0 \) have the same structure.

It is thus seen that if \( n_1^0 \geq 2 \) and \( n_2^0 \geq 2 \), then these \( k \) differences remain positive as \( c \) varies from \( \infty \) to \(-\infty \), with the consequence that the \( k_j \) are real for all \( c \) under these conditions. This also implies that the energy tends to a constant value for \( |c| \to \infty \), see Fig. 1. For these states, the delta function potential acts, for both very large positive and negative \( c \), effectively as an impenetrable barrier. That is, the wave function at the region boundaries, \( x_i = x_j \), tends to zero. This can also be deduced from the jump conditions, Eq. (4), since the derivatives produce only the
finite $k_j$ while $c$ becomes infinite, so that consistency requires that $\psi$ vanishes. The potential energy as a function of $c$ decreases from zero to an intermediate minimum and then grows again towards zero as $c \to -\infty$ and vice versa for $c > 0$, see the Appendix and Fig. 2.

The above deduced limitations on how the $\delta$’s change with $c$ allow a more detailed discussion of these changes from the point of Eqs. (30) and (31). An appropriate starting point is to consider the limit of these equations when $c \to 0$, namely

$$
\delta_1 = i \ln \left( \frac{\delta_1 - ic}{\delta_1 + ic} \right)^2 \frac{\delta_2 + ic}{\delta_2 - ic} \frac{(\delta_1 + \delta_2) - ic}{(\delta_1 + \delta_2) + ic} + 2\pi n_1^0 \quad (46)
$$

$$
\delta_2 = i \ln \left( \frac{\delta_2 - ic}{\delta_2 + ic} \right)^2 \frac{\delta_1 + ic}{\delta_1 - ic} \frac{(\delta_1 + \delta_2) - ic}{(\delta_1 + \delta_2) + ic} + 2\pi n_2^0 \quad (47)
$$

where the factors in the arguments have been rewritten to emphasize that the $\delta$’s are in this limit the leading terms. The identification of the $n_j^0$ is on the basis that, on expanding these equations as $c \to 0$, Eqs. (45) and (46) are obtained, namely

$$
\delta_1 = 2\pi n_1^0 + \frac{2n_1^0 n_2^0 + 2(n_2^0)^2 - (n_1^0)^2}{n_1^0 n_2^0 (n_1^0 + n_2^0) \pi} c + \cdots, \quad (48)
$$

with a symmetrical expression for $\delta_2$ on interchanging $n_1^0$ and $n_2^0$. These expansions are valid only if both $n_j^0 \neq 0$, while the exceptional cases are examined in Secs. VI and VII.

As $c$ increases positively [always assuming the order of Eq. (20)], the phases of the factors in the arguments of the logarithms change, compare the $\theta_{j,\ell}$ of Eq. (14) and the discussion of their behaviour. On tracing this behaviour as $c \to +\infty$, it is seen that the phase of the argument of each logarithm decreases by $2\pi$, so this can be taken into account when changing Eqs. (46) and (47) into Eqs. (30) and (31) by setting $n_j(c \to \infty) = n_j^0 + 1$. For negative $c$ the phase changes are the opposite and Eqs. (46) and (47) are appropriately changed into

$$
\delta_1 = i \ln \left( \frac{-c - i\delta_1}{-c + i\delta_1} \right)^2 \frac{-c + i\delta_2}{-c - i\delta_2} \frac{c - i(\delta_1 + \delta_2)}{c + i(\delta_1 + \delta_2)} + 2\pi(n_1^0 - 1) \quad (49)
$$

$$
\delta_2 = i \ln \left( \frac{-c - i\delta_2}{-c + i\delta_2} \right)^2 \frac{-c + i\delta_1}{-c - i\delta_1} \frac{c - i(\delta_1 + \delta_2)}{c + i(\delta_1 + \delta_2)} + 2\pi(n_2^0 - 1). \quad (50)
$$

These are appropriate for expansions when $c \to -\infty$, but may of course be used for all $c$ by analytic continuation. In the same vein, the related pair of equations with $n_j = n_j^0 + 1$ may be regarded as valid for all $c$ by analytic continuation across the logarithm branch cut.

In summary, provided both $n_j^0 \geq 0$, then

$$
\delta_j \xrightarrow{c \to -\infty} 2\pi(n_j^0 + 1) \left( 1 - \frac{6}{c} \right) + O(c^{-2}), \quad (51)
$$

while, provided both $n_j^0 > 1$, then

$$
\delta_j \xrightarrow{c \to -\infty} 2\pi(n_j^0 - 1) \left( 1 + \frac{6}{c} \right) + O(c^{-2}). \quad (52)
$$

In contrast, if $n_1^0 = 1$, then $\delta_1$ can approach 0 for finite negative $c$, see Fig. 3. For more negative values of $c$, the $k_j$’s can become complex. Similarly for $n_2^0 = 1$. Section V discusses this situation. If one of the $n_j^0 = 0$, then $\delta_j$ vanishes at $c = 0$, see Sec. VI.

