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Untouched Aspects of the Wave Mechanics of Two Particles in a Many Body Quantum System

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Abstract—The wave mechanics of a pair of hard core particles is critically analyzed to discover its several important untouched aspects. Identifying the possible weakness of the previous treatments in defining the relative dynamics of two hard core particles and related boundary conditions, it finds the correct form of their state function which can serve as an important basis of the microscopic theory of a system like liquid helium.

Keywords: two quantum particles — wave mechanics — many body systems

A: Introduction

The wave mechanics of two *hard core* (HC) identical particles (say P1 and P2) interacting through a central force forms an important subject of study because it serves as a basis of microscopic theories of *many body quantum systems* (MBQS) such as liquid helium[1–3]. The Schrodinger equation of P1 and P2 in *center of mass* (CM) coordinates can be written as

(1)

Here $V_{\mathrm{HC}}(r)$ represents the HC interaction (*i.e.* $V(r < \sigma) = \infty$ and $V(r \geq \sigma) = 0$ with σ being the HC diameter of a particle) between P1 and P2 and

(2)

describes their state of momenta, $\mathbf{k} = \mathbf{k}_2 - \mathbf{k}_1$ and $\mathbf{K} = \mathbf{k}_1 + \mathbf{k}_2$. All notations, including $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, $\mathbf{r} = (\mathbf{r}_2 - \mathbf{r}_1)$, *etc.,* have usual meaning. The $\psi_{\mathrm{k}}(r)$ representing the relative motion of P1 and P2 satisfies

(3)

with $E_k = E - h^2K^2/4m$. Since Equation 3 can not be solved as such due to non-analytic nature of $V_{\mathrm{HC}}(r)$ at $r < \sigma$, conventional approaches[1–3] use a boundary condition $\psi_k(r < \sigma) = 0$[3] or its equivalent (*viz.* the Jastrow correlation factor[4]) to find a $\psi_k(r)$ that agrees with the fact that two HC particles do not overlap. However, during the course of our recent work[5,6] on the theory of a system of interacting bosons such as liquid ^4He (our other paper in this issue[6]) we made a critical analysis of the wave mechanics of P1 and P2 and discovered its important untouched aspects (*cf.* Section B) and correct form of $\psi_k(r)$ (*cf.* Section C). Here we present a brief report of our analysis.

B: Important Aspects and Their Analysis

B(1): Real Dynamics of a Pair in a MBQS

To a good approximation particles in a MBQS like liquid helium represent hard balls moving freely on the surface of a constant negative potential, $-V_0$[5]. Naturally, P1 and P2 encounter $V_{HC}(r)$ only when they collide with each other. While this elastic collision leads to an exchange of momenta $\mathbf{k}_1$ and $\mathbf{k}_2$, the fact remains that P1 and P2 (before and after their collision) have free particle motion. Analysing another possible situation in which mutually colliding P1 and P2 also collide simultaneously with other particle(s), we find that $\mathbf{k}_1$ and $\mathbf{k}_2$ (or $\mathbf{k}$ and $\mathbf{K}$) after such collision may assume new values, $\mathbf{k}_1'$ and $\mathbf{k}_2'$ (or $\mathbf{k}'$ and $\mathbf{K}'$) but once again P1 and P2 retain their free particle motion. As such the inter-particle interactions make a pair embedded in a MBQS scatter/jump from its one state to another state of possible $\mathbf{k}$ and $\mathbf{K}$, while such a state of the pair in free space simply remains unchanged. Evidently, *the basic nature of the dynamics of a pair in two situations does not differ,* which means that the states of P1 and P2 in a MBQS, in spite of their interaction with other particles, can be described by Equation 1.

