Kicked Dirac particle in a box

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We study quantum dynamics of a kicked relativistic spin-half particle in a one dimensional box. Time-dependence of the average kinetic energy and evolution of the wave packet are explored. Kicking potential is introduced as the Lorentz-scalar, i.e., through the mass-term in the Dirac equation. It is found that depending on the values of the kicking parameters \( E(t) \) can be periodic, monotonically growing and non-periodic function of time. Particle transport in the system is studied by considering spatio-temporal evolution of the Gaussian wave packet. Splitting of the packet into two symmetric parts and restoration of the profile of the packet is found.

I. INTRODUCTION

Study of particle dynamics in confined systems is of fundamental and practical importance for variety of problems in mesoscopic and nanoscale physics. This causes monotonically growing interest to the problem and increasing the number of publications in the literature. The main difference between the physical properties of bulk and confined quantum systems is caused by the boundary conditions to be imposed for a quantum-mechanical wave equations describing their behavior. In the case of a bulk system these conditions are given in whole space, while for a confined system the boundary conditions should be imposed in spatially finite domains. This leads to considerable difference in the macroscopic properties of the bulk and confined systems making the latter size- and shape-dependent. Therefore the role of the quantum confinement in particle transport and its effects on the macroscopic properties of the system are among the key problems of nanoscale physics. Earlier particle dynamics in confined domains was the subject of extensive research in the context of nonlinear dynamics and quantum chaos theory (see, e.g., Refs. [1]-[4]). This is mainly done via modeling such systems by so-called billiard geometries [1, 7]. Billiards are hard-wall boxes that has become one of the paradigms in dynamical chaos theory [1, 6]. It was found that depending on the shape of billiard wall classical dynamics of the system can be regular, mixed or chaotic. In the case of quantum systems the effect of billiard size and shape appears in eigenvalues and eigenfunctions of the Schrodinger equation for which billiard boundary conditions are imposed.

For classically non-integrable (chaotic) billiards the effect of classical chaos is exhibited in statistical properties of the energy levels and wave function of the billiard particle [1, 6].

Apart from the quantum chaos theory, billiards found application in nanoscale physics as the models of quantum dots [2, 5]. Also, the wave dynamics in a microwave cavity is well described by quantum billiards [6]. Confined particle motion appear in different types of nanoscale and mesoscopic systems such as quantum dots, wells and wires, nanoscale networks, fullerene, CNT, graphene nanoribbons and many other structures. Most of these systems can be modeled by quantum billiards [2, 4, 5] or graphs [6]. In all cases, study of particle dynamics in confined quantum systems is reduced to solving of quantum mechanical wave equations with the box(billiard) boundary conditions.

Despite the fact that confined quantum systems are extensively discussed in the literature, the spectrum of the studied problems is mainly restricted by considering isolated (unperturbed) and nonrelativistic systems. However, quantum dynamics in driven confined systems is of importance for many nanoscale systems, as in many cases they are subjected to the actions of external static or time-dependent forces. Another restriction in the past studies of confined systems is related to nonrelativistic treatment: Most of the papers on this issue address the nonrelativistic quantum dynamics described by the Schrodinger equation.

However, confined particle dynamics in relativistic quantum systems is relevant to few important topics such as MIT bag model of particle physics [8], carbon nanotubes [9], graphene [10, 11] and Majorana fermions [12] in condensed matter. All these problems require solving of the Dirac equation with the box boundary conditions. We note that the Dirac equation for a particle confined in a box was earlier treated in detail by Alonso et.al in [13, 14], Berry and Mondragon [15]. Different formulations of the stationary Dirac equation for one dimensional box can be found also in the Refs. [16, 18].

