Physical behavior of a system representing a particle trapped in a box having flexible size

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Abstract

A critical study of the wave mechanics of a particle in a 1-D box having infinite potential walls and small flexibility in its size reveals its several important and hitherto unknown aspects which could be relevant for a better understanding of systems like quantum-dot/wire/well. Since most of these aspects arise from the zero point force coming into operation when the particle occupies its ground state in the box, they are expected to have great significance at low temperatures (i.e., $T < T_0$, -the $T$ equivalent of the ground state energy of the trapped particle). To demonstrate this point, we briefly analyze some important aspects of an electron bubble in liquid helium and its nano-droplets which represents a kind of unique quantum-dot. It is argued that our inferences should be equally significant for finding a correct microscopic understanding of the intriguing behavior of several many body quantum systems such as superfluids, superconductors, atomic nucleus, etc..

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1. Introduction

Soon after an important study of the quantum size effect in semiconductor micro-
crystals by Ekimov et.al. [1] reported in 1985, there has been manifold development in
the field of new systems like quantum-dot /wire/well which assumed importance for their
technological applications. While different authors in a recent book [2] elegantly review
different aspects of these systems, Borovitskaya and Shur [3] discuss the basic aspects of
the quantum size effects and their origin and relate the physical properties of these systems
with the wave mechanics of a particle (electron) trapped in a 1-D/2-D/3-D box which is
analyzed in many elementary texts on wave mechanics [4] and used to explain the basics of
the above said systems [3]. However, the set of standard results (SSR), [e.g. Eqns. 1
and 2 (below) expressing the eigen energy, and eigen function for a particle in 1-D box
and similar results for 2-D/3-D systems] available in [3,4] assume certain ideal situations :
(i) the boundary walls of the box are represented by infinite positive potential, and (ii)
the dimension(s) (or structure) of the box is considered to have infinite rigidity. But in
the world of real systems, a trapped particle (say an electron in systems like quantum-
dot /wire/well) encounters boundary walls of finite height and the box structure of finite
rigidity. Naturally, the said SSR are not expected to describe such a system accurately.
Of course, to a good approximation, one may use the SSR to understand the behavior
of a system if the particle energy is considerably lower than the height of the potential
well. However, since a particle trapped in a box exerts a real force (Eqn. 3, below) on
the walls of the box [4(c), p.67] and produces strain in the box size (i.e., finite increase
in the size of the box) and lowers the quantum energies of the trapped particle, SSR lose
their validity even for low a energy particle in a real system which happens to have finite
rigidity. Although, the wave mechanics of a particle trapped in a 1-D box of finite rigidity
has been analyzed in [5] by using WKB approximation, the problem has not been studied
for several important aspects of the system. For example, as concluded here, the strain in
the box size not only lowers the energy eigen values of the particle but also renders several
interesting (but hitherto unknown) properties of the system (cf. Section 4). In addition
the physics of a particle in a 1-D is also important for understanding the properties of
several many body systems, viz. an atomic nucleus [6]. As such we present a critical study
of different aspects of the system by using two model systems of a particle in a 1-D box
in Section 2 and summarize our results in Sections 3 and 4. In near future we also plan
to complete similar study of a particle trapped in 2-D and 3-D boxes. In Section 5 we
briefly analyze important experimental facts about an electron bubble (a kind of unique
quantum-dot) to demonstrate the accuracy of our inferences (drawn in Sections 3 and
4) and their significance for having a better understanding of systems like quantum-dot
/wire/well, helium droplets embedded with a particle (electron, atom or a molecule) and
other many body quantum systems where each constituent particle can be identified with
a particle trapped in a box.

2. Model Systems

A particle of mass \(m\) in a 1-D box of infinite potential walls and size \(d\) is characterized
by its quantum states of energy

\[ E_n = \frac{n^2 \hbar^2}{8md^2}, \]  

(1)
of n-th state (with n = 1,2,3, ... being its quantum number and \( h \) the Planck constant) represented by the eigenfunction

\[
\Psi_n = \sqrt{\frac{2}{d}} \sin \left( p_n x / h \right), \quad \text{for} \quad 0 < x < d, \quad \text{else} \quad \Psi_n = 0,
\]

where \( p_n \) could be identified as the momentum of the particle. Two models S1 and S2 of the system (a particle in a 1-D box of infinite potential walls) used in the present study are, respectively, shown in Fig.1(A) and 1(B). In defining S1 and S2, we identify the following facts:

(i) The size of the box in any real system is expected to increase under the action of the force \([4(c), \text{p.67}]\)

\[
F_n = - \frac{\partial E_n}{\partial d} = \frac{n^2 h^2}{4md^3}
\]

exerted by the trapped particle on the walls of the box. and

(ii) The increase in size \( d \) is, obviously, opposed by a force \( F_\zeta \) (Cf. Eqn 4 below) arising from the inherent elasticity of the structure of the box.

To include (i) and (ii) in S1 and S2, we make an assumption that the left wall of the box is rigidly fixed at \( x = 0 \) while the right wall located at \( x = d \) has some flexibility in its position provided and controlled by a spring whose one end is attached to the right wall and the other end to a rigidly fixed block. Since a change in the box size means a shift in the position of one wall relative to that of the other wall, our assumption remains valid for any 1-D box whose two walls may have equal or unequal flexibility for their positions under the action of a force \( F_n \). When the right wall stays at \( x = d \), the spring has its relaxed state (neither compressed nor extended). After going through the following discussion, one should find that the spring in S1 and S2 merely represents the elasticity of the structure of the box which provides the flexibility in its size.

