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Quantum dynamics of hydrogen-like atom in one-dimensional box with oscillating walls

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The quantum dynamics of a hydrogen-like atom confined in one-dimensional box with oscillating walls is studied. The description of the system is reduced to a one-dimensional Schrödinger equation for Coulomb potential with time-dependent boundary conditions, which is solved numerically. Using the obtained solution, the average kinetic energy and binding energies are calculated as a function of time. It is found that both the average kinetic energy and the binding energies are periodic in time with the period depending on the wall's oscillation parameters. The probability density is also analyzed as a function of time and coordinate.

Keywords: confined atom, time-dependent box, average kinetic energy, atom-optic billiards.

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1. Introduction

The behavior of matter under the spatial confinement is of importance for many topics in contemporary nanoscale physics. Macroscopic properties of confined matter are considerably different than those of bulk matter. Such a difference is caused by underlying microscopic phenomena implying the difference between the quantum mechanical properties of atoms and molecules in confined and bulk spaces. The latter means that quantum mechanical wave equations describing atoms and molecules in bulk and confined spaces have different solutions which depend on the boundary conditions for such spaces. As the macroscopic characteristics (e.g., heat capacity, dielectric constant, thermal conductance, etc.) are obtained by statistical averaging of the microscopic quantities (to be calculated using the solution for the quantum mechanical wave functions) the results for confined and bulk matters should be different. Therefore, study of the behavior of atoms and molecules under confinement at the quantum mechanical level is of importance for understanding macroscopic features of confined matter. In this work, we address the problem of atom confined in a hard wall box by considering a one dimensional system. Such hard wall confinement can be realized by putting the atom in a strong constant electric field or in a so-called atom-optic billiards [1-3]. Here, we focus on the time-dependent boundaries, i.e. when the wall of a box is harmonically oscillating. Earlier, the box with oscillating walls has been the subject for extensive research(see e.g., [4-14]). By solving the time-dependent Schrödinger equation with time-dependent boundary conditions for Coulomb potential, we compute the time-dependence of the average energy, and the evolution of the probability density . Before proceeding to the treatment of the time-dependent system, in the next section, we briefly recall the description of the static system.

2. The one-dimensional Coulomb atom

Consider electron motion in a one-dimensional singular Coulomb field (atomic system of units is used $\hbar = m = e = 1$):

$$V(x) = -\frac{Z}{|x|}. \tag{1}$$

Such system is described by one-dimensional Schrödinger equation given as [15-17]:

$$-\frac{1}{2}\frac{d^2\psi}{dx^2} - \frac{Z}{|x|}\psi = E\psi. \tag{2}$$

The general solution of this equation can be written as:

$$\psi(x) = N(Z,E)\exp\left\{-\alpha|x|\right\}{}_1F_1\left(1-\sqrt{-2E},2,\frac{2|x|}{\sqrt{-2E}}\right). \tag{3}$$

For an atom in bulk space, i.e. in the absence of confinement, one can require exponential decay of the wave function at $|x| \to \infty$ which leads to quantization condition of the form:

$$E_n = -\frac{Z^2}{2n^2}.$$

Then, the wave functions can be written as:

$$\psi(x) = \sqrt{\frac{2}{n^3}}|x|(sgn(n))^\sigma \exp\left\{-\frac{|x|}{n}\right\}{}_1F_1\left(1-n,2,\frac{2|x|}{n}\right), \tag{4}$$

where $n = 1, 2, ..., \infty$ and ${}_1F_1$ is the confluent hypergeometric function.

For an atom confined in a one-dimensional box, the problem can be solved by imposing boundary conditions given as:

$$\psi(x = L) = 0,$$

where L is the size (length) of the box. Then, from Eq.(3), we have quantization condition in the form:

$${}_1F_1\left(1-\sqrt{-2E},2,\frac{2|L|}{\sqrt{-2E}}\right) = 0, \tag{5}$$

which allows us to find eigenvalues(energy levels) for the confined atom. In Fig. 1, the first 7 eigenvalues of the hydrogen-like atom with charge $Z = 1$ in one dimensional box of size $L = 50$ are presented together with the Coulomb potential of the atomic nucleus.

3. Hydrogen-like atom confined in one-dimensional box with oscillating walls

Our purpose is to evaluate the quantum dynamics of the one-electron atom confined in a box with time-dependent walls. Such a system is described by the one-dimensional time-dependent Schrödinger equation for Coulomb potential. The time-dependence is caused by time-dependent boundary conditions imposed for the Schrödinger equation. Thus the Schrödinger equation we are going to treat can be written as:

$$i\frac{\partial\Psi(x,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2} - \frac{Z}{x}\Psi(x,t), \tag{6}$$

where the boundary condition is given as:

$$\Psi(L(t),t) = 0,$$

where $L = L(t)$.

