Dynamics of an electron in finite and infinite one dimensional systems in presence of electric field

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We study numerically, the dynamical behavior of an electron in a two site nonlinear system driven by dc and ac electric field separately. We also study, numerically, the effect of electric field on single static impurity and antidermic dynamical impurity in an infinite 1D chain to find the strength of the impurities. Analytical arguments for this system have also been given.

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I. INTRODUCTION

The dynamics of an electron in presence of electric field, in a two level system as well as in a linear chain has been a subject of recent interest. It is well known that for a double-well heterostructure in the absence of driving forces the electron can visit either well due to quantum tunneling. However, if the double well structure is biased, i.e. driven by a dc field the electron in an eigenstate will be naturally localized in one of the wells because of the superposition of the coherent tunneling between two wells. When the double well system is exposed to a pure ac field the electron gets frozen in the initially populated well, provided the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the ac field strength to the field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero. In presence of both ac and dc field, the electron gets trapped in the initially populated site when the ratio of the field strength to field frequency becomes a root of Bessel’s function of order zero.

On the other hand a lot of studies have been done on the dynamics of a charged particle subjected to a periodic potential in presence of dc, ac as well as in the presence of both dc and ac electric fields. It is well known that, in presence of dc field, a charged particle executes oscillatory motion in the reciprocal lattice. This, in turn, confines the particle spatially.

In presence of ac field, the particle is generally delocalized except for the cases when the ratio of the field magnitude to the field frequency is a root of the ordinary Bessel function of order zero. In presence of both ac and dc field, the localization induced by the dc field can be suppressed by the ac field when the stark frequency becomes equal to an integral multiple of the frequency of the ac field.

Recently, Nazareno et. al. had studied the dynamics of an electron in a 1D chain in the presence of a single static impurity subjected to a dc electric field. They had shown that when the impurity potential is such that it coincides with the on-site energy due the field on a particular site n, i.e., eEan = ε0, where e is the charge of the particle and a is the lattice parameter, the packet oscillates resonantly between the impurity site and the particular site n. Therefore, when the electric field E = cos(ωt), the charged particle oscillates resonantly between the impurity site and it’s neighboring site. However, we find that this condition is valid only if the particle is strictly confined to the impurity site and its neighboring site. On the other hand, in a 1D chain there is a probability for the particle to tunnel to other sites. Because of this tunneling probability the resonance condition gets modified.

We also study the dynamics of an electron in a 1D perfect chain in presence of two nonlinear impurities which are next to each other, subjected to dc electric field. We suggest a possible means of measuring the strength of the nonlinear impurity.

The organization of the paper is as follows. In Sec. II, we deal with a two site nonlinear system, in presence of electric fields. In Sec. III, we consider a one dimensional infinite chain with a static impurity and the dynamics of an electron in presence of a dc electric field. In Sec. IV, we consider a 1D chain with two consecutive nonlinear impurity sites and the dynamics of an electron in presence of a dc electric field. Finally, in Sec. V we give a summary of our investigations.

II. TWO SITE SYSTEM

The time evolution of the electron in a two site nonlinear system in presence of both ac and dc fields is governed by the equations given by,

\[ \frac{dC_1}{dt} = V C_2 + \left( -\frac{E_0}{2} - \frac{E}{2}\cos(\omega t) + \chi_1|C_1|^2 \right) C_1 \]

\[ \frac{dC_2}{dt} = V C_1 + \left( \frac{E_0}{2} + \frac{E}{2}\cos(\omega t) + \chi_2|C_2|^2 \right) C_2. \]
Here $C_1$ and $C_2$ are the probability amplitudes of the particle to stay at site 1 and 2 respectively. $V$ is the hopping amplitude of the particle between the two sites, $E_0$ is the amplitude of the dc field, $E$ is the amplitude of the ac field and $\omega$ is the frequency of the ac field. The kind of nonlinearity we consider here arises from the interaction of the electron with the vibration of the local oscillators in the system. $\chi_1$ and $\chi_2$ are the nonlinear parameters determining the strength of the interaction of the particle with the local oscillators at site 1 and 2 respectively.

In the absence of both dc and ac electric fields (i.e. $E_0 = E = 0$), the two site system is completely isolated from any external perturbations and the dynamics of the particle is governed completely by the strength of the nonlinearity at the two sites and the hopping matrix element between the two sites.