When \( F_n \) (Eqn.3) pushes the right wall to its right by \( \zeta \) (say), the spring gets compressed by equal amount and this calls for a force \( F_\zeta \) by which the compressed spring opposes \( F_n \) and tries to restore the wall at \( \zeta = 0 \) and we call \( F_\zeta \) as restoring force. Assuming that \( \zeta \) is a small increase in the box size, we define \( F_\zeta \) as

\[
F_\zeta = - k\zeta,
\]

by using Hook’s law of elasticity. While the \(-ve\) sign in Eqn.(4) signifies that \( F_\zeta \) tries to decrease \( \zeta \), \( k \) represents the spring constant (force per unit \( \zeta \)). The origin of \( F_\zeta \) lies with the amount of energy \( U \) stored in the spring as an increase in its internal energy. We have

\[
U = \frac{1}{2} k\zeta^2 = \left[ \frac{1}{2} kl^2 s^2 \right].
\]

where the term in square bracket \([ \quad ]\) uses \( \zeta = sl \) or \( s = \zeta / l \) which represents the strain in the spring with \( l \) being its length in its relaxed state. \( U \) is also known as strain energy of the spring for its \( s \)-dependence (Eqn.5). For a change in the box size from \( d \) to \( d + \zeta \), \( F_n \) (Eqn.3) changes to

\[
F_n(\zeta) = \frac{n^2 h^2}{4m(d + \zeta)^3}
\]
which finds equilibrium with $F_\zeta$ (Eqn. 4) when $\zeta = \delta_n$ (say); this implies that the net force on the wall $(F_n(\zeta) + F_\zeta)|_{\zeta=\delta_n} = 0$ or

$$\frac{n^2\hbar^2}{4m(d + \delta_n)^3} - k\delta_n = 0, \quad \text{or} \quad \delta_n \approx \frac{n^2\hbar^2}{4md^3}k$$

(7)

where we use $d >> \delta_n$ to get $\delta_n$. While for $k = \infty$, we find $\delta_n = 0$ for all $n$ (Case S1, Fig.1(A)) which certifies that the box in S1 has a truly fixed size, for $k \neq \infty$ we get $\delta_n \neq 0$ (Case S2, Fig.1(B)) indicating that the box size changes from $d$ to $d + \delta_n$. This shows that S1 is a special case of S2. To keep the clarity of depiction in Fig.1(B), we opt to show the displaced position of the right wall only for $n = 1$ and use $\delta_1 = \Delta d$ to emphasize that this much increase in box size $d$ is specifically consequential for four important intrinsic aspects of our system (see Sections 4.1-4.4).

Since a box, whose size assumes no change under the action of $F_n$, is not expected to exist in nature, S1 can better be identified as an ideal system, while S2 can provide a better description to a real system. The physical behavior of such a system is, therefore, expected to have a better agreement with our results (cf. Sections 3 and 4). However, the following analysis implicitly presumes that the energy of the particle due to flexibility of the box does not change significantly from $E_n$ (Eqn.1) and this holds to a good approximation only for large $k$ [5] which renders $\delta_n << d$.

3. Common Aspects of S1 and S2

In a recent study [7] of the wave mechanics of two $\delta$-size hard core particles in a 1-D box (also shown to be valid for the hard core particles of finite size), we discovered that: (i) each particle in a quantum state of the system assumes its self-superposition and an effective size of $\lambda/2 = \pi/q$ (with $q$ being the magnitude of momentum wave vector of two particles having equal and opposite momenta $p$ and $-p$ where $p = \hbar q$), (ii) the range of their hard core mutual repulsion increases from the characteristic 0 value (in classical description) to $\lambda/2$ (in quantum description), and (iii) the relative motion of two particles in their excited states represents collisional motion, while the same in their ground state is found to be collision-less. Since these inferences have an important role in finding the intrinsic properties of our system (cf. Section 4), we rediscover them (Sections 3.2-3.5) from a similar analysis of the present system with a view to: (i) affirm their relevance to its intrinsic behavior as concluded in Section 4, (ii) provide these inferences a stronger foundation, and (iii) have a better understanding of the structure of the ground state of an electron bubble and the process of its formation (cf. Section 5). In Section 3.1, we also discuss the signature of wave particle duality on the description of $F_n$ (Eqn.3) because it helps in understanding what we conclude in Sections 3.2-3.5.

3.1 Force $F_n$ and wave-particle duality

The fact, that none of the quantity in $F_n = -\partial_d E_n$ (Eqn.3) and $E_n$ (Eqn.1) depends (explicitly or implicitly) on time, indicates that $F_n$ should be an all time persisting constant force that the particle exerts on both the walls of the box. However, we also find the same expression

$$F_n = \frac{2p_n}{\tau_n} = 2p_n \frac{v_n}{2d} = \frac{n^2\hbar^2}{4md^3},$$

(8)
using a classical model of the particle bouncing back and forth which explicitly means that the particle (in its n-th quantum state), moving with a velocity \( v_n = p_n/m \), has periodic collision on each wall at time interval \( \tau_n = 2d/v_n \) and transfers \( 2p_n \) momentum to the wall of the box at its each collision. This indicates that \( F_n \) is a time average of the force(s) exerted by the particle on a wall with a periodicity of \( \tau_n \). Alternatively, \( F_n \) is an instantaneous force exerted by the particle during its collision and it has an identity with the force that a gas molecule (as a classical entity) exerts on a wall of its container and contributes to the gas pressure which tends to inflate the size of the container. This means that \( F_n \) has two different descriptions: (i) a time average of forces (as implied by Eqn.8) which agrees with particle nature, and (ii) an all time persisting constant force (as evident from the derivation of Eqn.3) which agrees with the wave nature of particle; it may be underlined that only due to this nature, a particle in the box assumes discrete quantum states described by \( \Psi_n \) (Eqn. 2) and \( |\Psi_n|^2 \) (representing the probability of finding the particle at a point \( x \)) has time independent non-zero values at infinitely many different points in the box \( 0 \leq x \leq d \). We note that the said difference of two descriptions of \( F_n \) can be easily resolved by using wave-particle duality, -the particle moves like a wave and leaves its impact like a particle which means that our analysis, for the first time, demonstrates how a physical quantity like \( F_n \) has two different descriptions due to wave-particle duality.

3.2 Self-superposition of the particle

Following the principle of superposition of waves [8], \( \Psi_n \) (Eqn.2) represents the superposition of two plain waves, viz., \( u_n = A \exp (ip_nx/\hbar) \) and \( w_n = A \exp (-ip_nx/\hbar) \) (with \( A \) being the normalization constant) of momenta \( p_n \) and \( -p_n \). We call this superposition as self-superposition of the particle because both these waves \((u_n \text{ and } w_n)\) represent one and the same particle. As discussed in [7], particles also have their self-superposition in the quantum states of two hard core particles in 1-D box. However, to add further clarity to this meaning, we may mention that the self-superposition of a particle, as defined here and in [7], does not differ significantly from the self-interference of a particle as defined in [9] because in both cases we have the superposition of two plane waves of one and the same particle but the two phenomena do differ in their physical situations. In the former case \( u_n \) and \( w_n \) travel in opposite direction and render standing wave like \( \Psi_n \) (Eqn.2), while in the latter case they reach the point of their superposition in nearly the same direction.

