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On the energy density in quantum mechanics

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Francisco Ricardo Torres Arvizu¹, Adrian Ortega^{2,3} and Hernán Larralde¹

¹ Instituto de Ciencias Físicas, UNAM, Av. Universidad s/n, CP 62210 Cuernavaca Morelos, Mexico

² Wigner RCP, Konkoly-Thege M.u. 29-33, H-1121 Budapest, Hungary

³ Departamento de Física, Universidad de Guadalajara, Blvd. Gral. Marcelino García Barragán 1421, C.P. 44430, Guadalajara, Jalisco, Mexico

E-mail: hernan@icf.unam.mx

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Abstract

There are several definitions of energy density in quantum mechanics. These yield expressions that differ locally, but all satisfy a continuity equation and integrate to the value of the expected energy of the system under consideration. Thus, the question of whether there are physical grounds to choose one definition over another arises naturally. In this work, we propose a way to probe a system by varying the size of a well containing a quantum particle. We show that the mean work done by moving the wall is closely related to one of the definitions for energy density. Specifically, the appropriate energy density, evaluated at the wall corresponds to the force exerted by the particle locally, against which the work is done. We show that this identification extends to two and three dimensional systems.

1. Introduction

In many textbooks on quantum mechanics [1–3] we are taught that an important consequence that emerges from the fact that the wave function that describes a quantum particle satisfies the Schrödinger equation, is that the probability density for finding the particle at a given position satisfies a continuity equation. This reflects the fact that probability is locally conserved [1–3]. However, and rather surprisingly, there is very little discussion in the literature regarding the concept of energy density in quantum mechanics, how to define it, how it evolves, whether it is conserved, and what is its physical significance [4–14]. In these few works, different expressions for the energy density have been proposed. These densities differ locally from one another, though they all integrate to the same value of the expected energy. It has been argued that there is no ‘physical’ way to choose which of these different densities is physically meaningful, and that it essentially comes down to a matter of preference [7, 8]. In this paper we present what we believe are the minimum conditions that the energy density must satisfy and we discuss two different possible definitions that satisfy the conditions. A similar problem was investigated in relation to the electromagnetic energy density in a dispersive and dissipative metamaterial [15–17]. We illustrate a way to probe the systems locally in order to identify which of the energy densities has a physical manifestation. To do this, we consider particles trapped in simple infinite well systems and probe the systems by changing the size of the well. We show that the expected work done to change the size of the well is directly related to the local value of one of the energy densities at the boundary. This density can be interpreted as the effective force exerted by the particle in the well. The other density is irrelevant in this respect as it vanishes identically at the walls. We remark that the work required to change the size of a system is in itself also a quantity of physical interest, since it characterizes the exchange of mechanical energy of the system with its surroundings,—as in thermodynamics— and should be amenable to experimental measurement in principle.

2. The probability density and the energy density

If we consider a quantum particle in a region I , in the position representation it is described by a wave function $\Psi(\mathbf{r}, t)$ that satisfies the Schrodinger equation

$$i\hbar \frac{\partial}{\partial t} \Psi = \hat{H} \Psi \quad (1)$$

where

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}) \quad (2)$$

$V(\mathbf{r})$ is a potential and the wave function is normalized:

$$\int_I |\Psi(\mathbf{r}, t)|^2 d\mathbf{r} = 1.$$

The integrand $|\Psi(\mathbf{r}, t)|^2 \equiv \rho_D(\mathbf{r}, t)$ is interpreted as the probability density of finding the particle at position $\mathbf{r}$ at time t . Then, as is well-known, the probability density fulfills a continuity equation

$$\frac{\partial}{\partial t} \rho_D + \nabla \cdot \mathbf{J}_D = 0, \quad (3)$$

where the flux $\mathbf{J}_D$ is given by

$$\mathbf{J}_D = \frac{\hbar}{2\mu i} (\Psi^* \nabla \Psi - \Psi \nabla \Psi^*). \quad (4)$$

This implies that the probability density is locally conserved [1, 3]. By the same token, the expected energy of a quantum particle can be expressed as

$$\langle E \rangle = \int_I \Psi^* \hat{H} \Psi d\mathbf{r} \quad (5)$$

This expression suggests that the integrand might be interpreted as an energy density, akin to the probability density discussed above. If this was the case, the energy density in the system would be given by

$$\rho_1^E = \Psi^* \hat{H} \Psi = \Psi^* \left(-\frac{\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}) \right) \Psi. \quad (6)$$

Unfortunately, the choice ρ_1^E above is not satisfactory as there is no guarantee that this density is real at every point where it is defined, though it is easy to see that the imaginary part always integrates to zero [10].

It would be reasonable to expect that a physically acceptable definition of quantum energy density should, at least, meet the following conditions:

1. it should be a local, real-valued function in the position representation;
2. its integral over the system must be equal to the expected energy $\langle E \rangle$.

However, an infinite number of different expressions for the energy density satisfying these conditions can still be defined.

One possible definition of energy density, that does satisfy the above conditions, is

$$\rho_2^E = \frac{1}{2} (\Psi^* \hat{H} \Psi + \Psi \hat{H} \Psi^*), \quad (7)$$

which is obviously real, and integrates to $\langle E \rangle$. We cannot guarantee that ρ_2^E is non-negative, even when the potential is positive for all $\mathbf{x}$. Nevertheless, it has been argued that the negative kinetic energies that this entails are not necessarily unphysical [18], and may even be measured [19]. Another possible choice for the energy density is

$$\rho_3^E = \frac{\hbar^2}{2\mu} (\nabla \Psi^*) \cdot (\nabla \Psi) + \Psi^* V(\mathbf{r}) \Psi \quad (8)$$

which is real and also integrates to $\langle E \rangle$. In contrast to ρ_2^E , this choice is nonnegative if the potential $V(\mathbf{x})$ is nonnegative itself. Note that ρ_3^E can be derived from the definition of the expectation value of the energy after an integration by parts [10]. Another option is to obtain ρ_3^E from one of the components of the energy momentum tensor [20, 21]. In appendix A we show this derivation explicitly. Both derivations hinge on the fact that in the position representation, the Hamiltonian acts as a second-order differential operator. In contrast, in the definition of the densities ρ_1 and ρ_2 no explicit dependence on the form of the Hamiltonian is required.

The energy densities defined above are locally conserved in the sense that they satisfy a continuity equation for appropriate energy fluxes:

$$\frac{\partial \rho_2^E}{\partial t} = -\frac{i\hbar}{4\mu} \nabla \cdot (-\Psi^* \nabla [\hat{H} \Psi] + \Psi \nabla [\hat{H} \Psi^*] + (\nabla \Psi^*) \hat{H} \Psi - (\nabla \Psi) \hat{H} \Psi^*), \quad (9)$$

$$\frac{\partial \rho_3^E}{\partial t} = -\frac{i\hbar}{2\mu} \nabla \cdot ((\nabla \Psi^*) \hat{H} \Psi - (\nabla \Psi) \hat{H} \Psi^*). \quad (10)$$

The derivation of these equations can be found in the appendix B.

Clearly, however, both expressions for the energy density differ locally, so the question of whether there are physical grounds to choose one over the other, or neither, arises naturally. Further, the physically meaningful density will be associated to an energy flux, which is central to the description of energy transport in quantum systems.