In the special case when the strengths of nonlinearity at the two sites are equal (i.e. $\chi_1 = \chi_2 = \chi$), there exists a critical value of $\chi$ (i.e. $\chi_{cr} = 4V$), below which the particle remains delocalized between the two sites and above which the particle gets trapped at the initially populated site. Thus, there is an abrupt transition from one across the critical value of the nonlinear parameter.

The other interesting situation arises when the local oscillators oscillate in opposite phase but interact with the particle with same strength. In this case, the time evolution of the probability of the particle at the initially populated site is given by,

$$P_1(t) = \frac{\chi^2}{\chi^2 + 4V^2} + (1 - \frac{\chi^2}{\chi^2 + 4V^2}) \cos(\omega t).$$ (2)

In this limit, the transition is a continuous one, where, as the nonlinearity increases, the particle continuously gets trapped at the initially populated site. This is obvious from Eq. (2) where $P_1(t) \to 1$ as $\chi \to \infty$.

We can, on the other hand, put $\chi_1 = \chi_2 = 0$ and $E = 0$. This is the case when nonlinearity is absent and a pure d.c. field is applied to the two site problem. In this case, the two site problem effectively reduces to a two level problem, where the degeneracy of the two levels (due to equal site energies) is lifted by the externally applied dc electric field. It has been shown that, in this situation, the particle remains localized at the initially populated site provided the hopping matrix element is small compared to the strength of the electric field (i.e. $V/E_0 \ll 1$).

In the absence of nonlinearity and dc electric field ($\chi_1 = \chi_2 = 0$, $E_0 = 0$) and in the presence of an ac electric field (given by $E \cos(\omega t)$), the particle remains delocalized between the two sites except when the ratio of the amplitude of the a.c. filed ($E$) to its frequency ($\omega$) is such that the zeroth order Bessel function $J_0(E/\omega)$ is identically equal to zero. Here too, the condition for localization is satisfied only when $V/E \ll 1$.

The question naturally arises as to what happens to the dynamics of the electron in the nonlinear two site system in presence of field. Here, we consider the case where the nonlinear parameters are of equal strength but are opposite in sign. As mentioned earlier, this kind of situation arises when the local oscillators oscillate in opposite phase but interact with the particle with same strength. Therefore, we consider $\chi_1 = \chi$ and $\chi_2 = -\chi$. In this situation, the site energies of both the sites vary with time. Now, we consider the effect of a dc and ac electric field on the dynamics of an electron in the nonlinear two site system, separately.

In presence of a pure dc electric field of strength $E_0$, the time evolution of the probability of the electron in the system is governed by the equations,

$$\frac{dP}{dt} = 2VR$$
$$\frac{dQ}{dt} = -(E_0 - \chi)R$$
$$\frac{dR}{dt} = -2VP + (E_0 - \chi)Q$$ (3)

where $P = \rho_{11} - \rho_{22}$, $Q = \rho_{12} + \rho_{21}$, $R = i(\rho_{12} - \rho_{21})$ and $\rho_{ij} = C_i C_j^*$, i,j=1,2. On solving Eqs. (3), the probability difference of the particle between the two sites is given by,

$$\rho_{11} - \rho_{22} = \frac{(E_0 - \chi)^2}{\Omega^2} + \frac{4V^2}{\Omega^2} \cos(\Omega t)$$ (4)

where $\Omega = \sqrt{4V^2 + (E_0 - \chi)^2}$. For the sake of discussion, we take $\chi$ and $E_0$ to be positive. Thus Eq. (4) explicitly shows that the particle becomes fully delocalized only when $\chi = E_0$. The field direction can be reversed by replacing $E_0$ by $-E_0$. In this case however, there is no delocalization for any field strength, since $\chi$ is still positive.

We now consider the case of a pure ac electric field applied to the same nonlinear two site system. The dynamics of the particle in this system is governed by the following equations.

$$\frac{dP}{dt} = 2VR$$
$$\frac{dQ}{dt} = -(E \cos(\omega t) - \chi)R$$
$$\frac{dR}{dt} = -2VP + (E \cos(\omega t) - \chi)Q.$$ (5)

where $P$, $Q$ and $R$ are defined earlier. We cannot decouple these equations and hence solve them numerically, using fourth order Runge-Kutta method. We have checked the probability conservation of the particle at each time step. We find that, as long as $V/E \ll 1$, the particle becomes
fully delocalized only when $\chi = n\omega$ where $n$ is a positive integer and $E/\omega$ is such that the $n^{th}$ order Bessel function becomes nonzero (i.e. $J_n(E/\omega) \neq 0$). On the other hand, the particle gets fully trapped at the initially populated site only when $\chi = n\omega$ and $E/\omega$ is such that the $n^{th}$ order Bessel function is identically equal to zero (i.e. $J_n(E/\omega) = 0$).

