Classical and quantum dynamics of a kicked relativistic particle in a box

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We study classical and quantum dynamics of a kicked relativistic particle confined in a one dimensional box. It is found that in classical case for chaotic motion the average kinetic energy grows in time, while for mixed regime the growth is suppressed. However, in case of regular motion energy fluctuates around certain value. Quantum dynamics is treated by solving the time-dependent Dirac equation with delta-kicking potential, whose exact solution is obtained for single kicking period. In quantum case, depending on the values of the kicking parameters, the average kinetic energy can be quasi periodic, or fluctuating around some value. Particle transport is studied by considering spatio-temporal evolution of the Gaussian wave packet and by analyzing the trembling motion.

I. INTRODUCTION

Particle dynamics in confined quantum systems has attracted much attention in the context of nanoscale physics [1–5] and quantum chaos theory [4–6]. Usually, studies of confined quantum dynamics within the chaos theory have been focused on two types of problems. First type deals with the analysis of the spectral statistics (so-called quantum chaos) by solving Schrödinger equation in confined geometries (quantum billiards) [6–9]. Second type deals with the quantum dynamics in periodically driven systems by studying average kinetic energy as a function of time [10–11].

Despite the fact that confined quantum systems are widely studied in the literature, most of the researches are mainly focused on the nonrelativistic systems. In this paper we address the problem of delta-kicked relativistic particle confined in a one-dimensional box. Nonrelativistic counterpart of such system have been considered earlier in classical and quantum chaos contexts by considering kicked particle in infinite square well [12–14]. For kicked systems, the main feature of the dynamics is the diffusive growth of the average kinetic energy as a function of time in classical case and its suppression for corresponding quantum system. The latter is called quantum localization of classical chaos [10–11]. The dynamics of the kicked nonrelativistic system is governed by single parameter, product of the kicking strength and kicking period. However, as we will see in the following, the dynamics of the relativistic system is completely different than that of its nonrelativistic counterpart: There is no single parameter which governs the dynamics.

Usually, confined relativistic quantum systems appear in particle physic models such as MIT bag model [15] and the quark potential models [16]. However, recent progress made in fabrication of graphene and studying its unusual properties made possible experimental realization of Dirac particle confined in one- [17] and two-dimensional boxes [18–21]. Such condensed matter realization of a Dirac particle in a box can be also realized in graphene nanoribbon ring [22–30] or dot [22–23] which is extensively studied recently both theoretically and experimentally. Graphene nanoribbon is a strip of graphene having different edge geometries. The quasiparticle dynamics in such material is effectively one-dimensional, i.e. can be described by one dimensional Dirac equation [17]. When its length is finite, it becomes ”Dirac particle in a 1D box”. “Kicked” version of such system, i.e., kicked Dirac particle in a box can be realized, e.g., by putting it in a standing laser wave. One of such models has been recently studied in [18] by focusing on transport phenomena.

We note that earlier, the Dirac equation for a particle confined in a box was considered in detail in the Refs. [31–36]. Unlike the Schrödinger equation for a box, introducing confinement in the Dirac equation via infinite square well or box faces some difficulties caused by the Klein tunneling and the electron-positron pair creation [37]. To avoid such complication, in the Ref. [34] the authors considered the situation when confinement is provided 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 [15] and the potential models of hadrons [16]. Another way to avoid such 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. [31] the types of the box boundary conditions, providing vanishing current at the box walls and keeping the Dirac Hamiltonian as self-adjoint are discussed.

The paper is organized as follows. In the next section we consider classical dynamics of a relativistic particle confined in a one dimensional box. In section 3, following the Ref. [31], we briefly recall the problem of stationary Dirac equation for one dimensional box. In section 4 we treat the time-dependent Dirac equation with delta-kicking potential with the box boundary conditions. In section 5 we discuss wave packet dynamics and trembling motion. Finally, section 6 presents some concluding remarks.

II. CLASSICAL DYNAMICS

Classical relativistic particles whose motion is spatially confined may appear in plasma [19] and astrophysical sys-
The energy in Fig. 2 (b) grows in time and the growth rate in time and the growth of the average kinetic energy does not grow in time (assumption of Eqs. (2)).

The dynamics of the particle is regular. For this case, the average kinetic energy (b) of a kicked relativistic particle in a box is Lorentz invariant, since it is a discretized version of Eqs. (2).

For integer part and sign of the argument respectively. It is clear that this map (as the equations of motion themselves) is Lorentz invariant, since it is a discretized version of Eqs. (2).

Fig. 1 presents phase-space portraits (a) and the time-dependence of the average energy vs the number of kicks (b) for the classical system. The average energy grows almost monotonically for this case in the considered time period. This regime can be considered as an acceleration mode. Existence of the acceleration modes can be clearly seen from the Fig. 4, where the average kinetic energy is plotted vs kicking parameters, ε and T. Maximum values of E(t) and acceleration are possible around certain values of the kicking period T = 100 while the growth of E(t) is not “sensitive” with respect to the values of ε. Our numerical experiments showed that the growth of E(t) depends on the parameters $K = \frac{2\pi \varepsilon T}{\lambda}$.

