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# Kicked Dirac particle confined in one-dimensional box

Bachelor diploma thesis

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# 1 Introduction

Driven quantum systems under a confinement appear in many practically important problems in nanoscale and particle physics. The latter deal with the hadrons, where quarks are bound due to the strong interaction, while in nanoscale systems huge variety of confined quantum systems appear in different structures and devices. The main factor making different physical properties of confined and bulk quantum systems is caused by the boundary conditions of the quantum mechanical wave equations (e.g. Schrodinger, Dirac, Klein-Gordon equations). Due to such difference in the boundary conditions macroscopic properties (e.g., heat capacity, thermal conductance, dielectric penetrability, optical conductivity etc.) of bulk and confined systems may be completely different. This makes important treatment of confined quantum dynamics under different boundary conditions with different wave equations. Up to now the time-dependent and stationary Schrodinger equations are studied for different confined systems both from nanoscale and particle physics frameworks. Remarkable feature of the confined systems is the dependence of their (both classical and quantum) dynamics of the geometry of the boundary conditions. During last few decades such systems have been extensively studied in the context of nonlinear dynamics and quantum chaos theory [1]-[2]. In particular, quantum billiards were one of the hot topics both in the context of quantum chaos theory [40, 41, 43, 44]. Driven quantum systems under the confinement are studied by considering kicked rotor [15, 16, 22]. Despite the great progress made in the study of confined quantum systems both unperturbed and driven ones, most of the studies are restricted mainly by consideration of nonrelativistic systems. Relativistic driven systems under the confinement are explored in

few works (see, e.g., [66, 95, 47]). It is clear that the driven relativistic dynamics can be much richer than its nonrelativistic counterpart. One of the reason for that is caused by different ways for choosing driving potential. In particular, it can be as a pure scalar (i.e. as the scalar component of the 4-potential), vector (magnetic field) and Lorentz scalar. The latter implies that potential is included into the mass term in the Dirac equation. In this work we explore quantum dynamics of a relativistic Dirac particle confined in a one dimensional box and simultaneously driven by delta-kicking potential. In particular, we obtain exact analytical formula for the evolution of the wave function during single kicking period. In the next section following to the Ref.[45], we will briefly describe corresponding unperturbed problem, i.e., Dirac particle in one dimensional box in the absence of driving force. Next to the next section represents description of corresponding nonrelativistic system, i.e., kicked nonrelativistic particle confined in a box by recalling the results of the Ref.[12]. Section 4 presents results of our study obtained within this dissertation, i.e. quantum dynamics of the kicked Dirac particle confined in a one dimensional box. Finally, the last section presents some concluding remarks.

## 2 Treatment of the nonrelativistic system

Study of the quantum dynamics of confined systems subjected to the influence of external time-dependent forces is of fundamental and practical importance. A textbook paradigm of this kind is the kicked quantum rotor [1, 3]. For certain values of system parameter, the map, describing the evolution of such system, possesses special kind of orbits called Accelerator Modes(AM) [4]. If an initial state of the rotor corresponds to the AM, then it is uniformly accelerated after each kick. In other words, momentum of the rotor increases linearly with time. This is to be contrasted with generic chaotic orbits that diffuse in momentum, i.e., momentum variance of an ensemble of chaotic orbits increases linearly in time leading to normal diffusion. AM are seen in phase space as small regular islands embedded in a chaotic sea. They are separated from chaotic region by cantori (partial barriers). If a chaotic orbit enters through the cantori, it sticks to the cantori for very long time and thus is accelerated along with the modes. Considering  $n$  as time, such a long excursion of a chaotic orbit is an example Levy flight [5]. Levy flight, some times called as super-diffusion, is characterized by  $\langle p_n^2 \rangle \sim n^\gamma$  with  $\gamma > 1$ . AM assisted anomalous transport of this kind has been already studied with different motivations [6]. It should be noted that the above mechanism of anomalous effect is numerically ascertained. Further studies have shown that these modes influence corresponding quantum system as well [7, 8]. In particular, the existence of regular islands in chaotic sea significantly alter the localization of quasienergy states in angular momentum, leading to enhancement in quantum transport. Developments on confining atoms in magneto-optical traps have opened experimental feasibility for atom-optics realizations of the kicked rotor. One such realization, in which

an ensemble of cold cesium atoms are exposed to a periodically pulsed standing wave light, has shown that for certain values of the kick amplitude the momentum distribution of the atomic sample is non-exponentially localized [9]. This then is shown as an effect of AM in the quantum system, in contrast to the generic exponential localization. Semiconductor based technological developments, on the other hand, have shown that it is possible to fabricate potential wells on atomic scales. Motion of electrons in such quantum wells in presence of an external electromagnetic field has been studied for experimental signatures of quantum chaos [10]. A simple model of this kind is a particle confined in a one-dimensional infinite square well exposed to a time periodic pulse field. This system is known to be one generalization of the kicked rotor [11]. The virtue of this generalization arises from two length scales of the system, namely, width of the well and field wavelength. If the well width is an integer multiple of the field wave-length, kick to kick dynamics of the particle is equivalent to that of the rotor. Otherwise, the dynamics is described by a discontinuous map resulting in a new scenario for transition to chaos even for weak field strengths [11]. Here we briefly recall the results of previous investigations of this model in the context of AM following to the Ref. [12] where it is shown that the generalization leads to a larger parametric space, in comparison to the standard map, for existence of the AM. In particular, it is demonstrated in the Ref. [12] that when the border of AM (which we call a beach) exposes a chain of islands of a lower order resonance, stickiness of the beach increases significantly leading to anomalous transport.

## 2.1 Classical dynamics in a kicked well

Let us consider a particle confined in an one-dimensional infinite square-well potential  $V_0(x)$  of width  $2a$  and the Hamiltonian is

$$H_0 = \frac{p^2}{2M} + V_0(x),$$

$$V_0(x) = \begin{cases} 0 & \text{for } |x| < a, \\ \infty & \text{for } |x| > a \end{cases} \quad (1)$$

The particle is subjected to a time periodic pulsed field of period  $T$ . The perturbed system is governed by the Hamiltonian

$$H = H_0 + \epsilon \cos\left(\frac{2\pi x}{\lambda}\right) \sum_n \delta\left(n - \frac{t}{T}\right), \quad (2)$$

where  $\epsilon$  and  $\lambda$  are strength and wavelength of the field respectively; a train of delta functions accomplishes the time periodic pulse. Kick to kick dynamics of the particle can be described by the map

$$\begin{aligned} X_{n+1} &= (-1)^{B_n}(X_n + P_n) + (-1)^{B_n+1} \text{Sgn}(P_n) B_n \\ P_{n+1} &= (-1)^{B_n} P_n + \frac{K}{2\pi} \sin(2\pi R X_{n+1}), \end{aligned} \quad (3)$$

where  $B_n = [\text{Sgn}(P_n)(X_n + P_n) + 1/2]; [\dots]$  and  $\text{Sgn}(\dots)$  stand for integer part and sign of the argument respectively.  $B_n$  is the number of bounces of the particle between the walls during the interval between  $n$  th and  $(n+1)$  th kick. This dimensionless map is related to physical variables by the scaling:

$$\begin{aligned} X_n &= \frac{x_n}{2a}, \\ P_n &= \frac{p_n T}{2aM} \\ K &= \frac{2x_n}{2a}, \end{aligned}$$

$$R = \frac{2a}{\lambda} \quad (4)$$

where  $K$  is effective field strength and  $R$  is ratio of two length scales of the system. Henceforth we refer to the classical mapping (3) as the well map. The well map can be studied by invoking a Generalized Standard Map (GSM)

$$\begin{aligned} J_{n+1} &= J_n + \frac{K}{2\pi} \sin(2\pi R\theta_n), \\ \theta_{n+1} &= \theta_n + J_{n+1} \pmod{1}, \end{aligned} \quad (5)$$

since time reversal of GSM and (3) are quantitatively related. GSM is defined on a cylinder  $(-\infty, \infty) \times [-1/2, 1/2)$  and the standard map is a special case with  $R = 1$ . A detailed study of GSM can be found in our earlier work [9]. The GSM is highly chaotic for strong field strength (large  $K$ ). In addition, it exhibits chaotic motion even for weak field strength (small  $K$ ) depending on the parameter  $R$ . In order to study the AM in the well map, we invoke the GSM which is amenable to a detailed analysis. Periodicity of the GSM  $J$  and  $\theta$  (with unit period) implies existence of AM. These are located at  $(J', \theta')$

$$\begin{aligned} J' &= m, \\ \frac{K}{2\pi} \sin(2\pi R\theta'_n) &= l \end{aligned} \quad (6)$$

where  $m$  and  $l$  are integers. They are also termed as step- $|l|$  AM as the acceleration is  $|l|$  at each iteration. Fixed points belong to the family of AM with  $l = 0$ . For stable AM, required stability condition is

$$\frac{4}{KR} < \cos(2\pi R\theta'_n) < 0, \quad (7)$$

and using (6) this becomes

$$|l| < \frac{K}{2\pi} < \sqrt{l^2 + \left(\frac{2}{\pi R}\right)^2}. \quad (8)$$