3.3 Effective size of the particle:

Our experience with classical objects tells us that the size of a material particle (say \( b \)) means the size of the real space it exclusively occupies. Evidently the particle of our system has \( b = 0 \) since it is implicitly assumed to be a point particle. In wave mechanics, however, a particle is believed to manifest itself as a wave packet [4] of size \( \approx \lambda/2 \) which implies that its \( b(\approx \lambda/2) \) has non-zero value that depends on its energy/momentum. Guided by this observation, we analyze \( E_n \) (Eqn.1) and its relation with box size to find useful information that improves our understanding of the particle size in quantum description.
Recasting Eqn.(1), we have

\[ E_n = \frac{\hbar^2}{8m(d/n)^2} = \frac{s^2\hbar^2}{8m(sd/n)^2}, \]

which leads us to infer the following:

I(1): The particle has \( E_n \) energy also when it occupies \( s \)-th quantum state in the box of size \( sd/n \) (where the integer \( s < n \)) indicating that the smallest size of the box in which the particle can have \( E_n \) energy is \( d/n \).

I(2): Since \( E_n \) is equal to the ground state energy of the particle for a box of size \( d/n \), it needs to have a higher value, if the box size is reduced below \( d/n \). This implies that the said particle can not be placed in a box of size smaller than \( d/n \) if its energy \( < E_n \); in other words, the particle with \( E_n \) energy exclusively occupies a space of size \( b = d/n = \lambda_n/2 \).

Generalizing I(2) we may conclude that a point particle (with energy \( E \) or momentum \( p \)) in its self-superposition state (such as \( \Psi_n \)) behaves like a wave packet of an effective size \( \lambda/2 \) which depends on \( E \) and \( p \) through \( \lambda/2 = \hbar/2p = \hbar/2\sqrt{2mE} \). This inference not only shows its variance with classical picture where particle size is believed to be independent of its \( E \) or \( p \) but also renders \( b = \lambda/2 \) which differs from \( b \approx \lambda/2 \) (concluded from the definition of wave packet) for its precise magnitude. In addition it agrees with an identical inference of our recent study on the wave mechanics of two hard core particles in 1-D box [7].

3.4 Effective Range of Repulsion

The particle in our system experiences a potential \( V(x) \) defined by \( V(0 < x < d) = 0 \), and \( V(x) = \infty \) at all other points; in other words it interacts with the walls through infinitely strong repulsion only when it presumably occupies \( x = 0 \) or \( x = d \) position of the infinite potential wall. One uses this understanding to determine the dynamics of the particle in classical (see Ref.[8]) as well as in quantum frameworks [4]. However, in variance with the fact that a classical particle in a 1-D square box has only kinetic energy, the \( d \) dependence of the allowed energy values of a quantum particle \( (E_n) \) indicates that it can be identified as a potential energy from which we derive the force \( F_n \) (Eqn.3). In order to examine the nature and range of this force we note that the particle can also have same \( E_n \) when the separation between the two walls of the box has any of the \( n-1 \) possible values \( (sd/n \) with integer \( s < n \)) which is valid for any \( n \) (including infinitely large value). This indicates that the particle in its \( n \)-th state does not experience an effective force which supports or opposes a change in the box size in units of \( d/n \) which has infinitely small value for infinitely large \( n \).

However, when we try to reduce the box size below \( d/n = \lambda_n/2 \) \( (i.e. \) when the particle is in its ground state with energy \( E_n) \), we need to increase particle energy above \( E_n \) since the ground state energy of the particle in a box of size \( < \lambda_n/2 \) is, obviously, expected to be higher than \( E_n \). This concludes that the particle opposes any reduction in the box size below \( \lambda_n/2 \) implying that the particle in its ground state experiences a real force which pushes it away from the infinite potential walls toward \( < x > = d_n/2 = \lambda_n/4 \) or the
particle pushes the two walls away from its expected position \(<x> = d_n/2\). Generalizing this inference and using the fact that \(<x>\) in the ground state satisfies \(<x> = \lambda/4\), it may be concluded that an infinite potential wall experiences the pushing action of \(F\) (or the particle experiences a repulsion from the wall) when the distance between the particle and the wall is \(\leq \lambda/4\); the potential energy that serves as the origin of \(F\) is nothing but the ground state energy of a particle \((\varepsilon_0, \text{Eqn.1})\) which varies as \(d^{-2}\). Evidently, While \(F_1\) always satisfies the condition for its persistent pushing action on the two walls of the box, \(F_{n\geq2}\) satisfies the condition for its periodic action (as experienced during periodic collision of particle). Alternatively, the particle experiences persisting impact of its interaction \((V(x = 0/d) = \infty)\) with the two walls when it rests in its ground state but in the higher energy states it experiences such an impact with a periodicity of \(\tau_n\) when its distance from a wall is \(\leq \lambda/4\).

In summary the range of the impact of the infinite potential walls felt by the particle is changed from its zero value (in classical description) to \(\lambda/4\) (in quantum description) due to wave particle duality. This agrees with a similar inference of our recent study [7] which concludes that two particles, interacting though an infinitely strong \(\delta-\)potential, have \(<x> \geq \lambda/2\) where \(x\) represents the relative position of one particle with respect to that of the other.