The case in which $n_1^0 = n_2^0$ is particularly simple to analyze. It follows from Eqs. (46) and (47), analytically continued for all $c$, that $\delta_1$ and $\delta_2$ satisfy the same equation and thus are equal, with the consequence that the three $k$’s for such an eigenstate remain equally spaced as $c$ varies. After dropping the subscripts, and formally written for $c > 0$, the equation for the common $\delta$ is

$$
\delta = i \ln \left( \frac{(c + i\delta)(c + 2i\delta)}{(c - i\delta)(c - 2i\delta)} \right) + 2\pi(n^0 + 1). \quad (53)
$$
Fig. 4 illustrates how \( \delta \) varies with \( c \). By implicit differentiation,

\[
\frac{d\delta}{dc} = \frac{6\delta(c^2 + 2\delta^2)}{c^2(c^2 + 5\delta^2) + 4\delta^4 + 6c(2\delta^2 + c^2)}.
\]  

(54)

If \( n_1^0 = n_2^0 \neq 0 \), Eq. (48) is consistent with the \( c \to 0 \) limit of this result.

V. STATES WITH AT LEAST ONE \( n_j^0 = 1 \); DIMER STATES

If one \( n_j^0 = 1 \), for definiteness \( n_1^0 = 1 \), then from Eqs. (54) and (55), there is a possibility that \( \delta_1 \) becomes 0 for some critical negative value \( C(1, n_1^0) \) of \( c \). Note that the equations for \( \delta_1 \) and \( \delta_2 \) are independent of \( p \), so the critical value \( C(1, n_0^0) \) has nothing to do with the value of \( p \). [The discussion for the degenerate partner \((n_0^0, 1)\) follows similar lines substituting \( n_1^0 \) by \( n_0^0 \), \( \delta_1 \) by \( \delta_2 \) and \( p \) by \( -p \), see the discussion of the symmetries of this parameterization in Sec. III.] At a critical point \( C(1, n_0^0) \), \( k_1 \) and \( k_2 \) become equal (if \( n_0^0 = 1 \) as well, all three \( k \)'s become equal) and the Bethe ansatz (13) form for the wavefunction is no longer valid because it vanishes. Of course the normalization constant also vanishes so that the normalized wavefunction does not vanish, but merely has a different functional form obtained by taking the limit as \( c \to C(1, n_0^0) \) using the rule of l'Hospital. A similar case was found by Lieb and Liniger for one particular root in the case \( N = 2 \).

Two different cases arise, according to whether \( n_2^0 > 1 \), or if \( n_1^0 = n_2^0 = 1 \). These cases are discussed in turn.

A. The case when \( n_2^0 > 1 \).

The value of the critical point \( C(1, n_2^0) \) and the behaviour in its neighborhood can be obtained by expanding Eqs. (49) and (50) for \( \delta_1 \to 0 \). For such a purpose it is useful to introduce the factors \( u_j \equiv \delta_j/c, j = 1, 2 \), and define \( u_1 \equiv u_2(c = C) \) as the critical value of \( u_2 \). After fairly extensive algebra, it follows that

\[
c = C(1, n_2^0) + \frac{21 + 24u_0^2 + 8u_0^4}{6(1 + u_0^2)^2}u_1^2 + \cdots
\]

(55)

with

\[
C(1, n_2^0) = -4 - \frac{2}{1 + u_0^2},
\]

(56)

where \( u_0 \) is determined by the transcendental equation

\[
3i \ln \frac{1 + iu_0}{1 - iu_0} + 2\pi(n_2^0 - 1) + 4u_0 + \frac{2u_0}{1 + u_0^2} = 0.
\]

(57)

In the neighborhood of the critical point, \( u_2 \) changes according to

\[
u_2 = u_0 - \frac{1}{2}u_1 + \frac{3 + 6u_0^2 + 2u_0^4}{6u_0(1 + u_0^2)}u_1^2 + \cdots.
\]

(58)

It is seen that \( \delta_1(c) \) has a square root singularity at the critical point, being real for \( c > C(1, n_2^0) \) and pure imaginary for \( c < C(1, n_2^0) \). An analytic connection between real and imaginary branches of \( \delta_1 \) can be made by attributing \( c \) with a small imaginary part. The association that is used in the following parameterization is consistent with \( c \) having a small negative imaginary part, essentially adding a small dissipative contribution to the Hamiltonian. It is also noticed from Eq. (57) that all the critical values of \( c \) lie between \(-6 \) and \(-4 \). Actually, to three decimal places, the lowest critical value is \( C(1, 2) = -4.163 \), increasing towards \(-4 \) as \( u_0 \), and \( n_0^0 \), increases. These aspects are illustrated in Fig. 3.

For \( c < C(1, n_2^0) \), \( k_1 \) and \( k_2 \) become a complex conjugate pair, while \( k_3 \) remains real. The discussion of the root in this region is better examined by using a new set of real variables, \( \alpha \) and \( \gamma \), defined by

\[
\delta_1 = -2i\alpha,
\]

\[
\delta_2 = i\alpha - 3\gamma,
\]

(59)
so that

\[ k_1 = i\alpha + \gamma + p/3 \]
\[ k_2 = -i\alpha + \gamma + p/3 \]
\[ k_3 = -2\gamma + p/3. \]  

(60)

This is consistent with Eq. (58) for \( \alpha \to 0 \), on the basis that both \( \alpha \) and \( \gamma \) are real. This parametrization could of course be used for all \( c \) [with \( \alpha \) possibly imaginary], since \( \delta_1/2 = -i\alpha \) has the physical meaning of the relative momentum between particles 1 and 2 while \( 2\gamma \) is the relative momentum between the pair 12 and particle 3,

\[ -i\alpha = \delta_1/2 = \frac{k_2 - k_1}{2} \]  

(61)

\[ 2\gamma = k_3 - \frac{p}{3} = 2\left(k_3 - \frac{k_1 + k_2}{2}\right). \]  

(62)

For real \( \alpha \), \( 1/\alpha \) gives a measure of the size of the “bound states” formed. Of course, in a finite box all states are, strictly speaking, bound, i.e., their energies are discrete and their spatial extension is limited by the box length. But when \( \alpha \) is real, the state is localized even further so that the probability of a pair of particles being close together has been significantly enhanced. As well, the energy has a negative contribution, see (63) below, so that an energy gap arises in the spectrum between states with real or imaginary \( \alpha \), see Fig. 1. Since these are all basic ingredients of proper bound states, this terminology seems justified.