B(2): Correct Description of Relative Motion

We note that the non-relativistic dynamics of two particles interacting through a central force can be separated mathematically into two components[7] expressing their relative motion ($\psi_k(r)$) and CM motion ($\exp[i \cdot \mathbf{K} \cdot \mathbf{R}]$) (*cf.* Equations 1–3). Notably, while $\Psi(R, r)$ defines a general state of the pair with P1 and P2 having their relative as well as CM motions, $\exp[i \cdot \mathbf{K} \cdot \mathbf{R}]$ represents a state in which its relative motion is absent (*i.e.,* the pair can be treated as a single body of mass $2m$) and, similarly, $\psi_k(r)$ describes *that motion of* P1 *and* P2 *in which their* CM *does not move* which means

$$\mathbf{K} = 0 \quad \text{and} \quad \mathbf{k}_1 = -\mathbf{k}_2 = \mathbf{q} \quad \text{(say)} \tag{4}$$

Evidently, P1 and P2 in their relative dynamics have equal and opposite momenta ($\mathbf{q}, -\mathbf{q}$) and their distance from their CM, $\mathbf{r}_{CM}(1)$ and $\mathbf{r}_{CM}(2)$, obviously, satisfies

$$\mathbf{r}_{CM}(1) = -\mathbf{r}_{CM}(2) \tag{5}$$

where $\mathbf{r}_{CM}$ represents a position vector in the frame attached to the CM. As such, Equations 4 and 5 define an important feature of $\psi_k(r)$ and conclude that the relative motion of P1 and P2 maintains a center of symmetry at their CM. However, these microscopic details of $\psi_k(r)$, that we use to find its correct form, are not used by conventional theories[1–3].

B(3): Relative Motion in General Perspective

Since the basic fact, that $\psi_k(r)$ of Equation 2 represents that motion of P1 and P2 in which their CM does not move, holds good even for a case of two particles having unequal masses ($m_1 > m_2$, say), $\psi_k(r)$ of such particles too would hold Equation 4 as well as

$$m_1 \cdot \mathbf{r}_{CM}(1) = -m_2 \cdot \mathbf{r}_{CM}(2) \tag{6}$$

which is corroborated by all experiments that can reveal the $\psi_k(r)$ of a two body system such as single electron atom/ion (*e.g.*, H atom and He^+ ion), diatomic molecules (*e.g.*, HCl), etc. As stated by Schiff[7] we, apparently, have two different choices (CH1 and CH2) of a frame of observation to construe $\psi_k(r)$. In CH1, we observe $\psi_k(r)$ as a motion of P2 relative to P1 or *vice versa*, while in CH2 we detect it as a motion of two particles relative to their fixed CM. Evidently, only CH2 choice is consistent with Equations 4 and 5/6. The CM can be at rest in CH1 also provided P1 is infinitely heavy (*i.e.*, $m_1 \; m_2$) or it is rigidly fixed at one point. However, since these conditions do not apply to particles in a MBQS like liquid *He*, use of CH1 choice to define their $\psi_k(r)$ in[1–3] can not render its correct form. The simple fact that $\Psi(R, r)$ can be mathematically separated into $\psi_k(r)$ and $\exp[i \cdot \mathbf{K} \cdot \mathbf{R}]$, does not ensure the consistency of a $\psi_k(r)$ with Equations 4 and 5/6 and a $\psi_k(r)$ determined as such by solving Equation 3 would fail to embody the useful details defined by Equations 4 and 5.

B(4): Correct Boundary Condition

The boundary condition, $\psi_k(r \leq \sigma) = 0$ (or its equivalent Jastrow correlation factor[4]) used in conventional theories[1–3], implicitly presumes that $r = \sigma$ can be determined precisely (*i.e.*, with an uncertainty $\Delta r = 0$) which implies that momentum uncertainty Δk is infinitely large. However, since $\Delta k = (\langle k^2 \rangle - \langle k \rangle^2)^{1/2}$ for the pair can be at the most equal to k itself[8], $\Delta r = 0$ would not hold with uncertainty principle unless k is infinitely large. Naturally, the degree of inconsistency would assume prominence, particularly, for particles of low momentum, *viz.*, $q < \pi/\sigma$ (*i.e.*, $\lambda/2 > \sigma$ with $\lambda = 2(\pi/q)$, for which uncertainty in the positions of each particle, $\Delta r = \lambda/2$, becomes much larger than r ($\leq \sigma$) and the statement $r \leq \sigma$ as well as the boundary condition, $\psi_k(r \leq \sigma) = 0$, lose their meaning. Evidently, one needs to find its correct alternative. In this context we take cognizance of the fact that a particle in wave mechanics manifests itself as a *wave packet* (WP) of size $\lambda/2$ (*i.e.*, a *sphere* of diameter $\lambda/2$) and because two HC particles do not overlap, their representative WPs should also have no overlap. Thus, the separation ($\langle r\rangle$) between two particles should satisfy $\langle r\rangle \geq \lambda/2$ (*i.e.*, $k\langle r\rangle \geq 2\pi$) which is also demanded by uncertainty relation, $\Delta k\Delta r \geq 2\pi$, because we expect $k \geq \Delta k$, and $\langle r\rangle \geq \Delta r$.