3.5 Collisional and collision-less motion

A classical particle (when made to move) has collisions with walls of the box if its size \(b < d\) but such collisions cease to exist if \(b = d\). Guided by this observation, we use the well known inference of wave mechanics that a particle manifests itself as a wave packet of size \(\approx \lambda/2\) (or to be more precise \(\lambda/2\) in the present case, cf., Section 3.3), we conclude that the particle has: (i) periodic collisions (time period \(\tau_n\)) with the walls of the box when it occupies higher energy states \(\Psi_{n\geq2}\) and (ii) no collisions in \(\Psi_1\) because the size of its representative wave packet satisfies \(\lambda_{n>1}/2 = d/n \ll d\) and \(\lambda_1/2 = d\), respectively. In other words, the particle motion (evident from non-zero value of all \(E_n\) representing the expectation values of the kinetic energy operator of the particle) in \(\Psi_{n>1}\) states could be identified as collisional motion, while that in \(\Psi_1\) as collisionless. To add clarity to the origin of this difference, we note that while \(\Psi_{n>1}\) having \(n \geq 2\) anti-nodal loops provide more than one point \((x = (2s + 1)\lambda_n/4\) with \(s = 0, 1, 2, 3, n-1\) where the probability \(|\Psi_{n>1}|^2\) has maximum and identically equal value \((2/d)\) and, as a result of this, the particle has a chance to move from one such point to another, but the chances of its similar movement do not exist in \(n=1\) state because \(\Psi_1\) has only one anti-nodal loop. The inference is also corroborated by the observation of identical difference identified in relation to the forces, \(F_1\) and \(F_{n>1}\), exerted by the particle on the walls of the box (\(F_1\) acting as an all time persisting force, while \(F_{n>1}\) acting periodically with a period of \(\tau_n\), cf., Section 3.4).

4. Important Aspects Related to S2

In this section we try to examine four important aspects of the system arising due to the possibility of a change in the box size. While three of these (cf., Sections 4.1, 4.3 and 4.4) are expected from the quantum description (not from classical description) of the
particle in the box, the fourth related to thermal expansion of the box (cf., Section 4.2), can be expected from classical description but not in the way we find from the quantum description.

4.1 Deviation of Particle energy from $E_n$

When the right wall tends to shift from $x = d$ to $x = d + \zeta$ under the action of $F_n(\zeta)$ against $F_c$, our system to a good approximation represents a particle trapped in a 1-D box of impenetrable walls. In the equilibrium state of these forces, the box size becomes $d + \delta_n$, since $\zeta = \delta_n$ and corresponding energy eigenvalues, $E_{S2,n}$, can be obtained by replacing $d$ in Eqn.2 with $d + \delta_n$ by using the procedure followed by Gea-Banacloche for obtaining his Eqns. 6 and 7 in [10] for the energies of a particle in a box whose size is approximately halved. To a good approximation this renders

$$E_{S2,n} = \frac{n^2h^2}{8md^2(1 + \delta_n/d)^2}.$$  \hfill (10)

We note that $E_{S2,n} < E_{S1,n}$ ($= E_n$, Eqn 1), -valid for the ideal case (S1) where the box has infinitely rigid size [4]. Subscripts S2 and S1 indicate that the particle energy is related to S2 and S1 systems, respectively. The fall in energy $\Delta E_n^{(I)} = E_{S2,n} - E_{S1,n}$ can be obtained, to a first order approximation (indicated by the superscript $(I)$), by using $(1 + \delta_n/d)^{-2} \approx 1 - 2\delta_n/d$ in Eqn.10. We have

$$\Delta E_n^{(I)} = -\frac{4n^4E_1^2}{kd^2}.$$  \hfill (11)

The fact that it vanishes for $k = \infty$ shows its consistency with our inference that S1 is identical to the system studied in [4]. We note that similar deviations from the predictions of ideal models are also seen in several other cases. For example, the energy of a rotational level of a molecule has lower value than that predicted by ideal rigid rotator model [11] because the centrifugal force increasing with increasing rotational velocity (i.e. rotational quantum number) increases the molecular dimensions and moments of inertia which lower the energy of rotational levels.

4.2 Strain and Thermal Expansion of the Box

In this section we analyze the results of our thought experiment in which we monitor the temperature ($T$) dependence of the increase in the box size (forced by $F_n$, Eqn.3) when our system is kept in contact of a thermal bath whose $T$ is slowly reduced to zero. The main objective of this analysis is to demonstrate how the said increase in box size and related thermal expansion coefficient [$\alpha = (1/d')\partial_T d'$] depends on $T$ and at what $T$ the quantum effects dominates the thermal behavior of our system.

Since $F_n$ depends on the quantum state occupied by the particle which occupies different quantum states at a given $T$ with a probability [12] $W_n \propto \exp(-E_n/k_B T)$ ($k_B$ being the Boltzmann constant), the experimental value of the said increase in the box size should be statistical average of $\delta_n$ (Eqn.7). Following standard relation for obtaining such an average, it can be expressed as
\[\delta(t)_{QP} = \frac{\hbar^2}{4md^3k} \sum_{n=1}^{\infty} n^2 W_n \]  
where \( W_n \) representing Maxwell-Boltzmann distribution [13] is given by

\[ W_n = Ae^{-E_n/k_BT} = Ae^{-n^2\varepsilon_o/k_BT} = Ae^{-n^2T_o/T} = Ae^{-n^2/t}. \]

with \( A = [\sum_{n=1}^{\infty} \exp (-E_n/k_BT)]^{-1} \), (ii) \( t = T/T_o \) which represents the temperature of the bath in units of \( T_o(=\varepsilon_o/k_BT) \) (the \( T \) equivalent of zero point energy \( \varepsilon_o \)) and (iii) subscript \( QP \) to emphasize that the particle in the box is a quantum particle having discrete \( E_n \) (Eqn.1) and to distinguish it from

\[ \bar{\delta}(t)_{CP} = \frac{2}{kd} \int_0^\infty EW(E)dE = \frac{2\varepsilon_o}{kd} \int_0^\infty E' e^{-E'/t}dE' \quad \text{with} \quad E' = \frac{E}{\varepsilon_o}, \]

which represents similar quantity for the box containing a classical particle. Eqn.14 uses the fact that the force exerted by a classical particle on a wall of 1-D box is \( F = 2p/\tau = 2E/(d+\zeta) \) (with \( \tau \) being the time of a round trip of the box of size \( d+\zeta \)) which finds its equilibrium with the force of spring \((=k\zeta)\) at \( \zeta = \delta \approx 2E/kd. \)

