Quasiadiabatic analysis for ionization of a particle in a periodically perturbed $\delta(x)$ potential

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We study an ionization process for a particle bound by an attractive $\delta(x)$ potential of a certain depth defined on a finite lattice under an external periodic force. Ionization coincides with the time when first two time dependent energy eigenvalues get close to each other. We use a slow driving force away from the resonance frequency. We also observe intermittent high frequency oscillation which can be analyzed with two level approximation.

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I. INTRODUCTION

The ionization process is a transition from bound to free states of a system and it is of importance in many areas of physics. Quantum description of atoms can be most sensible in predicting parameters necessary for ionization processes. It is not clear, however, what the conditions are for a time dependent external field to ionize an atom when the field is beyond the perturbation regime. Floquet theory, numerical solutions of the time dependent Schrödinger equation are known approaches for this problem.

We study the time evolution of the wave function of a particle bound by an attractive δ potential of a certain depth under an external periodic forcing [1]. We use a nonperturbative method [2], where for a given time, thus, for a fixed value of the external forcing, the eigenvalues and the eigenspectrum are known. For a frozen value of the external forcing for a given time, the Hamiltonian has an adiabatic spectrum parametrized by the frozen external potential. When the energy levels approach each other, the system shows an extreme nonadiabatic behavior. In this paper, we show an ionization process by way of this method.

The particle in this system is confined in $x\epsilon(-L,L)$. This can be directly applicable to a systems of quantum dots where electrons are usually confined in a finite dimension and the energy levels are discrete. The Hamiltonian for our system is given by

$$H=\frac{p^2}{2m}-g_0[1+\epsilon\sin(\omega t)]\delta(x), \tag{1}$$

where g_0 is the depth of the δ potential, ϵ is the amplitude of an external driving force, and ω is the driving frequency. We first consider an energy spectrum when there is no time dependent periodic forcing, i.e., $\epsilon=0$. Due to the finite dimension of the system, we apply boundary conditions

$$\phi(\pm L)=0,$$

$$\phi(0^+)=\phi(0^-), \tag{2}$$

$$\phi'(0^+)-\phi'(0^-)=-\frac{2mg_0\phi(0)}{\hbar^2}.$$

From now on we set $h=\hbar$. This system has one bound state and an infinite number of discrete states. The wave function for the bound state is given by

$$\phi_\kappa(x)=\frac{\kappa}{1-4\kappa L\exp(-2\kappa L)-\exp(-4\kappa L)}[\exp(-\kappa|x|) -\exp(-2\kappa L)\exp(\kappa|x|)], \tag{3}$$

where g_0 and κ are related by the equation

$$g_0=\frac{h^2}{m}\kappa\coth(\kappa L),$$
$$E_\kappa=-\frac{h^2\kappa^2}{2m}, \tag{4}$$

in which E_κ is the energy for the bound state. For discrete states, the wave functions are written as

$$\phi_{k_n}(x)=\frac{1}{2\sqrt{L-\dfrac{\kappa_0}{\kappa_0^2+k_n^2}}}[\exp(-ik_n|x|) -\exp(-2ik_nL)\exp(ik_n|x|)], \tag{5}$$

where

$$\kappa_o=\frac{mg_0}{h^2},$$

$$\sin(2k_nL)=\frac{2k_n\kappa_0}{\kappa_0^2+k_n^2}, \tag{6}$$

$$\cos(2k_nL)=\frac{\kappa 0^2-k_n^2}{\kappa_0^2+k_n^2}.$$

The energy for each k_n is given by $E_{k_n}=h^2k_n^2/2m$.

If we introduce the time dependent forcing, i.e., $\epsilon\neq0$, we can set

$$g'=g_0[1+\epsilon\sin(\omega t)]. \tag{7}$$

For a given instant of time $t=t'$, we have a value of g'. The energy spectrum can be recalculated based on g'. At every instant, the dynamics can be described by the eigenspectrum that depends on the given time this new eigenspectrum.