It is important to note that unlike to the Schrodinger equation for box, corresponding Dirac equation encounters with some additional complications. These difficulties are caused by the fact that for infinitely square well the Dirac equation cannot be treated as a single particle equation that is the result of the Klein tunneling and spontaneous electron-positron pair creation [19, 20]. To avoid such complication, in the Ref. [13] the authors considered the situation when confinement is caused by a Lorentz-scalar potential, i.e., by a potential coming in the mass term. Such a choice of confinement is often used in MIT bag model [21] and the potential models of hadrons [8]. Another way to avoid this complication is to impose box boundary conditions in such a way...
that they provide zero-current and probability density at the box walls. In the Ref. [14] the types of the box boundary conditions, providing vanishing current at the box walls and keeping the Dirac Hamiltonian as self-adjoint are discussed. We note that in condensed matter physics such boundary conditions are often used to describe the quasiparticle motion in graphene nanoribbons [10, 11].

In this paper, to treat delta-kicked relativistic particle dynamics confined in a one-dimensional box, we will use the boundary conditions formulated in the Ref. [14]. The kicking potential is considered as to be Lorentz scalar i.e. coming through the mass-term.

This paper is organized as follows. In the next section, following the Ref. [14], we briefly recall the problem of stationary Dirac equation for one dimensional box. In section 3 we treat time-dependent Dirac equation with delta-kicking potential with the box boundary conditions. Section 4 presents some results and their analysis. Finally, section 5 presented some concluding remarks.

II. DIRAC PARTICLE IN A ONE DIMENSIONAL BOX

Before starting treatment of the kicked Dirac particle dynamics, we briefly recall the description of the one dimensional stationary Dirac equation in a box following the Ref. [14]. In nonrelativistic case the box boundary conditions for the Schrödinger equation are introduced through the infinite square well, either by requiring zero-current at the box walls. In case of the Dirac equation introducing of infinite well leads to pair production from vacuum. Therefore the problem cannot be treated within the one-particle Dirac equation that makes impossible using the infinite well based description of the particle-in-box system. The second approach, i.e. requiring zero-current at the boundary can be used, if it does not lead to the breaking down of the self-adjointness of the problem. In case of the Schrodinger equation the boundary condition, \( \psi = 0 \) keeps the Schrodinger operator as self-adjoint. However, for Dirac equation the boundary conditions at the box walls should be determined carefully.

The stationary Dirac equation for free particle in a one-dimensional box given on the interval \((0, L)\) can be written as (in the system of units \(m_e = \hbar = c = 1\))

\[
H_0 \psi = (-i \alpha_x \cdot \frac{d}{dx} + \beta) \psi = E \psi
\]  

where \(\alpha_x\) and \(\beta\) are the Dirac matrices. The wave function, \(\psi\) can be written in two component form as

\[
\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}
\]  

where large, \(\phi\) and small, \(\chi\) components are also two-component semi-spinors:

\[
\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad \chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}
\]

respectively.

The system of first order differential equations can be reduced to second order, Helmholtz-type equation by eliminating one of the components:

\[
\left( \frac{d^2}{dx^2} + k^2 \right) \phi_i = 0 \quad i = 1, 2
\]  

Here

\[
k = [E^2 - 1]^{1/2}.
\]

The small and large components are related to each other through the expression

\[
\begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = \frac{-i}{E + 1} \begin{pmatrix} 0 & \frac{d}{dx} \\ \frac{d}{dx} & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}
\]

Then one of the positive energy solutions can be obtained by taking \(\phi_2 = 0\) and therefore \(\chi_1 = 0\). Thus the general solution for \(\phi_1\) can be written as

\[
\phi_1 = A_1 e^{ikx} + B_1 e^{-ikx}
\]
where $A_1$ and $B_1$ are complex constants. For $\chi_2$ one can obtain

$$
\chi_2 = \frac{k}{E+1} \left( A_1 e^{ikx} - B_1 e^{-ikx} \right).
$$

(7)

Now let us come back to one-dimensional box problem. Since large and small components are related through Eq. (5), it is enough to impose boundary conditions for one of them only, for example, for large component [14]:

$$
\phi_1(0) = \phi_1(L) = 0
$$

(8)

Then we the eigenfunctions, corresponding to these boundary conditions can be written as [14]

$$
\psi = 2A_1 \begin{pmatrix} i \sin(kx) \\ 0 \\ 0 \\ \frac{E}{k^2+1} \cos(kx) \end{pmatrix}
$$

(9)

with $k = N\pi/L$, $N = 1, 2, \ldots$. It was shown in the Ref. [14] that the boundary conditions given by Eq. (8) correspond, in the non-relativistic limit, to the familiar condition of a vanishing wave function at the walls of the box: $\phi_1^{NR}(0) = \phi_1^{NR}(L) = 0$.

