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Wave mechanics of two hard core quantum particles in A 1-D box

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Abstract: The wave mechanics of two impenetrable hard core particles in a 1-D box is analyzed. Each particle in the box behaves like an independent entity represented by a *macro-orbital* (a kind of pair waveform). While the expectation value of their interaction, $< V_{HC}(x) >$, vanishes for every state of two particles, the expectation value of their relative separation, $< x >$, satisfies $< x >\geq \lambda/2$ (or $q \geq \pi/d$, with $2d = L$ being the size of the box). The particles in their ground state define a close-packed arrangement of their wave packets (with $< x >= \lambda/2$, phase position separation $\Delta\phi = 2\pi$ and momentum $|q_o| = \pi/d$) and experience a mutual repulsive force (*zero point repulsion*) $f_o = h^2/2md^3$ which also tries to expand the box. While the relative dynamics of two particles in their excited states represents usual collisional motion, the same in their ground state becomes collisionless. These results have great significance in determining a correct microscopic understanding of widely different many-body systems.

Keywords: Wave mechanics, δ-particles, hard core particles, 1-D box, macro-orbital
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1 Introduction

The wave mechanics of two *hard core* (HC) identical particles in a 1-D box can serve as an important basis for understanding a many-body 1-D system and can simplify our understanding of the relatively complex dynamics of similar 2-D and 3-D systems. The problem has been studied elegantly by Girardeau [1] and Lieb and Liniger [2] as a part of their analysis of N-body 1-D systems of HC bosons. While Girardeau [1] studied a 1-D gas of finite size impenetrable bosons, Lieb and Liniger [2] studied a system of δ-size

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bosons with varying strength of δ-repulsion. Useful results can also be obtained from an equally elegant study of similar systems of δ-size bosons and fermions by Yang [3]. In their scheme for solving the problem, these authors assume a Bethe ansatz for N-body wave function, impose bosonic/fermionic symmetry (as the case demands) and use approximation methods or periodic boundary conditions. However, in our scheme for studying two δ-size HC particles in a 1-D box, we first use the *center of mass* (CM) coordinate system to separate the relative motion involved with δ-repulsion from the CM motion representing a kind of free particle motion. We next solve the Schrödinger equation of the pair to find its solution(s) and analyze these solution(s) to identify wave function(s) (which we propose be called *macro-orbital(s)*) that represent particles as independent entities. To this effect, we use the standard method of step potential to deal with δ-repulsion. Interestingly, this renders exact solutions. Initially, we solve the Schrödinger equation for two particles in free space and on such solutions later impose the boundary conditions associated with the locations of the two walls of our 1-D box to determine the desired eigenvalues and eigenfunctions. By establishing an equivalence between infinitely strong δ-repulsion ($A\delta(x)$ where $\delta(x)$ is Dirac's delta function and A reaches ∞ as x reaches zero) and HC interaction $V_{HC}(x)$ ($V_{HC}(x<\sigma)=\infty$ and $V_{HC}(x\geq\sigma)=0$ with σ being the HC diameter of a particle), we conclude that our results can be used for particles of any σ— particularly, when their $\lambda\approx\sigma$, *i.e., when the wave nature dominates their particle nature.* Finally, we also find (*cf.* Section 5) that this paper provides a sound mathematical foundation for our logical arguments used to analyse the 3-D dynamics of two HC particles [4] and helps in establishing our scheme as a means to discover a microscopic understanding of many-body systems such as liquid ^4He [5,6], as well as unifying the physics of widely different bosonic and fermionic systems [7].

2 Schrödinger Equation

The Hamiltonian for the mechanics of two identical particles (say P1 and P2) interacting through impenetrable δ-repulsion can be written as

$$H(2)=-(\hbar^2/2m)\left(\bigtriangledown_1^2+\bigtriangledown_2^2\right)+A\delta(x). \tag{1}$$