With given g', $\phi_{\kappa'}(x)$ is the wave function for the bound state and $E_{\kappa'}$ is the energy state for the bound state. The transcendental relationship for the eigenvalue is with κ' substituted for κ, and g' for g_0 in Eq. (4). $\phi_{k_n'}(x)$'s are the wave functions for discrete states with k_n' instead of k_n in Eq. (6). We also set $\kappa_o'=mg_0'/h^2$.

In Sec. II, we show two representations of the wave function, where in one picture, the evolution is described by a fixed eigenfunction set, and in the other, the dynamics can be viewed in time dependent eigenbasis. The time dependent eigenbasis are the eigenfunctions for the Hamiltonian parametrized by the external forcing at each time. This idea is very similar to the Schrödinger picture, versus the interaction picture. Time dependent energy levels in the Hamiltonian system can get close to each other, but do not cross each other [3]. When the levels become close, we observe the nontrivial energy mixing behaviors. We focus on the energy levels varying with a parametrized external forcing. We capture the ionization behavior when the time dependent energy levels for the bound state and the first excited state approach each other. We show the dynamics can be reduced to a two-level approach when the two levels are close.

In Sec. III, we show a result of the first few amplitudes of the wave function when ϵ is comparable to one. The ionization occurs as the time varying energy levels get close. The time evolution was calculated with many levels and compared with the approximation with two-levels only. We report an intermittent high frequency oscillation during the exchange of energy levels. We have a conclusion in Sec. IV.

II. QUASIADIABATIC VERSUS. DIRECT TIME DEPENDENT PICTURE

The time evolution for a quantum system is given by the Schrödinger equation. For a frozen value of $g'=g_0[1+\epsilon\sin(\omega t)]$, for a given time $t=t'$, one must first solve the stationary problem

$$ih\partial_t\Psi(t)=[H_0+H'(t')]\Psi(t')=E_n\Psi(t'),$$

$$H_0=p'2m, \tag{8}$$

$$H(t')=-g'\delta(x),$$

where $H(t')=H_0(t')+H'(t')$ is the time dependent Hamiltonian for the system. The wave function for evolution can be expanded in an eigenbasis set of $H_0+H'(t')$, such that

$$\Psi(t)=\sum_{n=0}^{\infty}\tilde{a}_n(t)\tilde{\phi}_n(x,t). \tag{9}$$

The eigenvalues are $E_n(g')$'s. By inserting Eqs. (9) to (8), we obtain

$$\begin{aligned} ih\partial_t\sum_{n=0}^{\infty}\tilde{a}_n(t)\tilde{\phi}_n(x,t)&=\sum_{n=0}^{\infty}\dot{\tilde{a}}_n(t)\tilde{\phi}_n(x,t)\\ &\quad+\tilde{a}_n(t)\frac{d}{dg'}\tilde{\phi}_n(x,t)\frac{dg'}{dt}\\ &=\sum_{n=0}^{\infty}E_n(g')\tilde{a}_n(t)\tilde{\phi}_n(x,t). \end{aligned} \tag{10}$$

Using the orthonormality property for the eigenbasis, and the relationship [2]

$$\int\tilde{\phi}_n(x,t)\frac{d}{dg'}\tilde{\phi}_m(x,t)=\frac{\int\tilde{\phi}_n(x,t)\delta(x)\tilde{\phi}_m(x,t)}{E_n(g')-E_m(g')}, \tag{11}$$

we obtain a set of ordinary differential equations for the amplitudes for the evolution of the system, i.e.,

$$\dot{\tilde{a}}=-\frac{i}{h}E_{\kappa'}\tilde{a}-\sum_{n=0}^{\infty}\tilde{a}_{kn}\frac{\langle k_n,\kappa_0'|\delta(x)|\kappa'\rangle^*}{E_{\kappa'}-E_{k_n}}, \tag{12}$$