In what follows, we propose a simple scheme to probe locally a particle in a box. Specifically, we calculate the work done by moving one of the box's walls a distance $d\ell$. The idea is that if this movement is done quickly, then the work will be due to interaction of the wall with the system at its immediate vicinity. As it turns out, the work done is independent of the speed at which the wall moves.

2.1. One dimensional system

Following one of the procedures described in [22, 23], we begin by considering a particle of mass μ in a one dimensional infinite square well of size $L(t)$ (the extension to higher dimension 'cubic' wells is straight forward). We can write the wave function of the particle as

$$\Psi(x, t) = \sum_{n=1}^{\infty} b_n(t) e^{-\frac{i}{\hbar} \int_0^t E_n(\tau) d\tau} \phi_n(x, t) \quad (11)$$

where $\phi_n(x, t)$ are the instantaneous eigenfunctions of the Hamiltonian,

$$\phi_n(x, t) = \sqrt{\frac{2}{L(t)}} \sin\left(\frac{n\pi x}{L(t)}\right) \quad n = 1, 2, \dots, \quad (12)$$

corresponding to eigenvalues (instantaneous energies)

$$E_n(t) = \frac{\hbar^2 n^2 \pi^2}{2\mu L^2(t)}, \quad (13)$$

and the coefficients $b_n(t)$ are chosen so that $\Psi(x, t)$ satisfies the time dependent Schrodinger equation. Substituting $\Psi(x, t)$ into equation (1) and using the orthonormality of the eigenfunctions $\phi_n(x, t)$, we find

$$\dot{b}_n(t) = - \sum_{n'=1}^{\infty} b_{n'}(t) e^{i(\theta_n(t) - \theta_{n'}(t))} \int_0^{L(t)} \phi_n(x, t) \dot{\phi}_{n'}(x, t) dx \quad (14)$$

where $\theta_n(t) = \frac{1}{\hbar} \int_0^t E_n(\tau) d\tau$. The initial values of the $b_n(t)$ are fixed when we prepare the initial state:

$$\Psi(x, 0) = \sum_{n=1}^{\infty} b_n(0) \phi_n(x, 0). \quad (15)$$

The expected energy of the particle is given by

$$\langle \Psi | \hat{H} | \Psi \rangle \equiv \mathcal{E}(t) = \sum_{n=1}^{\infty} |b_n(t)|^2 E_n(t). \quad (16)$$

We are interested in the change in energy of the particle due to the motion of the wall after a time δt , i.e. $\mathcal{E}(\delta t) - \mathcal{E}(0) \approx \dot{\mathcal{E}}(0) \delta t$. From equation (16) we can calculate

$$\dot{\mathcal{E}}(0) = \sum_{n=1}^{\infty} E_n(0) (b_n^*(0) \dot{b}_n(0) + \dot{b}_n^*(0) b_n(0)) + \dot{E}_n(0) |b_n(0)|^2 \quad (17)$$

where $\dot{E}_n(0)$ is

$$\dot{E}_n(0) = - \frac{\hbar^2 n^2 \pi^2}{\mu L(0)^3} v, \quad (18)$$

$L(0)$ is the initial length of the well, and $v \equiv \dot{L}(0)$ is the initial speed at which the wall moves. The $\dot{b}_n(0)$ can be calculated using equation (14), where the time derivatives of the instantaneous eigenfunctions can be obtained from equation (12) and the resulting integrals appearing in equation (14) can be evaluated directly

$$\int_0^{L(t)} \phi_{n'}(x, t) \dot{\phi}_n(x, t) dx = \begin{cases} \frac{2nn'(-1)^{n-n'}}{L(t)(n'^2 - n^2)} v, & n' \neq n, \\ 0, & n' = n. \end{cases} \quad (19)$$

Then, after a little algebra, $\dot{\mathcal{E}}(0)$ can be expressed in terms of the initial conditions of the system as

$$\dot{\mathcal{E}}(0) = - \frac{\hbar^2 \pi^2 v}{\mu L(0)^3} \left| \sum_{n=1}^{\infty} b_n(0) (-1)^n n \right|^2 \quad (20)$$

Now we compare this expression with the value of the value of energy density ρ_2^E and ρ_3^E evaluated at the wall. For this system we have

$$\rho_2^E(x, t) = \frac{\hbar^2 \pi^2}{2\mu L(t)^3} \operatorname{Re} \left[\sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} n^2 b_n^*(t) b_n(t) e^{i(\theta_{n'}(t) - \theta_n(t))} \sin\left(\frac{n'\pi x}{L(t)}\right) \sin\left(\frac{n\pi x}{L(t)}\right) \right]. \quad (21)$$

Evaluating at the wall, $x = L(t)$, we see that $\rho_2^E(L(t), t) = 0$ trivially for all time. On the other hand, for $\rho_3(x, t)$ we have

$$\rho_3^E(x, t) = \left(\frac{\hbar^2}{\mu L(t)} \right) \left[\sum_{n'=1}^{\infty} e^{i\theta_{n'}(t)} b_{n'}^*(t) \frac{n'\pi}{L(t)} \cos\left(\frac{n'\pi x}{L(t)}\right) \right] \left[\sum_{n=1}^{\infty} e^{-i\theta_n(t)} b_n(t) \frac{n\pi}{L(t)} \cos\left(\frac{n\pi x}{L(t)}\right) \right]. \quad (22)$$

Evaluating this expression at the wall, $x = L(t)$, at $t = 0$ we get

$$\rho_3^E(L(0), t = 0) = \frac{\hbar^2 \pi^2}{\mu L(0)^3} \left| \sum_{n=1}^{\infty} b_n(0) (-1)^n n \right|^2. \quad (23)$$

Thus, the average amount of work $\delta\mathcal{W}$ done by the the motion of the wall during a time interval δt is

$$\delta\mathcal{W} = \mathcal{E}(\delta t) - \mathcal{E}(0) = \dot{\mathcal{E}}(0) \delta t = -\rho_3^E(L(0), 0) \delta\ell \quad (24)$$

where $\delta\ell = v\delta t$ is the distance the wall moves. Both the particle density ρ_D and ρ_2^E vanish at the wall, thus, this result suggests that the wall transfers energy to, or receives energy from the particle as if the wall interacted with the system through the energy density ρ_3^E . In particular, in this one dimensional example, $\rho_3^E(L(0), 0)$, being an energy per unit length, can be thought of as the mean force exerted locally and instantaneously by the particle on the wall.

2.2. Two and three dimensional systems

For completeness, we show that these results extend to a quantum particle in a circular box in two dimensions and in a spherical box in three dimensions.