This inequality can also be rewritten as

$$0 < R < R_1, \quad (9)$$

where  $R_1 = (2/\pi) \left( (K/2\pi)^2 - l^2 \right)^{-1/2}$ . For stable AM

$$|\theta'| = \frac{1}{2R} \left( 2j + 1 \mp \frac{1}{\pi} \sin^{-1} \left( \frac{2\pi|l|}{K} \right) \right), \quad (10)$$

where  $j$  is an integer. Thus the AM are characterized by two integers  $l$  and  $j$  and we call them as  $(l, j)_{\mp}$  type modes. Since the cylindrical phase space of GSM has the constraint  $|\theta'| < +1/2$  (equivalent to restriction of the particle dynamics to between walls of the well), zero cannot be lower limit in the above inequality. The parameter  $R$  in GSM is recognized as frequency of the sinusoidal force term. As  $R$  increases from zero  $|\theta'|$  decreases such that  $(l, j)_{-}$  type modes first appear in the phase space followed by the  $(l, j)_{+}$  type. In a similar way, as  $R$  decreases  $|\theta'|$  increases such that  $(l, j)_{+}$  type is the first to disappear from the phase space while the  $(l, j)_{-}$  type mode is the last to disappear. Hence, lowest limit for the inequality (9) is set by the disappearance of  $(l, j)_{-}$  type modes. From Eq.(10), the constraint  $|\theta'| \leq 1/2$  for  $(l, j)_{-}$  becomes  $R_0 \leq R$ , where

$$R_0 = 2j + 1 - \frac{1}{\pi} \sin^{-1} \left( \frac{2\pi|l|}{K} \right)$$

Thus, the inequality (9) is replaced by

$$R_0 \leq R < R_1, \quad (11)$$

We emphasize that both the inequalities (8) and (11) must be simultaneously satisfied for existence of AM in the phase space. This is in contrast to the standard map for which the inequality (8) with  $R=1$  it-self is sufficient. Thus the two control parameters,  $K$  and  $R$ , provide a larger parametric space, in

comparison to that of the standard map, for the existence of AM. At  $K = 2\pi|l|$ , the lower bound of the inequality (8) ,  $R_0 = 1/2$  and this is the minimum possible value of  $R_0$ . In other words, for  $R < 1/2$  AM do not exist. In fact, GSM is hyperbolic for  $R < 1/2$  and there are only unstable orbits in the phase space. Since the well map and the GSM are quantitatively related, location of AM are same for both the maps, i.e.,  $(X', P') = (\theta', J')$  and all the above arguments hold for well map also. However, AM of the well map differ only in the following way due to the reflective boundary condition. When particle is on the AM,  $n$ th kick causes the particle to undergo  $n$  bounces between the walls. If  $n$  is odd momentum changes its sign, in turn sign of the particle position is also flipped. Phase space of a mixed system generally has many intricate structures. In particular, boundaries of regular region embedded in chaotic sea have structures at all scales and all of them are hard to discern. Stable AM islands are believed to be separated from the remaining chaotic region by cantori (partial barriers). Phase

space in the vicinity of the cantori is sticky as it retains long time correlations. When chaotic orbits explore all parts of the phase space, there are occasions that they pass through the cantori. When such an event occurs, chaotic orbits stick to the vicinity of cantori for long time. Thus they are dragged along the modes ballistically [13]. This is a mechanism which is known to enhance momentum transport. Below we demonstrate that the beaches around the AM island when occupied by a large resonance of small order are highly sticky. This in turn implies that the cantori surrounding these must have large gaps to allow larger penetration of itinerant chaotic orbits. Before we dwell more on AM assisted super diffusion, it is instructive to look at some of the

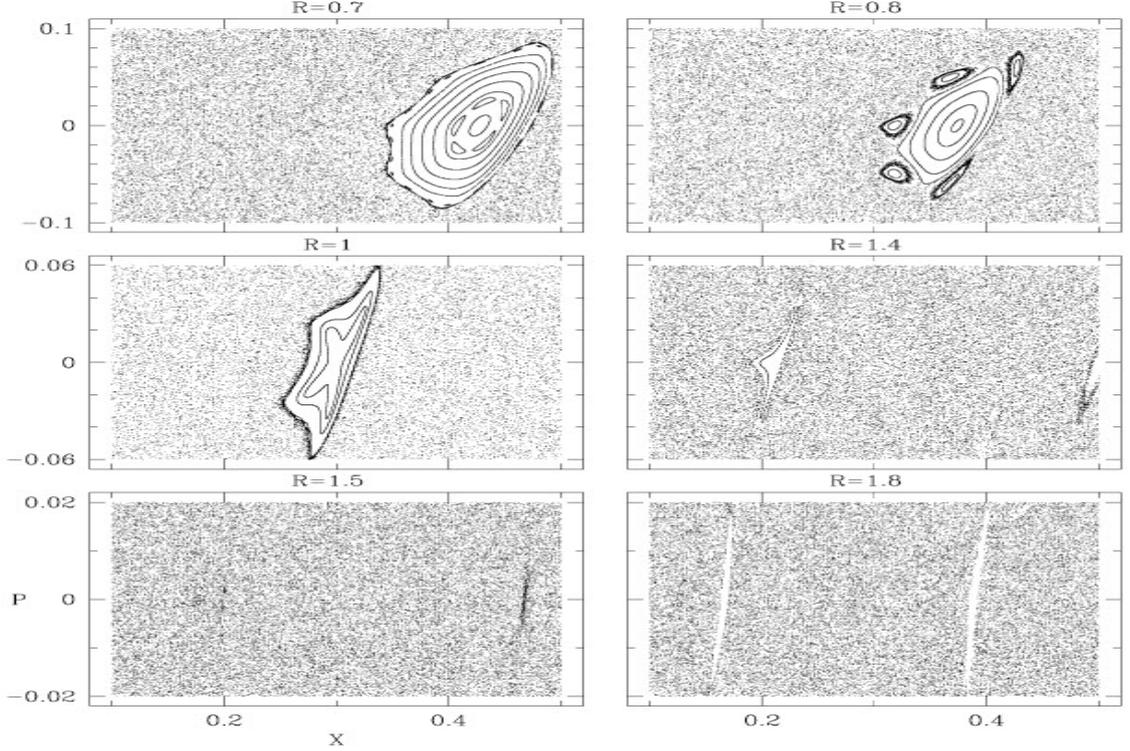


Figure 1: Stable regions embedded in chaotic sea are the accelerator modes of the well map ( $K/2\pi = 1.05$ ) whose  $P' = 0$  and  $X'$  is positive. For  $R=0.7, 0.8$  and  $1$ , we observe  $(1, 0)_-$  type mode. For  $R=1.4$ , one more mode just appears in the phase space which is  $(1, 0)_+$  type. For further increase of  $R$ , both the types are fully visible. Since  $X' \propto 1/R$ , as  $R$  increases the accelerator islands move towards interior of the square well. Note the three different scales on  $P$ -axis.

modes of the well map. Fig. 1 shows islands for different  $R$  values. In the given range of phase space we find one  $(1, 0)_-$  type mode for  $R=0.7, 0.8$  and  $1$ . As  $R$  increases the islands move towards interior of the well. For  $R=1.4$ , one more mode just appears at boundary of the well. This is a  $(1, 0)_+$  type mode. For further large values of  $R$  both the types fully appear and they

For (i) the ensemble consists of points with  $P_0 = 0$  and  $X_0$  distributed uniformly between  $-1/2$  and  $1/2$ . The range of  $R$  given by the Eq.(11) with  $R_0 = 0.598$  and  $R_1 = 1.988$  is seen as  $\gamma \cong 2$  due to ballistic evolution of the accelerating points contained in the ensemble. For (ii) the ensemble is chosen from

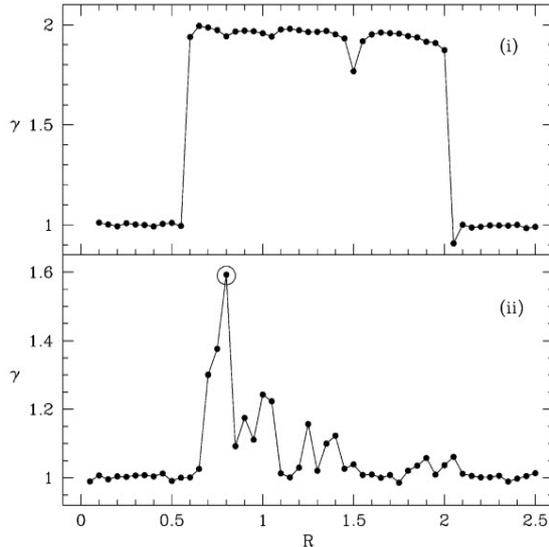


Figure 2: Exponent  $\gamma$  is plotted with respect to the parameter  $R$  for  $K/2\pi = 1.05$ . To obtain the exponent, an initial ensemble of 10 000 phase space points is iterated by the well map for 5000 time steps.

chaotic region of the phase space. Maximum exponent observed for  $R = 0.8$ , marked by circle, is due to the beaches around the AM island. move into the interior of the well. Evidently, parameter  $R$  also changes the size of the islands. In order to quantify the role of  $R$  in AM assisted anomalous transport, we consider  $\langle (P_n - P_0)^2 \rangle n^{-\gamma}$ . Here the angular bracket stands for an ensemble average and the exponent can be evaluated by iterating an ensemble of phase space points for long time under the well map. We perform numerical calculations for two different initial ensembles: (i) phase space points uniformly distributed along the line  $P_0 = 0$  which correspond to both accelerator and chaotic orbits; (ii) phase space points from a chaotic region which include only chaotic orbits. The ensemble (i) contains more chaotic orbits than the regular (accelerator) orbits. Chaotic orbits exhibit normal diffusion in momentum, i.e., like the random walk, until they are dragged along the mode. On the other hand, the

accelerator orbits exhibit ballistic behaviour ( $\gamma = 2$ ). Hence, in the long time limit, evolution of accelerator orbits dominate the ensemble average. Fig. 2(i), shows the characteristic exponent  $\gamma$

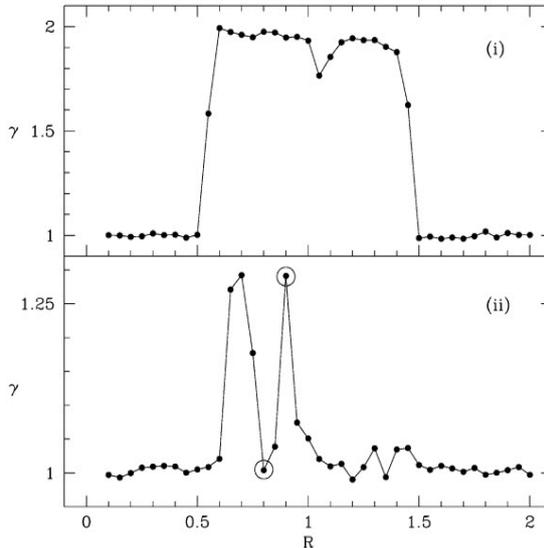


Figure 3: Exponent  $\gamma$  is plotted with respect to the parameter  $R$  for  $K/2\pi = 2.05$ . Rest of the calculation details are similar to the Fig. 2. In (i) the range of  $R$  given by the Eq.(11) with  $R_0 = 0.57$  and  $R_1 = 1.41$  is seen as  $\gamma \cong 2$ . In (ii) the exponents for  $R=0.8$  and  $0.9$  are marked by circles. Corresponding AM islands for these two cases are shown in Fig. 4.

for different  $R$  values. As we see, for the range of  $R$  in Eq.(11)  $\gamma \cong 2$ , confirming the existence of AM islands. Here the lesser  $\gamma$  for  $R=1.5$  is attributed to small size of AM (see Fig. 1). On contrary, for parameters outside the range of Eq. (11), diffusion is normal as there are no AM in the phase space. Fig. 2(ii) corresponds to the ensemble which contains only chaotic orbits. Within the parametric range where AM exist, the exponent? shows large fluctuations. There are also occasions wherein presence of AM does not enhance the diffusion significantly. It is natural to attribute the observed fluctuations to size of the islands and stickiness of their neighbourhood. That is, big AM islands with very sticky neighbourhood can significantly enhance the transport. For  $R=0.8$ ,

the exponent  $\gamma$  is found to be maximum ( $\cong 1.6$ ). As seen from Fig. 1, in this case AM island is surrounded by a chain of  $1/5$  resonance zones. These zones are also step-1 accelerators and they are separated from chaotic region by their boundary, the so-called beaches. Dynamics on the beach is chaotic, but very sticky with longer classical stay-ing time. If a wandering chaotic orbit happens to approach the beach region, it stays there for long time and thus gets accelerated along the modes resulting in very large enhancement in momentum