Using the CM coordinate system, we write the corresponding Schrödinger equation as

$$[-(\hbar^2/4m)\bigtriangledown_X^2-(\hbar^2/m)\bigtriangledown_x^2+A\delta(x)]\Psi(x,X)=E\Psi(x,X) \tag{2}$$

with

$$\Psi(x,X)=\psi_k(x)\exp\left[i(KX)\right] \tag{3}$$

which describes a general state for P1 and P2 with $\psi_k(x)$ representing their relative motion and $\exp\left[i(KX)\right]$ the CM motion. Note that $\psi_k(x)$ satisfies

$$[-(\hbar^2/m)\bigtriangledown_x^2+A\delta(x)]\psi_k(x)=E_k\psi_k(x) \tag{4}$$

with $E_k=E-\hbar^2K^2/4m$. All notations in Eqns. 2–4 including

$$x=\mathrm{x}_2-\mathrm{x}_1 \quad \text{and} \quad k=\mathrm{k}_2-\mathrm{k}_1, \tag{5}$$

$$X = (\mathrm{x}_1 + \mathrm{x}_2)/2 \quad \text{and} \quad K = \mathrm{k}_1 + \mathrm{k}_2 \tag{6}$$

have their usual meaning.

3 Important Aspects of Two-Body Dynamics

3.1 Characteristic details of $\psi_k(x)$

Without loss of generality, we may define

$$\mathrm{k}_1 = -q + K/2 \quad \text{and} \quad \mathrm{k}_2 = q + K/2 \tag{7}$$

which after the collision become $\mathrm{k}_1 = q + K/2$ and $\mathrm{k}_2 = -q + K/2$. If x_{CM} and k_{CM} represent, respectively, the position and momentum of a particle with respect to the CM, we have

$$\mathrm{k}_{CM}(1) = -\mathrm{k}_{CM}(2) = q \quad \text{and} \quad \mathrm{x}_{CM}(1) = -\mathrm{x}_{CM}(2). \tag{8}$$

Eqn. 8 implies that P1 and P2 in their relative dynamics have: (i) equal and opposite momenta $(q, -q)$ and (ii) maintain a center of symmetry at their CM. As such, Eqns. 7 and 8 define the characteristic details of $\psi_k(x)$ and imply that two particles in a laboratory frame have $(q, -q)$ momenta at their CM which itself moves with momentum K.

3.2 Functional form of $\psi_k(x)$

We consider $A\delta(x)$ as a step potential which has two different values over two different ranges of x, *viz.*, (i) $A\delta(x) = 0$ for $x \neq 0$ and (ii) $A\delta(x) = \infty$ for $x = 0$. Since P1 and P2 at $x \neq 0$ experience zero interaction, each of them can be represented by a plane wave, $u_{\mathrm{k}_i}(\mathrm{x}_i) = \exp(i\mathrm{k}_i\mathrm{x}_i)\exp[-iE_it/\hbar]$ (assumed to have unit normalization) and their state can be expressed, in principle, by

$$\Psi(\mathrm{x}_1, \mathrm{x}_2)^{\pm} = 1/\sqrt{2}[u_{\mathrm{k}_1}(\mathrm{x}_1)u_{\mathrm{k}_2}(\mathrm{x}_2) \pm u_{\mathrm{k}_2}(\mathrm{x}_1)u_{\mathrm{k}_1}(\mathrm{x}_2)] \tag{9}$$