With this parametrization, the total energy is decomposed into separate quadratic contributions from the three variables,

\[ E = -2\alpha^2 + 6\gamma^2 + p^2/3, \]  

(63)

and the system of transcendental equations takes the form

\[-2\alpha = \ln \left[ \left(-c - 2\alpha\right)^2 -c - 2\alpha - 3i\gamma -c - 2\alpha - 3i\gamma \right] \]  

\[-c - 2\alpha - 3i\gamma \]

\[ i\alpha - 3\gamma = i \ln \left[ \left(-c + 2\alpha + 3i\gamma -c + 2\alpha - 3i\gamma \right)^2 -c + 2\alpha - 2\alpha - 3i\gamma -c + 2\alpha - 3i\gamma \right] + 2\pi(n_2^0 - 1) \]  

(64)

(65)

which corresponds to the correct phase form for \( c < 0 \), according to Eqs. (49) and (50). It is consistent to solve these equations maintaining \( \alpha \) and \( \gamma \) real, which is also consistent with the local behaviour, Eq. (55), as \( \alpha \to 0 \). Before entering into the detailed analysis of the equations, it is worth examining Figures 5 and 6 to quickly visualize the behaviour of these two parameters with \( c \). Solid lines correspond to \( n_1^0 = 0 \) and dashed lines to \( n_1^0 = 1 \), whereas the numbers close to the different lines give \( n_2^0 \). As \( c \) becomes more negative \( \alpha \) increases. This concentrates the wavefunction to where the particles are close together and \( \langle V \rangle \) and \( \langle E \rangle \) become very large and negative, see in Figs. 1 and 2 the lines for \( n = 0, 1 \). A prominent feature in Fig. 5 is the grouping into two asymptotic behaviours for \( \alpha \) as \( c \to -\infty \). These will be later associated with dimer and trimer configurations. Note also that all states with \( n_1^0 = 0 \) have a common critical point at \( c = 0 \) (where \( \alpha = 0 \)), while for \( n_1^0 = 1 \) the critical points spread from \( c = -6 \) to \( c = -4 \). Another interesting point is the quasi-invariance of \( \alpha \) with respect to \( n_2^0 \) for \( n_2^0 \geq 2 \) at fixed \( c \). These states have essentially the same binding strength and differ only by pair-single relative momentum, and possibly by total momentum. Fig. 6 for \( \gamma \) has a simpler structure based on a rather regular pattern of lines with equally spaced asymptotic values. Except for the two cases \( (0, 0) \) and \( (1, 1) \) with \( \gamma = 0 \) for all \( c \), which corresponds to no relative motion between a particle pair and a single particle, when \( c \) becomes more negative, \( \gamma \) varies smoothly and tends to a constant value. When \( \gamma \) is essentially constant, \( c \) changes the strength of the attraction between the pair (i.e., the value of \( \alpha \)), but not the motion of the third particle with respect to the pair.

The structure of the spectrum of energy levels can be described in terms of how the energy varies as the three quantum numbers \( n_1^0, n_2^0, n_p \) change. This can be attributed to several types of “elementary excitations” which are associated with different physical effects. Within the central momentum strip, for states with complex \( k_j \)'s and for \( -c \) large, these are:

a) As \( n_2^0 \) varies, a change of relative pair-single motion by \( \Delta_\gamma \approx \pi/3 \), with \( \alpha \) essentially constant and \( |p| \) constant. In Fig. 6 this is not possible between all contiguous levels of \( \gamma \), but only for those where \( n_p = 1 \) and \( n_{p'} = -1 \), see Eq. (37). If one of the states has momentum zero, a jump to the nearest level necessarily implies in addition to \( \Delta_\gamma \), an elementary total momentum jump \( \Delta_p = 2\pi \); b) Transitions between a trimer and a dimer state or from a dimer to a
pair-absent state, with \( \delta_{n} \approx -c/2; \) c) A minimum total momentum jump by 2\( \pi \), with \( \alpha \) and \( \gamma \) constant. This may only occur between the states (0,0) and (0,1) or (1,0). Any other transition changes \( \gamma \). But \( \alpha \) and \( \gamma \) may also stay constant if the system changes to a different momentum strip by a total momentum translation of \( \Delta_{p} = 6\pi \). Of course multiples or combinations of these elementary excitations are possible and complicate the spectrum considerably.