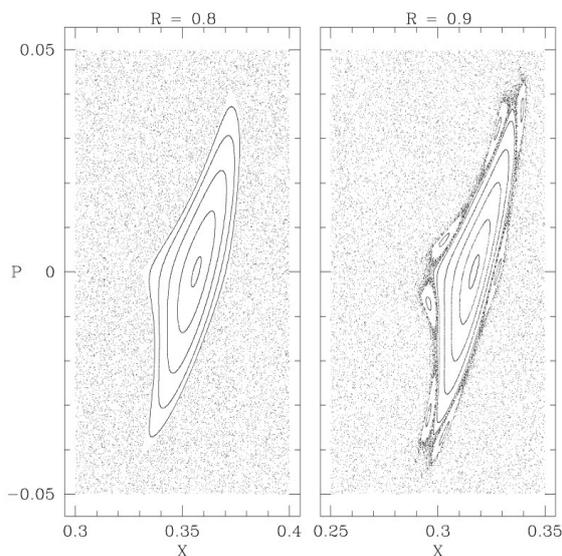


Figure 4: Step-2 AM are shown for  $K/2\pi = 2.05$ . For  $R = 0.9$ , the AM island is accompanied by a chain of  $2/7$  resonance zones and sticky beaches. On the other hand, AM island for  $R = 0.8$  is not accompanied by any beach regions.

transport. This maximum transport is a generic behaviour, i.e., independent of choice of the chaotic ensemble. From Fig. 1 we note that, although size of the AM for  $R = 0.7$  is larger than that for  $R = 0.8$ , exponent  $\gamma$  is maximum for the latter. This shows that the emergence of lower order resonance zones are chiefly responsible for the stickiness of the beach regions, leading to AM assisted anomalous transport. Thus the well map or equivalently GSM has a control

parameter  $R$  by tuning which AM induced super diffusion can be maximized. More over, longer the period of resonance zones lesser the stickiness of associated beach regions. Upon magnifying boundaries of AM islands for  $R = 0.7$  and  $1$ , we found long chain of resonance zones and their beach regions. As seen from Fig. 2(ii), enhancement is limited for both these cases. Further, we explore step-2 AM which are smaller in size than the step-1 modes. We choose  $K/2\pi = 2.05$  and step-2 modes exist in the range  $0.57 < R < 1.41$ . Nearly ballistic evolution in this range and the otherwise normal diffusion are shown in Fig. 3(i). In Fig. 3(ii) the exponent exhibits large fluctuations. In order to appreciate the role of beach regions in large scale transport, we focus our attention on two distinct cases where the exponent shows a minimum and a maximum. As we see from Fig. 4, when the enhancement is minimum (or absent) AM islands do not have the surrounding beach regions. On the other hand, transport is maximum when AM island is surrounded by short chain of resonance zones and their beach regions. These results reinforce that the expose of lower order resonance zones around the AM are chiefly responsible for stickiness of the beach and thus the resulting enhanced momentum transport.

## 2.2 Quantum kicked well

Analogous to the classical system, the kick to kick quantum dynamics can be studied using quantum map by solving Schrodinger equation for one period  $T$  as

$$|\psi(t + T)\rangle = U|\psi(t)\rangle, \quad (12)$$

where

$$U = \exp\{-ik \cos(2\pi x/\lambda)\} \exp\{-iH_0T/\hbar\}$$

with  $k = \varepsilon T/\hbar$ , being the effective field strength. Eigenvalue equation of the unperturbed system is  $H_0|\psi_n\rangle = E_n|\psi_n\rangle$ . The eigenstates and eigenvalues are given by

$$\langle X|\psi_n\rangle = \begin{cases} \sqrt{2} \cos(n\pi X) & \text{for } n \text{ odd,} \\ \sqrt{2} \sin(n\pi X) & \text{for } n \text{ even} \end{cases}$$

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

with  $n = 1, 2, 3, \dots$ . Considering unperturbed eigenstates as the basis, time evolution of an arbitrary quantum state is  $|\psi(t)\rangle = \sum_n A_n(t)|\phi_n\rangle$ , where  $A_n(t) = \langle\phi_n|\psi(t)\rangle$ . With following substitution

$$\tau = \frac{E_n T}{\hbar n^2}, \quad (14)$$

quantum map (12) takes the form

$$A_m(t+T) = \sum_n U_{mn} A_n(t), \quad (15)$$

where  $U_{mn} = e^{-i\tau n^2} \langle\phi_m|\exp\{-ik \cos(2\pi R X)\}|\phi_n\rangle$ . Dimensionless quantum parameters,  $t$  and the classical parameters are related through  $K/R = 8kt$ . Since  $k \propto 1/\hbar$  and  $t \propto \hbar$ , semiclassical limit for given classical system can be achieved by taking the limits  $k \rightarrow \infty$  and  $t \rightarrow 0$ . In the following numerical calculations, quantum map (15) is implemented with a finite, say  $N$ , number of unperturbed basis states. By obtaining the limit

$$\lim_{N \rightarrow \infty} \sum_{n=1}^N |A_n(t)|^2 \rightarrow 1 \quad (16)$$

we ensure that such a truncation of basis does not influence the quantum system. As seen from Eq.(15), unperturbed motion of the particle between successive kicks just adds phase to the wave function components through the parameter

$t \pmod{2\pi}$ . If  $t = 2\pi$ , unperturbed motion is absent and this is called quantum resonance. Under this condition, without loss of generality, we can write

$$|\psi(t)\rangle = e^{-ik \cos 2\pi R X t} |\psi(0)\rangle \quad (17)$$

where  $t$  represents the number of kicks. Then in the limit  $t \rightarrow \infty$ , kinetic energy of the particle grows quadratically, i.e.,  $\langle E \rangle_t \propto t^2$  [14]. This phenomenon is similar to that of the quantum kicked rotor [15]. An earlier study has shown that quantum resonance of kicked rotor occurs when  $t$  is rational multiples of  $2\pi$  [16]. This non-generic pure quantum phenomenon does not have any classical analogue. In order to investigate signatures of AM in the quantum system, it is necessary to suppress the resonance effect. This can be accomplished by taking  $t$  as an irrational multiple of  $2\pi$ .

One natural way to study the quantum signatures of the AM is using the time evolution of an initial wave packet localized in chaotic region of the classical phase space. We take a Gaussian wave packet confined in the square well as the initial state. In position representation it is given by

$$\langle X | \psi(0) \rangle = C \exp \left\{ -\frac{(X - \langle X \rangle)^2}{2\sigma^2} + \frac{i\langle P \rangle X}{\hbar_e} \right\}, \quad (18)$$

where  $\sigma$  measures width of the wave packet, centred at  $\langle X \rangle$  with momentum  $\langle P \rangle$ . Here  $\hbar_e = 2\tau/\pi^2$  is the effective Planck constant. Normalization constant,  $C$ , is obtained from the condition

$$\int_{-1/2}^{1/2} |\langle X | \psi(0) \rangle|^2 dX = 1$$

as

$$C = \left( \frac{2/\sigma\sqrt{\pi}}{\text{erf}(y_+) - \text{erf}(y_-)} \right)^{1/2}$$

with

$$y_{\pm} = \frac{\pm 1/2 - \langle X \rangle}{\sigma}. \quad (19)$$

As the quantum map is described in unperturbed basis states, the initial wave packet is represented in this basis. For evaluating  $A_n(0)$  we consider following integral

$$G_n = \sqrt{2} \int_{-1/2}^{1/2} e^{in\pi X} \langle X | \psi(0) \rangle dX \quad (20)$$

With change of variable  $u = (X - \langle X \rangle) / \sqrt{2}\sigma$  the integral becomes

$$G_n = 2\sigma C e^{iz_n \langle X \rangle} \int_{u_-}^{u_+} e^{-(u^2 - i\sqrt{2}\sigma z_n u)} du, \quad (21)$$

where  $z_n = n\pi + \langle P \rangle / \hbar$  and  $u_{\pm} = y_{\pm} / \sqrt{2}$ . Using the standard integral [17]

$$\int e^{-(a_0 x^2 + 2bx + x)} dx = \frac{1}{2} \sqrt{\frac{\pi}{a_0}} \exp\left(\frac{b^2 - ca_0}{a_0}\right) \operatorname{erf}\left(\frac{a_0 x + b}{\sqrt{a_0}}\right), \quad (22)$$

$G_n$  is represented in terms of complex error function, which can be computed using the algorithm [18]. The wave packet in the unperturbed basis is then given by

$$A_n(0) = \begin{cases} (G_n + G_{-n})/2 & \text{for } n \text{ odd,} \\ (G_n - G_{-n})/2i & \text{for } n \text{ even} \end{cases} \quad (23)$$

It should be noted that because of the spatial confinement, the initial state is a truncated Gaussian and hence it is not a minimum uncertainty wave packet. However, it can be made close to the minimum uncertainty wave packet provided mean  $\langle X \rangle$  is not close to boundary of the well and  $\Delta X \ll 1$ , i.e., spread in position is much less than the width of the square well. With this condition on the wave packet we consider the uncertainty relation  $\Delta X \Delta P = \hbar_e / 2$  for the following exercise. We take  $\Delta X = 0.02$  throughout. The initial wave packet is chosen with  $(\Delta X, \Delta P) = (0, 0.5)$  such that it is placed in a chaotic region. We take  $\hbar_e = 0.008$  and hence  $\Delta P = 0.2$ . For these choice of parameters, the initial state is squeezed in position and elongated in momentum. The number of basis states considered is as high as  $N=7500$ . Dimension-less kinetic energy

of the time evolved state is then given by

$$\langle E \rangle_t = \langle \psi(t) | P^2 | \psi(t) \rangle = \left( \frac{2\tau}{\pi} \right)^2 \sum_{n=1}^N |A_n(t)|^2 n^2, \quad (24)$$

which is equivalent to the classical energy  $\langle P_t^2 \rangle$ . Shown in Fig. 5 are typical quantum evolutions for  $K/2\pi = 1.05$  with varying  $R$  values. In all the cases, initially the quantum energy increases and then attains a quasiperiodic saturation. However, the saturation is much higher for  $R = 0.8$  than for  $R = 0.7$  and 1. It should be noted that even though effective field strength  $k$  is larger for  $R = 0.7$  than for  $R = 0.8$ ,