which can be arranged as

$$\Psi(x, X)^{\pm} = \psi_k(x)^{\pm} \exp(iKX), \tag{10}$$

$$\psi_k(x)^{+} = \sqrt{2}\cos(kx/2), \tag{11}$$

$$\psi_k(x)^{-} = \sqrt{2}\sin(kx/2). \tag{12}$$

Note that $\psi_k(x)^+$ and $\psi_k(x)^-$ represent a kind of *stationary matter wave* (SMW) which modulates the relative phase positions ($\phi = kx$) of P1 and P2. Although, $\psi_k(x)^-$ is a desired solution of Eqn. 4 because it satisfies the condition that a state function of two impenetrable HC particles must vanish at $x = 0$, its odd symmetry for an exchange of P1 and P2 fits with a fermionic pair but not with a bosonic one. However, we also have an even symmetry solution, $\phi_k(x)^+ = |\sin(kx/2)|$, of Eqn. 4. Since $\phi_k(x)^+$ has zero value and continuous character at $x = 0$, it can be used for two HC bosons. To get $\phi_k(x)^+$, we first use the even symmetry of $A\delta(x)$ to identify that the solutions of Eqn. 4 should have even or odd symmetry. We next consider $\omega_{k_o}(x) = \cos(k_o x/2)$ (with unit normalization) representing an even symmetry solution of Eqn. 4 for the $A = 0$ case, and analyse its changes under increasing A. When A assumes non-zero value, the pair is expressed by $\eta_{k'}(x)$ which deviates from $\omega_{k_o}(x)$ for a cusp like dip at $x = 0$. $|\eta_{k'}(x = 0)|$ decreases smoothly with increasing A and vanishes when $A = \infty$. In this limiting process, $\eta_{k'}(x)$ maintains *even symmetry* around $x = 0$ and reaches the form of $\phi_k(x)^+ = |\sin(kx/2)|$ when $A = \infty$; one can also use an alternative approach [8] to get $\phi_k(x)^+$. While it is evident that $\phi_k(x)^+$ and $\psi_k(x)^-$ have major differences with respect to the discontinuity of $\partial_x\phi_k(x)^+|_{x=0}$ and continuity of $\partial_x\psi_k(x)^-|_{x=0}$, the fact that $|\psi_k(x)^-|^2 = |\phi_k(x)^+|^2$ reveals that the modulation of the relative positions of two HC fermions by $\psi_k(x)^-$ is exactly identical to that of two HC bosons by $\phi_k(x)^+$. This renders an important result that the relative configuration and dynamics of two HC particles are not influenced by their fermioninc or bosonic nature and these aspects can be determined by analysing either $\psi_k(x)^-$ or $\phi_k(x)^+$. In this context we also note that $\psi_k(x)^- \exp[-iE_kt/\hbar]$ and $\phi_k(x)^+ \exp[-iE_kt/\hbar]$, as stationary waves, have exactly identical structures (a chain of sinusoidal antinodal loops of size $\lambda/2$ with nodal points at $x = s\lambda/2$, with $s = 0, \pm1, \pm2, \pm3,$ *etc.*

3.3 $< A\delta(x) >$ and $< H(2) >$

Following what has been concluded above, we find

$$< \zeta(x,X)|A\delta(x)|\zeta(x,X) >= |\psi_k(x)^-|^2_{x=0} = |\phi_k(x)^+|^2_{x=0} = 0 \tag{13}$$

with

$$\zeta(x,X) = \zeta_k(x)\exp(iKX), \tag{14}$$

where $\zeta_k(x)$ stands either for $\psi_k(x)^-$ or $\phi_k(x)^+$. Using Eqn 2, this renders

$$< \zeta(x,X)|H(2)|\zeta(x,X) >= (\hbar^2/4m)(K^2 + k^2) = (\hbar^2/2m)(\mathrm{k}_1^2 + \mathrm{k}_2^2). \tag{15}$$

However, Eqn. 15 should not be believed to imply that $< H(2) >$ for P1 and P2 interacting through $A\delta(x)$ are identical to those having no interaction. We address this issue in Section 4.1.

4 Dynamics of Two Particles in a 1-D Box

4.1 Eigenvalues and eigenfunctions

According to the boundary conditions of the problem, $\exp(iKX)$ as well as $\zeta_k(x)$ (Eqn. 14) should be zero at the impenetrable walls of our 1-D box. The locations of the two walls can be identified with two nodal points of $\zeta_k(x)$ (one on the left hand side and the other on the right hand side of a nodal point synonymous with the CM of P1 and P2). We do not locate a wall at the nodal point identified with the CM because this would keep one particle outside the box. Since the symmetry of the relative configuration of the pair demands that its CM, which for *a pure relative motion* of P1 and P2 has $K = 0$, should rest at the midpoint of the box, and P1 and P2, for their relative motions, make the two halves of the box. While one half is exclusively occupied by P1, the other is occupied by P2. This agrees with the excluded volume condition envisaged by Kleban [9] and implies that the q value for a particle in its n-th quantum state can be obtained from

$$q_{\mathrm{n}} = k_{\mathrm{n}}/2 = (\mathrm{n}+1)\pi/d \quad (\mathrm{n} = 0, 1, 2, .. \quad) \tag{16}$$

with $d = L/2$. However, the CM of P1 and P2 need not be at rest in their general motion. Since the CM motion can be identified as a motion of a single body of mass $2m$ constrained to move within the box of size L, the allowed K values in its N-th quantum state would be [10]

$$K_{\mathrm{N}} = (\mathrm{N}+1)\pi/L \quad (\mathrm{N} = 0, 1, 2, .. \quad). \tag{17}$$