The detailed quantitative features of \( \alpha \) and \( \gamma \) as functions of \( c \) are now examined. On the basis that \( \alpha \) and \( \gamma \) are real, the real part of Eq. (65) is

\[
\alpha \rightarrow \text{constant if the system changes to a different momentum strip by a total momentum translation of } \Delta_{p} = 6\pi. \text{ Of course}
\]

The asymptotic behaviour as \( c \rightarrow -\infty \) is now investigated. According to Eq. (67), \( \gamma \) remains finite while \( \alpha \) satisfies Eq. (64). Both positive and negative \( \alpha \) are solutions to this equation, but since these just correspond to an interchange of \( k_{1} \) and \( k_{2} \), only the positive root is examined. Eq. (64) can be rewritten as an equation involving only real quantities, namely

\[
-2\alpha = \ln \left( \frac{(-c - 2\alpha)^{2}(-c + 2\alpha)}{(-c + \alpha)^{2} + 9\gamma^{2}} \right). \tag{70}
\]

The obvious (but invalid) approach to try when making an asymptotic expansion, is to expand in powers of \( \gamma^{2} \) since the other factors involve \( c \). This implies that \( \alpha \) must also remain finite and leads to the requirement that \( c \rightarrow -6 \), an inconsistency. It follows that either \( (-c - 2\alpha) \rightarrow 0 \) or \( (-c - \alpha) \rightarrow 0 \) in the Limit \( c \rightarrow -\infty \). But it is noticed that as \( c \) changes from its critical value \( C(1, n_{0}^{2}) \) to \( -\infty \), \( \alpha \) changes from 0 to its asymptotic behaviour, yet the factors in the argument of the logarithm, \( -c \pm 2\alpha \) and \( (-c + 2\alpha)^{2} + 9\gamma^{2} \), must remain positive or an imaginary phase factor must be added to the right hand side. Since such a case would imply that \( \alpha \) becomes complex, this is not allowed. Another way to understand the preservation of sign of all factors is that if one of them became zero for a finite \( c \) (and \( \alpha \) the logarithm, and the left hand side of the equation, would be infinite in absolute value, which is again inconsistent with the finite value of \( \alpha \) on the right hand side. The only form of \( \alpha \) that maintains all factors positive, is \( \alpha = -\frac{1}{2}c + \beta \), with \( \beta < 0 \) and \( \beta/c \rightarrow 0 \) asymptotically. A straightforward expansion then gives

\[
\beta = 3c e^{c/2} - 9c^{2} e^{c} + \cdots, \tag{71}
\]

and from Eq. (68),

\[
\gamma = -\frac{2\pi}{3} (n_{2}^{0} - 1) \left( 1 - \frac{8}{c} + \cdots \right), \tag{72}
\]

as the asymptotic expansions for both \( \alpha \) and \( \gamma \).
B. The case when \( n_2^0 = n_1^0 = 1 \).

As previously mentioned, this implies that \( \delta_1 = \delta_2 \) for all \( c \), and the common \( \delta \) is determined by Eq. (53), which is appropriate for \( c > 0 \). Reexpressing this for \( c < 0 \), retaining a continuous relation for the phase, gives

\[
\delta = i \ln \left[ \frac{(-c - i\delta)(-c - 2i\delta)}{(-c + i\delta)(-c + 2i\delta)} \right],
\]

and taking into account that \( n_1^0 = 1 \). Clearly \( \delta = 0 \) is a solution of this equation. But to find the corresponding critical value \( C(1,1) \) of \( c \) and the behaviour in the neighborhood of this critical point, an expansion is needed. This is easily accomplished to yield

\[ c = -6 + \frac{1}{6} \delta^2 + \cdots. \tag{74} \]

This immediately shows that the critical value is \( C(1,1) = -6 \), and that there is a square root singularity of \( \delta \) as a function of \( c \). For \( c < -6 \), \( \delta = -i\delta_0 \) is pure imaginary [negative imaginary if the same connection around the singularity is used as in the last subsection]. It follows that the \( k_j \) are given in terms of this parameterization by

\[
k_3 = -i\alpha + p/3 \]
\[
k_2 = p/3 \]
\[
k_1 = i\alpha + p/3, \tag{75}\]

while \( \alpha \) is determined by

\[
\alpha = \ln \left( \frac{1 - 3\alpha' + 2\alpha'^2}{1 + 3\alpha' + 2\alpha'^2} \right), \tag{76}\]

where \( \alpha' = \alpha/c \). [Contrast this with Eq. (58).] The associations made for the \( k_j \) in (53) are more natural here, since \( \delta_1 = \delta_2 \) and the three \( k_j \) change continuously across the critical point, but in fact (54), with \( \gamma = 0 \) could be used as well because the state is defined by the three “momenta” regardless of the ordering convention.]

Clearly, if \( \alpha' \to 0 \) as \( c \to -\infty \), then \( \alpha \to 0 \). But on expanding to look at the correction terms, this assumption implies that \( c \to 6 \), an inconsistent result. It follows that \( \alpha \) grows to \( \infty \) asymptotically. On the basis that only \( \alpha > 0 \) solutions are needed (\( \alpha' < 0 \)), the vanishing of the denominator in the argument of the logarithm requires either \( \alpha' \to -1 \) or \( \alpha' \to -\frac{1}{2} \) as \( c \to -\infty \). Only the latter is consistent with no accumulation of phase as \( c \) changes from \( -6 \) to \( -\infty \), and the reality of \( \alpha \). (Note that, by a similar argument to the one below Eq. (71), numerator and denominator in (70) must preserve their sign as \( c \) varies from \( -6 \) to \( -\infty \) which implies the bound \( 2\alpha < -c \).) On setting \( \alpha = -\frac{1}{2}c + \eta \), it follows on expansion that

\[
\alpha = -\frac{1}{2}c + 3ce^{\eta/2} + \cdots \tag{77}\]

as the asymptotic behaviour of \( \alpha \) in this case.