The values of \( \delta(t)_{QP} \) (Eqn.12) and \( \bar{\delta}(t)_{CP} \) (Eqn.14) calculated in units of \( \delta_1 = \Delta d = \hbar^2/4md^3k \) are, respectively, depicted in Fig.2 by Curves A1 and B1 with corresponding \( \alpha(t) \) depicted by A2 and B2. While \( \bar{\delta}(t)_{CP} \) (Curve B1), having linear dependence on \( t \) reaches its zero value at \( t = 0 \), \( \delta(t)_{QP} \) (Curve A1), having similar dependence for \( t > 1 \), deviates smoothly at \( t \approx 1 \) to have unit value at \( t = 0 \). Consequently, \( \alpha(t) \) in the former case remains constant for all values of \( t \) (Curve B2), while in the latter case it deviates around \( t \approx 1 \) from its constant value at all \( t > 1 \) to assume zero value at \( t = 0 \) (Curve A2). This shows that the signatures of the quantum and classical nature of the particle on the thermal behavior of the system differ significantly at low \( T(<T_o) \) at which the particle has very high probability [as indicated by \( W_1 \approx 95\% \) (at \( T = T_o \)) to 100\% (at \( T = 0 \)) obtained by using Eq.13 for \( n=1 \)] to occupy its ground state which is characterized by \( \lambda/2 = d' \approx d \).

It appears that helium atoms in liquid helium also assume a physical state which can be identified with a particle trapped in a spherical cavity formed by neighboring atoms when the temperature of the liquid during the process of its cooling tends to cross \( T_o \) at which number of particles in their excited states \((n>1)\) are negligibly small. Obviously, under such situations, the \( F_i \) is the only force that tries to expand the cavity. To understand the \( T \)-dependence of the strain under these situations with our system, we calculate

\[ \bar{\delta}_1(t)_{QP} = \frac{\hbar^2}{4md^3k} \frac{W_1}{\sum_{n=1}^{\infty} W_n} = \frac{\hbar^2}{4md^3k} \sum_{n=1}^{\infty} e^{-1/t} \]

in units of \( \delta_1 = \Delta d = \hbar^2/4md^3k \) and plot it in Fig.3 (Curve A) along with the corresponding \( \alpha(t) \) (Curve B). We note that: (i) \( \bar{\delta}_1(t)_{QP} \) increases smoothly with decreasing \( t \) and reaches its maximum value \( \Delta d \) at \( t = 0 \) where the particle rests in its ground state with 100\% probability; in fact as depicted by Curve A, \( \bar{\delta}_1(t)_{QP} \) assumes \( \Delta d \) value closely
around $t = 1$, and (ii) the corresponding $\alpha(t)$ has $-ve$ values with a peak around $t \approx 1$ (Curve B).

We note that this simple exercise beautifully demonstrates that: (i) the $t-$dependence of $\delta_1(t)$ and corresponding $\alpha(t)$ (Fig. 3) represent unique signature of wave particle duality on the thermal expansion of our system when $F_1$ is the only operational force, and (ii) $-ve$ values of $\alpha(t)$ peaking around $t \approx 1$ (when observed experimentally) should prove that the constituent particle(s) of a system represent a particle trapped in a box and the particle in its ground state has collision-less motion. As observed from Fig. 2, the results depicted in Fig.3 also reveal that the thermal behavior of the system is greatly influenced by the quantum nature of the particle when its $T \approx T_o$ or $\lambda/2 \approx d$. Interestingly, as discussed in Section 5, these conclusions are found to be consistent with the observed $-ve$ thermal expansion of liquids $^4He$ and $^3He$ [15].

4.3 Bound state of the particle and the strained box

In order to conclude that the particle and the strained box form an energetically bound system when the particle occupies the ground state, we follow a standard method which can establish whether two atoms interacting through certain inter-atomic potential can form a diatomic molecule (i.e. a bound state of two atoms) [16] or not. We start with the total energy of our system where the particle rests in its ground state in the strained box and we consider that: (i) the particle and (ii) strained box (strained spring) represent its two constituents like two atoms in a diatomic molecule. Indicating the ground state by subscript ‘1’, we have

$$E_{S2,1}(\zeta) = \frac{\hbar^2}{2md} + \frac{1}{2}k\zeta^2$$

(16)

where we use Eqn.(1) for the particle energy in the strained box of size $d' = d + \zeta$. We now determine $\zeta = \Delta d$ (say) for which $E_{S2,1}(\zeta)$ has a minimum/ maximum by setting

$$\frac{\partial E_{S2,1}(\zeta)}{\partial \zeta} |_{\zeta=\Delta d} = -\frac{\hbar^2}{4md^3} + k\Delta d = 0$$

(17)

This renders

$$k\Delta d = \frac{2\varepsilon_o}{d} \left[ 1 + \frac{\Delta d}{d} \right]^{-3},$$

(18)

and $E_{S2,1} = \varepsilon'_o + \varepsilon_s$ with $\varepsilon'_o = \hbar^2/8md^2$ being the ground state energy of the particle in the strained box, $\varepsilon_s = (1/2)k\Delta d^2$ being the strain energy of the box, and $d' = d + \Delta d$. We now determine

$$\frac{\partial^2 E_{S2,1}(\zeta)}{\partial \zeta^2} |_{\zeta=\Delta d} = \frac{3\hbar^2}{4md^4} + k$$

(19)

whose $+ve$ value establishes that $E_{S2,1}(\zeta)$ has a minimum at $\zeta = \Delta d$ with a depth which can be found from : (i)

$$\varepsilon'_o = \varepsilon_o \left[ 1 - 2\frac{\Delta d}{d} + 3 \left( \frac{\Delta d}{d} \right)^2 - 4 \left( \frac{\Delta d}{d} \right)^3 \right]$$

(20)
which represents the binomial expansion of $\varepsilon'_o = (h^2/8md^2)(1 + \Delta d/d)^{-2}$, and (ii)

$$\varepsilon_n = \frac{1}{2}k(\Delta d)^2 = \varepsilon_o \left[ \frac{\Delta d}{d} - 3 \left( \frac{\Delta d}{d} \right)^2 + 6 \left( \frac{\Delta d}{d} \right)^3 - \ldots \right]$$  \hspace{1cm} (21)

which is obtained by multiplying $\Delta d/2$ with the binomial expansion of Eqn.(18). We find the said depth ($\Delta E_{s2,1}$) of minimum in $E_1(\zeta)$ at $\zeta = \Delta d$ by using Eqns.20 and 21 in 16. We have $\Delta E_{s2,1} = [E_{s2,1}(\zeta = \Delta d) - E_{s2,1}(\zeta = 0)]$ expressed in detail as

$$\Delta E_{s2,1} = \frac{h^2}{8md^2} + \frac{1}{2}k\Delta d^2 - \frac{h^2}{8md^2} \approx \varepsilon'_o + \frac{1}{2}k\Delta d^2 - \varepsilon_o = -\varepsilon_o \Delta d/d$$  \hspace{1cm} (22)