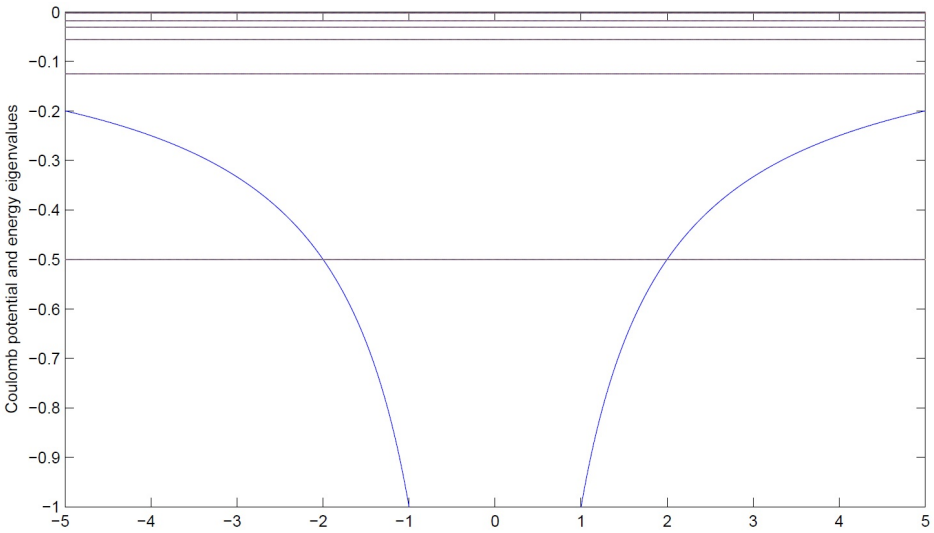

FIG. 1. Energy eigenvalues of the one-dimensional hydrogen-like atom confined in a box compared with Coulomb potential acting on an atomic electron

Using the coordinate transformations given by:

$$y = \frac{x}{L(t)}, \tag{7}$$

one can reduce these boundary conditions into time-independent form which can be written as:

$$\Psi|_{y=1} = 0.$$

Then Eq.(6) can be written as

$$i\frac{\partial\Psi(y,t)}{\partial t} = -\frac{1}{2L^2}\frac{\partial^2\Psi(y,t)}{\partial y^2} + i\frac{\dot{L}}{L}y\frac{\partial\Psi(y,t)}{\partial y} - \frac{Z}{Ly}\Psi(y,t). \tag{8}$$

This equation contains an imaginary term that breaks self-adjointness of the problem. To restore the self-adjointness we use the following transformation for the wave function:

$$\Psi(y,t) = \sqrt{\frac{1}{L}}e^{\frac{i}{2}L\dot{L}y^2}\Phi(y,t). \tag{9}$$

Then, inserting this into Eq.(8), we have:

$$i\frac{\partial\Phi}{\partial t} = -\frac{1}{2L^2}\frac{\partial^2\Phi}{\partial y^2} + \frac{1}{2}L\ddot{L}y^2\Phi - \frac{Z}{Ly}\Phi. \tag{10}$$

To solve Eq.(10), we expand $\Phi(y,t)$ in terms of a complete set of the eigenfunctions of the static one-dimensional box: $\varphi_n(y)$:

$$\Phi(y,t) = \sum_n C_n(t)\varphi_n(y), \tag{11}$$

where $\varphi_n(y)$ are the eigenfunctions of the stationary Schrödinger equation for one-dimensional box of size $L = 1$:

$$-\frac{1}{2L^2}\frac{d^2\varphi_n(y)}{dy^2} = E_n\varphi_n(y), \tag{12}$$

obeying the following normalization conditions:

$$\int_0^1 \varphi_n(y)\varphi_m^*(y)dy = \delta_{nm}.$$

Inserting expansion (11) into Eq.(10), we obtain a system of first order differential equations with respect to the expansion coefficients, $C_n(t)$:

$$i\dot{C}_n(t) = E_n C_n(t) + \sum_m V_{nm} C_m(t), \tag{13}$$

where:

$$V_{nm} = \frac{1}{2}L\ddot{L}\int_0^1 y^2\varphi_n(y)\varphi_m^*(y)dy - \frac{Z}{L}\int_0^1 \frac{1}{y}\varphi_n(y)\varphi_m^*(y)dy.$$

