Quantum dynamics in a time-dependent hard-wall spherical trap

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Abstract – Exact solution of the Schrödinger equation is given for a particle inside a hard sphere whose wall is moving with a constant velocity. Numerical computations are presented for both contracting and expanding spheres. The propagator is constructed and compared with the propagator of a particle in an infinite square well with one wall in uniform motion.

Exact solution. – Consider a particle with mass $\mu$ inside a hard sphere with a time-dependent radius $L(t)$. The potential energy function is zero if $r < L(t)$ and infinity otherwise. The Schrödinger equation is then

$$i\hbar \frac{\partial}{\partial t} \Psi(r,t) = -\frac{\hbar^2}{2\mu} \nabla^2 \Psi(r,t),$$

with the boundary condition $\Psi(r,t)|_{r=L(t)} = 0$.

The instantaneous energy eigenfunctions and eigenvalues are, respectively,

$$u_{lnm}(r,t) = \sqrt{\frac{2}{L^3(t)}} \frac{1}{|j_{l+1}(x_{ln})|} j_l \left( \frac{x_{ln} r}{L(t)} \right) Y_{lm}(\theta,\phi),$$

$$E_{ln}(t) = \frac{\hbar^2 x_{ln}^2}{2\mu L^2(t)},$$

for $l = 0, 1, 2, \ldots; n = 1, 2, 3, \ldots$ and $m = -l, -l+1, \ldots, l-1, l$, where $j_l(x)$ and $Y_{lm}(\theta,\phi)$ are, respectively, spherical Bessel functions and harmonics. $x_{ln}$ is the $n$-th zero of the spherical Bessel function of order $l$, i.e., $j_l(x_{ln}) = 0$. It must be noted that all Bessel functions with $l \neq 0$ have a zero at the origin, but to have a non-zero wave function these zeros must be excluded.

Using the method of “separation of variables” for solving the partial differential equation (1), we propose the solution

$$\Psi(r,t) = \frac{U(r,t)}{r} Y_{lm}(\theta,\phi),$$

where we have used the spherical symmetry of the Hamiltonian.
Putting eq. (4) into eq. (1) one gets
\[ i\hbar \frac{1}{r} \frac{\partial U(r,t)}{\partial t} = \frac{\hbar^2}{2\mu} \left[ \frac{\partial^2 U(r,t)}{r \partial r^2} - \frac{l(l+1)}{r^2} U(r,t) \right]. \tag{5} \]

The radial part of the proposed wave function, \( R(r,t) = U(r,t)/r \), must be zero on the shell, thus the boundary conditions on \( U(r,t) \) are \( U(r,t)|_{r=0} = 0 = U(r,t)|_{r=L(t)} \).