To show this, we have plotted $P_1$ as a function of time, where, $V = 0.8, \omega = 2, E/\omega = 1.9155$ such that $J_1(E/\omega) \neq 0$. The dotted curve, solid curve and the dashed curve are for $\chi = 1.8, 2.0$ and 2.1 respectively.

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{The probability of the electron at site 1 ($P_1$) as a function of time, where, $V = 0.8, \omega = 2, E/\omega = 1.9155$ such that $J_1(E/\omega) \neq 0$. The dotted curve, solid curve and the dashed curve are for $\chi = 1.8, 2.0$ and 2.1 respectively.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig2.png}
\caption{The probability of the electron at site 1 ($P_1$) as a function of time, where, $V = 0.8, \omega = 2, E/\omega = 1.9155$ such that $J_1(E/\omega) = 0$.}
\end{figure}

To show this, we have plotted $P_1 = \frac{1+P}{2}$ (probability of the particle to stay at the site 1) as a function of time in Figs. (1) and (2). In Fig. (1), we have taken $V = 0.8, \omega = 2$ and $E/\omega = 1.9155$ such that $J_1(E/\omega) \neq 0$. The dotted curve corresponds to $\chi = 1.8 < \omega$, the solid curve is for $\chi = 2.0 = \omega$ and the dashed curve for $\chi = 2.1 > \omega$. The dotted and dashed curves show that, as long as the nonlinearity strength ($\chi$) is not an integral multiple of the frequency ($\omega$) of the field, the electron remains mostly localized at the initially populated site. As soon as the nonlinearity parameter matches with the $n^{th}$ multiple of the frequency of the ac field (solid curve), the electron gets fully delocalized. On the other hand, in Fig. (2), we have taken $V = 0.8, \omega = 1$ and $E = 3.831$ such that $J_1(E/\omega) = 0$. The figure clearly shows that the electron gets completely frozen at the initially populated site. Thus, a two site system in presence of this kind of nonlinearity and ac field gives the same kind of dynamical behavior of the electron as is the case of a two level system subjected to dc and ac fields simultaneously. Here, the nonlinearity plays the role of a dc field in a two level system.

The complete delocalization of the electron in this system can be understood by the following physical reasoning. Because of the presence of nonlinearity, the site energies of the two sites become different. Thus, the nonlinearity maps the two site system to a two level system. Since site energy at both the sites depends on the probability of the particle to stay at the respective sites, they fluctuate with time. However, the energy difference between the sites, $\Delta = \chi (\rho_{11} + \rho_{22}) = \chi$ which is constant. This is because the total probability of the particle in the system is conserved. Therefore, when the particle is in one of the sites it can absorb an amount of energy $\chi = n\omega$, where $n$ is an integer, from the ac field and jump to the other site and thus, full delocalization is obtained for this condition.

\section{III. 1D Chain with Single Static Impurity}

In this section, we consider a one dimensional infinite perfect chain with a single static impurity at the middle ($0^{th}$) site. Our interest here is to find the dynamics of an electron initially populated at the impurity site in presence of a dc electric field. The governing equation for the electron dynamics in presence of the dc electric field is given by a set of differential equations, as,

$$i \frac{dC_n}{dt} = e_n \delta_{n,0} C_n + e a E_0 n C_n + V(C_{n+1} + C_{n-1}),$$

$$n = -N, -N+1, \ldots, N-1, N. \quad (6)$$

$C_n$ is the probability amplitude of the particle to stay at the $n^{th}$ site, $e_n$ is the site energy at the $n^{th}$ site, $e$ is the electronic charge, $a$ is the lattice spacing, $E_0$ is the strength of the dc electric field and $V$ is the hopping integral between neighboring sites. $N$ is chosen such that the particle does not feel the boundaries, which in turn
ensures the infiniteness of the chain. Without any loss of generality, we choose $c = 1, a = 1$ and normalize all energies with respect to the hopping matrix element $V$. The delta function implies that the site energy of all sites except the zeroth site have been taken to be zero, in absence of the dc electric field. To know the time evolution of the electron probability at site $n$ we need to solve Eqs. (6). Since, it is not possible to solve them analytically, we use fourth order Runge Kutta method to solve them numerically. Here also, conservation of the probability of the particle has been checked at each time step.