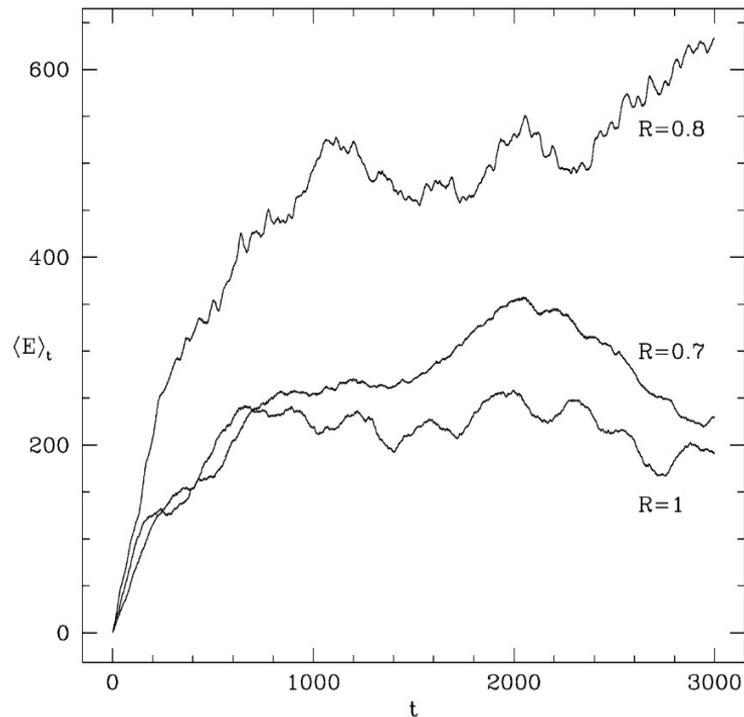


Figure 5: Kinetic energy of the quantum particle for  $K/2\pi = 1.05$ . For  $R = 0.7, 0.8$  and 1 the effective field strengths are  $k = 30.3, 26.5$  and  $21.2$ , respectively.

energy saturation for the later is much higher. We may compare these results with the corresponding phase space shown in Fig. 1. Thus, we obtain a clear evidence that the expose of lower order resonance zones and the associated

sticky beach around the AM are mainly responsible for AM assisted enhanced transport in quantum system also. Thus the treatment of the accelerator modes done in the Ref.[12] for a particle inside a 1D infinite square well in presence of a pulsed external field shows that when the border of AM (beach) exposes short periodic resonance zones, stickiness of the beach region is significantly increased, leading to AM assisted super diffusion in momentum. It also appears that longer the period of resonance lesser is the stickiness of the beach, results to less enhancement in transport. The corresponding quantum system is studied using time evolved wave packet. We showed that the presence of lower order resonance around the modes are responsible in enhancing the quantum transport as well. Some investigations on standard map show that for certain magic values of system parameter, AM is-lands are accompanied with hierarchy of self-similar structures. The vicinity of these structures are known to be regions of stickiness for the chaotic orbits [19, 20] causing enhancement in transport. Further, various multi-island structures in the near threshold regime of the map are identified as trapping zones for wandering orbits [21] leading to Levy-like flights. All these results collectively support that island-around-island structures are greatly responsible for anomalous transport in the mixed phase space.

### 3 Dirac equation for one-dimensional box

In non-relativistic quantum mechanics a vanishing normal component of the probability current is a sufficient condition to obtain an impenetrable boundary surface. This might be accomplished by imposing Dirichlet, Neumann or mixed boundary conditions upon the wavefunction. In the well known problem that we all learn in elementary quantum mechanics, the free particle in a one-dimensional box, the Dirichlet boundary condition,  $\psi = 0$ , is the simplest one. With this boundary condition the formal free Schrodinger Hamiltonian is a well defined self-adjoint operator. However, besides the above boundary condition, there exists a family of self-adjoint extensions each labelled by four parameters [23, 24]. In relativistic quantum mechanics the wavefunction is a spinor of four complex components, which are coupled in a system of first-order differential equations. Imposing the Dirichlet condition at the boundary is too restrictive; it leads to incompatibility in the relativistic scattering [25] as well as in the energy eigenvalues problem, as will be shown below. However, non-trivial solutions may be obtained by using appropriate boundary conditions for the wavefunction [26, 27], in such a way that self-adjointness of the formal Dirac operator is maintained. According to the principles of quantum mechanics, for each quantum mechanical system one defines a Hilbert space  $\mathcal{H}$ . Every measurable quantity is called an observable (e.g. energy, momentum, angular momentum, etc.) and has to be represented by a self-adjoint operator acting on  $\mathcal{H}$ . One might be interested in studying the Lorentz-covariant Dirac equation with covariant boundary conditions, but without losing any generality, the formal Lorentz covariance of a dynamical equation can be used to choose the privileged frame in which the intrinsic nature of the physical system is the simplest one. For a

particle in a box, if we want to know its energy eigenvalues, the convenient privileged frame is that in which the spacetime Lorentz transformations are frozen and the box is at rest in a determined space region. Once we have obtained the energy spectrum in the privileged frame, the energymomentum 4-vector may be calculated in any inertial frame. So, the state of the system is a normalized spinor, i.e. a four-component vector  $\Psi \in \mathcal{H}$ . Its time evolution is determined by the family of operators  $U(t) = e^{-iHt/\hbar}$ . Conservation of probability requires the operator  $U(t)$  to be unitary and, consequently, the Hamiltonian  $H$  to be self-adjoint. This is a very special observable because it generates the time evolution of the states and its spectrum represents the energy of the system. To define the Hamiltonian properly, besides the formal expression as a differential operator, its domain, in particular the boundary conditions, must be specified. In fact, by changing the boundary conditions of a given operator, one modifies the operator itself without changing its formal expression, not to mention the risk of losing the self-adjointness property (see appendix A). For example, in the Aharonov-Bohm effect, by choosing different boundary conditions, which preserve self-adjointness, one obtains different cross sections [26]; aside from other considerations, it is the experimental arrangement which selects the appropriate observable. In section 2 we give several physically acceptable boundary conditions, some of which were already proposed in scattering problems [26, 27]. We find non-trivial solutions of the Dirac equation for a particle with a fixed mass localized in a box. These results, as well as the eigenvalues and eigenfunctions for a family of self-adjoint extensions of the free Dirac Hamiltonian were obtained in [28]. It is worth pointing out that, as far as we know, the problem of the several boundary conditions that may be imposed for a free particle in-

side a box in relativistic quantum mechanics, has not been considered in the widely used textbooks for exact solutions of the Dirac equation [?]. However, the problem of a Dirac fermion in a one-dimensional box interacting with a scalar solitonic potential was considered earlier with periodic [32], as well as with more general boundary conditions [33] to elucidate the phenomenon of fractional fermion number. For the case of the Dirac free massless operator, also in 1C1 dimensions, eigenvalues and eigenfunctions were obtained for a family of self-adjoint extensions in [34] and the case with a non-zero vector potential was examined in [35]. Another particular solution to this problem has been obtained by considering the Dirac equation with a Lorentz scalar potential; here the rest mass can be thought of as an  $x$ -dependent mass [31]. This allows us to solve the infinite square well problem as a particle with a changing mass that becomes infinite outside the box, which avoids the Klein paradox [36]. A detailed study of the possible boundary conditions, i.e. self-adjoint extensions, for a relativistic particle inside a box, as well as their non-relativistic limits, has been considered by two of us (VA and SDeV) and will be submitted for publication elsewhere. The principal motivation in this pedagogical note is to call attention to the fact that the boundary conditions used in non-relativistic quantum mechanics should not be extrapolated to the relativistic case, without proving beforehand that the relativistic Hamiltonian will be self-adjoint for them. In section 2 we verify that the Dirac spinor cannot vanish at the boundary of a non-permitted region in our case, the walls of a one-dimensional box. We find non-trivial solutions upon imposing several boundary conditions on the wavefunction. The non-relativistic limit of these results is also discussed. In section 3 we solve the problem of a particle in a spherical box using a boundary

condition that cancels the large component of the spinor at the walls of the box. We propose various boundary conditions that lead to non-trivial solutions. Let us consider a free electron in a one-dimensional box in the interval  $\Omega = [0; L]$ . The three-dimensional Dirac equation for stationary states reads

$$H_0\psi = (-i\hbar c\boldsymbol{\alpha} \cdot \nabla + mc^2\beta)\psi = E\psi \quad (25)$$

where  $\alpha, \beta$  are the well known Dirac matrices. In this paper we restrict ourselves to positive relativistic energies. In the Dirac representation, the four-valued Dirac spinor can be expressed in terms of the large and small two-valued semi-spinors,  $\phi = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$  and  $\chi = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}$ , respectively; that is

$$\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \quad (26)$$

Equation (25) is equivalent to the following coupled equations:

$$-i\hbar c\boldsymbol{\sigma} \cdot \nabla\chi + mc^2\beta\phi = E\phi \quad (27)$$

$$-i\hbar c\boldsymbol{\sigma} \cdot \nabla\phi - mc^2\beta\chi = E\chi \quad (28)$$

where  $\sigma$  are the Pauli matrices. Eliminating  $\chi$  from (27) and (28), and taking  $\phi = \phi(x)$  and  $\chi = \chi(x)$ , with

$$k = [E^2 - (mc^2)^2]^{1/2}/\hbar c \quad (29)$$

, one obtains

$$\left(\frac{d^2}{dx^2} + k^2\right)\phi_i = 0 \quad (30)$$

$$i = 1, 2$$

which is independently satisfied by the large components. The small components may be obtained by means of

$$\begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix} = \frac{-i\hbar c}{E + mc^2} \begin{pmatrix} 0 & \frac{d}{dx} \\ \frac{d}{dx} & 0 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} \quad (31)$$

One of the positive energy solutions is obtained by taking  $\phi_2 = 0$  and therefore  $\chi_2 = 0$ . From equation (30), the general solution for  $\phi_1$  is

$$\phi_1 = A_1\phi_1^{(1)} + B_1\phi_1^{(2)} = A_1e^{ikx} + B_1e^{-ikx} \quad (32)$$

where  $A_1$  and  $B_1$  are complex constants. The solutions  $\phi_1^{(1)}$  and  $\phi_1^{(2)}$  are independent and verify the following relation in the interval  $\Omega$ :

$$\phi_1^{(1)} \frac{d\phi_1^{(2)}}{dx} - \phi_1^{(2)} \frac{d\phi_1^{(1)}}{dx} = 0 \quad (33)$$