$$\begin{aligned} \dot{\tilde{a}}_{k_n}&=\frac{i}{h}E_{k_n}\tilde{a}_{k_n}+\tilde{a}\frac{\langle k_n,\kappa_0'|\delta(x)|\kappa'\rangle^*}{E_{\kappa'}-E_{k_n}}\dot{g}'\\ &\quad-\sum_{n'\neq n,n'=1}^{\infty}\tilde{a}_{k_{n'}}\frac{\langle k_n,\kappa_0'|\delta(x)|k_{n'},\kappa_0'\rangle}{E_{k_n}-E_{k_{n'}}}\dot{g}', \end{aligned} \tag{13}$$

where $\dot{g}'=g_0\epsilon\omega\cos(\omega t)$, $\tilde{a}$ is the amplitude for the bound state ($\tilde{a}_0=\tilde{a}$), and $\tilde{a}_{k_n}$'s are the amplitudes for the discrete states. They are the amplitudes for the eigenstates which are stationary for a give $t=t'$. We call the states *quasiadibatic states*. We can prove that

$$|\tilde{a}(t)|^2+\sum_{n}^{\infty}|\tilde{a}_{k_n}(t)|^2=1, \tag{14}$$

for all time.

If we use the amplitudes for the eigenfunctions $\phi_n(x)$ for H_0 for all time, the amplitudes for the eigenfunctions evolve according to

$$ih\partial_t\Psi(t)=[H_0+H'(t)]\Psi(t). \tag{15}$$

$\Psi(t)$ is expanded into the eigenbasis for H_0 of which eigenvalues are E_κ, E_{k_n}'s, such that

$$\Psi(t)=\sum_{n=0}^{\infty}a_n(t)\phi_n(x). \tag{16}$$

With the similar procedures to the above and $a_0=a$, we obtain a set of differential equations for $a_n(t)$'s.

$$\dot{a} = -\frac{i}{h}E_\kappa a + \frac{i}{h}g_0\epsilon\sin(\omega t)a\langle\kappa|\delta(x)|\kappa\rangle + \frac{i}{h}g_0\epsilon\sin(\omega t)\sum_{n=1}^{\infty} a_{k_n}(t)\langle\kappa|\delta(x)|k_n,k_0\rangle, \quad (17)$$

$$\dot{a}_{k_n} = -\frac{i}{h}E_{k_n} + \frac{i}{h}g_0\epsilon\sin(\omega t)a_{k_n}\langle k_n,\kappa_0|\delta(x)|\kappa\rangle + \frac{i}{h}g_0\epsilon\sin(\omega t)\sum_{m=1}^{\infty} a_{k_n}\langle k_n,\kappa_0|\delta(x)k_m,\kappa_0\rangle. \quad (18)$$

Note, for the summation in the second equation, we do not exclude the term $n \neq m$. This *direct time dependent* method uses the fixed eigenfunctions for all time, and the only time dependent parts are amplitudes. Since our time dependent driving force is periodic, for every period of the driving, the amplitudes for *direct time dependent* method coincide with those from *quasiadiabatic* method, i.e., for the driving period of T,

$$a(t) = \tilde{a}(t), \quad (19)$$

$$a_{k_n}(t) = \tilde{a}_{k_n}(t), \quad (20)$$

for $\mathrm{mod}(t,T) = 0$.

III. RESULTS

The equivalence of the two representations in the above chapter is shown for the parameters for $g_0 = 2.5, \epsilon = 0.5, L = 1, \omega = 11.74$ in Fig. 1. We see a brief ionization after about three periods. (The probability that the particle stays in an excited state decays afterwards.) The solid line is the occupation probability for the ground state in time, and the dashed line is the occupation probability for the first excited state in the direct time dependent method. The results are compared with the quasiadiabatic picture where $+$'s are values for occupation probability for the ground state, and X's are values for occupation probability for the first excited state in every period up to three periods. They coincide at every driving period when $g' = g_0$. The amplitudes from Eqs. (12) and (17) are solved numerically.