VI. STATES WITH ONE \( n_j^0 = 0 \): DIMER AND TRIMER STATES

This group of states are of the form \((0,n_j^0)\), and of course their degenerate partners. Only the case \((0,n_1^0)\) is explicitly treated here since their corresponding partner states are simply obtained by symmetry, specifically for the states when \( c < 0 \) by changing the sign of \( \gamma \). For \( c \to \infty \), these states fit into the formulation of Eq. (51), so no further discussion of this limit is needed.

As \( c \to 0 \), the starting point for the analysis is the pair of equations, (40) and (47). Since \( n_2^0 = 0 \), \( \delta_1 \) and \( c \) are to simultaneously approach 0, and it is to be expected by analogy with the other cases, that \( c \) will be proportional to \( \delta_1^2 \). This is confirmed by the following argument: Since \( \delta_1 \to 0 \), then the argument of the logarithm in Eq. (40) must approach 1. For the ratios of the terms involving \( \delta_2 \), these approach 1 since they are dominated by the common non-zero value of \( \delta_2 \). That leaves the square term. For this to approach 1, each factor must be dominated by the common \( \delta_1 \), which implies that it is the ratio \( c/\delta_1 \) that is small and can be used as a variable for which the logarithm is expanded, as well as the ratios \( c/\delta_2 \) and \( \delta_1/\delta_2 \), all of which vanish as \( c \to 0 \). Explicitly, the expansions of Eqs. (40) and (47) are
\[
\delta_1 = \frac{4c}{\delta_1} - \frac{4c^3}{3\delta_1^3} - 2\frac{c\delta_1}{\delta_2} + O(\delta_1^4) \\
\delta_2 = 2\pi n_2^0 - 2\frac{c}{\delta_1} + \frac{2c^3}{3\delta_1^3} + 6\frac{c}{\delta_2} - 2\frac{c\delta_1}{\delta_2} + O(\delta_1^4).
\] (78)

It follows that \( c \) is proportional to \( \delta_1^2 \), as was to be deduced. Rearrangement of these series for \( c \to 0 \) gives the expansion in powers of \( \delta_1 \) as

\[
c = \frac{1}{4}\delta_1^2 + \left[ \frac{1}{192} + \frac{1}{32(\pi n_2^0)^2} \right]\delta_1^4 + \cdots \\
\delta_2 = 2\pi n_2^0 - \frac{1}{2}\delta_1 + \frac{3\delta_1^3}{4\pi n_2^0} + \cdots.
\] (79)

For \( c < 0 \), the parameterization of Eq. (79) is appropriate. In the limit \( c \to -0 \), the ratio \( c/\delta_1 \) transforms according to

\[
\frac{c}{\delta_1} \to \frac{1}{4}\delta_1 \to -\frac{1}{2}i\alpha \leftarrow \frac{c}{2\alpha}.
\] (80)

with the consequence that Eqs. (46) and (47) become

\[
-2\alpha = \ln \left[ \frac{(2\alpha + c)}{(2\alpha - c)} \frac{(\alpha + c)^2 + 9\gamma^2}{(\alpha - c)^2 + 9\gamma^2} \right] \\
i\alpha - 3\gamma = i\ln \left[ \frac{2\alpha - c}{2\alpha + c} \frac{(i\alpha - ic - 3\gamma)^2}{(i\alpha + ic - 3\gamma)^2} \left( \frac{1}{3} \right) \right] + 2\pi n_2^0.
\] (81) (82)

It is also important to note that, as a consequence of the analytic continuation into the \( c < 0 \) region, \( 2\alpha + c > 0 \), and \( \gamma \to -\delta_2/3 < 0 \). To avoid further singularities in the logarithmic expressions (which would lead to inconsistency between right and left sides of the transcendental equations), these constraints must hold for all \( c < 0 \).

For exploring the behaviour as \( c \to -\infty \), Eq. (81) for \( \alpha \) has an appropriate form for expansion about the large \( -c \) and \( \alpha \). But if one term in each of the factors is to dominate the expansion, then the result would imply that the logarithmic expression becomes finite, a result inconsistent with the left hand side approaching \( -\infty \). As a consequence, since \( \alpha > -c/2 \), either \( \alpha \to -c/2 \) or the combination, \( \alpha \to -c \) and \( \gamma \to 0 \), must occur. The first alternative is now shown to be valid only for \( n_2^0 > 1 \), while the second alternative is valid only if \( n_2^0 = 1 \).

The limiting case \( \alpha = -\frac{1}{2}c + \beta \) leads to a straightforward expansion of Eq. (81),

\[
-2\alpha = c - 2\beta = 2\ln \left( \frac{\beta}{-3c} \right) + \frac{22\beta}{3c} + \cdots,
\] (83)

which can be rewritten as the equation

\[
\beta = -3ce^{c/3} + 9c^2e^c + \cdots.
\] (84)

for \( \beta \). As \( c \to -\infty \), this vanishes exponentially. The behaviour of \( \gamma \) is to be obtained from Eq. (82). But the dominant quantity \( c \) is multiplied by the phase factors \( \pm i \), so that an asymptotic expansion carries along a phase change for the logarithm. On carefully analyzing how the various factors change as \( c \) changes from 0 to \( -\infty \), a phase change of \( e^{i\pi i} \) in the argument of the logarithm is found. The real part of Eq. (82) determines \( \gamma \), which after expanding and rewriting gives

\[
\gamma = -\left( \frac{2}{3}n_2^0 - 1 \right) \pi \left( 1 - \frac{8}{c} \cdots \right).
\] (85)

Since it is required that \( \gamma < 0 \), it is seen that this expansion is only valid for \( n_2^0 > 1 \).