Solving Eqs.(13), one can find the wave function for the hydrogen-like atom confined in a one-dimensional box with oscillating walls. Having found the wave function, we can calculate physically observable quantities, such as time-dependent average kinetic energy, $\langle E(t)\rangle$ and the binding energy $\langle\varepsilon(t)\rangle$. The average kinetic energy can be calculated as:

$$E(t) = \int_0^{L(t)} \Psi^*(x,t)\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}\right)\Psi(x,t)dx = \frac{1}{2}\int_0^{L(t)}\left|\frac{\partial\Psi}{\partial x}\right|^2 dx \tag{14}$$

or as:

$$E(t) = \sum_n |C_n(t)|^2 E_n + \frac{1}{2}\dot{L}^2\sum_n\sum_m C_n^*(t)C_m(t)\int_0^1 y^2\varphi_n^*(y)\varphi_m(y)dy + \\ + \frac{\dot{L}}{4L}\mathrm{Im}\left(\sum_m C_n^*(t)C_m(t)\int_0^1 y\frac{\partial\varphi_n(y)}{\partial y}\varphi_m(y)dy\right). \tag{15}$$

In Fig. 2, the average kinetic energy, $\langle E(t)\rangle$ and the binding energy, $\langle\varepsilon(t)\rangle$ are plotted as a function of time for the wall's oscillation frequency $\omega = 1$ and amplitude $a = 0.4$ for the box size $L = 1$. Fig. 3 presents similar plots for the wall's oscillation parameter values $\omega = 3$ and amplitude $a = 0.4$ ($L = 1$). As it can be seen from these plots, both the average kinetic and average binding energies show a certain periodicity in time and the period depends on that of wall's oscillation; that is, the longer the wall's oscillation frequency, the shorter the period for its average kinetic energy. Such a correlation between the behavior of the average kinetic energy and wall's oscillation parameters allows one to tune the atomic electron's acceleration, the pressure on the atom and electronic state transitions.

An important quantity which can be measured in experimentally by realizing the above model in atom-optic billiards, is the probability density. Fig. 4 presents plots of the probability density corresponding to Figs. 2 and 3. Periodicity in the temporospatial localization of an atomic electron can be observed from these plots. This explains the periodicity of the average kinetic energy as a function of time.

4. Conclusions

In this work, we studied the quantum dynamics of the one-electron atom confined in a one-dimensional box with oscillating wall. Time-evolutions of the average kinetic and binding energies are analyzed by solving the time-dependent Schrödinger equation for Coulomb potential with time-dependent boundary conditions. The latter is solved numerically by expanding the wave function in terms of static system eigenfunctions. Both the average kinetic and the binding energies were found to be periodic in time. Additionally, the temporospatial evolution of the probability density was computed. The probability density clearly exhibits

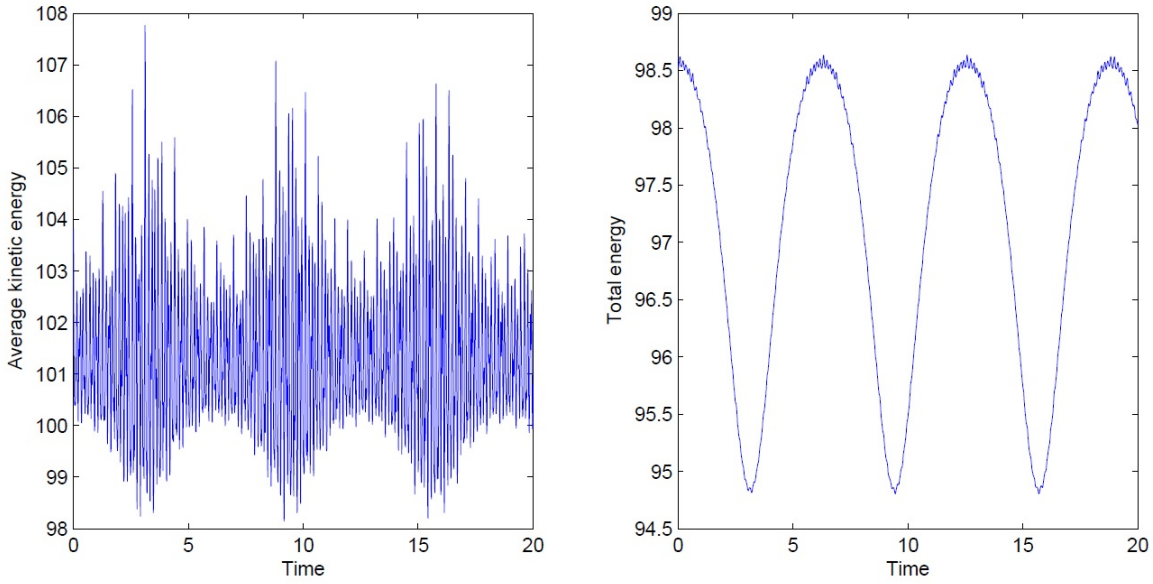

FIG. 2. Time dependence of the average kinetic and total energy ($\omega = 1, A = 0.4$)