Now, we follow [2] to solve the eq. (5). By defining a new coordinate
\[ s = \frac{r}{L(t)}, \tag{6} \]
we get
\[ i\hbar \frac{\partial U(s,t)}{\partial t} = i\hbar \frac{\partial }{ \partial s } U(s,t) - \frac{\hbar^2}{2\mu} \frac{1}{L^2(t)} \frac{\partial^2 U(s,t)}{\partial s^2} - \frac{l(l+1)}{s^2} U(s,t), \tag{7} \]
where \( L(t) = \frac{dL(t)}{dt} \) and moving boundary conditions are replaced by fixed-boundary ones; \( U(s,t)|_{s=0} = 0 = U(s,t)|_{s=1} \). When the transformation
\[ U(s,t) = \sqrt{\frac{2}{L(t)}} \exp \left[ \frac{i\mu}{2\hbar} L(t) \frac{s^2}{2} \right] \phi(s,t), \tag{8} \]
is introduced in eq. (7), one obtains
\[ i\hbar \frac{\partial \phi(s,t)}{\partial t} = -\frac{\hbar^2}{2\mu} \frac{1}{L^2(t)} \frac{\partial^2 \phi(s,t)}{\partial s^2} - \frac{l(l+1)}{s^2} \phi(s,t), \tag{9} \]
for the uniform motion of the wall, \( \tilde{L}(t) = 0 \). Boundary conditions on \( \phi(s,t) \) are \( \phi(s,t)|_{s=0} = 0 = \phi(s,t)|_{s=1} \). Defining the new time variable \( \tau \) as
\[ \tau(t) = \int_0^t \frac{dt'}{L(t')} \Rightarrow \frac{\partial }{ \partial \tau } = \frac{1}{L(t)} \frac{\partial }{ \partial t }, \tag{10} \]
eq (9) transforms to
\[ i\hbar \frac{\partial \phi(s,\tau)}{\partial \tau} = -\frac{\hbar^2}{2\mu} \left[ \frac{\partial^2 \phi(s,\tau)}{\partial s^2} - \frac{l(l+1)}{s^2} \phi(s,\tau) \right]. \tag{11} \]
Inserting \( \phi(s,\tau) = \exp(-iE'\tau/\hbar)\psi(s) \) in (11), one gets
\[ E'\psi(s) = -\frac{\hbar^2}{2\mu} \left[ \frac{\partial^2 \psi(s)}{\partial s^2} - \frac{l(l+1)}{s^2} \psi(s) \right]. \tag{12} \]
By introducing new variable \( k^2 = 2\mu E'/\hbar^2 \), we obtain
\[ \frac{\partial^2 \psi(s)}{\partial s^2} + \left( k^2 - \frac{l(l+1)}{s^2} \right) \psi(s) = 0. \tag{13} \]
The solutions of this equation are the spherical Bessel functions
\[ \psi(s) = s[c_1 j_l(ks) + c_2 n_l(ks)]. \tag{14} \]
If the radial wave function \( R(r) \) is finite at the origin, \( c_2 = 0 \). The requirement that \( \psi(s) = 0 \) at \( s = 1 \) means that \( k \) can take on only those special values
\[ k_n = x_n \quad (n = 1, 2, 3, \ldots). \tag{15} \]
For the uniform change of the radius with velocity \( u \)
\[ L(t) = a + ut, \tag{16} \]
where \( a \) is the initial radius, one has
\[ \tau(t) = \frac{t}{a(a + ut)}. \tag{17} \]
By using eqs. (17), (16), (15), (8) and (6) one obtains
\[ R_{ln}(r,t) = c_1 \sqrt{\frac{2}{L(t)}} \exp \left[ \frac{i\mu}{2\hbar} \frac{r^2}{L(t)} - \frac{i}{2\mu} \frac{\hbar^2}{aL(t)} \right] \times j_l \left( x_n \frac{r}{L(t)} \right), \tag{18} \]
for the radial part of the wave function. Unknown coefficient \( c_1 \) is determined by the normalization condition
\[ \int_0^{L(t)} dr \int d\Omega |\Psi_{lnm}(r,t)|^2 = 1, \tag{19} \]
where
\[ \Psi_{lnm}(r,t) = R_{ln}(r,t)Y_{lm}(\theta, \phi). \tag{20} \]
are the solutions of the Schrödinger equation (1) for a particle in a spherical box with a wall in uniform motion and
\[ \int d\Omega = \int_{-1}^1 d(cos \theta) \int_0^{2\pi} d\phi. \]
Using the orthogonality of the spherical Bessel functions [11]
\[ \int_0^1 ds \, s^2 j_l(xlns) j_l(xlns) = \frac{1}{2} [j_{l+1}(xln)]^2 \delta_{nm}, \tag{21} \]
one obtains
\[ |c_1|^2 = \frac{1}{L(t)} \frac{1}{[j_{l+1}(xln)]^2}. \tag{22} \]
Thus, apart from a phase factor, one obtains
\[ \Psi_{lnm}(r,t) = \frac{1}{L(t)} \sqrt{\frac{2}{L(t)}} \frac{1}{[j_{l+1}(xln)]} \]
\[ \times \exp \left[ \frac{i\mu}{2\hbar} \frac{r^2}{L(t)} - \frac{i}{2\mu} \frac{\hbar^2}{aL(t)} \right] \]
\[ \times j_l \left( x_n \frac{r}{L(t)} \right) Y_{lm}(\theta, \phi) \equiv \exp \left[ i\alpha \xi(t) \left( \frac{r}{L(t)} \right)^2 - i\frac{\hbar^2}{aL(t)} \frac{1-1}{4\alpha} \right] \]
\[ \times u_{lnm}(r,t), \tag{23} \]
where we have introduced new dimensionless parameters \( \alpha = \mu au/(2\hbar) \) and \( \xi(t) = L(t)/a \).
Functions $\Psi_{lnm}(r, t)$ vanish at $r = L(t)$, remain normalized as the radius changes, and form a complete orthogonal set. The general solution of eq. (1) is a superposition of functions (23),