From equation (31) one gets

$$\chi_2 = \frac{-i\hbar c}{E + mc^2} \left( A_1 \frac{d\phi_1^{(1)}}{dx} + B_1 \frac{d\phi_1^{(2)}}{dx} \right) = \frac{\hbar ck}{E + mc^2} (A_1 e^{ikx} - B_1 e^{-ikx}). \quad (34)$$

If  $\phi(0) = \begin{pmatrix} \phi_1(0) \\ 0 \end{pmatrix} = 0$  and  $\chi(0) = \begin{pmatrix} 0 \\ \chi_2(0) \end{pmatrix} = 0$  one obtains the homogeneous system

$$A_1\phi_1^{(1)}|_{x=0} + B_1\phi_1^{(2)}|_{x=0} = 0 \quad (35)$$

$$A_1 \frac{d\phi_1^{(1)}}{dx}|_{x=0} + B_1 A_1 \frac{d\phi_1^{(2)}}{dx}|_{x=0} = 0 \quad (36)$$

the determinant of which cannot be zero due to (33). Thus  $A_1 = B_1 = 0$ , that is, the only solution is the trivial one. A similar result is obtained if  $\psi = 0$  at  $x = L$ . From equation (31), it can be seen that the vanishing of the small component  $\chi_2$  at  $x = 0$  is equivalent to  $d\phi_1/dx|_{x=0} = 0$ . The non-existence of non-trivial solutions for the given boundary condition is certainly

a consequence of the fact that (30) is an elliptic equation, so that there are no non-trivial solutions if the function  $\phi_1$  and its derivative  $\chi_2$  have to vanish simultaneously at the boundaries of the interval  $\Omega$ . Certainly, the vanishing of the entire relativistic wave function at the beginning of an impenetrable barrier is not admissible. Though in non-relativistic quantum mechanics a vanishing wave function at the boundaries is one of the self-adjoint extensions of the free Hamiltonian, in relativistic quantum mechanics it is not so. Indeed, the formal Dirac free Hamiltonian does not have this boundary condition as one of its self-adjoint extensions. However, taking only the large component as zero is a physically acceptable boundary condition, because this condition is a self-adjoint extension of  $H_0$ . In the problem of an electron inside a one-dimensional box, by imposing upon the large component

$$\phi_1(0) = \phi_1(L) = 0 \quad (37)$$

one obtains inside the interval  $\Omega$

$$\psi = 2A_1 \begin{pmatrix} i \sin(kx) \\ 0 \\ 0 \\ \frac{\hbar ck}{E+mc^2} \cos(kx) \end{pmatrix} \quad (38)$$

with  $k = N\pi/L$ ,  $N = 1, 2, \dots$ . From appendix B, it can be seen that condition (37) corresponds, in the non-relativistic limit, to the familiar condition of a vanishing wavefunction at the walls of the box; that is,  $\phi_1^{NR}(0) = \phi_1^{NR}(L) = 0$ . Likewise, and according to the SchrodingerPauli problem, the small components of (38) are of the order of  $v^{NR}/c$  and  $k^{NR} = (2mE^{NR})^{1/2}/\hbar$ . The Dirac probability density and current are given by

$$\rho = \bar{\phi}_1 \phi_1 + \bar{\chi}_2 \chi_2 \quad (39)$$

$$j = ec\psi^\dagger\alpha_x\psi = ec(\bar{\phi}_1\chi_2 + \bar{\chi}_2\phi_1) \quad (40)$$

where  $\psi^\dagger$  is the Hermitian conjugate spinor and  $\bar{\phi}$  is the complex conjugate of  $\phi$ . With the boundary condition (37), these quantities verify

$$\rho(0) = \rho(L) \quad (41)$$

$$j(0) = j(L) = 0 \quad (42)$$

In this case, the electron is actually enclosed inside the box there is no particle for  $x < 0$  or  $x > L$ . There are a variety of other ways of satisfying (42), even though the four components of the Dirac spinor cannot be equal to zero simultaneously. In fact, in addition to (37), the impenetrability condition  $j = 0$  can be achieved, for example, in any of the following three cases:  $\phi_1(0) = \chi_2(L)$ ,  $\phi_1(L) = \chi_2(0)$  and  $\chi_2(0) = \chi_2(L) = 0$ . The vanishing of the relativistic current density at the walls of the box has been used in the MIT bag model, see e.g. [39]. The relativistic boundary condition used in this model is  $\pm(-i)\beta\alpha_x\psi = \psi$ , where the minus sign corresponds to  $x = 0$  and the plus sign to  $x = L$ . This boundary condition in the Dirac representation is precisely  $\chi_2(L) = \phi_1(L) = -\chi_2(0) = \phi_1(0) = i$ . All these conditions, which can be used if we consider the walls of the box to be impenetrable barriers, are self-adjoint extensions for the free Dirac Hamiltonian. It may argued that the mixed boundary conditions  $\phi_1(0) = \chi_2(L) = 0$  and  $\phi_1(L) = \chi_2(0) = 0$  are not physical because their symmetry is not the same at the walls of the box. In fact, the probability density  $\rho$  is such that  $\rho(0) \neq \rho(L)$ ; therefore these boundary conditions are not symmetric and consequently the corresponding wave functions exhibit a set of eigenvalues,  $k = (N - \frac{1}{2})\pi/L$  with  $N = 1, 2, 3, \dots$ , which are different from those of the wave function (38). In the non-relativistic limit these conditions correspond to a vanishing of  $\phi_1^{NR}$  at  $x = 0(x = L)$  and a vanishing of  $d\phi_1^{NR}/dx$  in  $x = L(x = 0)$ .

On the other hand, the boundary condition

$$\chi_2(0) = \chi_2(L) = 0 \quad (43)$$

yields the eigenfunction in  $\Omega$

$$\psi = 2A_1 \begin{pmatrix} \cos(kx) \\ 0 \\ 0 \\ \frac{i\hbar ck}{E+mc^2} \sin(kx) \end{pmatrix} \quad (44)$$

which has the same eigenvalues as the wave function (38) and satisfies the same relations (41) and (42). In the non-relativistic limit this state corresponds to a vanishing of  $d\phi_1^{NR}/dx$  at  $x = 0$  and  $x = L$ . The spinor (44) describes a positive energy electron; however, one may consider the charge conjugate of this spinor which has a vanishing large component, which may be regarded as describing a negative energy positron. It is important to emphasize that by taking into account only the physical symmetry (41), the requirement of impenetrability (42) and the corresponding energy spectrum, one cannot distinguish between the boundary conditions (37) and (43); that is,  $\phi_1(0) = \phi_1(L) = 0$  and  $\chi_2(0) = \chi_2(L) = 0$ . Hence, the wavefunctions (38) and (44) should be regarded as equivalent, although not trivially equivalent inasmuch as they cannot be taken one into the other by means of a symmetry operation which commutes with the Hamiltonian. Indeed, we consider that it is not possible to distinguish physically between these two solutions, despite the fact that they exhibit different probability densities. We assume that the probability prediction can be verified experimentally only in regions of size  $\Delta x$  sufficiently large so as to comply with the uncertainty relation  $\Delta x \Delta p \geq \hbar = 2$ , with  $\Delta p$  corresponding to the quantum state not perturbed by the measurement of localization. According to

this criterion, the localization of the points, which in the non-relativistic limit corresponds to a zero probability of the stationary wave, is not possible. It is worth to mention that, in relativistic quantum mechanics, one cannot localize the electron in a region of size less than the Compton wavelength, because otherwise the electron energy would be sufficient for pair production. Clearly,  $L$  must be much larger than the Compton wavelength. Finally, the boundary condition

$$\frac{\chi_2(L)}{\phi_1(L)} = -\frac{\chi_2(0)}{\phi_1(0)} = i \quad (45)$$

yields the following eigenfunction in  $\Omega$ :

$$\psi = 2A_1 e^{i\delta/2} \begin{pmatrix} \cos(kx - \delta/2) \\ 0 \\ 0 \\ \frac{i\hbar ck}{E+mc^2} \sin(kx - \delta/2) \end{pmatrix} \quad (46)$$

where  $\delta = \arctan(-\hbar k/mc)$ . In this case the eigenvalues are obtained from the transcendental equation  $\tan(kL) + (\hbar k/mc) = 0$ . It is worth pointing out that these results are the same as those obtained in [36]. There the authors give a mathematical justification for treating the problem of a particle absolutely confined in a box, without requiring the continuity of the wavefunction at the wall of the box. In [36] where a scalar potential is used, the particle mass becomes infinite in the external region of the box. However, we just impose adequate boundary conditions such that the Hamiltonian be self-adjoint. Taking the non-relativistic limit of (45), as is done in appendix B, we obtain  $\lambda \left( d\phi_1^{(NR)}/dx \right) (0) = -\left( \phi_1^{(NR)} \right) (0)$  and  $\lambda \left( d\phi_1^{(NR)}/dx \right) (L) = \left( \phi_1^{(NR)} \right) (L)$ . The non-relativistic energy eigenvalues are obtained from  $\tan(k^{(NR)}L) + (\hbar k^{(NR)}/mc) = 0$ . Obviously, by eliminating the term of order  $v^{(NR)}/c$  and allowing the size of the box to grow, we obtain that the spectrum, the wavefunction and the bound-

ary condition tend to their usual non-relativistic values [36]. Another way of getting a well defined self-adjoint problem is by extending the domain of  $H_0$  to that of periodic or anti-periodic functions in the interval  $\Omega$ . In fact, we may consider

$$\psi(0) = \pm\psi(L). \quad (47)$$

The corresponding plane-wave eigenfunctions have the form

$$\psi = C_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{\hbar ck}{E+mc^2} \end{pmatrix} e^{ikx} \quad (48)$$

and the energy eigenvalues are obtained from  $k = 2n\pi/L$  with  $n = 0, \pm 1, \pm 2, \dots$  for the periodic condition and from  $k = (2n - 1)\pi/L$  for the anti-periodic one. On the other hand, taking the non-relativistic limit of these boundary conditions, we obtain  $\phi_1^{(NR)}(0) = \pm\phi_1^{(NR)}(L)$ ,  $(d\phi_1^{(NR)}/dx)(0) = \pm(d\phi_1^{(NR)})/dx(L)$ , where the plus (minus) sign corresponds to the non-relativistic periodic (anti-periodic) condition. For these boundary conditions the density current in  $x = 0$  and  $x = L$  is not zero, and satisfies  $j(0) = j(L)$ . In this case the current at the box walls must be interpreted physically. One may say that the walls of the box are transparent to the particle, which is travelling through the box in a condition of resonance. As distinguished from the non-relativistic problem, the relativistic wavefunction at the boundaries of a non-permitted region cannot vanish entirely. A necessary and sufficient condition in order to find non-trivial solutions is to impose on the wavefunction boundary conditions that make the Hamiltonian self-adjoint. For some of these conditions the probability current vanishes at the walls of the box; they are just the conditions which can be

used in a model of an impenetrable barrier in place of the continuity of the wavefunction.