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FIG. 3. Time evolution of the probability of the electron in a 1D chain with a static impurity at the 0th site. $n$ represents the site index. The z-axis represents $|C_n|^2$. Here $\epsilon_0$ (strength of the impurity) = $E_0$ (strength of the electric field) = 2.

FIG. 4. Same as Fig. 3 except $E_0 = 2.67$.

For a fixed value of $\epsilon_0$ there is a particular value of the electric field strength ($E_0^{res}$) at which the electron oscillates resonantly between the impurity site and one of its nearest neighbor sites. We observe that, when $\epsilon_0$ is small, then the electric field strength required for the resonance condition is larger than $\epsilon_0$. We also find that, for smaller value of $\epsilon_0$, the departure of this electric field strength ($E_0^{res}$) from $\epsilon_0$ is larger and it decreases as $\epsilon_0$ increases. Thus, for very large values of $\epsilon_0$, the resonance condition reduces to $E_0^{res} = \epsilon_0$. We plot the time evolution of the probability of the electron in the system for $E_0 = \epsilon_0 = 2$ in Fig. (3) and the same for $E_0 = 2.67, \epsilon_0 = 2$ in Fig. (4). It is obvious from Fig. (3) that for $E_0 = \epsilon_0 = 2$, the electron propagates through the system and gets confined among many sites. On the other hand, Fig. (4) shows that the particle oscillates mainly between the impurity site and one of its nearest neighbors. Therefore, for $\epsilon_0 = 2, E_0 = 2.67$ is the electric field required for resonance between the impurity site and its neighbor.

In Fig. (5) we have also plotted the probability of the electron at the impurity site and its nearest neighbor site as a function of time for $\epsilon_0 = 4.0, E_0 = 4.0$ (dashed curves) and $\epsilon_0 = 4.0, E_0 = 4.37$ (solid curves). Here too, it is clear, that for $\epsilon_0 = 4.0$ and $E_0 = 4.37$ the particle oscillates more strongly between the impurity site and its nearest neighbor than for $\epsilon_0 = E_0 = 4.0$. Therefore, for $\epsilon_0 = 4.0$ one needs the field strength, $E_0 = 4.37$, to get the resonant motion of the particle between the impurity site and its neighbor. In order to understand this deviation from the normally expected resonance condition (i.e. $\epsilon_0 = E_0$) we find the resonance condition for general impurity strength as a function of electric field strength analytically. For this, we need to confine the particle between the impurity site (site 0) and its nearest neighbor site (site 1). To do this, we renormalize the hopping elements between the sites 0 and -1, and between sites 1 and 2 respectively. This in turn renormalizes the site energies...
at sites 0 and 1. The effective hopping between sites 0 and -1 and that between sites 1 and 2 thereby decreases. The effective energies at site 0 and 1 are given by

\[
eff_0 = \epsilon_0 + V^2/E_0 \\
\eff_1 = E_0 - V^2/(2E_0)
\]  

(7)

By putting \(\eff_0 = \eff_1\) we get the condition for resonance given by

\[
E_{\text{res}} = \frac{\epsilon_0 + \sqrt{\epsilon_0^2 + 6}}{2}
\]  

(8)

This condition is in contrast to the condition for resonance given by Nazareno et.al. [11] Eq. (6) explicitly shows that the resonance condition reduces to \(\epsilon_0 = E_0\) only when \(\epsilon_0 \gg \sqrt{6}\). Thus, to get a resonant motion of the particle between the sites 0 and 1, a higher value of electric field is required as compared to the impurity strength. We have plotted \(E_{\text{res}}^0 - \epsilon_0\) as a function of \(\epsilon_0\) obtained from Eq. (6) (solid curve) along with the corresponding numerical plot (dotted line) in Fig. 6.

![FIG. 6. \(E_{\text{res}}^0 - \epsilon_0\) as a function of \(\epsilon_0\). The dotted curve and the solid curve represent the numerical and analytical estimates, respectively.](image)

We see a good agreement between the numerical and analytical estimates. One can estimate the higher order corrections to Eq. (6) by further renormalizing the hopping matrix elements. However, the contribution from the higher order corrections is negligibly small. We therefore, restrict ourselves only upto the first order correction. Upto the first order, the strength of the static impurity can be evaluated using Eq. (6), once there is resonant oscillation between the impurity site and its nearest neighbor, which is characterized by the emission of a photon for the particular value of the dc electric field (\(E_{\text{res}}^0\)), as remarked by Nazareno et.al. [11]