$$\Psi(r, t) = \sum_{l' = 0}^{\infty} \sum_{n' = 1}^{\infty} \sum_{m' = -l'}^{l'} c_{l'n'm'}(r, t) \Psi_{l'n'm'}(r, t),$$  \tag{24}$$

with time-independent coefficients $c_{l'n'm'}$ determined from the relation

$$c_{l'n'm'} = \int_0^a dr r^2 \int d\Omega \Psi_{l'n'm'}^*(r, 0) \Psi(r, 0).$$ \tag{25}$$

The general solution can also be expanded in terms of instantaneous eigenfunctions as

$$\Psi(r, t) = \sum_{l' = 0}^{\infty} \sum_{n' = 1}^{\infty} \sum_{m' = -l'}^{l'} b_{l'n'm'}(t) u_{l'n'm'}(r, t),$$ \tag{26}$$

now with time-dependent coefficients $b_{l'n'm'}(t)$ determined from the relation

$$b_{l'n'm'}(t) = \int_0^{L(t)} dr r^2 \int d\Omega u_{l'n'm'}^*(r, t) \Psi(r, t).$$ \tag{27}$$

Using eqs. (27) and (24) and the orthogonality of the spherical harmonics, one finds

$$b_{l'n'm'}(t) = \frac{2}{[j_{l' + 1}]^2} \sum_{n'' = 1}^{\infty} c_{l'n'm'} \frac{1}{[j_{l' + 1}]} \exp \left[-i\xi^2 \frac{1 - 1/n}{4a} \right] I_{l'n'm'}(t, \alpha),$$ \tag{28}$$

where

$$I_{l'n'm'}(t, \alpha) = \int_0^1 ds s^{2} e^{-i\alpha \xi s} j_{l'}(x_{l'n'm'} s) j_{l'}(x_{l'n'm'} s).$$ \tag{29}$$

This integral is not elementary and following the procedure of [8], can be reduced to a combination of terms involving the Fresnel integrals and the derivative of the Legendre polynomials.

The expectation value of the energy of the particle is obtained from

$$\langle E(t) \rangle = \sum_{l'n'm'} |b_{l'n'm'}|^2 E_{l'n'm'}(t).$$ \tag{30}$$

If the particle is initially in an energy eigenstate, i.e., $\Psi(r, 0) = u_{l'm'}(r, 0)$, then

$$c_{l'n'm'} = \delta_{l'l} \delta_{m'm'} \frac{2}{[j_{l'+1}]} \frac{1}{[j_{l'+1}]} I_{lm}(0, \alpha),$$ \tag{31}$$

which is not an unexpected result as the quantum numbers $l$ and $m$ do not change.

Fig. 1: (Color online) Transition probabilities vs. $\xi(t)$ for different values of the velocity parameter $\alpha$: (a) $\alpha = -2$; (b) $\alpha = -4$; (c) $\alpha = -6$ and (d) $\alpha = -10$. In each part the black curve shows $|b_{111m}|^2$, the red one $|b_{122m}|^2$, the green one $|b_{133m}|^2$ and the blue one $|b_{144m}|^2$.