Evidently, the net energy, $E(\mathrm{n}, \mathrm{N}) = (\hbar^2/4m)(k_{\mathrm{n}}^2 + K_{\mathrm{N}}^2)$ of the pair should be

$$E(\mathrm{n}, \mathrm{N}) = (h^2/16mL^2)\left[16(\mathrm{n}+1)^2 + (\mathrm{N}+1)^2\right] \tag{18}$$

and its *ground state* (G-state) should be characterised by

$$q_o = \pi/d \qquad \text{and} \qquad K_o = \pi/L, \tag{19}$$

$$E_o = E(0,0) = h^2/8md^2(17/8) = 2.12\varepsilon_o. \tag{20}$$

Here $\varepsilon_o = h^2/8md^2$ is the G-state energy of a particle in a box of size d. It is interesting to note that K-motion contributes a small fraction ($\approx 6\%$) to E_o. The eigenfunction of the general state should be

$$\zeta(\mathrm{n}, \mathrm{N}) = \zeta_{q_{\mathrm{n}}}(x)\zeta_{K_{\mathrm{N}}}(X), \tag{21}$$

with $\zeta_{q_{\mathrm{n}}}(x) = \psi_{q_{\mathrm{n}}}(x)^-$ [or $\phi_{q_{\mathrm{n}}}(x)^+$] and

$$\zeta_{K_{\mathrm{N}}}(X)_{\mathrm{odd-N}} = \sqrt{2/L}\sin(K_{\mathrm{N}}X), \tag{22}$$

$$\zeta_{K_{\mathrm{N}}}(X)_{\mathrm{even-N}} = \sqrt{2/L}\cos(K_{\mathrm{N}}X). \tag{23}$$

While x in $\zeta_{q_{\mathrm{n}}}(x)$ varies from $x = 0$ at the midpoint of the box (defined by $\mathrm{x}_1 = 0$ and $\mathrm{x}_2 = 0$) to $x = L$ when P1 and P2 are at $\mathrm{x}_1 = -L/2$ and $\mathrm{x}_2 = L/2$ (the walls of the box), X in Eqns. 22 and 23 varies from $X = -L/2$ at one wall of the box to $X = L/2$ at the other wall. If P1 and P2 happen to be non-interacting particles, they have no means of identifying the presence of each other. Evidently, the G-state energy ($\varepsilon'_o = h^2/8mL^2$) and momentum ($q'_o = \pi/L$) of such particles satisfy $\varepsilon_o = 4\varepsilon'_o$ and $q_o = 2q'_o$, which proves that ε_o and q_o of each HC particle in the box is much higher than ε'_o and q'_o of a non-interacting particle. Further since neither $\zeta_{q_{\mathrm{n}}}(x)$ nor $\zeta_{K_{\mathrm{N}}}(X)$ in Eqns. 22 and 23 defines an eigenstate of momentum operators (∂_x and ∂_X), $k(=2q)$ and K cannot be fully determined in magnitude and direction by any experiment. If necessary, one may possibly obtain their magnitude from $E_k = \hbar^2k^2/4m$ and $E_K = \hbar^2K^2/4m$, implying that the directions of k as well as K lose meaning in the states defined by Eqn. 21. Evidently, we should avoid viewing k- and K-motions as motions with specific direction.

4.2 G-state configuration

Assuming that P1 and P2 remain confined within λ, as observed for their G-state in the box ($n = 0$, $N = 0$, $q = 2\pi/\lambda$ and $\lambda = L = 2d$), we have

$$< x >^o = < \zeta_k(x)|x|\zeta_k(x) > / < \zeta_k(x)|\zeta_k(x) > = \lambda/2 = d \tag{24}$$

which represents the least possible $< x >$ for two particles of given q. Here x is chosen to vary from its least possible value $x = 0$ to the maximum possible value $x = \lambda = 2d$ in the box. However, if P1 and P2 are allowed to move out of the λ-size region, we have