Here we assume that the terms having $\Delta d/d$ with powers more than 2 in Eqns.20 and 21 are negligibly small. The fact that $\zeta$ is a common factor in: (i) $h^2/8m(d + \zeta)^2$ representing the energy of the trapped particle (the kinetic energy of particle affected by the presence of infinite potential walls leading to $d$ dependence) and (ii) $(1/2)k\zeta^2$ representing the strain energy of the box/spring, clearly shows that the trapped particle and the strained box/spring are energetically inter-dependent. Further since $E(\zeta)$ has a minimum with a depth $\Delta E_{s2,1} = -\varepsilon_o \Delta d/d$, the two form a physically bound state like two atoms in a diatomic molecule [16]. They remain in this state unless $\Delta E_{s2,1}$ energy is supplied from outside. Although, one may similarly find a minimum in $E_{s2,n}(\zeta)$ at $\zeta = \delta_n$, and corresponding depth $\Delta E_{s2,n} = -n^2E_{S1,n}\delta_n/d$ for any state $\Psi_{n>1}$, but the particle and the strained box/spring would not have their stable bound state for $n > 1$ because the particle in $\Psi_{n>1}$ states is free to jump to a lower energy state by releasing out the difference in their energies which implies that the particle in a $\Psi_{n>1}$ always has an excess energy to overcome corresponding binding energy $-\Delta E_{s2,n}$. However, the particle in $\Psi_1$ does not have this option and it assumes a stable bound state with the strained box/spring.

4.4 Oscillations and Energy exchange

Since, as discussed in Section 4.3, the energies of two constituents [(1) trapped particle and (2) the strained box/spring] of our system depend on a common factor $\zeta$ and they have their mutually bound state for $\zeta = \Delta d$ at which the total sum of their energies has minimum value, one expects this system to oscillate around $\zeta = \Delta d$ if it is disturbed to have different $\zeta$ for a moment. To study these oscillations, we start our analysis by evaluating $E_{s2,1}(\zeta)$ (Eqn.16) for $\zeta = \Delta d$ (the point of equilibrium, Eqn.17). We have

$$E_{s2,1} = \frac{h^2}{8md^2} + \frac{1}{2}k\Delta d^2$$  \hspace{1cm} (23)

Assuming that the said equilibrium is disturbed by changing $d'$ to $d' \pm \eta$ (with $|\eta| < \Delta d$) (Fig 1B), we write the corresponding energy as $E_{s2,1}(\eta)$ to have

$$E_{s2,1}(\eta) = \frac{h^2}{8m(d' \pm \eta)^2} + \frac{1}{2}k(\Delta d \pm \eta)^2$$  \hspace{1cm} (24)

Using

$$\frac{h^2}{8md^2} \left[ 1 \pm \frac{\eta}{d} \right]^{-2} = \frac{h^2}{8md^2} \left[ 1 \mp 2\left( \frac{\eta}{d} \right) + 3\left( \frac{\eta}{d} \right)^2 - \ldots \right]$$  \hspace{1cm} (25)
in Eqn.24 after dropping all terms containing \( \eta/d \) with powers more than two, we find

\[
E_{S2,1}(\eta) \approx \varepsilon'_o + \varepsilon_s + \left[ \frac{2\varepsilon'_o}{d'} - k\Delta d \right] \eta + \frac{1}{2}k'\eta^2
\]  

(26)

where we use \( \varepsilon_s = \frac{1}{2}k\Delta d^2 \) (Eqn.21) and modified force constant

\[
k' = k + \frac{6\varepsilon'_o}{d^2}
\]  

(27)

Since the sum \( \varepsilon'_o + \varepsilon_s \) (Eqn.27) is independent of \( \eta \) and the condition for equilibrium (Eqn.17) renders

\[
\left[ \frac{2\varepsilon'_o}{d'} - k\Delta d \right] \eta = 0
\]  

(28)

we are left with only one \( \eta \)-dependent term (i.e., \( k'\eta^2/2 \)) in Eqn.(26). This concludes that the box (occupied with a particle in its ground state) can sustain harmonic oscillations in its size and such oscillations are governed by an increased value of spring constant \( k' \) (Eqn.27). Further since \( \mp(2\varepsilon'_o\eta/d') \) (Eqn.26) represents a linear change (in terms of \( \eta \)) in \( \varepsilon'_o \) and \( \pm k\Delta d\eta \) (Eqn. 26) is a similar change in \( \varepsilon_s = k\Delta d^2/2 \) and these changes are equal and opposite (Eqn. 28), it is obvious that the particle in \( \Psi_1 \) state and strained box/spring keep exchanging energy with each other during \( \eta \)-oscillations.

5. Results and Discussion

Our results expected to be of great significance to understand the quantum behavior of widely different physical systems whose constituent particles can be identified with a particle trapped in a box. For example, their application to an electron in a quantum-well (a thin film of certain semiconductor sandwiched between two slabs of other suitable semiconducting material and a good representative of a particle (electron) trapped in a 1-D box) can help in having a complete and better understanding of its behavior. However, to testify our inferences (Sections 3 and 4), we prefer to compare them with relevant aspects of an electron bubble [17,18] comprising only single electron, although it represents a quantum particle trapped in a 3-D spherical cavity. The extent to which our inferences agree with relevant aspects of a quantum-dot /wire/well would be discussed in our forth-coming paper since a large number of electrons in such a system constitute a gas of trapped particles which, obviously, have their collective impact on its behavior, -not expected to have a simple correlation with our inferences (Sections 3 and 4) for a single trapped particle.

