High-frequency blockade in tight-binding one-dimensional lattice with single vibrating site

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Abstract – A one-dimensional tight-binding lattice, the single site of which possesses a harmonically vibrating level is studied. The states of non-interacting electrons are considered both numerically and (in the case of narrow band) analytically. It is shown that at definite conditions the site reflects electrons incident from infinity absolutely and elastically. This phenomenon, called high-frequency blockade, is accompanied by the vanishing of the system static conductance when the Fermi level crosses the blockade states. Together with these states we have found local and reflectionless states. Possible realizations of the system as a lattice of quantum dots or a linear polymer are discussed.

We study a 1D tight-binding lattice expressed by a system of equations

\[ ia_m - \delta_m,0 (u + v \cos(\omega t)) a_0 + \frac{\Delta}{2} (a_{m+1} + a_{m-1}) = 0. \]

Here \(a_m\) is the amplitude of the wave function on the \(m\)-th lattice site, \(\Delta/2\) is the transition amplitude between neighboring sites, the energy is counted from the levels of sites with \(m \neq 0\), the quantities \(u, v, \Delta, E\) are measured in units of the frequency \(\omega\); \(\hbar = 1\). If \(u = v = 0\) the system of equations (1) represents an ideal 1D tight-binding lattice with eigenstates \(a_m = e^{ipm-iE(p)\tau}\), which have quasi-momentum \(p\) and energy \(E(p) = -\Delta \cos(p)\). Real \(p\) corresponds to propagating states with energy within the allowed band \(-\Delta < E < \Delta\). If \(v = 0\) the site \(m = 0\) can be treated as an “impurity” which produces scattering of propagating electrons and the impurity state above or below the allowed band. The presence of vibrations \((v \neq 0)\) leads to energy non-conservation: the energy is changing by some quanta \(\omega\).

We consider two kinds of states, namely, the scattering problem with a given energy of the incident electron and local Floquet states characterized by a quasienergy. It should be emphasized that the tight-binding model allows the existence of the local states, unlike the free-electron model with a vibrating delta-potential.

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The general solution of the scattering problem reads
\[ a_{m \leq 0} = \sum_n \left( \delta_{n,0} e^{ip_0 n} + r_n e^{-ip_0 n} \right) e^{-i(E+n)t}, \]
\[ a_{m \geq 0} = \sum_n t_n e^{ip_0 n} e^{-i(E+n)t}. \]  

(2)

Here \( n \) denotes the transmission channel with absorption \((n > 0)\) or emission \((n < 0)\) of \(|n|\) quanta of the alternating field; \( t_n \) and \( r_n = t_n^* - \delta_{n,0} \) are the transmission and reflection amplitudes in the channel \( n \); \( p_0 \) is the solution of the equation \( E + n = -\Delta \cos p_n \), corresponding to the positive velocity of the electron states inside the allowed band, in accordance with causality. Some of the states \( E + n \) get to the forbidden band; for them the positive imaginary value of \( p_n \) should be chosen to guarantee the decay of states apart from the zero site.

The transmission amplitudes \( t_n \) satisfy the equation
\[ t_n (\Lambda(E + n) - u) - \frac{v}{2} (t_{n+1} + t_{n-1}) = \Lambda(E) \delta_{n,0}. \]  

(3)

Here \( \Lambda(E) = i\sqrt{\Delta^2 - (E + i\cdot 0)^2} \) (the term \( i \cdot 0 \) reflects the causality). In general, the system of equations (3) can be solved numerically.

The system under consideration can be treated as a quantum wire constructed from a long chain of quantum dots, the ends of which are connected to electron seas (source and drain). Suppose, that the source and the drain of the device have equilibrium electron gas at zero temperature. The chemical potentials of seas are different due to the applied dc voltage. The solutions of the scattering problem determine the system linear conductance:
\[ G = G_0 \int dE \sum_n |t_n|^2 \left( \frac{\partial f(E)}{\partial E} \right). \]  

(4)

Here \( f(E) \) is the Fermi distribution function; \( G_0 = 2e^2/h \) is the conductance quantum.

The presence of the mentioned blockade states reflects in the vanishing of the conductance at definite conditions.