It was also shown in [14] that probability ($\rho$) and current ($j$) densities defined as

$$
\rho = \bar{\phi}_1 \phi_1 + \bar{\chi}_2 \chi_2
$$

(10)

$$
\rho(0) = \rho(L)
$$

(12)

$$
\rho(0) = \rho(L)
$$

(13)

This implies that the particle is confined inside the box. Dirac particle confined in a one-dimensional box, whose periodically driven dynamics we are going to explore in the next section, defined though the above boundary conditions.

III. KICKED DIRAC PARTICLE CONFINED IN A ONE DIMENSIONAL BOX

Now consider the relativistic spin-half particle confined in a box and interacting with the external delta-kicking potential of the form

$$
V(x, t) = -\varepsilon \cos\left(\frac{2\pi x}{\lambda}\right) \sum_l \delta(t - lT)
$$

where $\varepsilon$ and $T$ are the kicking strength and period, respectively. The dynamics of the system is governed by the time-dependent Dirac equation which is given as

$$
\frac{i}{\hbar} \frac{\partial \Psi(x, t)}{\partial t} = \left[ -i \alpha \frac{d}{dx} + \beta (1 + V(x, t)) \right] \Psi(x, t),
$$

(14)

for which the box boundary conditions are imposed. One should note that in this equation, to avoid the above mentioned complications related to becoming of the Dirac equation multi-particle, the kicking potential is introduced as a Lorentz-scalar, i.e. through the mass term. Exact solution of Eq. (14) can be obtained within a single kicking period as in the case of kicked rotor [22] and kicked particle in infinite potential well [24]. Indeed, expanding the wave function, $\Psi(x, t)$ in terms of the complete set of the eigenfunctions given by Eq. (9) as

$$
\Psi(x, t) = \sum A_n(t) \psi_n(x)
$$

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and inserting this expansion into Eq.(14), by integrating the obtained equation within one kicking period we have

\[ A_n(t + T) = \sum_l A_l(t)V_{ln}e^{-iE_l T}, \]  

(15)

where

\[ V_{ln} = \int \psi^\dagger_n(x)e^{i\epsilon \cos(\frac{2\pi x}{\lambda})}\psi_l(x)dx \]

and \( E_l \) are defined by Eq. (4). Using the relation

\[ e^{i\epsilon \cos x} = \sum_{m=-\infty}^{\infty} b_m(\epsilon)e^{imx}, \]

(16)

where \( b_m(\epsilon) = i^m J_m(\epsilon) \), the matrix elements \( V_{ln} \) can be calculated exactly and analytically. It is clear that the norm conservation in terms of expansion coefficients, \( A_n(t) \) reads as

\[ N(t) = \sum_n |A_n(t)| = 1, \]

that follows from

\[ \int_0^L |\Psi(x, t)|^2 dx = 1 \text{ and } \int_0^L \psi^\dagger_m(x)\psi_n(x)dx = \delta_{mn}. \]