An electron bubble is an electron trapped in a self created cavity in helium liquid [17] or its nano-droplets where it is also identified as a unique quantum-dot [18]. Under the condition of zero external pressure, it is energetically described [19] by

\[
E(R) = \frac{A}{R^2} + BR^2 = \frac{A}{(R_1 \pm \zeta)^2} + B(R_1 \pm \zeta)^2
\]  

(29)

where \( R_1 \) represents the radius of the bubble for the electron in its ground state identified by subscript '1'), \( A = \hbar^2/8m_e \) (with \( m_e \) = mass of electron), and \( B = 4\pi\sigma \) (with \( \sigma = \)...
surface tension of the liquid). While the first term on the right hand side of Eqn.29 is electron energy for its confinement in the spherical cavity of radius \( R = R_1 \pm \zeta \), the second term stands for the surface energy of the bubble. The process of its formation with a high energy electron entering into liquid helium (or its nano-droplet) and losing its excess energy (above its ground state energy) through collisions with surrounding He atoms [17-19], indicates that the bubble maintains a spherical shape [17] from its incipient state having \( R_i \approx 3.5 \) Å to final state of \( R = R_1 \approx 17\) Å. Since the lowest possible energy \( E = E_> \) of a particle trapped in a spherical cavity is related to cavity radius \( R \) through

\[
R = \frac{\lambda}{2} \quad \text{with} \quad \lambda = \frac{h}{\sqrt{2mE_>}} \quad (30)
\]
a decrease in \( E_> \) is possible only when \( R \) can have corresponding increase. A system like liquid helium provides this possibility since a cavity in a liquid is expected to have flexible size because its constituent atoms do not have rigidly fixed positions and the electron, in accordance with Eqn.(29), exerts a force \( F(R) = 2AR^{-3} \) on the walls of the cavity and tries to expand its size against the force \( F_R = -2BR \) arising from the surface energy. In the state of equilibrium, we have

\[
F(R) + F_R|_{R=R_1} = 0 \quad \text{or} \quad R_1 = \left( \frac{A}{B} \right)^{1/4} = \left( \frac{h^2}{32\pi m_e \sigma} \right)^{1/4}. \quad (31)
\]

This shows that the expansion of the bubble from its incipient state \( (R = R_i \text{ and } E_> = E_i) \) to final state \( (R = R_1 \text{ and } E_> = E_1) \) is an act of \( F(R) \) which assumes equilibrium with \( F_R \) when \( R = R_1 \) and the electron, at every stage of this transformation, stays in a state that can be identified as the ground state of a particle trapped in a spherical cavity of radius \( R \) with least possible energy \( E_> \) (cf. Eqn.30) which decreases with increase in \( R \) unless \( R = R_1 \). Since the electron occupies the bubble exclusively its effective size (by definition of the size of a particle) can be identified with the size of the bubble which means that the electron in a 3-D cavity behaves effectively like a spherical body of size (diameter) \( \lambda \) which depends on \( E_> \) as a result of wave particle duality. However, on the quantitative scale, this size differs by a factor of two from: (1) the effective size \( (\lambda/2) \) inferred for a particle trapped in 1-D cavity (cf. Section 3.3) as well as (2) the size \( (\approx \lambda/2) \) of the representative wave packet of a quantum particle. While it should be interesting to discover the reasons for such a difference with wave packet size (2), particularly when (1) matches closely with (2), but this point would be examined at a later date.

Use of Eqn.(31) in Eqn.(29) to analyze the state of equilibrium (i.e. \( R = R_1 \) or \( \zeta = 0 \)), renders

\[
E(R_1) = 2\sqrt{AB} = \sqrt{\frac{\pi h^2 \sigma}{2m_e}}. \quad (32)
\]

which implies that a decrease in \( \sigma \) decreases \( E(R_1) \), while as evident from Eqn.(31), it increases \( R_1 \) and this agrees with the fact that a particle (trapped in a spherical cavity) in its ground state satisfies Eqn.(30). Interestingly, an analysis of Eqn.(29) for the excited states, for which \( A \) needs to be replaced by \( A^* = \beta_{n,l}^2 A \) (with \( n \) and \( l \), respectively, representing the principal quantum number of the state and angular momentum of the
particle, and $\beta_{n,l} > 1$ [20]), reveals that corresponding $R^*$ should increase with increasing $\beta_{n,l}$ indicating that $R^* > R_1$. Further the fact, that excited state energy $E^* > E_1$ and corresponding $\lambda^*/2 < \lambda_1/2$, implies that the effective size ($\lambda^*$) of the electron in an excited state would be shorter than the bubble size $2R_1$ and the electron in such a state can be visualized to have collisions with the walls of the bubble cavity even if an instantaneous excitation of the electron to such a state does not change the $R_1$ to $R^*$. However, such collisions would not be there in the ground state in which effective size of the electron $\lambda$ fits exactly with the bubble size $2R_1$. We also note that the electron in its ground state sits at a distance $R = \lambda/2$ from the walls of the cavity which implies that the range of repulsion (experienced by the electron with $He$ atoms constituting the walls of the cavity) gets increased to $\lambda/2$.

Evidently what follows from the above discussion, the electron bubble provides a clear experimental proof for the accuracy of our inferences pertaining to: (i) the force that a trapped particle exerts on the walls of the cavity/box (cf. Section 3.1), (ii) the self superposition state of a trapped particle (cf. Section 3.2), (iii) energy dependent effective size of a quantum particle (cf. Section 3.3), (ii) the increase in the effective range of repulsion between trapped particle and the boundary walls of the cavity (cf. Section 3.4), and (iv) the collisional motion of the particle in its excited state and collisionless motion (representing the motion corresponding to the zero point energy) in its ground state (cf. Section 3.5).