We note that there is no single parameter governing the dynamics of the system for relativistic kicked particle in a box. In other words, scaling of the map (2) in such way that it will depend on single parameter, $K = \varepsilon T$, is not possible. Instead, it depends on each parameter separately which makes the dynamics of the system more rich than that of the nonrelativistic counterpart. As shows the Fig. 4, the average energy and dynamics are more sensitive to the change of the kicking period, T than the kicking parameter, ε. Such a feature can be related to the fact that the underlying factor for the growth of the average kinetic energy is the “correlations” between the bouncing of the particle on the box walls and the kicks. Indeed, the dynamics of the particle depends on two interactions, bouncing from the walls and on the kicking pulses. In case, if the kicks and bounces are “synchronized”, the dynamics can be regular. Otherwise, chaotization of the system may occur. Moreover, our detailed numerical analysis of the map and phase-space portraits showed that unlike the classical nonrelativistic kicked particle in a box studied in Refs. 13, 14, for (classical) relativistic kicked particle in a box, the diffusion and growth of the energy does not occur for all values of the kicking parameters. Namely, diffusive growth is possible only for fully chaotic regime, while for regular dynamics the average kinetic energy does not grow at all.
III. DIRAC PARTICLE IN A ONE-DIMENSIONAL BOX

Unperturbed version of the system we are going to treat, i.e., Dirac particle confined in a one-dimensional box was considered earlier in the Refs. [31]-[12]. Here we briefly recall the description of such system following the Ref. [31]. In the nonrelativistic case the box boundary conditions for the Schrödinger equation are introduced through the infinite square well, either by imposing the boundary conditions providing zero-current at the box walls. In case of the Dirac equation introducing of infinite well leads the Klein paradox and to electron-positron pair production from vacuum [34, 37]. The latter implies that 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 [34, 37]. Instead, the box can be introduced through the boundary conditions, providing zero-current at the boundary and keeping the self-adjointness of the problem. In case of the Schrödinger equation the boundary condition, \( \psi = 0 \) keeps the Schrödinger operator as self-adjoint. However, for Dirac equation the boundary conditions at the box walls should be determined carefully [31]-[33] to keep the self-adjointness of the problem.

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 \( m = \hbar = c = 1 \))

\[
H_0 \psi = \left(-i \alpha \cdot \frac{d}{dx} + \beta\right) \psi = E \psi, \quad (4)
\]

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

\[
\psi = \left(\begin{array}{c} \phi \\ \chi \end{array}\right), \quad (5)
\]

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

\[
\phi = \left(\begin{array}{c} \phi_1 \\ \phi_2 \end{array}\right) \quad \chi = \left(\begin{array}{c} \chi_1 \\ \chi_2 \end{array}\right),
\]

respectively.

The system of first order differential equations (4) can be reduced to second order, Helmholtz-type equation by eliminating one of the components:

\[
\left(\frac{d^2}{dx^2} + k^2\right) \phi_i = 0 \quad i = 1, 2, \quad (6)
\]

Here

\[
k = (E^2 - 1)^{1/2}. \quad (7)
\]

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

\[
\left(\begin{array}{c} \chi_1 \\ \chi_2 \end{array}\right) = \frac{-i}{E + 1} \left(\begin{array}{c} 0 \\ \frac{d}{dx} \end{array}\right) \left(\begin{array}{c} \phi_1 \\ \phi_2 \end{array}\right). \quad (8)
\]

Therefore box boundary conditions should be imposed for one of the components only. 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

\[
\phi_1 = A_1 e^{ikx} + B_1 e^{-ikx}, \quad (9)
\]

where \( A_1 \) and \( B_1 \) are complex constants. For \( \chi_2 \) one can obtain

\[
\chi_2 = \frac{k}{E + 1} (A_1 e^{ikx} - B_1 e^{-ikx}). \quad (10)
\]
Imposing the box boundary conditions given by Eq. (11),
\[ \phi_1(0) = \phi_1(L) = 0, \]
we get the following eigenfunctions:
\[ \psi_n = 2A_n \begin{pmatrix} i \sin(k_n x) \\ 0 \\ 0 \end{pmatrix}, \]
where \( E_n \) determined by Eq. (7), \( A_n \) is the normalization constant, and \( k_n = \pi n/L, n = 1,2, \ldots \). It is clear that the boundary conditions given by Eq. (11) correspond, in the non-relativistic limit, to the familiar condition of a vanishing wave function at the walls of the box: \( \phi_1(0) = \phi_1(L) = 0 \) and the probability (\( \rho \)) and current (\( j \)) densities defined as
\[ \rho = \bar{\phi}_1 \phi_1 + \bar{\chi}_2 \chi_2, \]
\[ j = e\psi_1^\dagger \alpha_x \psi = ec \left( \bar{\phi}_1 \chi_2 + \bar{\chi}_2 \phi_1 \right). \]
satisfy the following boundary conditions:
\[ \rho(0) = \rho(L), \]
\[ j(0) = j(L) = 0. \]
This implies that the particle is confined inside the box.