$$< x > \geq \lambda/2 \quad \text{or} \quad k < x > \geq 2\pi, \tag{25}$$

which clearly shows that $< x >$ can be shortened only by shortening λ (*i.e.* by increasing q). When compared with $\Delta k \Delta x \geq 2\pi$, Eqn. 25 also shows that $< x > \geq \lambda/2$ is essentially a requirement of the uncertainty principle because for the relative configuration of two particles one would surely expect $k \geq \Delta k$ and $< x > \geq \Delta x$. Defining $\phi = kx$ and recasting $\zeta_k(x)$ ($\psi_k(x)^-$ and $\phi_k(x)^+$, Eqn. 14 or 21) as functions of ϕ, we also find that the ϕ-positions of P1 and P2 (confined to remain within λ) are locked at $< \phi > = 2\pi$, or else $< \phi > > 2\pi$. As such, P1 and P2 in their G-state define a close-packed arrangement of their equal size ($\lambda/2 = d$) wave packets. When this inference is used in association with the fact that the directions of $k = 2q$ and K lose meaning, we find that P1 and P2 cease to have collisions in their G-state. However, since the wave packet size decreases with increasing energy, P1 and P2, in their higher energy states, do not retain such a close-packed arrangement, and their dynamics becomes collisional. As such, the dynamics of P1 and P2 moving from their excited state (n $\geq$ 1) to their G-state (n=0) transforms from collisional to collisionless.

4.3 Range of zero-point repulsion

Eqn. 25 implies that two δ-size impenetrable HC particles cannot have a configuration of $< x > < \lambda/2$. To identify the force which prevents this, we examine the G-state energy $E(0) = 2\varepsilon_o = 2h^2/8md^2$ (Eqn. 20) of the relative configuration of P1 and P2. Evidently, P1 and P2 in this state experience a kind of mutual repulsion (or zero-point repulsion)

$$F = -\partial_d E(0) = h^2/2md^3 = 4h^2/mL^3 \tag{26}$$

which tries to increase d by increasing L. In view of Eqns. 24 and 25, this shows that due to the wave packet manifestation of particles, $\delta(x)$-repulsion changes to zero-point repulsion with an effective range of $x = \lambda/2$.

4.4 Impact of zero-point repulsion on the system

To understand this aspect, we perform a thought experiment where the system is kept in contact with a thermal bath whose temperature (T) is slowly reduced to zero. Since the probability for the pair to occupy its n-th quantum state goes proportionally with $\exp[-(E_{\mathrm{n}} - E_o)/k_B T] = \exp[-((\mathrm{n}+1)^2 - 1)2\varepsilon_o/k_B T]$, it can be shown that such probability even for the first excited state (n = 1) of the pair becomes an order of magnitude smaller than that for the ground state (n = 0) at $T \approx T_o$ (the T equivalent of ε_o). Evidently, to a good approximation, the pair at all $T \leq T_o$ stays in its ground state. Naturally, when T is lowered through T_o, the wave packet size of P1 and P2 tends to increase beyond d (the size of the exclusive half occupied by them). This tends to produce some overlap of P1 and P2 at the mid point of the box leading to their mutual repulsion by F (Eqn. 26) which tries to expand the size of the box (L). In all practical situations where forces restoring L are not infinitely strong, we expect non-zero strain (*i.e.*, its expansion by $+\delta L$) in the system at $T \approx T_o$. In other words, the system is expected to exhibit -ve thermal expansion coefficient $-(1/L)\partial_T L$, and the experimental observation of such effect particularly around T_o should conclude the fall of P1 and P2 into their G-state. It may be noted that K-motion energy in the ground state of the pair can also contribute to such expansion of the box; however, such energy ($\approx 0.12\varepsilon_o$) is very small in comparison to that ($\approx 2\varepsilon_o$) of k-motion (*cf.*, Eqn. 20).