In choosing of the initial conditions, i.e. the values of \( A_n(0) \) one should use this condition. Having computed \( A_n(t) \) we can calculate any dynamical characteristics of the system such as average kinetic energy or transport properties. In particular, the average kinetic energy as a function of time can be written as

\[ E(t) = \int \Psi^\dagger(x, t)(-i\alpha \cdot \frac{d}{dx})\Psi(x, t)dx, \]

where \( A_n(t) \) are given by Eq.(15). For classical periodically driven systems such as kicked rotor or kicked box, the average kinetic energy grows linearly in time. However, for quantum counterparts of these systems such a growth is suppressed [22, 23], which is caused by so-called quantum localization effect [23]. The latter implies that no unbounded acceleration of a nonrelativistic kicked quantum particle is possible (except the special cases of quantum resonances [22, 23]). We are interested to explore the behavior of \( E(t) \) in corresponding relativistic case described by the Dirac equation. Fig. 1 compares the average kinetic energy as a function of time for different values of the kicking strength \( \epsilon = 0.01; 0.05; \) and \( 0.1 \) at fixed kicking period \( T = 0.47 \). As is seen from these plots, \( E(t) \) is periodic in time for this set of kicking parameters. In Fig. 2 \( E(t) \) is plotted for \( \epsilon = 0.5 \)
FIG. 2: (Color online) Time-dependence of the average kinetic energy for different values of the kicking strength ($\varepsilon = 0.1$; and 0.5) at fixed kicking period $T = 10^{-2}$.

FIG. 3: (Color online) Time-dependence of the average kinetic energy for monotonically growing cases: ($\varepsilon = 0.1$; 0.5; 1) and $T = 10^{-4}$.

and 0.1 at $T = 0.01$. The periodicity in time completely broken in this case. In Fig.3 monotonically growing cases are presented for the values of kicking parameters $\varepsilon = 0.1$; 0.5; 1 and $T = 10^{-4}$. Fig.4 compares the plots of $E(t)$ for different kicking periods ($T = 0.1$; $10^{-2}$; and $10^{-4}$) and at fixed value of the kicking strength ($\varepsilon = 0.5$).

The difference in behavior of $E(t)$ for different regimes of external kicking force can be explained by the spatio-temporal localization of the particle with respect to the profile of the kicking potential. It is clear that depending on the coordinate, $x$ the kicking potential can be attractive or repulsive. In Fig. 5 profile of the kicking potential is plotted for the value of the wavelength $\lambda = 1$. If the motion of the particle is localized in the area where the kicking potential is positive, gaining of energy by particle and its acceleration occurs. When particle motion is localized on the area of the box where the kicking potential is attractive, it loses the energy. Therefore by tuning the kicking parameters such as $\varepsilon$, $T$ and $\lambda$ it is possible to achieve tunable dynamics of a kicked particle in a box. Fig. 6 presents plots of $\rho(x, t) = |\Psi(x, t)|^2$ for $\varepsilon = 0.5$ and $T = 10^{-4}$. As it can be seen, the wave function is localized near the walls and the maximum values are achieved along whole $t$–axis within the localization band. Fig. 7 presents time dependence of $E(t)$ and corresponding average velocity as a function of time which is defined as

$$\langle v_x \rangle = -i \int \Psi^\dagger \alpha_x \Psi dx$$

(17)

The velocity of a kicked Dirac particle confined in a box does not grow monotonically and suppressed after some growth. The above treatment shows that unlike to its nonrelativistic counterpart treated in [24], the quantum dynamics of kicked relativistic particle in a box does not depend on the product $\varepsilon T$, but depends on each kicking
FIG. 4: (Color online) Time-dependence of the average kinetic energy for different kicking periods ($T = 0.1; 10^{-2};$ and $10^{-4}$) and at fixed value of the kicking strength ($\varepsilon = 0.5$).

FIG. 5: (Color online) Profile of the kicking potential for the case of $\lambda = L$.

parameter separately. This provides more tools for manipulation by the dynamics of the system by playing $\varepsilon$, $T$ and $\lambda$. Fig. 8 presents plots of $V(x, t)$ for $\lambda = 0.5L$ and $E(t)$ for kicking parameters $T = 10^{-4}$ and $\varepsilon = 0.1$ and 0.5. If we compare $E(t)$ plotted in Figs. 3 and 8, the strong dependence of the dynamics of the average kinetic energy on $L/\lambda$ can be observed.