The limiting case \( \alpha = -c + \eta \) also allows a straightforward expansion of Eq. (81), but in this case the resulting equation for \( \eta \) involves \( \gamma \) in the lowest order term, namely

\[
\eta^2 + \gamma^2 = 36e^{-2\eta}e^{2c} \left( 1 - \frac{5\eta}{3c} \cdots \right).
\] (86)
Since both $\eta$ and $\gamma$ are real, this implies that both these quantities must vanish asymptotically as $c \to -\infty$. In this case, Eq. (82) accumulates a phase $e^{3\pi i/2}$ in the argument of the logarithm when transforming the factors so that they will be dominated by a positive real part in the limit. What is crucially different in this case from the previous one is the presence of finite complex factors $-3\gamma \mp i\eta$. As a result, the real part of Eq. (82) has the asymptotic expansion

$$-3\gamma = \frac{3}{2} \arctan \left( \frac{-\eta}{-3\gamma} \right) + \left( 2n_2^0 - \frac{3}{2} \right) \pi - \frac{9\gamma}{2c} + \cdots .$$  

(87)

As $c \to -\infty$, $\gamma$ must vanish for this case, as was deduced from the expansion of the $\alpha$ equation. Thus in the limit, the identity

$$\lim_{c \to -\infty} \arctan \left( \frac{\eta}{-3\gamma} \right) = \left( \frac{4}{3} n_2^0 - 1 \right) \pi$$  

(88)

must be satisfied. Since the magnitude of the arctangent is bounded by $\pi/2$, this identity can only be satisfied if $n_2^0 = 1$, in which case the limiting ratio of $\eta$ and $\gamma$ is determined by the condition $\eta = -3\gamma \tan(\pi/3)$. In summary, for $n_2^0 > 1$ the asymptotic behaviour of $\alpha$ is $\alpha \to -c/2$, which gives states of dimer type, while for $n_2^0 = 1$, $\alpha \to -c$ and all three particles are forced to be close to one another, a trimmer state. These associations will be discussed in Section VIII.

VII. THE GROUND STATE: $n_1^0 = n_2^0 = 0$

Since $n_1^0$ and $n_2^0$ are equal, it follows that $\delta_1 = \delta_2 \equiv \delta$. Near $c = 0$ and for $c > 0$, the appropriate equation for determining $\delta$ is Eq. (86), which is modified for equal $\delta$’s to be

$$\delta = i \ln \left[ \frac{(\delta - ic)(2\delta - ic)}{(\delta + ic)(2\delta + ic)} \right].$$  

(89)

The behaviour as $c \to \infty$ is covered by the expansion of Eq. (83), with asymptotic form identical to Eq. (51). Since $\delta \to 0$ as $c \to 0$, it is necessary that the argument of the logarithm must approach 1, which requires that $c \to 0$ faster than does $\delta$. Thus the expansion parameter is $c/\delta$, so that after expansion and rearrangement

$$c = \frac{1}{3} \delta^2 + \frac{1}{108} \delta^4 + \cdots .$$  

(90)

For $c < 0$, the parameterization of Eq. (73) is used, this being equivalent to $\delta = -i\alpha$ with $\alpha > 0$. The ratio $-ic/\delta$ for $c > 0$ thus becomes $c/\alpha$ for $c < 0$ and Eq. (89) becomes

$$\alpha = \ln \left[ \frac{(\alpha - c)(2\alpha - c)}{(\alpha + c)(2\alpha + c)} \right].$$  

(91)

This is identical to Eq. (70), but now the constraint is that $\alpha > -c$. This constraint requires that as $c \to -\infty$, $\alpha$ must become infinite and the expansion of the logarithm is about a singular point of the logarithm. The only possible form is $\alpha = -c + \eta$, with $\eta > 0$ approaching zero. After rearrangement, the resulting expansion gives

$$\eta = -6ce^c - 36e^2e^{2c} + \cdots .$$  

(92)

which is consistent with $\eta$ being positive.

VIII. TYPES OF STATES AND THEIR REPRESENTATION

The states are best represented as contour plots of the probability density (and of the phase if required) in a “ternary phase diagram” for the variables

$$r_{12} = x_2 - x_1$$
$$r_{23} = x_3 - x_2$$
$$r_{31} = 1 + x_1 - x_3 .$$  

(93)
constrained to the region $R_{123}$, $0 \leq r_{ij} \leq 1$. Note that these three coordinates always add to one. In this diagram the coordinate points are represented in an equilateral triangle. Each of the base lines corresponds to one of the coordinates $r_{ij}$ being zero, and each point in the base line corresponds to a particular location of the third particle at the right or left side of the pair $ij$ (the closer to the vertex, the closer the third particle is to the pair). The lines parallel to the base are lines of constant $r_{ij}$. The value of $r_{ij}$ increases from zero at the base to one at the opposite vertex (labeled as $r_{ij}$ in the figures). The center of the triangle is the point where the distance are equal to 1/3. Near the vertex $r_{ij}$ the distance between particles $j$ and $i$ is also small (and tends to zero at the vertex itself); the difference with the basis region is that now the third particle is between the particles $j$ and $i$.