4.5 Macro-orbitals

In what follows from the above discussion (Section 4.4), P1 and P2 in their quantum state either experience a repulsion when $< x >< \lambda/2$, or no force when $< x >\geq \lambda/2$, which implies that they have no binding in x-space and retain their independent particle state in spite of their inter-particle phase correlation, $g(\phi) = |\zeta_k(x)|^2$, which can keep them locked at $< \phi >= 2n\pi$ ($n = 1, 2, ..$) in the ϕ-space. Since P1 and P2 moving towards each other with (say) momenta $\mathrm{k}_1 = -q + K/2$ and $\mathrm{k}_2 = q + K/2$, respectively, have $\mathrm{k}_1 = q + K/2$ and $\mathrm{k}_2 = -q + K/2$ after their collision, they can be identified to either have their *self superposition* [*i.e.* the superposition of the plane waves of k_1 and $\mathrm{k}'_1(= \mathrm{k}_2)$ for P1 and of k_2 and $\mathrm{k}'_2(= \mathrm{k}_1)$ for P2] in their respective halves of the box they occupy, or exchange their positions to have their mutual superposition (which again is the superposition of the plane waves of k_1 and k_2). Since one has no means to decide whether particles have their self superposition or mutual superposition, what matters is the net result (*i.e.* the superposition of plane waves of k_1 and k_2) which however is identical for both types of superposition. We therefore assume that P1 and P2 have their self superposition and each of them is an independent entity in a state represented by a $(q, -q)$ pair moving with CM momentum K. In other words, the state of each particle of the pair can be described by a separate pair waveform, say $\xi(x_{(i)}, X_{(i)}) \equiv \zeta(x, X)$. This applies identically to (i) particles described by $\zeta(x, X)$ (Eqn. 14) which represents a general case where q and K can have any value, and (ii) those described by ζ(n,N) (Eqn. 21) pertaining to the specific situation in which $q = q_{\rm n}$ and $K = K_{\rm N}$ are quantized (Eqns. 16 and 17). To distinguish $\xi(x_{(i)}, X_{(i)})$ from $\zeta(x, X)$, we propose to call the former a *macro-orbital* because, as shown in [6], this helps in understanding *macroscopic* quantum effects such as superfluidity. One may also call it a *super-orbital*. We note that a macro-orbital for general usage can be obtained by using $\xi(x_{(i)}, X_{(i)}) \equiv \zeta(x, X)$ and replacing x, X, q and K, respectively, by $x_{(i)}$, $X_{(i)}$, $q_{(i)}$, and $K_{(i)}$ to make reference to the i-th particle. This renders

$$\xi(x_{(i)}, X_{(i)}) = B\zeta_{q_{(i)}}(x_{(i)}) \exp\left[K_{(i)}X_{(i)}\right] \tag{27}$$

where B is a normalization constant, and $\zeta_{q_{(i)}}(x_{(i)})$ is that part of the macro-orbital which does not overlap with a similar part of another macro-orbital. Note that a macro-orbital is a derived form of wave function which can describe a particle in its self superposition state. Since each particle in this state (*cf.* Eqn. 27) has two motions, *viz.*, the q-motion of energy $E(q_{(i)}) = \hbar^2 q_{(i)}^2/2m$ which decides the quantum size $\lambda_{(i)}/2 = \pi/q_{(i)}$ of the particle, and the K-motion of energy $E(K_{(i)}) = \hbar^2 K_{(i)}^2/8m$ which represents a kind of free motion of the particle, $\xi(x_{(i)}, X_{(i)})$ does not fit, as a solution, with the form of the Schrödinger equation expressed by Eqn. 2. However, Eqn. 1 can be rearranged to obtain a suitable form in which $\xi(x_{(i)}, X_{(i)})$ is compatible as a solution. To this effect, we define

$$h_i = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2_{x_i}} \qquad \text{and} \qquad h(i) = \frac{h_i + h_{i+1}}{2} \tag{28}$$

with $i = 1$ or 2 for a system of $N = 2$, $h_{N+1} = h_1$, h_i being the kinetic energy operator of the i-th particle in unpaired format of P1 and P2, and $h(i)$ is the same in their paired format. We have

$$h(i) = -\frac{\hbar^2}{8m}\frac{\partial^2}{\partial^2_{X_{(i)}}} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial^2_{x_{(i)}}} \tag{29}$$

which is such that

$$h(i)\xi(x_{(i)}, X_{(i)}) = [(E(q_{(i)}) + E(K_{(i)}))/2]\xi(x_{(i)}, X_{(i)}). \tag{30}$$

The way we can use N-macro-orbitals to construct an N-body wave function of bosonic or fermionic symmetries has been elegantly shown in [5, 6]. However, for two particles we have

$$\Psi(1,2)^{\pm} = B^2\Pi_{i=1}^2\zeta_{q_{(i)}}(x_{(i)})\sum_P(\pm 1)^P\Pi_{i=1}^2[\exp\left({}_PK_{(i)}X_{(i)}\right)] \tag{31}$$

where P represents the number of permutations of possible $K_{(i)}$ with $(+1)^P$ standing for bosons and $(-1)^P$ for fermions.