Fig. 2: (Color online) Ratio of the energy expectation value to the instantaneous first excited energy as a function of $\xi(t)$ for three different values of the velocity parameter.

**Numerical calculations.** – Numerical computations are shown in figs. 1 and 2 for a particle that is initially in the first excited state with threefold degeneracy. In this case we have

$$\frac{\langle E(t) \rangle}{E_{11m}(t)} = \sum_{n'} |b_{1n'm'}|^2 \left( \frac{x_{1n'}}{x_{11}} \right)^2,$$ \tag{32}$$

for the ratio of energy expectation value to the instantaneous first excited state energy.

Figure 1 shows the squares of energy eigenfunction expansion coefficients vs. $\xi(t)$ for three different contraction rates $\alpha$. For these values of $\alpha$, it was found that series (28) converges for the first ten terms.

Figure 2 shows the ratio of the expectation value of the energy to the energy the particle would have if it remained in the first excited state $u_{11m}$ for the sphere in contraction. Here fifteen terms in eq. (32) lead to convergency.

We have plotted the dimensionless radial probability density $p_{lnm}(\eta \bar{t}, T_{ln}) = \lambda_{lnm} \eta^2 [R(\eta, T_{ln})/2]^{2}$ in fig. 3 for a particle initially in the state $u_{l000}$, vs. the dimensionless position coordinate $\eta_{ln} = r/\lambda_{ln}$ at the dimensionless
where the dimensionless position coordinate \( \eta_n \) at the time coordinate \( T_{ln} \), for six different values of the expansion rate; \( \alpha = 0 \) (black curve), \( \alpha = 0.01\alpha_n \) (red curve), \( \alpha = \alpha_n \) (green curve), \( \alpha = 10\alpha_n \) (blue curve), \( \alpha = 15\alpha_n \) (yellow curve) and \( \alpha = 20\alpha_n \) (magenta curve); where \( \alpha_n = x_{ln}/2 \).

**Propagator.** – One can construct the propagator as follows:

\[
|\Psi(t)\rangle = S(t,t_0)|\Psi(t_0)\rangle
= \sum_{ln} \sum_{l'n'm'} |\Psi_{lnm}(t)\rangle \langle \Psi_{lnm}(t)|S(t,t_0)|\Psi_{l'n'm'}(t_0)\rangle \\
\times \langle \Psi_{l'n'm'}(t_0)|\Psi(t_0)\rangle
= \sum_{ln} |\Psi_{lnm}(t)\rangle \langle \Psi_{lnm}(t_0)|\Psi(t_0)\rangle,
\]

where \( S(t,t_0) \) is the time evolution operator and we have used the fact that if the particle is in the state \(|\Psi_{lnm}(t_0)\rangle\) at \( t_0 \), it remains in that state as the wall moves, i.e., \( S(t,t_0)|\Psi_{lnm}(t_0)\rangle = |\Psi_{lnm}(t)\rangle \). Now, we write this equation in the form

\[
\Psi(r,t) = \int_0^a \int_0^\pi d\phi d^2t' \int d\Omega K(r,t; x', t') \Psi(r', \theta', \phi', t'),
\]

where we have introduced the propagator as

\[
K(r,t; x', t') = \sum_{l=0}^\infty \sum_{n=1}^\infty \sum_{m=-l}^l \Psi_{lnm}(r,t)\Psi^*_{lnm}(r', t')
= \frac{2}{L^{3/2}(t)L^{3/2}(t')} \sum_{lm} \frac{1}{|j_{l+1}(x_{ln})|^2}
\times \exp \left[ \frac{ip\mu \alpha}{2\hbar} \left( \frac{r^2}{L(t)} - \frac{r'^2}{L(t')} \right) \right]
\times \exp \left[ -i\hbar \frac{x_{ln}}{2\mu \alpha} \left( \frac{t}{L(t)} - \frac{t'}{L(t')} \right) \right]
\times j_l \left( x_{ln} \frac{r}{L(t)} \right) j_l \left( x_{ln} \frac{r'}{L(t')} \right)
\times Y_{lnm}(\theta, \phi) Y^*_{lnm}(\theta', \phi').
\]