In summary, bases are associated with two particles being together (dimer configurations), and vertices with the three particles being together (trimers). However, in a general state with three real $k$’s, there is no bias towards these configurations. Recall that the wave functions in $R_{123}$ are linear combinations of six exponentials that can be obtained from the (123) form,

$$e^{i(k_1 x_1 + k_2 x_2 + k_3 x_3)},$$

(94)

by permuting $k$’s in all possible manners. The probability density (square modulus) of any of these real $k$ plane wave terms is constant; in other words, in these plane waves none of the particle configurations is favored. The interference between the six different plane waves however destroys the spatial homogeneity (except for the ground state at $c = 0$) and provides some structure with maxima and minima, see Fig. 7. The complex $k$ case is different, see Figs. 8 and 9 for examples of trimer and dimer states. Eq. (94) for the (123) exponential may now be written, using the parameterization in (100), as

$$e^{i(x_1 + x_2 + x_3)p/3} e^{i\gamma(x_1 + x_2 + x_3)} e^{\alpha(x_2 - x_1)},$$

(95)

where the plane wave for the center of mass motion, a plane wave for relative motion of the pair 12 with respect to particle 3, and a real exponential can be recognized; for $\alpha > 0$ the exponent is positive and it favors the trimer configuration of the vertex ($r_{12} = 1$). By permuting $k_1$ and $k_2$, one finds instead, in the term (213), a negative exponent that favors the dimer configurations $r_{12} = 0$. Of course the other two pairs, 13 and 23, have also a corresponding set of dimer and trimer contributions, so that the six terms of the wave function can be separated into two groups: Three of them, (123), (231) and (312), represent trimer configurations, and the other three, (213), (132) and (321), represent dimer configurations. The relative weights among them are determined by the amplitudes $a_{ijk}$. For “trimer states” the three trimer terms dominate the linear combination and the energy becomes, as $c \rightarrow -\infty$, the energy of an actual trimer state (for three particles on an infinite line). For “dimer states”, there is also significant density along the edges of the triangle (not only at the vertices), and the energy tends to the energy of the actual dimer (on the infinite line), plus the contributions from relative motion of the dimer with the free particle and of the center of mass motion. This is consistent with our expectation of reproducing infinite line results in the limit of a large box. As a concrete example, the (unnormalized) states $(0,0)$ and $(1,1)$ for $c \leq -6$ are examined: In both cases $\gamma = p = 0$ and they can be written, using Eqs. (12), (14), (16) and (91), as

$$\psi = e^{\alpha r_{12}} + e^{\alpha r_{23}} + e^{\alpha r_{31}}$$

$$+ \frac{2\alpha - c}{2\alpha + c} (e^{-\alpha r_{12}} + e^{-\alpha r_{23}} + e^{-\alpha r_{31}}).$$

(96)

As $c \rightarrow -\infty$ the factor multiplying the dimer terms in parenthesis tends to 3 for $(0,0)$ (which makes this contribution negligible) but to $\infty$ for $(1,1)$. Fig. 8 shows the ground state $(0,0)$ for negative $c$.

An important aspect of these associations is that the trimer or dimer character changes continuously along a given root as $c$ varies, and only asymptotically ($c \rightarrow -\infty$) is the separation between trimer and dimer states unambiguous. For any finite negative $c$ the complex $k$ roots have non-zero dimer and trimer components. Note for example how the state $(0,1)$ goes from a dimer dominated behaviour to trimer behaviour as $c$ becomes more negative in Fig. 5. In the same vein, even though the threshold between real and complex $k$ is well defined and it occurs at a critical value of $c$, there aren’t any dramatic (discontinuous) changes in the wave function, and the energy varies smoothly with $c$, see Fig. 1, in the neighborhood of the critical $c$ values. However, a different qualitative behaviour (of the energy and state probability density) becomes clear when comparing the state below and above the critical point as the distance from $C$ increases. Thus the critical values indicate a transition of the root from one character, without pair formation, to another where dimers or trimers can be recognized.
IX. SUMMARY

A model of three bosons subject to delta function interactions and periodic boundary conditions has been analyzed. In particular a description of the eigenstates and their behaviour has been given in terms of three momenta $k_i$, $i = 1, 2, 3$ or two sets of alternative parameterizations, $\delta_1, \delta_2$, $p$ and $\alpha, \gamma, p$, convenient, respectively, for the cases where the $k$'s are real or complex. The roots can be primarily classified according to whether the three momenta remain real, or not, for all $c$. In the second case the wave function tends to concentrate asymptotically around dimer or trimer configurations and the energy decreases quadratically with $c$ as $c \to -\infty$. The critical values of $c$ required to form the bounds (go from real to complex $k$'s) have been provided.

The main features of the root behaviour as $c$ varies are now summarized. (Using the symmetry properties or total momentum translations the behaviour of any other state is obtained from the ones we consider explicitly, namely states $(n_1^0, n_2^0)$, $n_1^0 \leq n_2^0$, in the central momentum strip, $n_p = 0, \pm 1$.) Relations satisfied by all roots are:

- The total momentum $p$ (within the central strip) is given from $n_1^0$ and $n_2^0$ by Eq. (12). It is constant as $c$ varies for a given root. The total energy varies according to Eq. (29) or (63).
- $\delta_j(c = 0) = 2\pi n_j^0$.
- $\delta_j \to 2\pi(n_j^0 + 1)$ as $c \to \infty$.