IV. KICKED DIRAC PARTICLE CONFINED IN A ONE DIMENSIONAL BOX

Consider the relativistic spin-half particle confined in a box and interacting with the external delta-kicking potential of the form
\[ V(x, t) = -\varepsilon \cos \left( \frac{2\pi x}{\lambda} x \right) \sum_l \delta(t - lT), \]
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
\[ i \frac{\partial}{\partial t} \Psi(x, t) = \left[ -i \alpha_x \frac{d}{dx} + \beta(1 + V(x, t)) \right] \Psi(x, t), \]
for which the box boundary conditions given by Eq. (11) are imposed. To avoid complications in the treatment caused by Klein paradox and pair creation, we choose the kicking potential as a Lorentz-scalar, i.e. as the mass term. Then the exact solution of Eq. (17) can be obtained within a single kicking period as in the Refs. [10, 13]. Expanding the wave function, \( \Psi(x, t) \) in terms of the complete set of the eigenfunctions given by Eq. (12) as
\[ \Psi(x, t) = \sum_n A_n(t) \psi_n(x), \]
and inserting this expansion into Eq. (17), by integrating the obtained equation within one kicking period we have
\[ A_n(t + T) = \sum_l A_l(t) V_l e^{-iE_l T}, \]
where
\[ V_l = \int \psi_1^\dagger(x) e^{i\varepsilon \cos(2\pi x/\lambda)} \psi_1(x) dx, \]
and \( E_l \) are defined by Eq. (7). Using the relation
\[ e^{i\varepsilon \cos x} = \sum_{m=-\infty}^{\infty} b_m(\varepsilon)e^{imx}, \]
where \( b_m(\varepsilon) = i^m J_m(\varepsilon) \), the matrix elements \( V_l \) 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
\[ \int_0^L |\Psi(x, t)|^2 dx = 1 \text{ and } \int_0^L \psi_1^\dagger(x)\psi_1(x) dx = \delta_{mm}. \]
In choosing of the initial conditions, i.e. the values of \( A_n(0) \) one should use the norm conservation.

Having found \( A_n(t) \), we can calculate any dynamical characteristics of the system such as average kinetic energy, probability density, wave packet evolution, etc. The average kinetic energy as a function of time can be written as
\[ \langle E(t) \rangle = \int \Psi^\dagger(x, t) \left( -i \alpha_x \cdot \frac{d}{dx} \right) \Psi(x, t) dx, \]
where \( A_n(t) \) are given by Eq. (18).

For the non relativistic counterpart of our model, non relativistic kicked particle in a box, the average classical kinetic energy grows linearly in time, while in quantum case such a growth is suppressed [13]. This is caused by so-called quantum localization effect [10, 11]. The latter implies that no unbounded acceleration of a nonrelativistic kicked quantum particle is possible (except the special cases of quantum resonances [10, 11]). Here we explore behavior of \( \langle E(t) \rangle \) in the relativistic case for the system described by Eq. (17) for different kicking regimes. In Fig. 6 time-dependence of the average kinetic energy (a) and spatio-temporal evolution of the probability density (b) are plotted for \( \varepsilon = 0.5 \) and \( T = 200 \). Time-dependence of the average kinetic energy shows the quasi-periodic behavior. Such behavior is confirmed by the plot of probability density which is also quasi-periodic both in space and time. Fig. 6 presents time-dependence of the average kinetic energy (a) and probability density (b) at the values of the kicking parameters \( \varepsilon = 1 \) and
The time dependence of $E(t)$ is neither periodic, nor monotonic and fluctuates around some value in this kicking regime. However, the plot of the probability density shows that particle is mostly localized in two areas within the box. Depending on the position of the particle in the box, the kicking potential can be attractive or repulsive, which caused by the presence of the factor $\cos x$. Therefore, the behavior of $E(t)$ in this system depends on the localization particle’s position inside the box and the synchronization of kicking and bouncing (at the wall) regimes. If the particle’s motion is localized in the area where the kicking potential is positive, the particle gains energy. Localization of the motion in the area, where the kicking potential is negative causes the loss of energy by particle. If the particle’s motion is time-periodically localized in these two areas, $E(t)$ will be time periodic (or quasiperiodic). For the regime when such localization time is different for the areas where the kicking potential is attractive and positive, the periodicity of $E(t)$ is broken and we have time dependence of the average kinetic energy presented in Fig.6

FIG. 5. (Color online) Time-dependence of the average kinetic energy (a) for the value of the kicking strength $\varepsilon = 0.5$ and period $T = 200$ and the corresponding probability density plot (b) for the time interval $[0 100T]$. The initial state chosen as the 40th positive energy level of the unperturbed system.