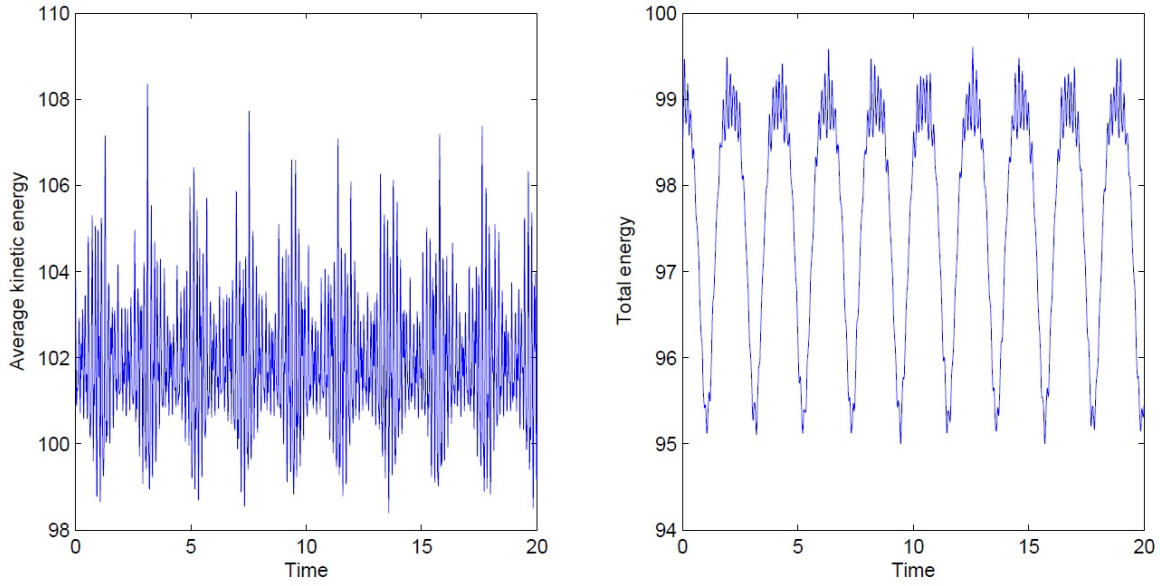

FIG. 3. Time dependence of the average kinetic and total energy ($\omega = 3, A = 0.4$)

periodicity in both space and time. The model studied in this paper can be realized for so-called atom-optic billiards which provide spatial confinement with the required boundary geometry. The obtained results are importance for the study of atomic behavior under high pressure confinement. That information is necessary for the engineering of mechanical and electric nanoscale devices with tunable properties.

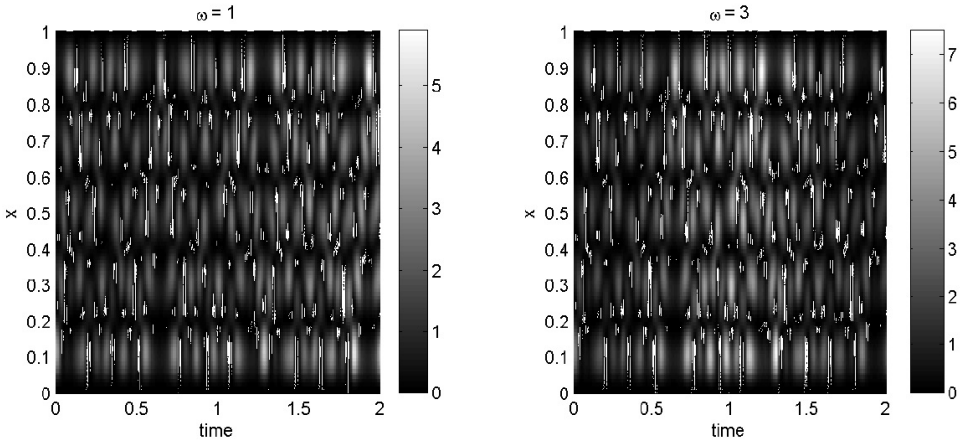

FIG. 4. Time and coordinate dependence of the probability density ($\omega = 1$ and $\omega = 3, A = 0.4$)

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