## 4 Kicked Dirac particle in a one-dimensional box

In this section we treat quantum dynamics of the Dirac particle confined to one dimensional box and simultaneously driven by delta-kicking potential. Study of particle dynamics in confined systems is of fundamental and practical importance for variety of problems in nanoscale physics. This causes monotonically growing interest to the different aspects of classical and quantum particle dynamics in confined systems. It should be noted that the main difference between the physical properties of bulk and confined systems is caused by the boundary conditions to be imposed for the quantum mechanical wave equations. In the case of bulk systems these conditions are given in whole space, while for confined systems 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. Thus the role of quantum confinement and size effects is one of the central problems of nanoscale physics. Earlier particle dynamics in confined domains was the subject of extensive research in the context of non-linear dynamics and quantum chaos theory (see, e.g., Refs. [40]-[43]). Particle dynamics in confined domains can be successfully described both in quantum and classical contexts by modeling so-called billiard geometries which became paradigm of quantum chaos theory [40, 44]. It was found that depending on the shape of the billiard walls classical dynamics of the system can be regular, mixed or chaotic. In the case of quantum systems, Later, in late nineties of the last century, different types of confined particle motion started to be explored in the context of mesoscopic and nanoscale physics, in such systems as quantum dots, wells and wires, nanoscale networks, fullerene, CNT (carbon nano tube), graphene and many other structures. However, despite certain progress

made in the study of confined particle dynamics, most of the studies are mainly restricted by non-relativistic systems. However, relativistic confined particles are of importance for particle and graphene physics. Consider a Dirac particle confined in a one dimensional box and interacting with external delta-kicking potential. Quantum dynamics of such particle is described by the following Dirac equation(in the system of units  $\hbar = m = c = 1$ ):

$$\frac{\partial \Psi(x, t)}{\partial t} = [-i\alpha \frac{d}{dx} + \beta + \varepsilon \cos x \sum_l \delta(t - lT)] \Psi(x, t), \quad (49)$$

for which the box boundary conditions are imposed. Exact solution of this equation can be obtained within the single kicking period as in the case of kicked rotor [1] and kicked particle in infinite potential well [12]. Indeed, expanding the wave,  $\Psi(x, t)$  can be in terms of the complete set of the solutions of Eq.(38)

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

and inserting this expansion into Eq.(49) after integrating the obtained equation we have

$$A_n(t + T) = \sum_l A_l(t) V_{ln} e^{-iE_l T}, \quad (50)$$

where

$$V_{ln} = \int \psi_n^*(x) e^{i\varepsilon \cos x} \psi_l(x) dx$$

and  $E_l$  is defined by Eq. (29). Using the relation

$$e^{i\varepsilon \cos x} = \sum_{m=-\infty}^{\infty} b_m(\varepsilon) e^{imx}, \quad (51)$$

where  $b_m(\varepsilon) = i^m J_m(\varepsilon)$  the matrix elements can be calculated exactly and analytically as. It is important to note that  $A_n(t)$  should satisfy norm conservation condition given as

$$\sum_n |A_n(t)| = 1; \quad \forall t,$$

and initial conditions for  $A_n(t)$  should be chosen on the basis of this condition. The quantity we are interested to treat is time-dependence of the average kinetic energy which can be calculated as

$$E(t) = \int \Psi^*(x, t) H_0 \Psi(x, t) dx = \sum |A_n(t)|^2 E_n,$$

where  $A_n(t)$  can be found from Eq.(50).

Another choice of the kicking potential is Lorentz-scalar-type kicking for which the Dirac equation can be written as

$$\frac{\partial \Psi(x, t)}{\partial t} = \left[ -i\alpha \frac{d}{dx} + \beta(1 + \varepsilon \cos x \sum_l \delta(t - lT)) \right] \Psi(x, t). \quad (52)$$

In this case kicking potential is included into the mass term in the Dirac equation that makes different its matrix structure. We explore particle dynamics for both cases by treating time-dependence of the average kinetic energy and wave packet evolution.

#### 4.1 Average kinetic energy

Calculations of the of average kinetic energy is quite important in the context of so-called quantum localization phenomenon [15] and quantum Fermi acceleration. Unlike classical kicked systems, in quantum kicked systems the growth of the energy is suppressed [15]

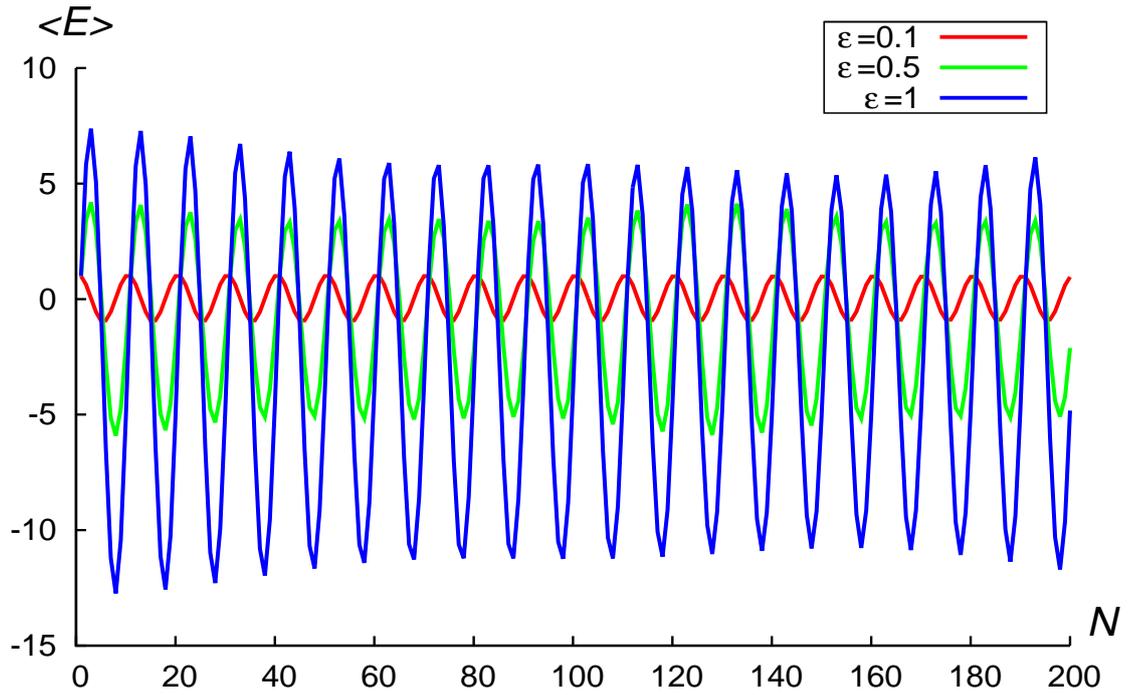


Figure 6: Time-dependence of the average kinetic energy for the fixed kicking period ( $T = 0.1$ ) at different kicking strengths in the case of scalar kicking potential (in the units of the kicking period).

Fig. 6 represents the average kinetic energy as a function of time for the value of kicking period  $T = 0.1$  and at different values of the kicking strength. As is seen from these plots, the average kinetic energy is a periodic function of time for these values of kicking parameters. This implies existence some synchronization between the particle motion and kicking force. It is clear that no monotonic particle acceleration is possible in this case.

In Fig. 7 the case of resonances at which  $E(t)$  monotonically grows in time are plotted for scalar kicking potential.

Fig. 8 represents the average kinetic energy as a function of time for the value of kicking period  $T = 0.1$  and at different values of the kicking strength for the case of Lorentz scalar potential. As is seen from these plots, the average

kinetic energy is strongly suppressed compared to that for scalar kicking and no Fermi acceleration is possible. We also found that no resonances are possible in the case of Lorentz scalar kicking.

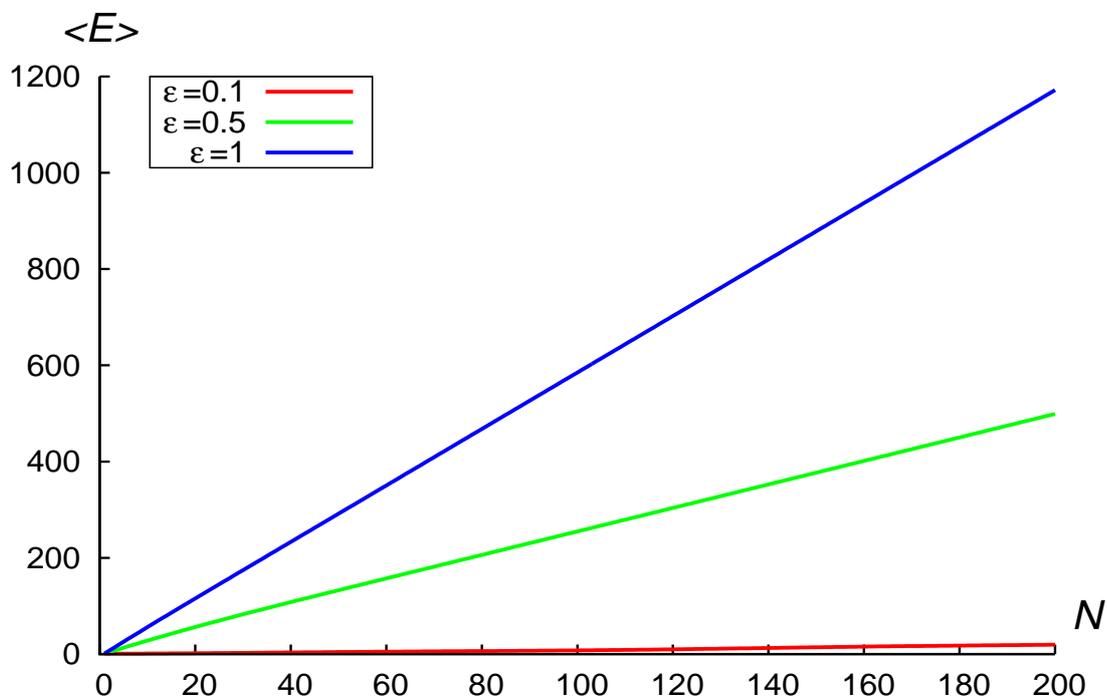


Figure 7: The case of the quantum resonance ( $T = 1$ ,  $\varepsilon = 0.1, 0.5$  and  $1$ )