In the two dimensional case we consider a particle with mass μ confined in an infinite circular potential

$$V(r) = \begin{cases} 0, & \text{if } r \leq R(t), \\ \infty, & \text{if } r > R(t), \end{cases} \quad (25)$$

where the radius varies in time $R(t) = R_0 + vt$. The wave function takes the form

$$\Psi(\mathbf{r}, t) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} b_{m,n}(t) e^{-i\theta_{m,n}(t)} \frac{1}{\sqrt{\pi} R(t) J_{m+1}(z_{m,n})} J_m(k_{m,n} r) e^{im\phi}, \quad (26)$$

where $z_{m,n}$ is the n th the zero of $J_m(x)$, the Bessel function of order m , $k_{m,n} = \frac{z_{m,n}}{R(t)}$ and $\theta_{m,n}(t) = \frac{1}{\hbar} \int_0^t E_{m,n}(t') dt'$ as before, with

$$E_{m,n}(t) = \frac{\hbar^2 z_{m,n}^2}{2\mu R(t)^2}. \quad (27)$$

Following the same procedure as above (see details in appendix C), we find that the average work done to move the wall a distance $\delta\ell = v\delta t$ is given by

$$\dot{\mathcal{E}}(0) \delta t = -\frac{\hbar^2}{\mu R_0^3} \delta\ell \sum_{m=-\infty}^{\infty} \left| \sum_{n=1}^{\infty} b_{m,n}(0) z_{m,n} \right|^2. \quad (28)$$

Now we check that this work is done against the mean total force exerted by the particle on the wall through the energy density ρ_3^E :

$$\mathcal{F} \equiv \int \rho_3^E(\mathbf{r}, t = 0) \delta(r - R_0) r dr d\phi \quad (29)$$

where

$$\begin{aligned} \rho_3^E(\mathbf{r}, t) &= \frac{\hbar^2}{2\mu} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{m'=-\infty}^{\infty} \sum_{n'=1}^{\infty} e^{(m-m')i\phi} \frac{b_{m,n}(t) b_{m',n'}^*(t)}{\pi R(t)^2 J_{m+1}(z_{m,n}) J_{m'+1}(z_{m',n'})} e^{i(\theta_{m,n'}(t) - \theta_{m,n}(t))} \\ &\times \left[\frac{\partial}{\partial r} J_m(k_{m,n} r) \frac{\partial}{\partial r} J_{m'}(k_{m',n'} r) + \frac{mm'}{r^2} J_m(k_{m,n} r) J_{m'}(k_{m',n'} r) \right] \end{aligned} \quad (30)$$

Evaluating at $t = 0$ and performing the integral in equation (29), we find

$$\mathcal{F} = \frac{\hbar^2}{\mu R_0^3} \sum_{m=-\infty}^{\infty} \left| \sum_{n=1}^{\infty} b_{m,n}(0) z_{m,n} \right|^2. \quad (31)$$

so indeed we have $\delta\mathcal{W} = -\mathcal{F}\delta\ell$

Finally, for the three dimensional case we consider a particle with mass μ in an infinite spherical moving well potential of radius $R(t) = R_0 + vt$. Now the wave function takes the form

$$\Psi(\mathbf{r}, t) = \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l b_{n,l,m}(t) e^{-i\theta_{l,n}(t)} \frac{\sqrt{2}}{R(t)^{3/2} j_{l+1}(z_{l,n})} j_l(k_{l,n}r) Y_{l,m}(\theta, \phi), \quad (32)$$

where $z_{l,n}$ is the n th zero of $j_l(x)$, the spherical Bessel function of order l , $Y_{l,m}(\theta, \phi)$ are the spherical harmonics, and $\theta_{l,n}(t) = \frac{1}{\hbar} \int_0^t E_{l,n}(t') dt'$, as before. For this case, the change in the total energy of the system caused by moving the boundary at a speed v for a time δt is (See appendix D):

$$\dot{E}(0) \delta t = -\frac{\hbar^2 v \delta t}{\mu R_0^3} \sum_{n'=1}^{\infty} \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l b_{n,l,m}(0) b_{n',l,m}^*(0) z_{l,n} z_{l,n'} \quad (33)$$

As in the previous examples, this change of energy is due to work done against the total force exerted by the particle on the boundary. In this case this is given by

$$\mathcal{F} = \int \rho_3(\mathbf{r}, t=0) \delta(r - R_0) r^2 dr d\Omega. \quad (34)$$

where

$$\begin{aligned} \rho_3^E(\mathbf{r}, t) = & \frac{\hbar^2}{2\mu} \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n'=1}^{\infty} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=l'} \frac{2b_{n,l,m}(t) b_{n',l',m'}^*(t)}{R(t)^3 j_{l+1}(z_{l,n'}) j_{l+1}(z_{l,n})} e^{i(\theta_{l,n'}(t) - \theta_{l,n}(t))} \\ & \times \left[\frac{\partial}{\partial r} j_l(k_{l,n}r) \frac{\partial}{\partial r} j_{l'}(k_{l',n'}r) \mathbf{Y}_{l',m'}^* \cdot \mathbf{Y}_{l,m} + \frac{1}{r^2} j_l(k_{l,n}r) j_{l'}(k_{l',n'}r) \mathbf{\Psi}_{l,m}^* \cdot \mathbf{\Psi}_{l',m'} \right]. \end{aligned} \quad (35)$$

Here $\mathbf{Y}_{l,m} = Y_{l,m}(\theta, \psi) \hat{r}$ and $\mathbf{\Psi}_{l,m} = r \nabla Y_{l,m}(\theta, \psi)$ are the vector spherical harmonics [24]. These satisfy the orthogonality relation $\mathbf{\Psi}_{l,m} \cdot \mathbf{Y}_{l,m} = 0$, and the integral relations $\int_0^{2\pi} \int_0^{\pi} \mathbf{\Psi}_{l,m}^* \cdot \mathbf{\Psi}_{l',m'} d\Omega = l(l+1) \delta_{l,l'} \delta_{m,m'}$ and $\int_0^{2\pi} \int_0^{\pi} \mathbf{Y}_{l,m}^* \cdot \mathbf{Y}_{l',m'} d\Omega = \delta_{l,l'} \delta_{m,m'}$. Thus, evaluating $\rho_3(\mathbf{r}, t)$ at $t=0$ and integrating, we have

$$\mathcal{F} = \frac{\hbar^2}{2\mu} \sum_{n'=1}^{\infty} \sum_{n=1}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{2b_{n,l,m}(0) b_{n',l,m}^*(0) z_{l,n} z_{l,n'}}{R_0^3 j_{l+1}(z_{l,n}) j_{l+1}(z_{l,n'})} [j_l'(z_{l,n}) j_l'(z_{l,n'})]. \quad (36)$$

Finally, using the properties of the Bessel functions, we get

$$\mathcal{F} = \frac{\hbar^2}{\mu R_0^3} \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n'=1}^{\infty} \sum_{n=1}^{\infty} b_{n,l,m}(0) b_{n',l,m}^*(0) z_{l,n} z_{l,n'} = \frac{\hbar^2}{\mu R_0^3} \sum_{l=0}^{\infty} \sum_{m=-l}^l \left| \sum_{n=1}^{\infty} b_{n,l,m}(0) z_{l,n} \right|^2 \quad (37)$$

Thus, we again have $d\mathcal{W} = -\mathcal{F} d\ell$, or equivalently, $d\mathcal{W} = -\mathcal{P} dV$, where the pressure is $\mathcal{P} = \mathcal{F}/A$, the differential of volume is $dV = A d\ell$, and $A = 4\pi R_0^2$ is the area of the surface.