C: Correct Form of $\psi_k(r)$ and Related Aspects

Using the inferences of Section B, this section concludes the correct form of $\psi_k(r)$ and analyzes other related aspects as follows.

C(1): ($\mathbf{q}$, - $\mathbf{q}$) *or SMW Pair Waveform*

Since two particles in their physically possible state always have $r \geq \sigma$ and $V_{\mathrm{HC}}(r \geq \sigma) = 0$, their dynamics can, possibly, be described by the hamiltonian of two non-interacting particles,

(7)

and its eigenfunction

with

(with unit normalisation constant and $\varepsilon_i = {}^2k_i^2/2m$) provided $U^{\pm}$ is subjected to the condition $\lambda/2 \leq \langle r\rangle$ to take care of $V_{\mathrm{HC}}(r)$. As such we have $\Psi(R, r) \equiv U^{\pm}$ and

(8)

with U^+ and U^- having usual meaning, $\alpha = 0$ for U^+, $\alpha = \pi$ for U^- and $\varepsilon(K) + \varepsilon(k) = {}^2[K^2 + k^2]/4m = {}^2[k_1^2 + k_2^2]/2m$. Comparing Equations 2 and 8 and using $\mathbf{k} = 2\mathbf{q}$ we have

(9)

We note that $\psi_k(r)^{\pm}$ is a kind of *stationary matter wave* (SMW) that modulates the probability ($|U^{\pm}|^2 = |\psi^{\pm}|^2$) of finding two particles at their relative phase position, $\phi = \mathbf{k} \cdot \mathbf{r}$. We have

(10)

where $g(\phi)$ represents *phase correlation factor* which will be analyzed in Section C(3). The fact that $\psi_k(r)^{\pm}$ is the superposition of two particles of momenta **q** and **- q** not only agrees with Equation 4 but also implies that $U^{\pm}$ represents a (**q**, **- q**) pair (proposed to be known as SMW pair) moving with CM momentum **K**.

C(2): Equivalence of $\psi_k(r)^{\pm}$

Since two particles always collide at their CM ($r = 0$), their $\psi_k(r)$ has to have its zero at $r = 0$. While this condition is satisfied as such by $\psi_k(r)^-$, whose antisymmetry for the exchange of two particles corroborates the contention[2] that HC particles in r-space behave the way fermions behave in k-space, we also find that $\psi_k(r)^+ \equiv \psi_k(r)^-$ because they differ only in the locations of the origin $\phi' = \alpha + \phi = 0$. For $\psi_k(r)^+$, it is located at $\phi = 0$—the central point of an *antinodal region* (AR), and for $\psi_k(r)^-$ at $\phi = \pi$ (the nodal point) of a SMW. To understand this equivalence of $\psi_k(r)^+$ and $\psi_k(r)^-$ we note that in a wave mechanical superposition, there is no way to find whether two particles after their collision have bounced back on the respective sides of their CM or they exchanged their positions across this point. Since the former case represents the *self superposition* (SS) of each particle, it can be best described by $\psi_k(r)^+$ because $V_{\mathrm{HC}}(r)$ does not operate in such superposition. However, the latter case implying *mutual superposition* (MS) of P1 and P2 should be represented only by $\psi_k(r)^-$ because the corresponding wave function has to vanish at $r = 0$ due to $V_{\mathrm{HC}}(r)$ operating between these particles. As such, $\psi_k(r)^+$ and $\psi_k(r)^-$ represent equivalent configuration.