One can see that when \( l = 0 \), eq. (7) reduces to eq. (4) of [2], i.e., \( l = 0 \) corresponds to a particle in a 1D box with the left wall at \( x = 0 \) and the right wall in uniform motion. In order to have the relation

\[
\Psi(x,t) = \int_0^a K_{1D}(x,t; x', 0)\Psi(x', 0)dx',
\]

in 1D, we must write the 1D propagator as

\[
K_{1D}(x,t; x', t') = \frac{r'^2}{4\pi} K(r,t; x', t')
\equiv \sum_{n=1}^\infty \frac{U_{ln}(r) U^*_{ln}(r')}{\sqrt{4\pi}}
\times \sqrt{4\pi}.
\]
By preserving just the terms with $l = 0$, eq. (34) becomes

$$K(r, t; r', t') = \frac{2}{L^{3/2}(t)L^{3/2}(t')} \sum_{n=1}^{\infty} \frac{1}{|j_1(x_{0n})|^2} \times \exp \left[ \frac{i\mu u}{2\hbar} \left( r^2 - L(t) - r'^2 - L(t') \right) \right] \times \exp \left[ \frac{-ih}{2\mu a} \left( \frac{t}{L(t)} - \frac{t'}{L(t')} \right) \right] \times j_0 \left( x_{0n} \frac{r}{L(t)} \right) j_0 \left( x_{0n} \frac{r'}{L(t')} \right) \times \frac{1}{\sqrt{4\pi}} \frac{1}{\sqrt{4\pi}},$$ (37)

where we have used $Y_0 = 1/\sqrt{4\pi}$. The first two Bessel functions are

$$j_0(x) = \frac{\sin x}{x}, \quad j_1(x) = \frac{\sin x}{x^2} - \cos x,$$ (38)

thus $x_{0n} = n\pi$ and $j_1(x_{0n}) = (-1)^{n+1}/n\pi$. Using these in eq. (37), we find

$$K(r, t; r', t') = \frac{1}{4\pi rr'} \frac{2}{\sqrt{L(t)L(t')}} \times \exp \left[ \frac{i\mu u}{2\hbar} \left( r^2 - L(t) - r'^2 - L(t') \right) \right] \times \sum_{n=1}^{\infty} \exp \left[ \frac{ih}{2\mu a} \left( \frac{1}{L(t)} - \frac{1}{L(t')} \right) \right] \times \sin \left( n\pi \frac{r}{L(t)} \right) \sin \left( n\pi \frac{r'}{L(t')} \right).$$ (39)

Now from eq. (36) we obtain

$$K_{1D}(x, t; x', t') = \frac{2}{\sqrt{L(t)L(t')}} \times \exp \left[ \frac{i\mu u}{2\hbar} \left( \frac{x^2}{L(t)} - \frac{x'^2}{L(t')} \right) \right] \times \sum_{n=1}^{\infty} \exp \left[ \frac{ih}{2\mu u} \left( \frac{1}{L(t)} - \frac{1}{L(t')} \right) \right] \times \sin \left( n\pi \frac{x}{L(t)} \right) \sin \left( n\pi \frac{x'}{L(t')} \right),$$ (40)

which is exactly eq. (32) of ref. [9] for the propagator of a particle in a 1D box. This equation can be written in a compact form as a combination of $\vartheta_3$ functions [10].

**Summary and discussion.** – In this letter we found solutions of the Schrödinger equation for a particle confined in a hard spherical trap with a wall moving at constant velocity. We see that in solutions (23), except for the phase factor $\exp(-i \int dt E_{inn}(t)/\hbar)$ which has no coordinate dependence, a coordinate-dependent phase $\exp[\frac{ih}{2\mu u} \frac{1}{2\pi}]$ appears. It has been shown that this factor leads to an effective quantum non-local interaction with the boundary: even though the particle is nowhere near the walls, it will be affected [1,12].