Two levels dynamics with a driving of the resonance frequency is well explained in Ref. [4]. We are interested in the ionization process away from resonance frequency. The driving frequency is far smaller than the resonance frequency. We set the parameters such that the quasiadiabatic energy levels get very close in one period. The parameters we use are $g_0 = 2.5, \epsilon = 0.9, L = 10, h = m = 1, \omega = 0.01$. In Fig. 2, the ground energy level gets close to the first excited state. The resonance frequency between the ground and the first excited state is $\omega_{01} = 0.1174$. With a slow driving, the ionization takes place when the quasienergy levels become close. We show the probability of the amplitude for the ground state for ten periods in Fig. 3. The ionization is not permanent, and

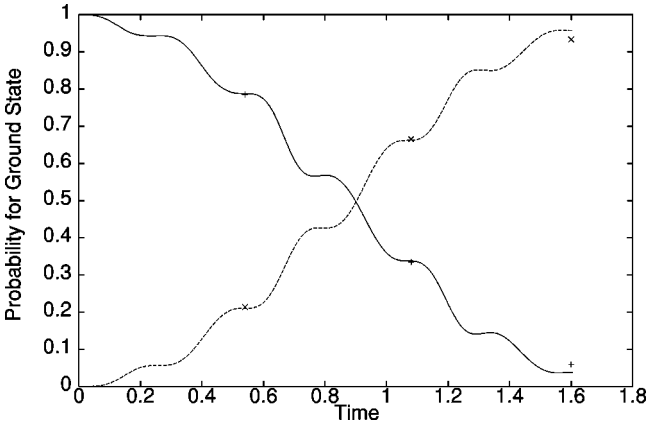

FIG. 1. Evolution for amplitudes for the quasiadiabatic and the direct time dependent methods. The ionization occurs after about three periods. The parameters are $g_0 = 2.5$, $\epsilon = 0.5$, $L = 1$, $h = m = 1$, $\omega = 11.74$. The quasiadiabatic amplitude for the ground state $+$, and the first excited state $\times$ are shown for every period of the driving forcing. The solid line is for the ground state, and the dashed line is for the first excited state from the direct time dependent method. Results from the two different methods coincide at every period when $g' = g_0$. For the direct time dependent method, we used the ground and the first five excited levels, and for the quasiadiabatic method we used the time dependent ground state and the first ten excited levels.

the occupation probability oscillates between two levels. We used $a(t)$, $a_{k_n}(t)$, and $\tilde{a}(t)$, $\tilde{a}_{k_n}(t)$ for $k = 1, \ldots, 10$, and for clarity, we only show the probability for the wave function to be in the ground state.

We observe a time region, where the occupation probability oscillates at a high frequency Figs. 4(a) and 4(b). This can be analyzed with two-level approximation of $a_0(t)$, $a_1(t)$, i.e.,

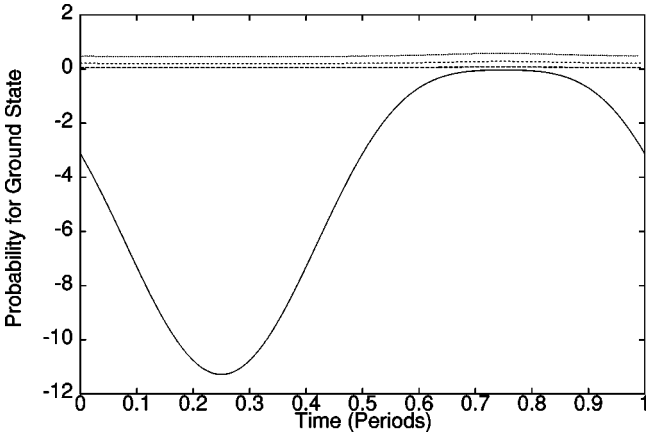

FIG. 2. The quasiadiabatic energy level in time (for one period). The parameters are $g_0 = 2.5$, $\epsilon = 0.9$, $L = 10$, $h = m = 1$, $\omega = 0.01$. The bottom solid line is the ground state, and from bottom up, we show the first, second, and third excited levels. When the ground state approaches the first excited state closely in every period, we expect ionization. The driving frequency used is much slower than the resonance frequency between the ground and the first excited level.