C(3): SMW Pair and Phase Correlation

The possibility that P1 and P2 may rest simultaneously in a single AR of $\psi_k(r)$ is ruled out because this does not satisfy the condition that $\psi_k(r)$ has to have its zero at their CM. Evidently, P1 and P2 in a configuration of their least separation can occupy two separate close by ARs of $\psi_k(r)^{\pm}$. We note that this configuration is consistent with *excluded volume condition* (a consequence of the HC nature of the particles)[9] and is characterized by $\langle r\rangle = \langle r_2\rangle - \langle r_1\rangle = \lambda/2$[10] which not only implies that $\Delta\phi = \langle\phi_2\rangle - \langle\phi_1\rangle = 2\pi$ but also shows that our condition $\langle r\rangle \geq \lambda/2$ is, naturally, satisfied by SMW formation. Further, since the phase correlation factor, $g(\phi) = |\psi_k(r)^{\pm}|^2$, varies periodically from $g(\phi) = 0$ at $\phi' = (2n + 1)\pi$ to $g(\phi) = 2.0$ at $\phi' = 2n\pi$ (with $n = 1, 2, 3, ...$) implies that SMW formation renders a kind inter-particle phase correlation or a kind of binding that binds P1 and P2 in ϕ-space at positions separated by $\Delta\phi = 2n\pi$ (with $n = 1, 2, 3, ...$). Our other paper[6] not only finds the potential equivalent of $g(\phi)$ but also concludes that particles also acquire a kind of collective binding in r-space when a weak attraction is switched on the state of HC particles in SMW configuration. It is obvious[10] that ϕ-correlations can be observed only when the physical condition of the system forces two particles to remain always in the state $\psi_k(r)^{\pm}$ of their wave mechanical superposition as found in superfluid phase of liquid ^4He but not in normal fluid phase where this requirement is not fulfilled[5,6].

C(4): Dominance of Wave/Particle Nature

While the least possible separation, $\langle r \rangle = \lambda/2$, between two particles of $q < \pi/\sigma$ or $\lambda/2 > \sigma$ depends on their q through $q\langle r \rangle = \pi$, similar separation, $r = \sigma$, between two particles of $q > \pi/\sigma$, is independent of q. Evidently, the wave nature fails to prevail over $V_{HC}(r)$ to have $q\langle r \rangle = \pi$ for high q particles of $q > \pi/\sigma$, and as such, $\lambda/2 > \sigma$ seems to precisely characterize a physical state in which two HC particles would behave like waves or otherwise as particles.

C(5): $V_{HC}(r)$ and its Equivalence with $\delta(r)$-Repulsion

We find that a $\psi_k(r)^{\pm}$ defining the superposition of two particles of $\lambda/2 > \sigma$ is independent of σ. This is consistent with: (i) the basic principle of image resolution which implies that P1 of $\lambda/2 > \sigma$ can not resolve a structure of size σ within the WP of size = $\lambda/2$ ($> \sigma$) of P2 or *vice versa* and (ii) the experimental fact that the patterns of interference and diffraction of even strongly interacting particles like electrons, neutrons, *He* atoms, *etc.,* do not depend on σ-size of these particles[11]. As such, the details of $\psi_k(r)^{\pm}$ would not change when σ is infinitely small. Evidently, two HC particles in $\psi_k(r)^{\pm}$ state may be considered to have δ-size HC or $\delta(r)$-repulsion. This implies that

(11)

where A represents the strength of $\delta(r)$ repulsion. Using U^- (Equation 8) as a function representing a $|K, q>$ pair state of $H(2)$ (Equation 11) along with the fact that two particles in their relative motion always have $r_1 = - r_2$ (Equation 5), which implies that $r_1 = r_2$ is possible only when $r_1 = r_2 = 0$ (the CM of the pair and a nodal point of U^- where $U^- = 0$), we can show by simple integration over the limit $r = 0$ to $r = \lambda$[10] that

(12)

and

(13)

Although, the real value of A is unimportant because of $\langle A \cdot \delta(r_1 - r_2) \rangle = 0$, however, we address it in Section 2.7 of our next paper[6].