**Numerical results.** – The calculated conductance at zero temperature is depicted in figs. 1–4 for different values of \( \Delta \). The Fermi energy, denoted below as \( E \), runs from the bottom \( -\Delta \) to the top \( \Delta \) of the allowed band.

The conductance oscillates with \( v \), that reflects the interference nature of the process. At \( u = 0 \) the pictures are symmetric about the band center (figs. 1, 2, 3a). This electron-hole symmetry can be easily deduced from eq. (3). For large \( \Delta > 1 \) (figs. 1b, 2) the picture exhibits singularities, connected with the thresholds \( \pm \Delta \), namely \( \pm (\Delta - n) \). The singularities \( n = 0, 1 \) are most pronounced. The other singularities (easing with \( n \)) arise as photon repetitions of these singularities. For a wide allowed band \( \Delta > 1 \) the behavior of the conductance near the band boundaries is similar to the model of free electrons interacting with the vibrating \( \delta \)-potential [19,20]. This is not the case for a narrow allowed band.

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**Fig. 1:** Conductance \( G \) (in units of \( G_0 \)) vs. the Fermi energy and parameter \( v \) at \( u = 0 \). \( \Delta = 0.5 \) (a) and \( \Delta = 2.5 \) (b). Panel (a), where \( \Delta < 1 \), distinctly shows the reflectionless state \( E = 0 \), \( G = 1 \). For \( \Delta > 1 \) (b) the reflectionless state disappears.

**Blockade states.** There are two other important features of the conductance dependence. One is the vanishing of the conductance at specific energies \( E(u, v) \) (blockade states). It means that at corresponding energy all the channels of transmission become closed, \( t_n = 0 \) for \( |E + n| < \Delta \).

These high-frequency blockade states can be found directly. Note that if for some \( n > 0 \) \( t_n = t_{n+1} = 0 \), then all \( t_k = 0 \) for \( k > n + 1 \). Hence, the condition \( t_0 = t_1 = 0 \) automatically solves all equations (3) with \( n > 0 \). The equations for \( n < 0 \) compose a homogeneous system, while the equation for \( n = 0 \) determines the value for \( t_{-1} \). This condition can be fulfilled if \( -\Delta + 1 > E > -\Delta \). If the energy satisfies the condition \( -\Delta - 1 < E < \Delta \), what mentioned above is valid with the change of sign in front of \( n \). The homogeneous system has solutions for some eigenvalues of the parameters. Practically, they can be found as eigenvalues for \( 1/v \), if one rewrites the system as
\[ \frac{1}{v} t_{n} - \frac{1}{2(\Lambda(E + n) - u)} (t_{n+1} + t_{n-1}) = 0, \quad n < 0. \]  

(5)

Figures 2, 3a show the dependence of the blockade states on the parameters for \( u = 0 \). If \( \Delta > 1 \) (fig. 2) the domains
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Fig. 2: Map of conductance levels (in units of $G_0$) as a function of the Fermi energy and the parameter $v$ at $u = 0$, $\Delta = 2$. The levels run equidistantly from $< 10^{-6}$ (white) to $\geq 1$ (black). The blockade states are depicted by dashed curves.

of existence of the blockade states adjacent to the left and right band boundaries do not overlap. If $\Delta < 1$ the blockade states cross, and if $\Delta < 1/2$ they also overlap the allowed band (fig. 3a).

**Reflectionless states.** Another feature is the existence of a state with absolute transmission when the conductance exactly equals 1. For $u = 0$ (fig. 3a) this reflectionless state corresponds to the center of the allowed band $E = 0$ and exists if $\Delta < 1$. It is interesting that there are essentially singular points where the blockade and reflectionless states coexist.

For $u \neq 0$ the relief of the conductance becomes asymmetric and, in particular, the line of the reflectionless state moves from the allowed band center $E = 0$ and curves (fig. 3b).

**Local states.** For finite $u$, besides the considered states, the local states appear in the forbidden band (fig. 4). These states are constructed from the waves decaying apart from the site $n = 0$. Their amplitudes obey eq. (2) with no incident wave. The energy should lie in the forbidden band (all $p_n$'s are chosen with positive imaginary part).