IV. NONLINEAR IMPURITIES IN A CHAIN

In this section we consider a system of 1 dimensional chain with two nonlinear impurities at two consecutive sites. The nonlinearity arises due to the interaction of the particle with lattice vibration. We consider a special case where the particle interacts with the local oscillator only when it is at site 0 or site 1. We denote the middle site as the 0th site. The interactions at both the sites (site 0 and 1) are equal in strength but opposite in nature. This may arise only when the oscillators at sites 0 and 1 oscillate in opposite phase. Assuming the presence of this kind of nonlinearity, we ask whether it is possible to find the strength of the interaction, by applying an external electric field, as was done for the single static impurity case in the previous section. Here, we give an answer to this question.

We start by applying a pure dc electric field to the system and see the time evolution of the electron populated initially at the 0th site. The dynamics of the electron is governed by the equations given by,

\[
\frac{dC_0}{dt} = \chi[C_0]^2C_0 + V(C_1 + C_{-1}) \\
\frac{dC_1}{dt} = (-\chi[C_1]^2 + E_0)C_1 + V(C_0 + C_2) \\
\frac{dC_n}{dt} = nE_0C_n + V(C_{n+1} + C_{n-1}), \quad n \neq 0, 1.
\]  

(9)

We solve these equations numerically by using fourth order Runge Kutta method. We check the conservation of probability here too. We observe that, as \(E_0\) increases, the particle becomes more and more confined between sites 0 and 1. The amplitude of oscillation between sites 0 and 1 increases and then at some \(E_0\) (say, \(E_0^r\)) it becomes maximum. If \(E_0\) is increased further, the particle gets trapped at the initially populated site. So, at \(E_0 = E_0^r\) the particle oscillates between sites 0 and 1 resonantly. Here also, as is the case with a single static impurity in an infinite chain, for any strength of nonlinearity, \(\chi\) the electric field needed to get the resonance condition is higher than \(\chi\). This situation can also be detected by the radiation emitted by the electron while oscillating resonantly between sites 0 and 1.

We now find the resonance condition analytically. For this we have to reduce the system into an effectively two site system. In other words we need to confine the motion of the particle between sites 0 and 1. Since, at resonance condition, the time average probability of the particle at sites 0 and 1 are approximately 1/2, we therefore replace the site energies arising from nonlinearity at site 0 and 1 by \(\frac{\chi}{2}\) and \(-\frac{\chi}{2}\) respectively. We then renormalize the hopping matrix element between sites 0 and its left neighbor and that between site 1 and its right neighbor (the sites are numbered in increasing order from left to right, with the middle site being the zeroth site). As a consequence
of this renormalization, the site energies at sites 0 and 1 get renormalized and are given by,

$$\epsilon_{0}^{\text{eff}} = \frac{\chi}{2} + \frac{V^2}{E_0}$$

$$\epsilon_{1}^{\text{eff}} = \frac{-\chi}{2} + E_0 - \frac{V^2}{2E_0}$$

(10)

Now equating these effective site energies we get the condition for the particle to oscillate resonantly between site 0 and 1. This condition is given by

$$\chi = E_0^r - \frac{3V^2}{2E_0^r}.$$  

(11)

We plot $E_0^r - \chi$ as a function of $\chi$ obtained analytically in Fig. (7). Now we take a point from the curve for resonance condition (Fig. (7)) which corresponds to $\chi = 4.0$ and $E_0 = 4.34$. For these values of $\chi$ and $E_0$ we see the the time evolution of the electron probability in the system. This is shown in Fig. (8). We notice that the electron mostly oscillates between sites 0 and 1 resonantly. This also confirms our analytical estimate for resonance condition. Thus tuning the electric field one can obtain the resonance condition and hence the strength of the nonlinear impurity can be estimated using Eq. (11) provided that special kind of nonlinearity is present in the system.

V. CONCLUSION

We have studied the dynamics of an electron in a two site nonlinear system in presence of externally applied dc and ac electric fields, separately. We have shown the localization-delocalization conditions in both the cases. We have also studied the dynamics of an electron in an infinite 1D chain having a single static impurity in presence of a dc electric field. We have given an analytic expression for the condition when the particle oscillates resonantly between the impurity site and its nearest neighbor. This, in turn, gives a possible method of measuring the impurity strength. A similar analysis has been performed for an antidimeric dynamical impurity present in an otherwise perfect chain.

VI. ACKNOWLEDGMENT

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