C(6): U^- Pair Waveform for a Single Particle

Each particle of a SMW pair, being a part and parcel of it, needs to be represented by U^+ or its equivalent U^- pair waveform. However, we propose to use

U^- because it embodies the fact that the pair waveform of two HC particles must vanish at their CM $r_1 = r_2 = 0$, more clearly than U^+. As such for the ith particle, we have

(14)

(with $i = 1$ or 2). However, in doing so R_i could, rightly, be identified as the position of the CM of ith particle (*not the* CM *of the pair*), and r_i as the coordinate of a point (within the WP of ith particle) measured from a nodal point of $\psi_k(r)^-$ on the line joining the two particles. Each particle seems to have two motions: (i) the q-motion of energy $^2q^2/2m$ and (ii) the K-motion of energy $^2K^2/8m$.

C(7): Rearrangement of H(2)

Use of U^- pair waveform for a single particle can be accepted without any difficulty because under the approximation $V_{HC}(r) \equiv A \cdot \delta(r)$, U^- has been shown to be an eigenfunction of $H(2)$ and $H_0(2) = H(2) - V_{HC}(r)$ (*cf.* Eqn.7) can be rearranged into a form compatible with Equation 14. We have

(15)

with $h_i = -(^2/2m) \cdot \nabla_i^2$ being the hamiltonian of ith free particle ($i = 1$ or 2) which can also be represented by $h(i)$ when the particle symbolizes a SMW pair. This gives

(16)

Using $|K_1, q_1\rangle\, |K_2, q_2\rangle$ as an eigenstate of $H(2)$ (Equation 16) with $|K_i, q_i\rangle$ being the state of ith particle defined by $U^-(i)$ (Equation 14)—an eigenfunction of $h(i)$, we find that

(17)

because the representation of two particles by separate $U^-(1)$ and $U^-(2)$ pair waveforms does not change the reality that their relative motion satisfies $r_1 = -r_2$ (Equation 5), which implies that $r_1 = r_2$ is possible only when $r_1 = r_2 = 0$ for which $U^-(1) = U^-(2) = 0$. Evidently, we have $\langle H(2)\rangle = 2\langle h(1)\rangle = 2\langle h(2)\rangle$ (= $E(2)$ given by Equation 13). The fact, that $E(2)$ is basically the kinetic energy of the pair evinces that the main role of $V_{HC}(r)$ is nothing but to scatter the pair from its one state to another state of **K** and **k** as envisaged in Section B(1). Our $\psi_k(r)$ and other results (Equations 11–13 and 17) are not expected to agree with those of pseudo-potential approach[3], which also concludes $V_{HC}(r) \equiv \delta(r)$-repulsion, because the latter[3] does not use $\lambda/2 \leq \langle r \rangle$ and the basic features (Equations 4 and 5) of $\psi_k(r)^{-}$.

D: Concluding Remarks

By using different aspects of wave mechanics in their right perspective, this paper concludes the correct form of the wave function (U^{-}, Equation 8) that can represent two HC particles in a state of their wave mechanical superposition. While it finds that each particle of the pair can also be represented by the pair waveform $U^{-}(i)$ (Equation 14) as a separate entity, the way particle-particle correlation effects can be treated in a MBQS like liquid ^4He is discussed in Jain[6].

One may find that: (i) the way $\psi_k(r)$, appearing in Equation 2, is obtained either as a solution[3] of the Schrodinger equation (*viz.* Equation 3) or by using Jastrow type approach[4], does not take cognizance of the basic characteristics of $\psi_k(r)$ (*i.e.,* Equations 4 and 5) and (ii) the boundary condition $\psi_k(r \leq \sigma) = 0$ or its equivalent as used in references 1–3 loses its meaning for low momentum particles of $\lambda/2 > \sigma$ (*cf.* Section B(4)). Obviously, because of all such weaknesses of these approaches[1–3], the direction for finding the correct microscopic theory of a system like liquid ^4He has been missed for so long. This point is clearly demonstrated by the fact that by using a new approach free from these weaknesses we succeeded[5,6] in formulating the long awaited theory of liquid ^4He which has unmatched accuracy, simplicity and clarity. Moreover, as discussed briefly in our third paper reported in this issue[12], we also find that the framework of our new approach can help us in developing a correct understanding of other MBQS and in unifying the physics of widely different systems of bosons as well as fermions.

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Notes

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