3. Discussion

If we have a quantum particle in a infinite well, changing the size of the well changes the energy of the system. Conservation of energy implies that this change of energy must be due to work done when moving the walls against the force exerted by particle. We have shown that the mean amount of work done when moving the wall is directly related to the energy density ρ_3^E at the wall. This energy density also satisfies the physical requirements of being local, and, of course, integrates to the expected value of energy. Further, this expression yields a positive definite value everywhere if the potential is also positive, and it satisfies a continuity equation, implying that it is locally conserved. In contrast, due to the boundary condition ρ_2^E vanishes identically at the wall (as does the probability density ρ_D), so its value cannot be probed by moving the wall, and though it is also conserved, it is not necessarily positive everywhere it is defined, even when the potential is nowhere negative, which implies that the particle may have negative kinetic energy in some regions of the system. We contend that these results imply that ρ_3^E can be considered as the actual physical energy density of the system, in the sense that it is measurable as the mean instantaneous local force (pressure) exerted by the particle on the wall. This would also imply that the energy flux associated to ρ_3^E is the relevant flux to describe energy transport in quantum systems. From a different perspective, ρ_3^E is analogous to the electromagnetic radiation pressure on a perfect absorber, as in that case too $P_{\text{rad}} = u$, where u is the energy density of the wave. Of course, if all that is wanted is the integral of the density to obtain the expected energy, then any one of the expressions discussed in this work can be used, even ρ_1^E , which may have complex values locally.

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Data availability statement

No new data were created or analysed in this study.

Appendix A. Derivation of ρ_3 from the energy-momentum tensor

An alternative derivation for ρ_3^E and its associated continuity equation follows from the principle of least action, for which the Lagrangian density reads [20]

$$\mathcal{L} = -\frac{\hbar^2}{2\mu} \nabla\Psi \cdot \nabla\Psi^* - V\Psi^*\Psi - \frac{\hbar}{2i}(\Psi^*\dot{\Psi} - \Psi\dot{\Psi}^*). \quad (\text{A1})$$

Here one considers the two independent fields $\eta_\gamma \in \{\Psi, \Psi^*\}$, and the Schrödinger equation is recovered using the Euler–Lagrange equations

$$\partial_\alpha \left(\frac{\partial \mathcal{L}}{\partial \eta_{\gamma,\alpha}} \right) - \frac{\partial \mathcal{L}}{\partial \eta_\gamma} = 0 \quad (\text{A2})$$

for the field $\eta_\gamma = \psi^*$ and $\alpha \in \{t, \mathbf{r}\}$. The energy-momentum tensor is defined as [25]

$$T_\alpha^\beta = \frac{\partial \mathcal{L}}{\partial \eta_{\gamma,\alpha}} \eta_{\gamma,\beta} - \mathcal{L} \delta_\alpha^\beta. \quad (\text{A3})$$

from which the energy density, is found to be

$$T_0^0 = \frac{\hbar^2}{2\mu} \nabla\Psi \cdot \nabla\Psi^* + V|\Psi|^2 = \rho_3^E. \quad (\text{A4})$$

The continuity equations are given by

$$\frac{dT_\alpha^\beta}{dx^\beta} = 0 \quad (\text{A5})$$

from which one can also obtain the flux (See equation (10)).

Appendix B. Derivation of the continuity equations for the energy densities

The time derivative of ρ_2^E can be calculated using the Schrodinger equation (1):

$$\frac{\partial \rho_2^E}{\partial t} = \frac{\partial}{\partial t} \frac{1}{2} [\Psi^* \hat{H} \Psi + \Psi \hat{H} \Psi^*] = \frac{i}{2\hbar} [\Psi \hat{H} \hat{H} \Psi^* - \Psi^* \hat{H} \hat{H} \Psi]. \quad (\text{B1})$$

Now

$$\hat{H} \hat{H} \Psi = \left(\frac{\hbar^2}{2\mu} \right)^2 \nabla^4 \Psi - \frac{\hbar^2}{2\mu} (\nabla^2 (V(\mathbf{r}) \Psi) + V(\mathbf{r}) \nabla^2 \Psi) + V^2(\mathbf{r}) \Psi, \quad (\text{B2})$$

where

$$\Psi^* \nabla^4 \Psi = \nabla \cdot [\Psi^* \nabla (\nabla^2 \Psi)] - \nabla \cdot [(\nabla \Psi^*) \nabla^2 \Psi] + (\nabla^2 \Psi^*) (\nabla^2 \Psi) \quad (\text{B3})$$

and

$$\begin{aligned} & \Psi^* \nabla^2 (V(\mathbf{r}) \Psi) + \Psi^* V(\mathbf{r}) \nabla^2 \Psi \\ &= \nabla \cdot (\Psi^* \nabla (V(\mathbf{r}) \Psi)) - \nabla \Psi^* \cdot \nabla (V(\mathbf{r}) \Psi) + \nabla \cdot [V(\mathbf{r}) \Psi^* \nabla \Psi] - \nabla \Psi \cdot \nabla (V(\mathbf{r}) \Psi^*). \end{aligned} \quad (\text{B4})$$

The complex conjugate of equation (B4) is

$$\begin{aligned} & \Psi \nabla^2 (V(\mathbf{r}) \Psi^*) + \Psi V(\mathbf{r}) \nabla^2 \Psi^* \\ &= \nabla \cdot (\Psi \nabla (V(\mathbf{r}) \Psi^*)) - \nabla \Psi \cdot \nabla (V(\mathbf{r}) \Psi^*) + \nabla \cdot [V(\mathbf{r}) \Psi \nabla \Psi^*] - \nabla \Psi^* \cdot \nabla (V(\mathbf{r}) \Psi). \end{aligned} \quad (\text{B5})$$

Taking the difference between equations (B4) and (B5) gives

$$\nabla \cdot [\Psi^* \nabla (V(\mathbf{r}) \Psi) + V(\mathbf{r}) \Psi^* \nabla \Psi - \Psi \nabla (V(\mathbf{r}) \Psi^*) - V(\mathbf{r}) \Psi \nabla \Psi^*].$$

Thus

$$\begin{aligned} \frac{\partial \rho_2^E}{\partial t} = \frac{1}{2i\hbar} \nabla \cdot \left(\left(\frac{\hbar^2}{2\mu} \right)^2 [\Psi^* \nabla (\nabla^2 \Psi) - (\nabla \Psi^*) \nabla^2 \Psi - \Psi \nabla (\nabla^2 \Psi^*) + (\nabla \Psi) \nabla^2 \Psi^*] \right. \\ \left. - \left(\frac{\hbar^2}{2\mu} \right) [\Psi^* \nabla (V(\mathbf{r}) \Psi) + V(\mathbf{r}) \Psi^* \nabla \Psi - \Psi \nabla (V(\mathbf{r}) \Psi^*) - V(\mathbf{r}) \Psi \nabla \Psi^*] \right). \end{aligned} \quad (\text{B6})$$

The above equation can be rewritten as

$$\frac{\partial \rho_2^E}{\partial t} = -\frac{i\hbar}{4\mu} \nabla \cdot (-\Psi^* \nabla [\hat{H} \Psi] + \Psi \nabla [\hat{H} \Psi^*] + (\nabla \Psi^*) \hat{H} \Psi - (\nabla \Psi) \hat{H} \Psi^*). \quad (\text{B7})$$