The local states originate from the local impurity state at $v = 0$ when the transitions into propagating modes caused by alternating field are not permitted by the energy conservation law. Accordingly, their quasienergy plus (or minus) any integer number should not get into the allowed band. The local states appear below or above the allowed band in dependence on the sign of $u$.

Similar to resonance tunneling in conservative systems, the local states transform to the reflectionless states when they go through the allowed band boundaries $E = \pm \Delta$ (fig. 4).

**Analytical results.** Let us consider the limit $\Delta \ll 1$. For energies $E \gg \Delta$ one can replace in the zero approximation $\Lambda(E)$ by $E$. Treating the remainder $\Lambda(E) - E$ as a perturbation, we shall rewrite the system (3) for $E \ll 1$ as

$$H_{n,n'} t_{n,n'} - \lambda t_n = \Lambda(E) \delta_{n,0},$$

(6)

where $\lambda = u - E$ and $H = H^{(0)} + V$,

$$H^{(0)}_{n,n'} = n \delta_{n,n'} - \frac{v}{2} (\delta_{n,n'} - 1 + \delta_{n,n'} + 1).$$

(7)

The perturbation $V$ is $V_{n,n'} = (\Lambda(E + n) - E - n) \delta_{n,n'}$. In the limit of small $\Delta$ all elements of $V_{n,n'}$ are negligible.
Fig. 4: (a) The same as in fig. 2 at $\Delta = 0.4, u = 0.38$. In this case the crossing point of the blockade and reflectionless states approach the allowed band boundary $E = 0.4$. The local states (solid lines) are situated to the right of this boundary. (b) The magnified neighborhood of the first crossing point of blockade states and reflectionless states illustrates how the local states convert to the reflectionless states (inside the black regions).

except for $V_{0,0} = (\Lambda(E) - E)$. Equation (6) with this local perturbation can be solved using the Green function. The eigenvectors $\psi_k$ of the Hamiltonian $H^{(0)}$ are given by the integer Bessel functions $\psi_k = J_{n-k}(v)$ whose eigenvalues are $k$. The Green function $G^{(0)} = 1/H^{(0)}$ is

$$G_{n,m}^{(0)} = \sum_k \frac{J_{n-k}(v)J_{n'-k}(v)}{-k - \lambda}.$$  

Using the Green function, we find

$$t_n = \frac{\Lambda(E)\sum_k \frac{J_{n-k}(v)J_{n'-k}(v)}{-k - \lambda}}{1 + [\Lambda(E) - E]\sum_k \frac{J_{n'(v)}^2}{-k - \lambda}}.$$  

(8)

In the considered case only the channel $n = 0$ belongs to the propagating states. Hence the zeros of $t_0$ determine the blockade states, the poles determine the localized states, and the condition $t_0 = 1$ determines the reflectionless states:

$$\sum_k \frac{J_k^2(v)}{-k - \lambda} = 0, \quad \text{for blockade states},$$  

(9)

$$1 + [\Lambda(E) - E]\sum_k \frac{J_k^2(v)}{-k - \lambda} = 0, \quad \text{for local states},$$  

(10)

$$1 - E\sum_k \frac{J_k^2(v)}{-k - \lambda} = 0, \quad \text{for reflectionless states}.$$  

(11)

Equations (9), (10) and (11) implicitly determine these discrete states. Below we shall denote them by superscripts $(b, l, r)$ for blockade, local and reflectionless states, respectively.

The local states join to the continuum if

$$1 + \Delta \sum_k \frac{J_k^2(v)}{k - u + \Delta} = 0.$$  

(12)

This threshold equation coincides with the condition when the reflectionless states come to the allowed band boundary. Hence, crossing the boundary they transform to the local states.

**Blockade states.** Let $u \ll 1$. Then the term $k = 0$ with the denominator $\lambda = u - E$ majorizes the sums, and the condition for blockade states eq. (9) holds if $v$ is close to some zero of the Bessel function $J_0(\nu_{0,m}) = 0$.