The different particular cases are characterized by the following properties:

- $(0,0)$: $C(0,0) = 0$, $p = 0$, $\gamma = 0$, $\alpha \sim -c$ as $c \to -\infty$. The ground state is a nondegenerate state with trimer character.
- $(0,1)$: $C(0,1) = 0$, $\alpha \sim -c$ and $\gamma \to 0$ as $c \to -\infty$. Asymptotic trimer character. Similar to the ground state but it has a degenerate partner and $p \neq 0$.
- $(0, n_2^0 > 1)$: $C(0, n_2^0) = 0$, $\gamma \to (-2/3n_2^0 + 1)\pi$ and $\alpha \sim -c/2$ as $c \to -\infty$. Dimer character.
- $(1, n_1^0 \geq 1)$: $-6 \leq C(1, n_1^0) < -4$, $\gamma \to -2\pi/3(n_1^0 - 1)$, $\alpha \sim -c/2$ as $c \to -\infty$. Also dimer character, but it takes a stronger interaction to achieve in comparison to the previous group.
- $(n_1^0 > 1, n_2^0 \geq n_1^0)$: Real $k_i$ for all $c$, $\delta_j(\pm \infty) = 2\pi n_j^0 \pm 1$. The energy tends to a constant value as $|c| \to \infty$.

It is hoped that the root structure found and the techniques developed for its study will be useful for the examination of variants of the model involving different interactions and/or an arbitrary number of particles. Since all eigenstates can be obtained for a given $c$, one of the possible applications of the present work is the simulation of time dependent rearrangement processes using a discretized basis. In this context it may serve as a reference exact model to compare with approximate wave function propagation methods based on periodic boundary conditions [3]. The model may also permit an explicit comparison between the classical concepts of “bound pair” and “free” particles and their collisional rearrangements with their quantum counterparts. The origin of the difficulties in the quantum case is that the Hamiltonian for the 3 (or $N$) body system does not commute with the Hamiltonian of a pair, so that using the concept of the bound pair in a gas (or in a box) is a delicate matter [31].

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APPENDIX A: NORMALIZATION AND POTENTIAL ENERGY

The expression for the wave function is not normalized. For the analysis of the energy spectrum this does not have any effect. However the calculation of physical expectation values, and in particular of the potential energy, requires a normalized function. This requires the evaluation of the inner product $\langle \psi | \psi \rangle$, where $|\psi\rangle$ is the unnormalized total wave function given explicitly by Eq. (12) in the region $R_{123}$. The contribution of the six regions is identical so
\[ \langle \psi | \psi \rangle = 6 \int_0^1 dx_3 \int_0^{x_3} dx_2 \int_0^{x_2} dx_1 |\psi(k_1, k_2, k_3; x_1, x_2, x_3)|^2 \] (A1)

This integral is decomposed into 36 terms with integrals of the general form

\[ \int_0^1 dx_3 \int_0^{x_3} dx_2 \int_0^{x_2} dx_1 e^{i(\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3)} \] (A2)

where the \( \alpha \)'s are combinations of momenta of the form \(-k_j^* + k_i\), \((i, j = 1, 2, 3)\). These integrals can of course be solved explicitly but the result is so lengthy that it is not reported here. In order to handle all terms efficiently, it is useful to classify the possible types of integrals. There are three cases: \((\alpha_j = 0, j = 1, 2, 3)\), \((\alpha_j = 0, \alpha_k + \alpha_i = 0)\), and \((\alpha_j \neq 0, j = 1, 2, 3)\). In all cases the sum of the \( \alpha \)'s is zero, \( \sum_j \alpha_j = p - p = 0 \).

Once \( \langle \psi | \psi \rangle \) is obtained, the (dimensionless) potential energy involves a simpler integration because of the delta functions, namely

\[ \langle V \rangle = \frac{6c}{\langle \psi | \psi \rangle} \int_0^1 dx_3 \int_0^{x_3} dx_1 |\psi(x_1, x_3)|^2 . \] (A3)

Again, all integrals involved can be carried out.

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FIGURE CAPTIONS

Fig. 1 $\langle E \rangle$ vs $c$ for $(n^0, n^0)$. From bottom to top, $n^0 = 0, 1, 2, 3$. The lines for $n^0 = 0$ and 1 extend to $-\infty$ as $c \to -\infty$.

Fig. 2 $\langle V \rangle$ vs $c$ for $(n^0, n^0)$. From bottom to top, $n^0 = 0, 1, 2, 3$. The lines for $n^0 = 0$ and 1 extend to $-\infty$ as $c \to -\infty$.

Fig. 3 $\delta_1$ vs $c$. The numbers close to each line correspond to $n^0_1$ and $n^0_2$. The figure for $\delta_2$ is identical by interchanging $n^0_1$ and $n^0_2$. The lines are only drawn up to the critical values of $c$ where $\delta_1 = 0$ [for (1,1), (1,2) and (1,3)], or $\delta_2 = 0$ [for (2,1) and (3,1)]. For more negative values of $c$, the $\alpha$-$\gamma$ parameterization is used, see Figs. 5 and 6.

Fig. 4 $\delta$ vs $c$ for $(n^0, n^0)$. From bottom to top, $n^0 = 0, 1, 2, 3$.

Fig. 5 $\alpha$ vs $c$. Solid lines: $n^0_1 = 0$; Dashed lines: $n^0_1 = 1$. The number close to the lines is $n^0_2$.

Fig. 6 $\gamma$ vs $c$. Solid lines: $n^0_1 = 0$; Dashed lines: $n^0_1 = 1$. The number close to the lines is $n^0_2$.

Fig. 7 Contour plot of the probability density of the state $(3,3)$ at $c = 1$. The interpretation of a “ternary phase” type of diagram is explained in the text.

Fig. 8 Contour plot of the probability density of the state $(0,0)$ at $c = -9$.

Fig. 9 Contour plot for the probability density of the state $(0,2)$ at $c = -9$. 