On the other hand, the time derivative of ρ_3^E is

$$\begin{aligned} \frac{\partial \rho_3^E}{\partial t} &= \frac{\hbar^2}{2\mu} \left[\nabla \left(\frac{\partial \Psi^*}{\partial t} \right) \cdot \nabla \Psi + \nabla \Psi^* \cdot \left(\frac{\partial \Psi}{\partial t} \right) \right] + \frac{\partial \Psi^*}{\partial t} V(\mathbf{r}) \Psi + \Psi^* V \frac{\partial \Psi}{\partial t} \\ &= \frac{\hbar^2}{2\mu} \frac{i}{\hbar} [\nabla (\hat{H} \Psi^*) \cdot \nabla \Psi - \nabla \Psi^* \cdot \nabla (\hat{H} \Psi)] + \frac{i}{\hbar} [(\hat{H} \Psi^*) V(\mathbf{r}) \Psi - \Psi^* V (\hat{H} \Psi)]. \end{aligned} \quad (\text{B8})$$

Now,

$$\begin{aligned} \frac{i}{\hbar} [(\hat{H} \Psi^*) V(\mathbf{r}) \Psi - \Psi^* V (\hat{H} \Psi)] &= -\frac{i\hbar}{2\mu} (\nabla \cdot (V(\mathbf{r}) \Psi \nabla \Psi^*) - \nabla (V(\mathbf{r}) \Psi) \cdot \nabla \Psi^*) \\ &\quad + \frac{i\hbar}{2\mu} (\nabla \cdot (V(\mathbf{r}) \Psi^* \nabla \Psi) - \nabla (V(\mathbf{r}) \Psi^*) \cdot \nabla \Psi), \end{aligned} \quad (\text{B9})$$

also

$$\begin{aligned} \frac{i\hbar}{2\mu} [\nabla (\hat{H} \Psi^*) \cdot \nabla \Psi - \nabla \Psi^* \cdot \nabla (\hat{H} \Psi)] &= \frac{i\hbar}{2\mu} \left[\nabla \left(-\frac{\hbar^2}{2\mu} \nabla^2 \Psi^* + V(\mathbf{r}) \Psi^* \right) \cdot \nabla \Psi \right. \\ &\quad \left. - \nabla \Psi^* \cdot \nabla \left(-\frac{\hbar^2}{2\mu} \nabla^2 \Psi + V(\mathbf{r}) \Psi \right) \right]. \end{aligned} \quad (\text{B10})$$

Thus, using the two equations above in equation (B8) we obtain

$$\begin{aligned} \frac{i\hbar}{2\mu} [\nabla (\hat{H} \Psi^*) \cdot \nabla \Psi - \nabla \Psi^* \cdot \nabla (\hat{H} \Psi)] + \frac{i}{\hbar} [(\hat{H} \Psi^*) V(\mathbf{r}) \Psi - \Psi^* V (\hat{H} \Psi)] \\ = \frac{i\hbar}{2\mu} \left[\nabla \cdot (V(\mathbf{r}) \Psi^* \nabla \Psi) - \nabla \cdot (V(\mathbf{r}) \Psi \nabla \Psi^*) + \frac{\hbar^2}{2\mu} \nabla \Psi^* \cdot \nabla (\nabla^2 \Psi) - \frac{\hbar^2}{2\mu} \nabla \Psi \cdot \nabla (\nabla^2 \Psi^*) \right]. \end{aligned} \quad (\text{B11})$$

The last two terms yield

$$\begin{aligned} \nabla \Psi^* \cdot \nabla (\nabla^2 \Psi) - \nabla \Psi \cdot \nabla (\nabla^2 \Psi^*) &= \nabla \cdot ((\nabla^2 \Psi) \nabla \Psi^*) - (\nabla^2 \Psi) (\nabla^2 \Psi^*) \\ &\quad - \nabla \cdot ((\nabla^2 \Psi^*) \nabla \Psi) + (\nabla^2 \Psi^*) (\nabla^2 \Psi) \end{aligned} \quad (\text{B12})$$

and therefore

$$\begin{aligned} \frac{\partial \rho_3^E}{\partial t} &= \frac{i\hbar}{2\mu} \nabla \cdot \left[\frac{\hbar^2}{2\mu} (\nabla^2 \Psi) \nabla \Psi^* - \frac{\hbar^2}{2\mu} (\nabla^2 \Psi^*) \nabla \Psi + V(\mathbf{r}) \Psi^* \nabla \Psi - V(\mathbf{r}) \Psi \nabla \Psi^* \right] \\ &= \frac{i\hbar}{2\mu} \nabla \cdot [(\nabla \Psi) \hat{H} \Psi^* - (\nabla \Psi^*) \hat{H} \Psi]. \end{aligned} \quad (\text{B13})$$

Appendix C. Two dimensional case

Consider a particle with mass μ in an infinite spherical potential moving well

$$V(r) = \begin{cases} 0 & \text{if } r \leq R(t) \\ \infty & \text{if } r > R(t) \end{cases} \quad (\text{C1})$$

where $R(t) = R_0 + vt$. The Hamiltonian operator is

$$\mathcal{H} = -\frac{\hbar^2}{2\mu} \left[\frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \phi^2} \right], \quad (\text{C2})$$

in this case, the instantaneous eigenfunctions are

$$\psi_{n,m}(r, \phi, t) = \frac{1}{\sqrt{\pi} R(t) J_{m+1}(z_{m,n})} J_m(k_{m,n} r) e^{im\phi}, \quad k_{m,n} = \frac{z_{m,n}}{R(t)}, \quad (\text{C3})$$

where $z_{m,n}$ is the n th the zero of $J_m(x)$, the Bessel function of order m . The wave function takes the form

$$\Psi(\mathbf{r}, t) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} b_{m,n}(t) e^{-i\theta_{m,n}(t)} \frac{1}{\sqrt{\pi} R(t) J_{m+1}(z_{m,n})} J_m(k_{m,n} r) e^{im\phi}, \quad (\text{C4})$$

where $\theta_{m,n}(t) = \frac{1}{\hbar} \int_0^t E_{m,n}(t') dt'$, with

$$E_{m,n}(t) = \frac{\hbar^2 z_{m,n}^2}{2\mu R(t)^2}. \quad (\text{C5})$$

Then, the expected energy is given by

$$\langle \Psi | \hat{H} | \Psi \rangle \equiv \mathcal{E}(t) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} |b_{m,n}(t)|^2 E_{m,n}(t),$$

and its derivative at $t = 0$

$$\dot{\mathcal{E}}(0) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \{E_{m,n}(0)(b_{m,n}^*(0)\dot{b}_{m,n}(0) + \dot{b}_{m,n}^*(0)b_{m,n}(0)) + \dot{E}_{m,n}(0)|b_{m,n}(0)|^2\}, \quad (\text{C6})$$

where $\dot{b}(t)$ and $\dot{E}_{m,n}(t)$ are

$$\dot{E}_{m,n} = -v \frac{\hbar^2 z_{m,n}^2}{\mu R(t)^3}, \quad (\text{C7})$$

$$\dot{b}_{m,n}(t) = - \sum_{m'=-\infty}^{\infty} \sum_{n'=1}^{\infty} b_{m',n'}(t) e^{i(\theta_{m,n}(t) - \theta_{m',n'}(t))} \int_0^{R(t)} \int_0^{2\pi} \psi_{m,n}(r, \phi, t) \dot{\psi}_{m',n'}(r, \phi, t) r dr d\phi, \quad (\text{C8})$$

respectively. The integral in the last expression when $n = n'$ satisfies

$$\int_{S_0} \psi_n \frac{\partial}{\partial t} \psi_n^* dS = - \int_{S_0} \psi_n^* \frac{\partial}{\partial t} \psi_n dS \quad (\text{C9})$$