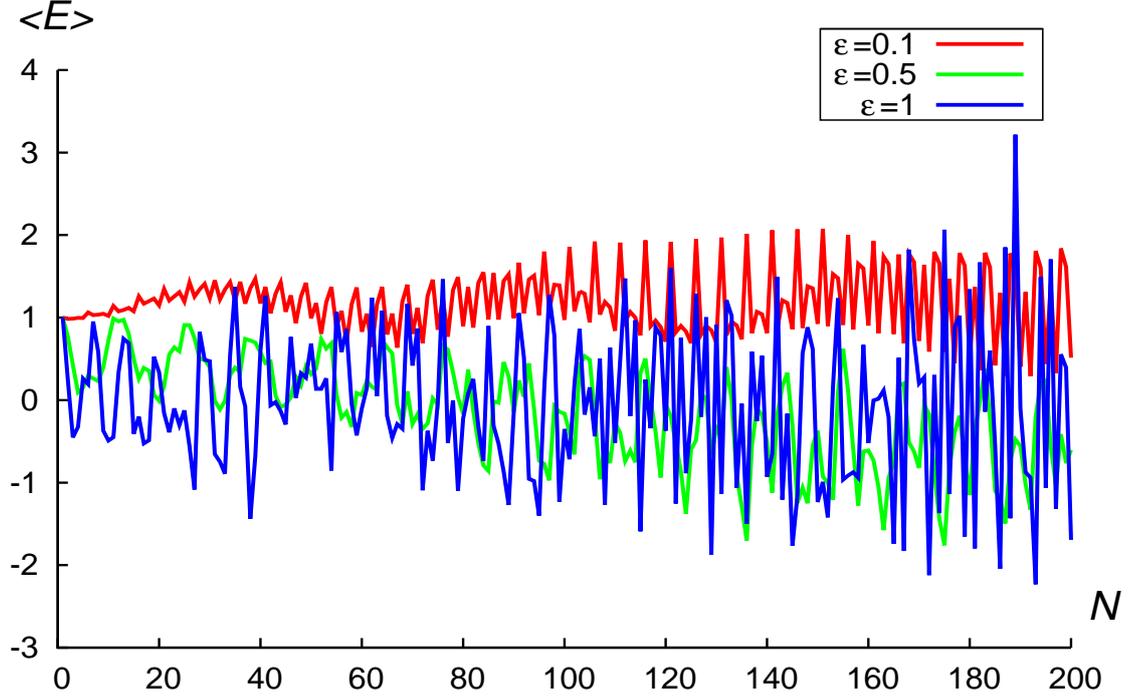


Figure 8: Time-dependence of average kinetic energy for fixed kicking period ( $T = 0.1$ ) at different values of the kicking strength ( $\varepsilon = 0.1, 0.5$  and  $1$ ) for Lorentz-scalar type kicking potential (in the units of kicking period).

## 4.2 Wave packet evolution

Another problem we explored in this work is the wave packet evolution. To treat the wave packet evolution in our system the initial condition is chosen in terms of the Gaussian wave packet as follows:

$$\Psi(x, 0) = \frac{f(x)}{\sqrt{|s_1|^2 + |s_2|^2 + |s_3|^2 + |s_4|^2}} \begin{pmatrix} s_1 \\ s_2 \\ s_3 \\ s_4 \end{pmatrix} \quad (53)$$

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

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

By multiplying each side of Eq.(53) to  $\psi_m^*(x)$  and integrating over  $x$  from 0 to  $L$ , we can get expression for initial values of the expansion coefficient as

$$A_n(0) = \int_0^L \psi_n^*(x) \Psi(x, 0) dx \quad (54)$$

In Figs. 9 and 10 evolution of the wave packet for the kicking parameters  $T = 0.1$  and  $\varepsilon = 5$  is presented for scalar and Lorentz scalar kicking potentials. As it can be seen from these plots, the picture of the evolution is completely different for scalar and Lorentz scalar potentials. Namely, in case of the the scalar kicking the splitting of the packet into two parts with different spins is possible, while for Lorentz scalar case the packet splits into more than two parts. Such splitting is possible due to the boundary conditions that mix the different spins.

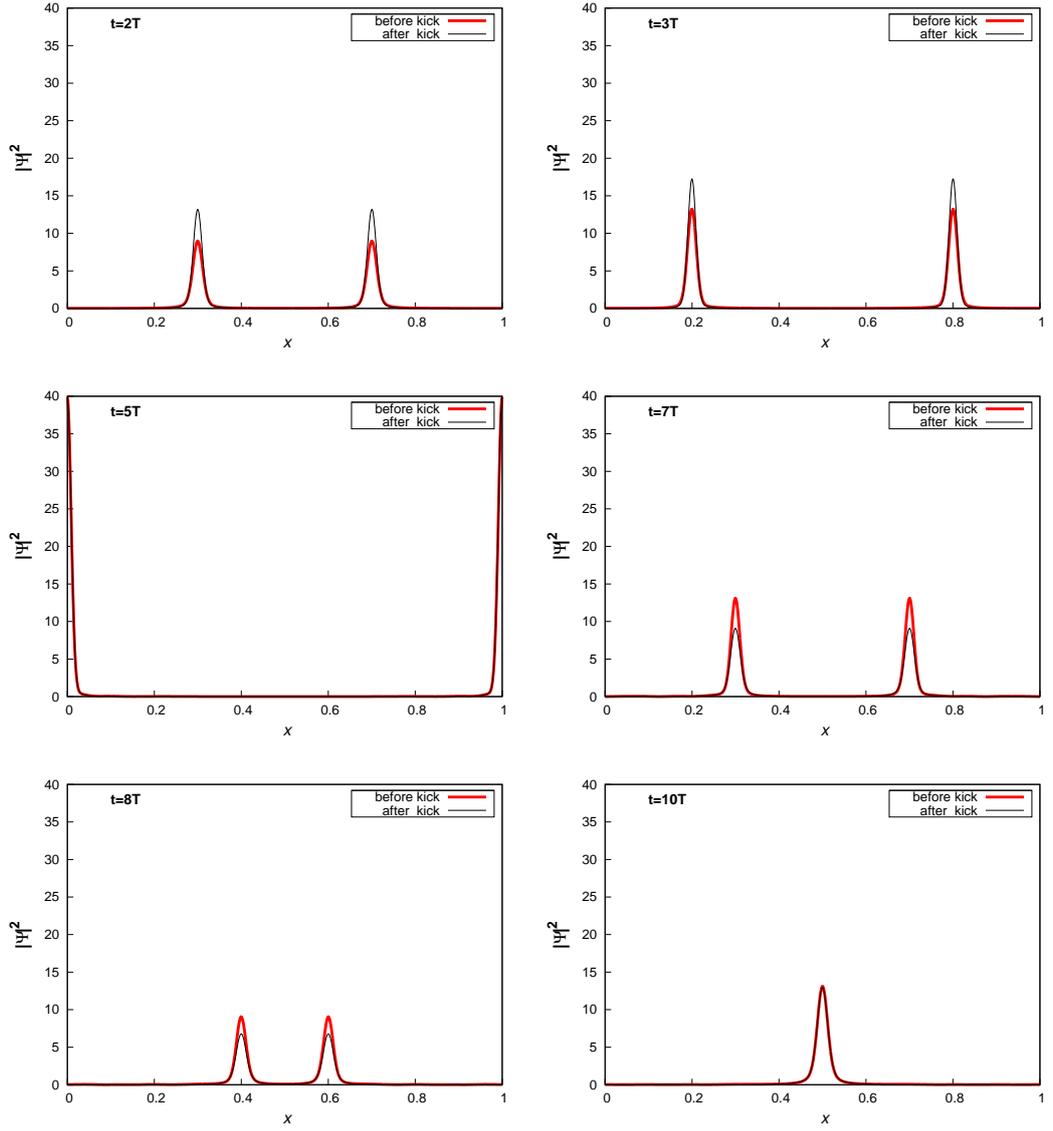


Figure 9: Gaussian wave packet evolution in delta-kicked one dimensional box for kicking parameters  $T = 0.1$  and  $\varepsilon = 5$ . Scalar kicking case is considered.

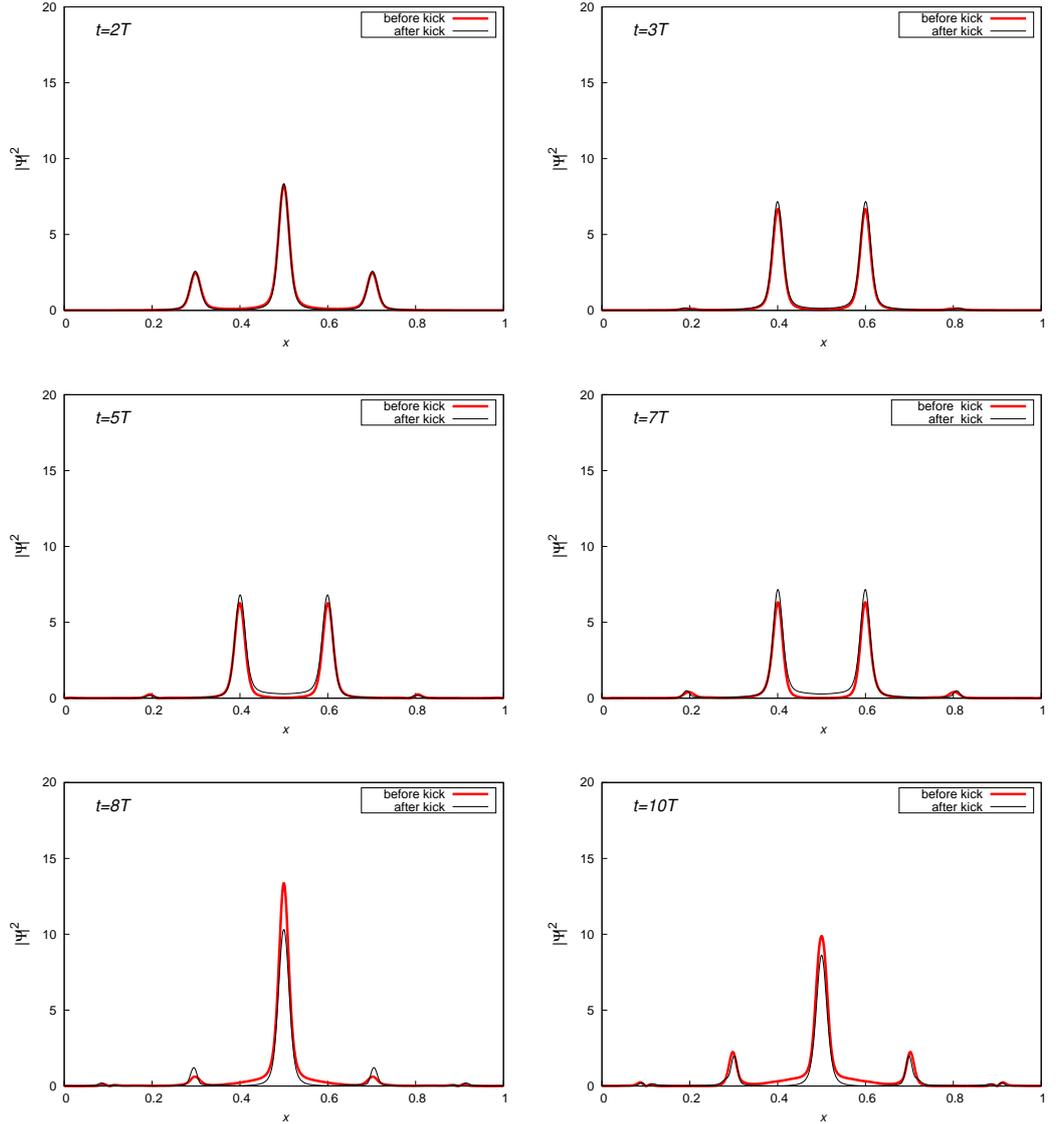


Figure 10: Gaussian wave packet evolution in delta-kicked one dimensional box for kicking parameters  $T = 0.1$  and  $\varepsilon = 5$ . Lorentz-Scalar kicking case is considered.