Let us expand eq. (9) by $v$.

$$\sum_k \frac{J_k^2(v)}{-k - \lambda} \approx -\frac{J_0^2(v)}{\lambda} + \lambda s_N^2(v) + \ldots,$$  

(13)

where $s_N(v) = \sum_{k \neq 0} J_k^2(v)/(k - N)^2$. Solving eq. (9) for small $v - \nu_{0,m}$ with the aid of eq. (13), we find the blockade states

$$E_m^b = u \pm (v - \nu_{0,m})J_1(\nu_{0,m})/s_0(\nu_{0,m}).$$  

(14)

Equation (14) can be generalized to the case of $u$ close to some integer $N$. $u = N + \bar{u}$ using the identity

$$\sum_{k \neq 0} J_k^2(v_{N,m})/(k - N)^2 = 0.$$  

and eq. (13), we find the blockade states

$$E_m^b = \bar{u} \pm (v - v_{N,m})J_{N+1}(v_{N,m})/s_N(v_{N,m}).$$  

(15)

In the case of $v \ll 1$ we can expand eq. (9) by $\lambda$ and $v$.

The blockade state exists for $N \neq 0$ (or for finite $u$). As a result, the blockade energy takes form

$$E_m^b = \bar{u} + \frac{N}{(N!)^2} \left(\frac{v}{2}\right)^{2N}, \quad N \neq 0.$$  

(16)

It should be emphasized that eqs. (14) and (15) are valid both inside (where they correspond to the blockade of propagating waves) and outside the allowed band. The blockade state has even dependence on the parameter $v$, due to symmetry of the alternating signal. If $|\bar{u}| < \Delta$ the blockade state exists for any small $v$, otherwise the quantity $v$ should be also large for the blockade state to exist. Finite $u$ makes the dependence asymmetric about the allowed band center.

Let us qualitatively discuss the origin of the blockade states. It is known, that the reflectionless states originate from destructive interference of waves reflected by different singularities of potential, for example, edges of rectangular potential well. By analogy, the disappearance of transmission in blockade states is caused by the destructive interference of different transition channels. Let the
alternating signal be weak and the process passes through a single intermediate state (local level or edge of allowed band). In this case one should collect two ways of transition: a direct transmission and an indirect transition via the local or the edge state by emission of a single quantum with consequent reabsorption. These two partial transmission amplitudes may have the same orders and cancel each other. Taking into account higher-perturbation terms evidently corrects the interference condition but cannot violate it.

The blockade states, together with reflectionless states, are discrete states on the continuum background. Interestingly, in spite of the fact that the oscillating potential does not conserve energy, the blockade state contains the reflected wave with incident energy only. When the high-frequency blockade occurs the connectivity between two parts of the wire becomes broken (for fixed electron energy), regardless of the fact that the potential remains limited. This leads to important consequences.

For example, two identical vibrating sites can confine an electron with energy in the allowed band between them. This is a classical picture, not accounting for the wave interference. The quantum picture needs some additional conditions for the phase of the wave function that quantizes the energy. Besides, the presence of overlapping evanescent modes makes these local states quasistationary [19,20]. However, the overlapping exponentially drops with the distance, so the widths of quasistationary states do.

Local states. In eq. (10) the quantity $E$ can be treated as the quasienergy chosen in the first Brillouin zone $|E| < 1/2$. Here we restrict ourselves to the case $E \ll 1$. For $\tilde{u} \ll 1$ the energies of local states satisfy the equation

$$E^l = \tilde{u} \left[ 1 - J_N^2(v) \frac{1 - \sqrt{1 - J_N^2(v)} \Delta^2 / u^2}{1 - 2J_N^2(v)} \right],$$

for $|\tilde{u}| \geq \Delta[1 - J_N^2(v)].$ (17)

If $v \rightarrow \infty$, $E^l \rightarrow \tilde{u}$. If the alternating signal $v = 0$, the local state for $N = 0$ is converted to the static impurity state $E^l = u\sqrt{1 + \Delta^2 / u^2}$. For small, but finite $v$, and $u \ll 1$ the level moves to the boundaries of the allowed band:

$$E^l = u \left[ \sqrt{1 + \Delta^2 / u^2} - \frac{u^2}{2} \left(1 - \frac{1}{\sqrt{1 + \Delta^2 / u^2}}\right) \right].$$

(18)

This result can be obtained from the perturbation series on the alternating signal.