which implies that these terms in $\dot{\mathcal{E}}(0)$ vanish, moreover when $n \neq n'$ we have

$$\begin{aligned} & \int_0^{R(t)} \int_0^{2\pi} \psi_{m,n}(r, \phi, t) \dot{\psi}_{m',n'}(r, \phi, t) r dr d\phi \\ &= \delta_{m,m'} \frac{2}{R(t)^2 J_{m+1}(z_{m,n}) J_{m'+1}(z_{m',n'})} \int_0^{R(t)} J_m(k_{m,n} r) \dot{J}_{m'}(k_{m',n'} r) r dr, \end{aligned} \quad (\text{C10})$$

substituting

$$\begin{aligned} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} E_{m,n}(t) \dot{b}_{m,n}(t) b_{m,n}^*(t) &= - \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{m,n'}(t) b_{m,n}^*(t) E_{m,n}(t) e^{i(\theta_{m,n}(t) - \theta_{m,n'}(t))} \\ &\times \frac{2}{R(t)^2 J_{m+1}(z_{m,n}) J_{m'+1}(z_{m,n'})} \int_0^{R(t)} J_l(k_{m,n} r) \dot{J}_l(k_{m,n'} r) r dr, \\ &= - \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{m,n'}^*(t) b_{m,n}(t) E_{m,n'}(t) e^{i(\theta_{m,n'}(t) - \theta_{m,n}(t))} \\ &\times \frac{2}{R(t)^2 J_{m+1}(z_{m,n}) J_{m'+1}(z_{m,n'})} \int_0^{R(t)} J_m(k_{m,n} r) \dot{J}_m(k_{m,n'} r) r dr, \end{aligned} \quad (\text{C11})$$

and

$$\begin{aligned} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} E_{m,n}(t) \dot{b}_{m,n}^*(t) b_{m,n}(t) &= - \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{m,n}(t) b_{m,n'}^*(t) E_{m,n}(t) e^{i(\theta_{m,n'}(t) - \theta_{m,n}(t))} \\ &\times \frac{2}{R(t)^2 J_{m+1}(z_{m,n}) J_{m'+1}(z_{m,n'})} \int_0^{R(t)} J_m(k_{m,n} r) \dot{J}_m(k_{m,n'} r) r dr. \end{aligned} \quad (\text{C12})$$

Thus,

$$\begin{aligned} & \frac{2}{R(t)^2 J_{m+1}(z_{m,n}) J_{m+1}(z_{m,n'})} \int_0^{R(t)} J_l(k_{m,n} r) \dot{J}_m(k_{m,n'} r) r dr \\ &= - \frac{2z_{m,n'} v}{J_{m+1}(z_{m,n}) J_{m+1}(z_{m,n'}) R(t)^4} \int_0^{R(t)} J_m(k_{m,n} r) J'_m(k_{m,n'} r) r^2 dr, \end{aligned} \quad (\text{C13})$$

using⁴ and the Leibnitz rule, we obtain

$$\int_0^{R(t)} J_{m+1}(k_{m,n} r) J'_{m+1}(k_{m,n'} r) r^2 dr = - \frac{R^3(t) z_{m,n}}{z_{m,n'}^2 - z_{m,n}^2} J_{m+1}(z_{m,n}) J'_m(z_{m,n'}). \quad (\text{C14})$$

⁴ Using Abramowitz 11.3.9

$$\int_z \left\{ (k^2 - l^2)t - \frac{(\mu^2 - \nu^2)}{t} \right\} \mathcal{C}_\mu(kt) \mathcal{D}_\nu(lt) dt = z \{ k \mathcal{C}_{\mu+1}(kz) \mathcal{D}_\nu(lz) - l \mathcal{C}_\mu(kz) \mathcal{D}_{\nu+1}(lz) \} - (\mu - \nu) \mathcal{C}_\mu(kt) \mathcal{D}_\nu(lt)$$

for two cylindrical functions $\mathcal{C}_\mu(kt)$ and $\mathcal{D}_\nu(lt)$, [26]

By the recurrence relation $J_p'(x) = \frac{p}{x}J_p(x) - J_{p+1}(x)$,

$$\int_0^{R(t)} J_m(k_{m,n}r)J_m'(k_{m,n'}r)r^2dr = \frac{R^3(t)z_{m,n}}{z_{m,n'}^2 - z_{m,n}^2}J_m'(z_{m,n})J_m'(z_{m,n'}), \quad (C15)$$

analogously we have

$$\int_0^{R(t)} J_m(k_{m,n'}r)J_m'(k_{m,n}r)r^2dr = -\frac{R^3(t)z_{m,n}}{z_{m,n}^2 - z_{m,n'}^2}J_m'(z_{m,n})J_m'(z_{m,n'}), \quad (C16)$$

evaluating $\mathcal{E}(t)$ at $t = 0$

$$\begin{aligned} \mathcal{E}(0) = & -\frac{\hbar^2}{\mu R_0^3}v \left\{ \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} z_{m,n}^2 |b_{m,n}(0)|^2 \right. \\ & \left. + \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n' \neq n}^{\infty} b_{m,n}^*(0)b_{m,n'}(0)z_{m,n}z_{m,n'} \frac{J_m'(z_{m,n})J_m'(z_{m,n'})}{J_{m+1}(z_{m,n})J_{m+1}(z_{m,n'})} \right\}, \end{aligned} \quad (C17)$$

using the recurrence formula again

$$\mathcal{E}(0) = -\frac{\hbar^2}{\mu R_0^3}v \left\{ \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} z_{m,n}^2 |b_{m,n}(0)|^2 + \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n' \neq n}^{\infty} b_{m,n}^*(0)b_{m,n'}(0)z_{m,n}z_{m,n'} \right\}. \quad (C18)$$

On the other hand, the energy density is given by

$$\rho_3(\mathbf{r}, t) = \frac{\hbar^2}{2\mu} \nabla \Psi^*(\mathbf{r}, t) \cdot \nabla \Psi(\mathbf{r}, t) \quad (C19)$$

in this case we take

$$\nabla \Psi(\mathbf{r}, t) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} e^{-i\theta_{m,n}} b_{m,n}(t) \frac{e^{im\phi}}{\sqrt{\pi} R(t) J_{m+1}(z_{m,n})} \left[\frac{\partial}{\partial r} J_m(z_{m,n}r) \hat{r} + \frac{im}{r} J_m(k_{m,n}r) \hat{\phi} \right]. \quad (C20)$$