## 5 Conclusion

Thus we have studied quantum dynamics of a kicked Dirac particle confined to one dimensional box by treating time-dependence of the average kinetic energy and wave packet evolution. The wave function is found analytically for

single kicking period. Using the obtained solution the average kinetic energy is computed as a function of time. Two types of the the kicking potentials are considered: Scalar and Lorentz-scalar kicking potentials. It is found that in the case of Lorentz scalar kicking the growth of the energy is strongly suppressed compared to that of scalar kicking. Also, resonances at which energy grows monotonically are found for scalar kicking case, while for Lorentz scalar case there are no resonances. Particle transport in the system is analyzed by exploring wave packet evolution. In case of the the scalar kicking splitting of the packet into two parts with different spins is possible, while for Lorentz scalar case the packet splits into more than two parts. The results obtained within this study can be used for the study of particle transport in hadrons driven by external forces and some carbon nanostructures (e.g. CNT, graphene, fullerene etc.) where particle dynamics is described by the Dirac equation.

## Appendix A

For the relativistic 'free' particle inside a one-dimensional box with fixed walls at  $x = 0$  and  $x = L$  the Dirac equation for stationary states may be written as

$$(H_0\psi)(x) = (-i\hbar c\alpha_x \frac{d}{dx} + mc^2\beta)\psi(x) = E\psi(x) \quad (\text{A1})$$

(A1)

where  $\psi$  is the four-component column Dirac spinor depending on  $x \in \Omega = [0; L]$  and

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The spinors  $\psi(x)$  and  $(H_0\psi)(x)$  belong to a dense proper subset of the Hilbert space  $H = L^2(\Omega) \oplus L^2(\Omega)$ ; that is, in this subset there exists a basis in which to expand every  $\psi \in \mathcal{H}$ , with a scalar product denoted by  $\langle, \rangle$ . Generally the domains of  $H_0$  and its adjoint  $H_0^*$  verify  $\text{Dom}(H_0) \subseteq \text{Dom}(H_0^*)$ , but  $H_0$  must be self-adjoint, so we look for self-adjoint extensions of the symmetric operator  $H_0$  (as we shall define below). Without using the machinery of Von Neumanns theory of self-adjoint extensions of symmetric operators [39] and without intending to be rigorous, let us briefly consider the construction of a self-adjoint operator from the formal Hamiltonian

$$H_0 = -i\hbar c\alpha_x \frac{d}{dx} + mc^2\beta \quad (\text{A2})$$

whose initial dense domain may be written as

$$\mathcal{D} = \psi \in \mathcal{H}, \quad \text{a.c. in } \Omega, \quad (H_0\psi) \in \mathcal{H}, \quad \text{with } \psi(0) = \psi(L) = 0 \quad (\text{A3})$$

where a.c. means absolutely continuous functions. With this domain  $H_0$  is a symmetric operator; that is, for all

$$\zeta, \eta \in \mathcal{D},$$

$$\langle H_0\zeta, \eta \rangle - \langle \zeta, H_0\eta \rangle = i\hbar c[(\zeta \dagger a_x \eta)(L) - (\zeta \dagger a_x \eta)(0)] = 0. \quad (\text{A4})$$

Since the quantum dynamics requires  $H_0$  to be a self-adjoint operator, it must be fulfilled that  $\text{Dom}(H_0) = \text{Dom}(H_0^*)$ , where  $(H_0^*)$ , defined by the same formal operator (A2), is the adjoint of the differential operator  $H_0$ . Its domain is defined by  $\text{Dom}(H_0^*) = v \in H, \text{ a.c. in } \Omega, (H_0^*v) \in H,$

$$\langle H_0\zeta, v \rangle - \langle \zeta, H_0^*v \rangle = i\hbar c[(\zeta \dagger a_x v)(L) - (\zeta \dagger a_x v)(0)] = 0. \quad (\text{A5})$$

for all  $\zeta \in \text{Dom}(H_0)$  and  $v \in \text{Dom}(H_0^*)$ . Clearly,  $(H_0^*)$  is defined on a manifold of spinors taking arbitrary values at the end points of the interval  $\Omega$ . So, the boundary conditions (BC) defined by equation (A3) are incompatible with the required self-adjointness of  $H_0$ . Now the problem consists in choosing a sufficiently general set of BC for which  $\text{Dom}(H_0)=\text{Dom}(H_0^*)$ . If  $\text{Dom}(H_0)$  is fixed,  $H_0^*$

will be the adjoint of  $H_0$  if

its maximal domain is consistent with the vanishing of  $(\zeta \dagger a_x v)(L) - (\zeta \dagger a_x v)(0)$ , for all  $\zeta \in \text{Dom}(H_0)$ . Taking into account our study on the general BC for this problem, we write here, as an example, the form of one of the families of BC,

$$\begin{pmatrix} \phi_1(L) \\ \phi_1(0) \end{pmatrix} = A \begin{pmatrix} -\chi_2(L) \\ \chi_2(0) \end{pmatrix}$$

$$A = -A^\dagger$$

$$\phi_2 = \chi_1 = 0 \tag{A6}$$

where

$$A = i(\sin \mu + \sin \tau \cos \theta)^{-1} \times \begin{pmatrix} \cos \mu + \cos \tau \cos \theta & e^{-i\gamma} \sin \theta \\ e^{i\gamma} \sin \theta & \cos \mu - \cos \tau \cos \theta \end{pmatrix} \tag{A7}$$

with the restrictions that  $\sin \mu + \sin \tau \cos \theta \neq 0$  and  $0 \leq \theta < \pi, 0 \leq \mu, \tau, \gamma < 2\pi$ . Among the BC included in this family are  $\phi_1(L) = \phi_1(0) = 0$  and  $\chi_2(L) = \phi_1(L) = -\chi_2(0) = \phi_1(0) = i$ .

These BC and all the others discussed in this paper are self-adjoint extensions for the free Dirac Hamiltonian. The eigenvalues and eigenfunctions for the most general BC of the Dirac Hamiltonian have been calculated in [28].

With respect to the problem of completeness, we remark that the set of eigenfunctions of a self-adjoint operator with a non-degenerate spectrum constitutes a basis of the Hilbert space. In our case we found eigenfunctions of positive energy, from which those of negative energy can easily be obtained.

## Appendix B

By considering  $\phi = \begin{pmatrix} \phi_1(x) \\ 0 \end{pmatrix}$  and  $\chi = \begin{pmatrix} 0 \\ \chi_2(x) \end{pmatrix}$ , equations (27) and (28) lead to the system

$$\begin{aligned} -i\hbar c \frac{d}{dx} \phi_1 &= (E + mc^2) \chi_2 \\ -i\hbar c \frac{d}{dx} \chi_2 &= (E - mc^2) \phi_1 \end{aligned} \quad (\text{B1})$$

Assuming that  $\phi_1(x, c) = \phi_1(x, -c)$ ,  $\chi_2(x, c) = -\chi_2(x, -c)$  and  $E(c) = E(-c)$ , the functions  $\phi_1(x, -c)$  and  $\chi_2(x, -c)$  satisfy equations (B1) with  $c \rightarrow -c$ ; consequently, we may write the following expansions in  $c$  for  $\phi_1(x, c)$  and  $\chi_2(x, c)$  [31]:

$$\begin{aligned} \phi_1 &= \phi_1^{(NR)} + \frac{1}{c^2} \phi_{1(1)}^{(NR)} + \frac{1}{c^4} \phi_{1(2)}^{(NR)} + \dots \\ \chi_2 &= \frac{1}{c} \chi_2^{(NR)} + \frac{1}{c^3} \chi_{2(1)}^{(NR)} + \frac{1}{c^5} \chi_{2(2)}^{(NR)} + \dots \end{aligned} \quad (\text{B2})$$

and for the energy

$$E = mc^2 + E^{(NR)} + \frac{1}{c^2} E_{(1)}^{(NR)} + \frac{1}{c^4} E_{(2)}^{(NR)} + \dots \quad (\text{B3})$$

Substituting relations (B2) and (B3) in (B1) and comparing the terms of lower order, we obtain the following system:

$$\begin{aligned}
i\frac{d}{dx}\phi_1^{(NR)} + \frac{2m}{\hbar}\chi_2^{(NR)} &= 0 \\
i\frac{d}{dx}\chi_2^{(NR)} + \frac{E^{(NR)}}{\hbar}\chi_2^{(NR)} &= 0.
\end{aligned}
\tag{B4}$$

Eliminating  $\chi_2^{(NR)}$ , we obtain the eigenvalue Schrodinger equation

$$\left[ \frac{d^2}{dx^2} + \left( k^{(NR)} \right)^2 \right] \phi_1^{(NR)} = 0
\tag{B5}$$

where  $\left( k^{(NR)} \right)^2 = 2mE^{(NR)}/\hbar^2$ . In the non-relativistic limit, the connection between the components  $\phi_1$  and  $\chi_2$  of the Dirac spinor and the SchrodingerPauli function  $\phi_1^{(NR)}$ , is obtained keeping only the first term of the expansions (B2), and using the first equation of (B4); that is

$$\begin{aligned}
\phi_1 &\rightarrow \phi_1^{(NR)} \\
\chi_2 &\rightarrow -\lambda i \frac{d}{dx} \phi_1^{(NR)}
\end{aligned}
\tag{B6}$$

where  $\lambda = \hbar/2mc$ . With these relations, we may calculate the non-relativistic limit up to the order of  $v^{(NR)}/c$  for any quantum mechanical expression in one spatial dimension.

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