Eqn.(29) not only represents a situation that can be identified with S2 (where structure of the box/cavity has finite rigidity, cf. Section 2) but also matches closely with Eqn.16/24 which evidently means that the electron bubble has all properties that we concluded in Section 4. For example: (i) the structure of the cavity (an arrangement of mutually bound $He$ atoms that constitute the inner layer of the cavity) assumes a strain which can be perceived with expanded state of $He$-$He$ bonds in the said structure, (ii) the bubble represents a kind of bound state of the trapped electron and the spherical cavity it creates in helium liquid or its nano-droplets; this is evident from the fact that the electron can be separated from the bubble only by increasing its energy [18]), (iii) the bubble can sustain oscillations (to a good approximation having simple harmonic nature) in its size/radius around $R_1$ and (iv) the electron energy for its confinement increases (decreases) with equal loss (gain) in strain energy of the structure of the cavity during such oscillations. As a strong evidence for the accuracy of (ii-iv) we note that the use of $R_1 = (A/B)^{1/4}$ (Eqn.31) in Eq.29 renders

$$E_e(R_1 + \zeta) = 2\sqrt{AB} + \frac{1}{2} \left(\frac{6A}{R_1^2} + 2B\right) \zeta^2,$$

which has first significant term with only $\zeta^2$ dependence; it does not have $\zeta$ dependent term because $E_e(R_1 + \zeta)$ has minimum value at $\zeta = 0$. In arranging Eqn.(32) we assume that all terms in the binomial expansion of $(A/R_1^2)(1 + \zeta/R_1^2)^{-2}$ having $\zeta$ with powers $\geq 3$ are negligible.

We may also mention that 3-D systems like liquid $^4He$ and liquid $^3He$ exhibit $-ve$ expansion coefficient [15] when their $T$ approaches $T_o$ (the $T$ equivalent of the ground state energy of a $He$ atom as a particle trapped in a cavity formed by other $He$ atoms in
the liquid) or the thermal de Broglie wave length [15] a $He$ atoms $\lambda_T = h/\sqrt{2\pi mk_BT}$ ($\approx a =$ the inter-particle separation). Since this condition can be compared with $\lambda/2 \approx d$ for the particle in 1-D box, the observation of the said $-ve$ expansion provides strong experimental support to our inference (Section 4.2) and an added conclusion that the particles in these systems at $T \leq T_o$ behave like a particle trapped in a cavity of size $a$.

6. Conclusions

Analyzing the wave mechanics of a particle trapped in a 1-D box having small flexibility in its size provided by the elasticity of its structure, we discovered its several intrinsic new aspects which are expected to help in having a better understanding of the effects of wave nature of a particle in several systems like quantum- (dot/wire/well) [2], electron in an electron bubble [17, 18], trapped atom [21], etc., as well as the quantum behavior of various many body systems. These aspects are found to have close consistency with relevant inferences of our recent study [7]. Several important aspects of an electron bubble provides strong experimental support to our inferences (Sections 3 and 4) at qualitative scale; a quantitative agreement is not expected because the bubble is a representative of a particle trapped in a 3-D (not a 1-D) cavity. Through the existence of an electron bubble, the Nature reveals two important facts: (A1) a quantum particle, like an electron in electron bubble, exclusively occupies a spherical cavity of radius $R = \lambda/2$ when it rests in its lowest possible energy state, and (A2) such a particle exerts a force which tries to expand the cavity against the inter-atomic forces among the constituents of the cavity wall. Although, to the best of our knowledge, A1 and A2 have been experimentally observed so clearly for an electron trapped in an electron bubble only but they can not be the exclusive properties of only this electron. In fact these should be intrinsic characteristics of any quantum particle. For example a conduction electron (in a superconductor) too should occupy exclusively a sphere of radius $\lambda/2$, -expected to increase with fall in $T$ and in this process it is likely to strain the lattice of the conductor by exerting its zero-point force against the inter-atomic forces which decide the symmetry and structure of the lattice and assume maximum possible size when it rests in its ground state in a self created cavity in the lattice. In a recent paper [22], we use this possibility to reveal the basic foundations of superconductivity and it is interesting to note that recent experimental studies [23] do confirm the occurrence of lattice strain in superconducting systems. In addition, one may find that liquids $^4He$ and $^3He$ exhibit [15] $-ve$ volume expansion when they are cooled through $T \approx T_o$ which clearly shows that the constituent particles ($He$-atoms) in their low temperature or superfluid states represent a particle trapped in a 3-D cavity. Guided by these facts, we believe that: (i) our important inferences (A1 and A2 as stated above) supported strongly by the existence of electron bubble would greatly help in having a better understanding of all systems like superfluids, superconductors and quantum-dot /wire/well, (ii) a microscopic theory of quantum fluidity (superfluidity/superconductivity [24]) or of similar behavior of other many body quantum systems would succeed in providing a complete and correct account of these phenomena and related properties if it incorporates (A1) and (A2) in its formulation, and (iii) the merit in our theoretical work (related to quantum fluidity of a system of interacting bosons/fermions [22, 25, 26]) which clearly incorporates (A1) and (A2) would have its due recognition sooner or later. As such we make several important and useful inferences (cf. Sections 3,
that are strongly supported by experimentally observed existence of an electron bubble. The fact, that the size of the bubble can be identified with the effective size of the electron or its representative wave packet, rightly emphasizes the importance of wave packet and its size in describing a quantum particle in its trapped state and a many body quantum system if its constituents behave like a particle trapped in cavity formed by neighboring particles.
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Fig. 1: Two model systems of a particle in a box of impenetrable walls (see section 2 for details). (A) Model system S1 where both walls are rigidly fixed, and (B) model system S2 where left wall is rigidly fixed, while the right wall has a flexibility (controlled by a spring of finite spring constant $k$) to have some displacement to the right. While $\Delta d =$ displacement of the right wall when force $F_1$ (Eqn.4 with $n = 1$) reaches equilibrium with $F_\zeta$ (Eqn.5), $\eta$ represents an arbitrary but small ($|\eta| < \Delta d$) displacement from the equilibrium position of the right wall from $x = d + \Delta d$ to set oscillation in the position of this wall (Section 4.4).
Fig. 2: The $t (= T/T_o)$ dependence of the increase in the box size. While Curve A1 represents $\tilde{\delta}(t)_{QP}$ (Eqn.12), Curve B1 represents $\tilde{\delta}(t)_{CP}$ (Eqn.14) obtained in units of $\Delta d = \delta_1 = h^2/4md^3k$; corresponding $\alpha(t)$ values are, respectively, depicted by Curves A2 and B2 (see Section 4.2 for details).
Fig. 3: The $t (= T/T_o)$ dependence of: (i) the increase in the box size $\delta_1(t)$ (Curve-A) forced by $F_1$ (Eqn. 4 with $n = 1$) and calculated in units of $\Delta d = \delta_1 = h^2/4md^3k$ by using Eqn.15, and (ii) corresponding $\alpha(t)$ (Curve B). (See Section 4.2 for details)