IV. WAVE PACKET EVOLUTION

An important characteristics of the particle transport in quantum regime is wave packet evolution. Changes of the profile of a packet in space and time can give useful information about the transport phenomena. As one of the most simplest and interesting case one can treat the evolution of the gaussian wave packet. In the relativistic case the Gaussian (spinor) wave packet can be written as follows [25]:

$$
\Psi(x, 0) = \frac{f(x)}{\sqrt{|s_1|^2 + |s_2|^2 + |s_3|^2 + |s_4|^2}} \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \end{pmatrix}
$$

(18)

where $s_1, s_2, s_3$ and $s_4$ determine the initial spin polarization and

$$
f(x) = \frac{1}{d\sqrt{\pi}} \exp\left[-\frac{(x-x_0)^2}{2d^2} + iv_0x\right].
$$
Multiplying each side of Eq. (18) by \( \psi_m^*(x) \) and integrating over \( x \) from 0 to \( L \), we obtain expression for the initial values of the expansion coefficients to used in Eq. (15):

\[
A_n(0) = \int_0^L \psi_n^*(x) \Psi(x,0) dx.
\] (19)

Fig. 9 presents profile of the Gaussian wave packet (for \( d = L/100, x_0 = L/2 \) and \( v_0 = 0 \)) at different time moments: \( t = 0, 20T, 50T \) and \( 80T \). Dispersion of the packet by simultaneous splitting into two symmetric parts can be observed for this regime of motion. Such splitting is caused by the existence of the spin of particle. In Fig 10. the regime of motion at which restoration of the Gaussian wave packet can be observed, is plotted. It is clear that the dynamics of the wave packet in relativistic spin-half system is considerably different than

FIG. 6: (Color online) Probability density as function of coordinate and time for the kicking parameters \( \varepsilon = 0.1 \) and \( T = 0.47, T = 10^{-2} \) and \( T = 10^{-4} \).
that in corresponding nonrelativistic system. Such a difference is caused by the spin of the system and other relativistic effects.

V. CONCLUSION

Thus we have studied kicked Dirac particle dynamics confined in one dimensional box. Box boundary conditions for the unperturbed Dirac equation are imposed in such a way that they provide zero-current at the box walls.

Kicking potential is taken as the Lorentz-scalar, i.e. included into the mass term in the Dirac equation. Time-dependence of the average kinetic energy is analyzed. It is found that depending on the values of the kicking parameters $E(t)$ can be periodic, monotonically growing and non-periodic function of $t$. Such different regimes of motion can be explained by the localization of the particle motion with respect to the profile of the kicking potential. In particular, if the particle motion is always localized in the area where potential is repulsive it gains the energy and acceleration occurs that corresponds to monotonically growing $E(t)$.

If the localization of the particle in repulsive and attractive areas periodically replace each other $E(t)$ becomes periodic function of $t$. When the motion of the particle is localized the the area where potential is attractive it looses the energy that leads to deceleration. Therefore the case when particle is localization in attractive and repulsive areas is non-periodic, the average energy becomes non-periodic and non-growing function of time. The average velocity as function of time is also analyzed and it is found that its growth as a function of time is suppressed even for monotonically growing $E(t)$. Particle transport in the system is studied by considering spatio-temporal evolution of the Gaussian wave packet. Splitting of the packet into two symmetric parts and restoration of the profile of the packet is found in this case.

The above results obtained in this paper can be useful for the study of time-dependent particle transport in different nanoscale systems (e.g. graphene nanoribbons, carbon nanotubes, Majorana wires etc) described
FIG. 8: (Color online) Probability density as function of coordinate and time $\varepsilon = 0.1$ and $T = 10^{-2}$.

by Dirac equation. Extension of the results for two- and three-dimensional cases is rather trivial.

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FIG. 9: (Color online) Profile of the Gaussian wave packet at different times for $\varepsilon = 1$ and $T = 10^{-2}$.

FIG. 10: (Color online) Profile of the Gaussian wave packet at different times for $\varepsilon = 1$ and $T = 0.25$. 
$\varepsilon = 0.1$
\( \epsilon = 0.1 \)