4.6 Superposition pushes P1 and P2 towards degeneracy

We note that P1 and P2 (which, as independent particles represented by plane waves before their superposition have unequal momenta k_1 and k_2 and unequal energy E_1 and E_2) have equal share in $E_k = \hbar^2k^2/4m$ and $E_K = \hbar^2K^2/4m$ after their wave mechanical superposition $\zeta(x, X)$ (*cf.* Section 4.5). Further, since $\zeta(x, X)$ is not an eigenfunction of the energy or momentum operator of independent P1 or P2 and E_k and E_K, representing the energy eigenvalues for $|\zeta(x, X) >$ have reference to both particles, it is clear that P1 and P2 find themselves in a state of two particles with equal share in $E = E_k + E_K$. As an important inference, this implies that the wave mechanical superposition of two particles pushes them towards degeneracy.

4.7 Equivalence of $A\delta(x)$ and $V_{HC}(x)$

Following a systematic analysis of a 3-D case of two HC particles of finite size hard core, Huang [11] establishes $V_{HC}(r) \equiv A\delta(r)$. Although, this result is sufficient to identify $V_{HC}(x) \equiv A\delta(x)$, to have a physical understanding of this equivalence we examine the possible configuration of P1 and P2 just at the instant of their collision. We find that while P1 and P2 keep their centers of gravity at $x = \sigma$ (with $x_2 = \sigma/2$ and $x_1 = -\sigma/2$), they register their physical touch at $x = 0$. Their encounter with $V_{HC}(x)$ in this process is a result of this contact at $x = 0$ beyond which two HC particles cannot be pushed. Naturally, in this process, σ has no importance either as the size of P1 and P2 or as a distance between their centers of gravity. The process of collision only identifies that particles are hard spheres, (whether of finite σ or of infinitely small σ) and this means $V_{HC}(x) \equiv A\delta(x)$. Evidently, our results obtained for particles having $A\delta(x)$-repulsion are also valid for particles of finite σ. However, it may be emphasized that this equivalence would not be applicable to situations where particle size assumes importance. For example, two particles of HC size σ cannot be compressed into a box of infinitely small size just because δ-size particles can be so accommodated, $\psi_k(x)^-$ or $\phi_k(x)^+$ would fail to modulate P1 and P2 at $< x >= \lambda/2$ if $\lambda/2 < \sigma$ [or $q > 2\pi/\sigma$] while particles of δ-size would have no such restriction, *etc.*

5 Concluding Remarks

This paper analyses the wave mechanics of a pair of impenetrable HC particles in a 1-D box by using a new scheme. It concludes that: (i) each particle in the box behaves like an independent entity represented by a *macro-orbital*, (ii) while $< V_{HC}(x) >$ vanishes for every state of the pair, $< x >$ satisfies $< x > \geq \lambda/2$ (or $q \geq \pi/d$), (iii) the particles in their ground state define a close-packed arrangement of their wave packets with $< x >= \lambda/2$, $\Delta\phi = 2\pi$ and $|q_o| = \pi/d$, (iv) while the relative dynamics of two particles in their excited states is collisional, the same in the G-state becomes collisionless, (v) the particles in their G-state experience mutual repulsion (*the zero-point force*, Eqn. 26) which also tries to expand the box, and (vi) the system, in certain situations (*cf.* Section 4.4), is expected to have -ve thermal expansion coefficient at $T \approx T_o$.

The paper also provides a sound mathematical basis for *certain results* of basic importance, *e.g.*, (i) $< x > \geq \lambda/2$ (or $q \geq \pi/d$) which implies that from an experimental point of view, two HC particles do not come closer than $\lambda/2$ which agrees with the uncertainty principle and our earlier results [4–6] obtained by using a logical argument following from the manifestation of a particle as a wave packet of size = $\lambda/2$; accordingly, since two HC particles do not share any point in configuration space, their representative wave packets should do likewise and remain at least at a distance $\lambda/2$, and (ii) the representation of a HC particle in a state of its wave mechanical superposition with an identical neighbouring particle by a *macro-orbital* (*cf.* Section 4.5) is a better approximation than a plane wave.