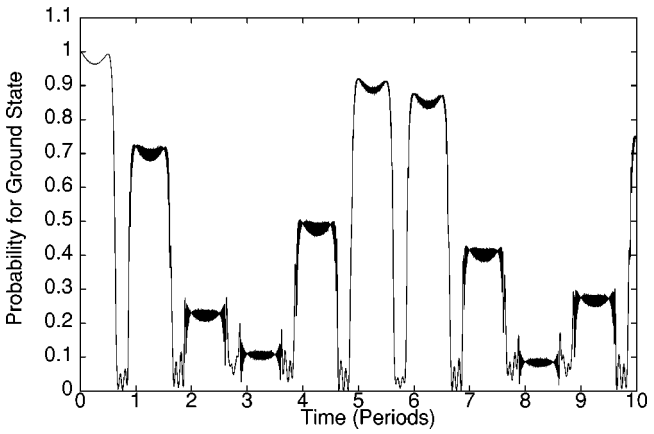

FIG. 3. Time evolution of the amplitude for the ground state from the direct time dependent method (for ten periods). The ionization occurs when the first two quasiadiabatic levels approach closely. The parameters are $g_0=2.5$, $\epsilon=0.9$, $L=10$, $h=m=1$, $\omega=0.01$.

$$\dot{a}_0 = -\omega_0 a_0 + i g_0 \epsilon \sin(\omega t)[\langle 0|\delta(x)|0\rangle a_0 + \langle 0|\delta(x)|1\rangle a_1], \tag{21}$$

$$\dot{a}_1 = -\omega_1 a_1 + i g_0 \epsilon \sin(\omega t)[\langle 1|\delta(x)|0\rangle a_0 + \langle 1|\delta(x)|1\rangle a_1],$$

where $\langle 1|\delta(x)|0\rangle = \int \phi_1(x)\,\delta(x)\,\phi_0(x)dx$, and $\langle 0|\delta(x)|1\rangle = \langle 1|\delta(x)|0\rangle^*$. Since this high frequency part is a result of mixing of the two levels, the natural frequency of ω_1, ω_2 are not relevant for finding how this high frequency arises. We assume that $\omega_1=\omega_2=\Omega$, and introduce a matrix $\mathbf{a}=(a_0,a_1)$ and $\mathbf{b}=e^{-i\Omega t}\mathbf{a}$. The equations reduce to

$$\frac{d}{dt}\mathbf{b} = i g_0 \epsilon \sin(\omega t) \begin{pmatrix} \langle 0|\delta(x)|0\rangle & \langle 0|\delta(x)|1\rangle \\ \langle 1|\delta(x)|0\rangle & \langle 1|\delta(x)|1\rangle \end{pmatrix} \mathbf{b}. \tag{22}$$

The solution for the equation is given by

$$\begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = e^{i g_0 \epsilon [1-\cos(\omega t)/\omega]\mathbf{M}} \begin{pmatrix} b_0(0) \\ b_1(0) \end{pmatrix}, \tag{23}$$

where the matrix $\mathbf{M}$ is given by

$$\mathbf{M} = \begin{pmatrix} \langle 0|\delta(x)|0\rangle & \langle 0|\delta(x)|1\rangle \\ \langle 1|\delta(x)|0\rangle & \langle 1|\delta(x)|1\rangle \end{pmatrix} \tag{24}$$

and the initial conditions are given by $[b_0(0),b_1(0)]=[a_0(0),a_1(0)]$. We can see that the slowdown of the high frequency occurs when the term $[1-\cos(\omega t)/\omega]$ in the exponent approaches zero. The exponent can be expressed by a 2×2 matrix using spinors [4], i.e.,