FIG. 6. (Color online) Time-dependence of the average kinetic energy (a) for the value of the kicking strength $\varepsilon = 1$ and period $T = 10$ and the corresponding probability density plot (b) for the time interval $[0 100T]$. The initial state chosen as the 40th positive energy level of the unperturbed system.

V. ZITTERBEGWUNG AND WAVE PACKET DYNAMICS

In this section we consider dynamics of the kicked Dirac particle in a box by exploring its transport properties. Very interesting feature of the Dirac particle is so called trembling motion (zitterbewegung), which is the pure relativistic effect. It was first studied by Schrödinger [42–45], who showed that the free relativistic electron experiences trembling motion in vacuum. Later it was shown that such motion can occur in the interaction of the electron with external field. Trembling motion is characterized by the time-dependence of the average position which is given by

$$\langle x(t) \rangle = \langle \Psi(x, t)|x|\Psi(x, t) \rangle.$$

Here we calculate the average position by choosing the initial wave function in the form of spinor Gaussian wave packet which can be written as [38]:

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

(20)

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

$$f(x) = \frac{1}{d\sqrt{\pi}} \exp \left[ -\frac{(x - x_0)^2}{2d^2} + iv_0x \right].$$

Then the initial conditions in terms of the wave packet can be written as:

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

(21)

In Fig.7 the average position of the kicked Dirac particle in a box is plotted for fixed $\varepsilon = 0.1$ at different values of the kicking period, $T$ and compared with that of unperturbed system. It can be seen from these plots that for unperturbed particle damping of motion occurs much faster compared to kicked one. Fig.8 presents similar plots for fixed $T$ at different values of the kicking parameter, $\varepsilon = 0.5$. The profiles of the average position are close to each other. Therefore we may conclude that the trembling dynamics is more sensitive to the change of $T$ rather than $\varepsilon$. Such sensitivity can be explained by existence (unlike, e.g., kicked rotor) of two factors acting on the trembling motion, bouncing and kicks. Synchronization or de-synchronization of these factors play important role in the dynamics of the particle. Thus in case of the unperturbed system trembling becomes damped and suppressed after some time, while for the kicked system such suppression is not possible. In calculation of the average position the initial wave packet parameters have been chosen as those in the second example in the section IV of the Ref. [40].
An important information about the particle transport in quantum regime can be extracted from the wave packet evolution. Fig. 9 presents plots of the profile of the Gaussian wave packet (for $d = L/100$, $x_0 = L/2$ and $v_0 = 0$) at different times $t = 0, 64T, 261T$ and $467T$). Dispersion of the packet and 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 which can have two values (up and down). Numerical experiments for different kicking regimes showed that revival of the Gaussian wave packet is not possible in this system.

VI. CONCLUSIONS

We have studied classical and quantum dynamics of relativistic particle confined in a 1D box and driven by external delta-kicking potential by considering spin-half Dirac particle.
atte around some value. Such behavior can be explained by the dependence of the particle dynamics on bouncing on the wall and interaction with the kicking potential. The latter can be attractive or repulsive depending on the position of particle inside the wall and may cause its acceleration or deceleration. When particle is trapped in the area where the kicking force is attractive it looses its energy, while being trapped in the repulsive kicking area it gains the energy. If the trapping times for these two areas are equal, the average kinetic energy is time-periodic. By tuning of the kicking parameters one can achieve that the amplitude and period of $E(t)$ can be as higher and longer as we want, i.e. the average kinetic energy can grow in time during very long time. However, no monotonic growth of the average kinetic energy is possible as in the case of quantum resonances appearing in non-relativistic counterpart of the system. The analysis of the Gaussian wave packet evolution shows that dispersion of the packet can occur via splitting into two symmetric part and no revival is possible. The trembling motion of the particle is also studied by considering unperturbed and kicked particles in a box. It is shown that damping in the trembling motion is more sensitive to kicking period than to kicking strength.

The above model can be used to describe Dirac particles in graphene quantum dot, graphene nanoribbon rings and carbon nanotubes driven by external time-periodic fields. Kicking potential can be realized by embedding these systems in a standing wave in generated by optical cavities. Particle physics realization of the kicked Dirac particle in a box comes from the MIT Bag models of quarks where quarks confined in a bag subjected to the influence of external time-periodic fields.

ACKNOWLEDGMENTS

This work is partially supported by a grant of the Committee for Coordination of Science and Technology of Uzbekistan (Ref. Nr F-2-003)
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