Analogously,

$$\nabla \Psi^*(\mathbf{r}, t) = \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} e^{i\theta_{m,n}} b_{m,n}^*(t) \frac{e^{-im\phi}}{\sqrt{\pi} R(t) J_{m+1}(z_{m,n})} \left[\frac{\partial}{\partial r} J_m(z_{m,n}r) \hat{r} - \frac{im}{r} J_m(k_{m,n}r) \hat{\phi} \right]. \quad (C21)$$

$$\begin{aligned} \rho_3(\mathbf{r}, t) = & \frac{\hbar^2}{2\mu} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{m'=-\infty}^{\infty} \sum_{n'=1}^{\infty} e^{(m-m')i\phi} \frac{b_{m,n}(t)b_{m',n'}^*(t)}{\pi R(t)^2 J_{m+1}(z_{m',n'}) J_{m'+1}(z_{m,n})} e^{i(\theta_{m,n'}(t) - \theta_{m,n}(t))} \\ & \times \left[\frac{\partial}{\partial r} J_m(k_{m,n}r) \frac{\partial}{\partial r} J_{m'}(k_{m',n'}r) + \frac{mm'}{r^2} J_m(k_{m,n}r) J_{m'}(k_{m',n'}r) \right] \end{aligned} \quad (C22)$$

we need to know $\rho(R_0, 0) = \int \rho_3(\mathbf{r}, t) \delta(r - R_0) r dr d\phi$. We know that $\int_0^{2\pi} e^{(m-m')i\phi} d\phi = 2\pi \delta_{m,m'}$, thus we have

$$\rho_3^E(R_0, 0) = \frac{\hbar^2}{2\mu} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \frac{2b_{m,n}(0)b_{m,n'}^*(0)z_{m,n}z_{m,n'}}{R_0^3 J_{m+1}(z_{m,n'}) J_{m+1}(z_{m,n})} [J_m'(z_{m,n})J_m'(z_{m,n'})]. \quad (C23)$$

Applying the same recurrence relation as above we get,

$$\rho_3^E(R_0, 0) = \frac{\hbar^2}{\mu R_0^3} \sum_{m=-\infty}^{\infty} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{m,n}(0)b_{m,n'}^*(0)z_{m,n}z_{m,n'}. \quad (C24)$$

Appendix D. Case for a spherical moving wall

Consider a particle with mass μ in an infinite spherical potential moving well

$$V(r) = \begin{cases} 0 & \text{if } r \leq R(t) \\ \infty & \text{if } r > R(t) \end{cases} \quad (D1)$$

where $R(t) = R_0 + vt$. The Hamiltonian operator is

$$\mathcal{H} = -\frac{\hbar^2}{2\mu} \left[\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{1}{\hbar^2 r^2} \hat{L}^2 \right], \quad (D2)$$

where $\hat{L}$ is the orbital angular momentum operator, which is given by

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \sin(\theta) \frac{\partial}{\partial \theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial \phi^2} \right], \quad (D3)$$

in this case, the instant eigenfunctions are

$$\phi_{n,l,m}(r, \theta, \psi, t) = \frac{\sqrt{2}}{R(t)^{3/2} j_{l+1}(z_{l,n})} j_l(k_{l,n} r) Y_{l,m}(\theta, \phi), \quad k_{l,n} = \frac{z_{l,n}}{R(t)}, \quad (\text{D4})$$

where $z_{l,n}$ is the n th zero of spherical Bessel function of order l ($j_l(x)$) and $Y_{l,m}(\theta, \phi)$ are the spherical harmonics. The wave function takes the form of

$$\Psi(\mathbf{r}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=1}^{\infty} b_{n,l,m}(t) e^{-i\theta_{l,n}(t)} \frac{\sqrt{2}}{R(t)^{3/2} j_{l+1}(z_{l,n})} j_l(k_{l,n} r) Y_{l,m}(\theta, \phi), \quad (\text{D5})$$

where $\theta_{l,n}(t) = \frac{1}{\hbar} \int_0^t E_{l,n}(t') dt'$, with

$$E_{l,n}(t) = \frac{\hbar^2 z_{l,n}^2}{2\mu R(t)^2} \quad (\text{D6})$$

Then, the expected energy is given by

$$\langle \Psi | \hat{H} | \Psi \rangle \equiv \mathcal{E}(t) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=1}^{\infty} |b_{n,l,m}(t)|^2 E_{l,n}(t),$$

and its derivative in $t = 0$

$$\dot{\mathcal{E}}(0) = \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=1}^{\infty} \{E_{l,n}(0)(b_{n,l,m}^*(0)\dot{b}_{n,l,m}(0) + \dot{b}_{n,l,m}^*(0)b_{n,l,m}(0)) + \dot{E}_{l,n}(0)|b_{n,l,m}(0)|^2\}, \quad (\text{D7})$$

where $\dot{b}(t)$ and $\dot{E}_{l,n}(t)$ are respectively

$$\dot{E}_{l,n} = -v \frac{\hbar^2 z_{l,n}^2}{\mu R(t)^3}, \quad (\text{D8})$$

$$\begin{aligned} \dot{b}_{n,l,m}(t) &= - \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \sum_{n'=1}^{\infty} b_{n',l',m'}(t) e^{i(\theta_{l,n}(t) - \theta_{l',n'}(t))} \\ &\times \int_0^{R(t)} \int_0^{\pi} \int_0^{2\pi} \phi_{n,l,m}(r, \theta, \psi, t) \dot{\phi}_{n',l',m'}(r, \theta, \psi, t) r^2 dr d\Omega, \end{aligned} \quad (\text{D9})$$

where $d\Omega$ is the solid angle differential. Analogously to the 2-dimensional case, we only work when $n' \neq n$ because when $n = n'$ the above integral vanishes. Now,

$$\begin{aligned} \int_0^{R(t)} \int_0^{\pi} \int_0^{2\pi} \phi_{n,l,m}(r, \theta, \psi, t) \dot{\phi}_{n',l',m'}(r, \theta, \psi, t) r^2 dr d\Omega &= \delta_{l,l'} \delta_{m,m'} \frac{2}{R(t)^3 j_{l+1}(z_{l,n}) j_{l'+1}(z_{l',n'})} \\ &\times \int_0^{R(t)} j_l(k_{l,n} r) \dot{j}_{l'}(k_{l',n'} r) r^2 dr, \end{aligned} \quad (\text{D10})$$

thus we have

$$\begin{aligned} \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=1}^{\infty} E_{l,n}(t) \dot{b}_{n,l,m}(t) b_{n,l,m}^*(t) &= - \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n'=1}^{\infty} \sum_{l'=1}^{\infty} b_{l,n',m}(t) b_{n,l,m}^*(t) E_{l,n}(t) e^{i(\theta_{l,n}(t) - \theta_{l',n'}(t))} \\ &\times \frac{2}{R(t)^3 j_{l+1}(z_{l,n}) j_{l'+1}(z_{l',n'})} \int_0^{R(t)} j_l(k_{l,n} r) \dot{j}_{l'}(k_{l',n'} r) r^2 dr, \\ &= - \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n'=1}^{\infty} \sum_{l'=1}^{\infty} b_{n',l,m}^*(t) b_{n,l,m}(t) E_{l,n'}(t) e^{i(\theta_{l,n'}(t) - \theta_{l,n}(t))} \\ &\times \frac{2}{R(t)^3 j_{l+1}(z_{l,n}) j_{l'+1}(z_{l',n'})} \int_0^{R(t)} j_l(k_{l,n'} r) \dot{j}_{l'}(k_{l',n'} r) r^2 dr, \end{aligned} \quad (\text{D11})$$

and

$$\begin{aligned} \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n=1}^{\infty} E_{l,n}(t) \dot{b}_{n,l,m}^*(t) b_{n,l,m}(t) &= - \sum_{l=0}^{\infty} \sum_{m=-l}^l \sum_{n'=1}^{\infty} \sum_{l'=1}^{\infty} b_{n,l,m}(t) b_{n',l,m}^*(t) E_{l,n}(t) e^{i(\theta_{l,n'}(t) - \theta_{l,n}(t))} \\ &\times \frac{2}{R(t)^3 j_{l+1}(z_{l,n}) j_{l'+1}(z_{l',n'})} \int_0^{R(t)} j_l(k_{l,n} r) \dot{j}_{l'}(k_{l',n'} r) r^2 dr. \end{aligned} \quad (\text{D12})$$