In principle, two particles described by plane waves have their superposition independent of their separation and wave length. However, the experimental fact that the wave nature of particles dominates the behaviour of a many-body system like liquid helium only when their λ compares with d [11,12], defines a condition for their effective wave mechanical superposition. In fact it is evident that a SMW such as $\zeta_k(x)$ assumes stability only when $\lambda/2 = d$. Since the formation of SMWs is an obvious result of the wave nature of particles, our results derived from the analysis of such SMWs are expected to be reasonably accurate. They are also expected to differ from those of [1,2] which use plane waves to represent different particles and do not incorporate the possible consequences (*e.g.*, $< x > \geq \lambda/2$), $\Delta\phi = 2n\pi$, *etc.*) of SMW formation. Broadly speaking, one may find that the spectrum of allowed k_1 and k_2, as per the results of [1,2], includes only integer multiples of $\pm\pi/L$, while as per our results it includes integer and half integer multiples of $\pm\pi/L$. However, a given k_1 (or k_2) from this spectrum pairs with *only select values* of such k_2 (or k_1) to define a set of states of our system. It may be mentioned that we derived the allowed k_1 and k_2 by using Eqns. 7, 16 and 17 just for the clarity of this comparison; otherwise the system, in our framework, does not have independent particle states. Of course, as the particles in their higher energy states ($\lambda << d$) do not have an effective wave mechanical superposition, they could equally well be described by plane waves as used in [1,2]. Evidently, the behaviour of P1 and P2 with increase in their energy changes slowly from that in their SMW states to one described by plane waves as considered in [1,2]. Hence two results are expected to have maximum difference in relation to the G-state. While, the G-state as per our conclusions represents the sum of their zero-point motions [*viz.*, the CM motion of $K = \pm\pi/L$ and relative motion of $k = 4\pi/L$ (*i.e.*, $k_2 = 5\pi/2L$ and $k_1 = -3\pi/2L$) which, however, differs from the G-state of two HC bosons [1,2] of $k_1 = -k_2 = \pi/L$, a comparison of these results with $k_1 = \pm\pi/L$ and $k_2 = \pm\pi/L$ defining the G-state of two non-interacting particles shows that the G-state derived in [1,2], unexpectedly, has no impact from the HC interaction. However, as shown in Section 4.1, our results for HC particles differ significantly from the G-state of non-interacting particles. Evidently, our results (including those of $N > 2$ [13]) supplement those of [1,2] in rendering a complete and correct understanding of 1-D systems.

Finally, we note that our results not only fall in line with our similar study of a simplest system, (*viz.*, single particle in a 1-D box [14]) but also agree with our findings in relation to the G-state of N HC quantum particles in 1-D box [13] and our other studies of larger 3-D systems like liquid helium [5-7]. It is important that our scheme has been used, successfully, to develop an almost exact theory of interacting bosons [6] which explains the properties of liquid ^4He with unmatched accuracy, simplicity and clarity. As outlined in [7], it also has great potential to unify our understanding of widely different many-body systems of interacting bosons and fermions.

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[8] Motions of P1 and P2 (HC size, σ) relative to their CM can be represented by a superposition of a plane wave of momentum q with one of momentum $-q$ (a reflected wave from $V_{HC}(x)$). Correcting such a waveform, $v_k(x) = \sin(qx) = \sin(kx/2)$, for σ size, we get $w'_k(\mathrm{x}_{CM}(1) \geq \sigma/2) = \sin[k(\mathrm{x}_{CM}(1) - \sigma/2)]$ (with $w'_k(\mathrm{x}_{CM}(1) < \sigma/2) = 0$) for P1 and $w''_k(\mathrm{x}_{CM}(2) \leq -\sigma/2) = \sin[k(|\mathrm{x}_{CM}(2)| - \sigma/2)]$) (with $w''_k(\mathrm{x}_{CM}(2) > -\sigma/2) = 0$) for P2. One can express both w' and w'' by a single waveform $w_k(|x| \geq \sigma) = \sin[k(|x| - \sigma)/2]$ with $w_k(|x| < \sigma) = 0$ which in the limit $\sigma \to 0$ becomes $w_k(x) = \sin(k|x|/2) = |\sin(kx/2)| = \phi_k(x)^+$; here we use Eqn. 8 with $x = \mathrm{x}_{CM}(1) - \mathrm{x}_{CM}(2)$. Note that $w_k(|x| < \sigma) = 0$ holds good if the occupancy of space by P1 and P2 is identified with the points occupied by the centres of their HC spheres, but the fact remains that all points (excluding $x = 0$) covered by $|x| < \sigma$ remain occupied by P1 and P2 when these centres are at $|x| = \sigma$.

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