$$\exp[i(\lambda \mathbf{a}\cdot\sigma)] = \cos(a\lambda)\sigma_0 + i\sin(a\lambda)\frac{\mathbf{a}\cdot\sigma}{a}, \tag{25}$$

where $a=|\mathbf{a}|$ and σ is given by

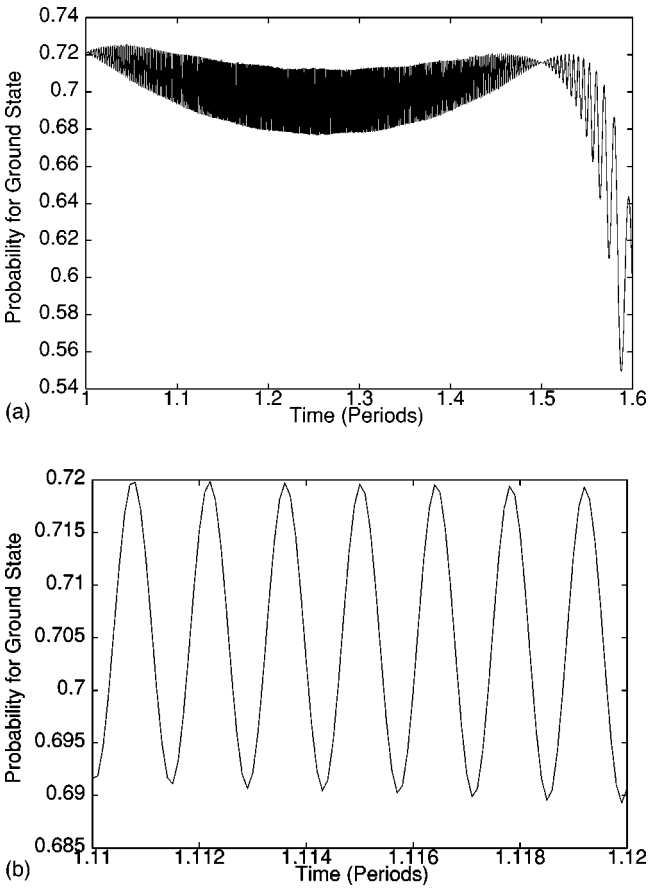

FIG. 4. (a) The high frequency region is observed intermittently. The frequency can be estimated with a two-level approximation. The high frequency behavior slows down before another ionization occurs. (b) The high frequency region zoom-in is shown.

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{26}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Once we obtain right coefficients for σ, we have the solution. The solution from this calculation for a_0,a_1 gives the period of 2.37. Our $1+10$ level numerical simulation gives a period of 1.67. The driving period is 628.

IV. CONCLUSION

We observe an ionization process from the bound state to one of the continuum level in a $\delta(x)$ potential. We use the ground level and the first ten excited levels for level dynamic calculation. When the two quasiadiabatic energy levels (the

bound, the first excited one) approach each other, the energy mixing is possible. The evolution of the system can be viewed from eigenstates which are fixed in all time, or from the eigenstates which change according to time. The quasiadiabatic energy levels are quite useful in terms of predicting the ionization process. The amplitudes in many levels from the direct time dependent method were calculated by numerically solving a set of ordinary differential equations.

Due to the finite size of the system, we did not observe the permanant ionization. A brief ionization is followed by a decay of the wave function back into the ground state. It is not clear what the conditions are for a complete ionization. The occupation probability of the ground state and the first excited state evolve in a very complicated manner in time. The evolution is not fully understood.

Occasional high frequency oscillations occur after partial ionization processes. This is due to the interaction of different states. We are able to show the estimate of the high frequency and subsequent slowdown with a simple two level dynamics approximation.

The purpose of this paper is to show a new way of solving ionization problems in quantum systems and giving an insight for use of time varying energy levels. Since the energy levels are not stationary in the time dependent Hamiltonian, when the quasienergy levels approach each other, one can observe the ionization.

ACKNOWLEDGMENT

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