Then,

$$\begin{aligned} & \frac{2}{R(t)^3 j_l(z_{l,n}) j_l'(z_{l',n'})} \int_0^{R(t)} j_l(k_{l,n} r) j_l'(k_{l',n'} r) r^2 dr \\ &= -\frac{2 z_{l,n'} v}{J_{l+3/2}(z_{l,n}) J_{l+3/2}(z_{l',n'}) R(t)^4} \int_0^{R(t)} J_{l+1/2}(k_{l,n} r) J_{l+1/2}'(k_{l',n'} r) r^2 dr \end{aligned} \quad (D13)$$

using the same relations as above for this type of integrals we have,

$$\int_0^{R(t)} J_{l+1/2}(k_{l,n} r) J_{l+1/2}'(k_{l',n'} r) r^2 dr = -\frac{R^3(t) z_{l,n}}{z_{l,n'}^2 - z_{l,n}^2} J_{l+3/2}(z_{l,n}) J_{l+1/2}'(z_{l',n'}). \quad (D14)$$

By the recurrence relations

$$\int_0^{R(t)} J_{l+1/2}(k_{l,n} r) J_{l+1/2}'(k_{l',n'} r) r^2 dr = \frac{R^3(t) z_{l,n}}{z_{l,n'}^2 - z_{l,n}^2} J_{l+1/2}'(z_{l,n}) J_{l+1/2}'(z_{l',n'}), \quad (D15)$$

hence,

$$\int_0^{R(t)} J_{l+1/2}(k_{l,n} r) J_{l+1/2}'(k_{l',n'} r) r^2 dr = -\frac{R^3(t) z_{l,n}}{z_{l,n}^2 - z_{l,n'}^2} J_{l+1/2}'(z_{l,n}) J_{l+1/2}'(z_{l',n'}), \quad (D16)$$

then $\dot{\mathcal{E}}(0)$ is

$$\begin{aligned} \dot{\mathcal{E}}(0) = & -\frac{\hbar^2}{\mu R_0^3} v \left\{ \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} z_{l,n}^2 |b_{n,l,m}(0)|^2 \right. \\ & \left. + \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{n,l,m}^*(0) b_{n',l,m}(0) z_{l,n} z_{l,n'} \frac{J_{l+1/2}'(z_{l,n}) J_{l+1/2}'(z_{l,n'})}{J_{l+3/2}(z_{l,n}) J_{l+3/2}(z_{l,n'})} \right\}, \end{aligned} \quad (D17)$$

that can be written as

$$\dot{\mathcal{E}}(0) = -\frac{\hbar^2}{\mu R_0^3} v \left\{ \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} z_{l,n}^2 |b_{n,l,m}(0)|^2 + \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{n,l,m}^*(0) b_{n',l,m}(0) z_{l,n} z_{l,n'} \right\}. \quad (D18)$$

The energy density in this case is

$$\rho_3(\mathbf{r}, t) = \frac{\hbar^2}{2\mu} \nabla \Psi^*(\mathbf{r}, t) \cdot \nabla \Psi(\mathbf{r}, t) \quad (D19)$$

where

$$\nabla \Psi(\mathbf{r}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} e^{-i\theta_{l,n}} b_{n,l,m}(t) \frac{\sqrt{2}}{R(t)^{3/2} j_{l+1}(k_{l,n} a)} \left[\frac{\partial}{\partial r} j_l(k_{l,n} r) \mathbf{Y}_{l,m} + \frac{1}{r} j_l(k_{l,n} r) \Psi_{l,m} \right] \quad (D20)$$

where $\mathbf{Y}_{l,m} = Y_{l,m}(\theta, \psi) \hat{r}$ and $\Psi_{l,m} = r \nabla Y_{l,m}(\theta, \psi)$ are the vector spherical harmonics [24], this follow the orthogonality relation $\Psi_{l,m} \cdot \mathbf{Y}_{l,m} = 0$. Analogously,

$$\nabla \Psi^*(\mathbf{r}, t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} e^{i\theta_{l,n}} b_{n,l,m}^*(t) \frac{\sqrt{2}}{R(t)^{3/2} j_{l+1}(k_{l,n} a)} \left[\frac{\partial}{\partial r} j_l(k_{l,n} r) \mathbf{Y}_{l,m}^* + \frac{1}{r} j_l(k_{l,n} r) \Psi_{l,m}^* \right] \quad (D21)$$

thus,

$$\begin{aligned} \rho_3(\mathbf{r}, t) = & \frac{\hbar^2}{2\mu} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{m'=l'} \sum_{n'=1}^{\infty} \frac{2 b_{n,l,m}(t) b_{n',l',m'}^*(t)}{R(t)^3 j_{l+1}(z_{l',n'}) j_{l'+1}(z_{l',n'})} e^{i(\theta_{l,n'}(t) - \theta_{l,n}(t))} \\ & \left[\frac{\partial}{\partial r} j_l(k_{l,n} r) \frac{\partial}{\partial r} j_{l'}(k_{l',n'} r) \mathbf{Y}_{l',m'}^* \cdot \mathbf{Y}_{l,m} + \frac{1}{r^2} j_l(k_{l,n} r) j_{l'}(k_{l',n'} r) \Psi_{l,m}^* \cdot \Psi_{l',m'} \right] \end{aligned} \quad (D22)$$

we want to know the total force exerted by the particle on the boundary $\mathcal{F} = \int_0^{2\pi} \int_0^\pi \rho_3(\mathbf{r}, t) \delta(r - R_0) r^2 dr d\Omega$.

The vector spherical harmonics satisfy the integral equations relations

$\int_0^{2\pi} \int_0^\pi \Psi_{l,m}^* \cdot \Psi_{l',m'} d\Omega = l(l+1) \delta_{l,l'} \delta_{m,m'}$ and $\int_0^{2\pi} \int_0^\pi \mathbf{Y}_{l,m}^* \cdot \mathbf{Y}_{l',m'} d\Omega = \delta_{l,l'} \delta_{m,m'}$, thus we have

$$\rho_3^E(R_0, 0) = \frac{\hbar^2}{2\mu} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \frac{2 b_{n,l,m}(0) b_{n',l,m}^*(0) z_{l,n} z_{l,n'}}{R_0^3 j_{l+1}(z_{l,n'}) j_{l+1}(z_{l,n'})} [j_l'(z_{l,n}) j_l'(z_{l,n'})]. \quad (D23)$$

Finally, using the properties of the Bessel functions, we get

$$\rho_3^E(R_0, 0) = \frac{\hbar^2}{\mu R_0^3} \sum_{l=0}^{\infty} \sum_{m=-l}^{m=l} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} b_{n,l,m}(0) b_{n',l,m}^*(0) z_{l,n} z_{l,n'} \quad (D24)$$

ORCID iDs

Adrian Ortega  <https://orcid.org/0000-0001-5816-7274>

Hernán Larralde  <https://orcid.org/0000-0002-6037-2629>

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