From fig. 1, one can see that as the velocity of the wall increases, larger amounts of energy states other than the initial one, i.e., $u_{11m}$, are mixed in. Figure 2 shows that for rapid contraction, the energy expectation value increases faster than the $1/L^2(t)$ increase which would be obtained in a quasi-static contraction. These results are in agreement with the ones of ref. [3] obtained for a particle in an infinite square well with one wall in uniform motion. Confinement of the particle to a smaller region leads to the enhancement of the energy expectation value. This can be explained by an application of the “old quantum theory” [13] or by uncertainty relations [14].

In the process of expansion, there are two characteristic times involved: $t_e$, over which the parameters of the system change appreciably, and $t_i$, representing the motion of the system itself. In our calculations, $t_e = a/u$ and $t_i = a/v_{in}$. Figure 3 shows that for $t_e \gg t_i$ ($u \ll v_{in}$), the particle, initially in the state $u_{0,0,0}$, will end up in the corresponding state of the expanded well. This process characterizes an adiabatic one for which external conditions change gradually [15], while, in the opposite limit, rapidly changing conditions prevent the system from adapting its configuration during the process, hence the probability density remains almost unchanged.

Looking at fig. 4, one can see a quasi-classical behavior in the high-energy limit [16] as the velocity of the wall increases. A non-monotonous increasing behavior of the density is seen for $T < T_1$ only when $u > v_{in}$, while for $T > T_2$ a non-monotonous decreasing behavior is seen irrespectively of the wall velocity. These results are in contrast to classical mechanics. The height of the first maximums decreases with $u$. The constructive interference with the reflected components from the wall for $u < v_{in}$ leads to this enhancement. The long-time behavior of the density in a given observation point, is the same for all values of the wall velocity, which is not an unexpected result considering the behavior of functions $\Psi_{inn}$ at long times.

The propagator of the problem was derived using the spectral decomposition.

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REFERENCES

[1] Makowski A. J., J. Phys. A: Math. Gen., 25 (1992) 3419.
[2] Makowski A. J. and Dembinski S. T., Phys. Lett. A, 154 (1991) 217.
[3] Doescher S. W. and Rice M. H., Am. J. Phys., 37 (1969) 1246.
[4] del Campo A., García-Calderón G. and Muga J. G., Phys. Rep., 476 (2009) 1.
[5] Moshinsky M., Phys. Rev., 88 (1952) 625.
[6] del Campo A., Muga J. G. and Kleber M., Phys. Rev. A, 77 (2008) 013608.
[7] Godoy S., Phys. Rev. A, 65 (2002) 42111; del Campo A. and Muga J. G., Europhys. Lett., 74 (2006) 965; Mousavi S. V., J. Phys. A: Math. Theor., 43 (2010) 035304.
[8] Godoy S., Phys. Rev. A, 67 (2003) 012102.
[9] da Luz M. G. E. and Cheng B. K., J. Phys. A: Math. Gen., 25 (1992) L1043.
[10] Grosche Ch., Phys. Lett. A, 182 (1993) 28.
[11] Arfken G. B. and Weber H. J., Mathematical Methods for Physicists (Elsevier Academic Press) 2005.
[12] Dodonov V. V. and Andrea M. A., Phys. Lett. A, 275 (2000) 173; Greenberger D. M., Physica B, 151 (1988) 374; Mousavi S. V., arXiv:1111.3962v3, preprint (2011).
[13] Pinder D. N., Am. J. Phys., 58 (1989) 54.
[14] Wilhelm H. E., J. Phys. A: Math. Gen., 16 (1983) 2149.
[15] Griffiths D. J., Introduction to Quantum Mechanics (Prentice Hall, NJ) 1994.
[16] Godoy S., Physica B, 390 (2007) 112.