If $\tilde{u} \ll 1$ the threshold equation for local states eq. (12) can be solved and yields the multiple solution

$$u = N \pm \Delta[1 - J_N^2(v)].$$

(19)

At $v \rightarrow 0$ the threshold values of $u$ tend to integers $N$ like $N + O(v)$. Reflectionless states. If $\tilde{u} \ll 1$, eq. (11) results in

$$E^r = \frac{\tilde{u}}{1 - J_N^2(v)}.$$  

(20)

Equation (20) is valid while the energy remains within the allowed band. If $u \ll 1$, and $v \ll 1$, this gives the energy $E^r = 2u/v^2$ valid until $u \ll v^2\Delta$. If $u \ll \Delta$ and $v \gtrsim 1$, $E^r = u/(1 - J_N^2(v))$.

Let us discuss the limits of weak and strong alternating signal. The behavior of the states at $v \rightarrow 0$ is conditioned by the perturbation character of the alternating signal. Taking into account its large frequency the action of this signal on the atomic states can be considered in the second approximation of the perturbation theory as static. This static perturbation leads to the quadratic shift of the levels as compared with the case of $v = 0$ (eq. (16) at $N = 1$ and eq. (18)). More weak dependence on $v$ in eq. (16) at $N \neq 1$ is explained by vanishing of the lower orders of perturbation series.

If $v \rightarrow \infty$ the alternating field distributes an electron on a large number of states $E + mv$, only one of which is resonant with other sites; that isolates the site 0 from the others, hence the energies of discrete states cease to depend on $v$ and $\Delta$ (see eqs. (17), (19), (20)).

The numerical results are in accord with the obtained formulae.

How to realize local high-frequency perturbation?. – The most interesting events considered here happen when the frequency is comparable with the band width and the Fermi energy. The application of a so high frequency is difficult by using ordinary electrodes. A more natural way is the utilization of a freely propagating electromagnetic wave (neglecting the corrections caused by the low-dimensional system itself). The wavelength of the electromagnetic wave for a typical frequency $\omega \gtrsim E$ exceeds the electron wavelength, that means non-locality of the electromagnetic perturbation. Nevertheless, the ways for locality exist. For example, it can be done using curved systems, in analogy with the way to produce an effectively non-uniform magnetic field.

Let us consider the 1D periodic chain of quantum dots with a single quantum dot number 0 shifted in the $y$-direction for a distance $b$: $U(x, y) = (1 + u/w) V(x, y - b) + \sum_{n \neq 0} V(x - na, y)$ (see fig. 5). Being placed into an electric field $F(t) = F_0 + F_1 \cos(\omega t)$ in the $y$-direction this system simulates the considered model with the parameters $u = F_0b$, $v = F_1b$. The action of the field on other quantum dots can be neglected if it is out of resonance with distance between their levels.
Another candidate for practical use is the linear oriented periodic polymer chain with different monomer (“impurity”) inside, considered within tight-binding approximation. One can produce local high-frequency perturbation by some sort of excitation of one site, in particular, in a resonant way with no impact to the others.

Let us consider the system depicted in fig. 6. The central site possesses three levels, a pair of which, 1 and 2 (filled and empty), lies in the forbidden band and one level 0 is situated near the allowed band. The presence of a strong alternating field connects the levels 1 and 2, pumping electrons between them. The frequency of light is resonant with the transition between the levels 1 and 2, which are out of resonance with levels of other sites. The state 0 is yet resonantly connected with the other sites. The resonance phototransitions between the levels 1 and 2 produces a dynamic Stark shift of the level 0. This results in the appearance of the effective equation (1) for electrons propagating along the lattice. The calculations within the perturbation approximation give for $v = d_{12}F_1 \cdot V_C$, where $d_{12}$ is the dipole momentum matrix element between the levels 1 and 2, the factor

$$V_C = \frac{1}{\sqrt{\delta^2 + \gamma^2}} |(\psi_1(r)\psi_2(r))U_C(r - r')|\psi_0(r')|^2$$

follows from the Coulomb interaction $U_C(r - r')$ of electrons in the states $\psi_1$ and $\psi_2$ with an electron in a state $\psi_0$ (resonant with the lattice sites), $\delta = E_2 - E_1 - \omega$ is the detuning, $\gamma$ is the damping of the 2-1 transition. The magnitude of $v$ is amplified near the resonance via the factor $V_C$ as compared with the direct dynamic Stark shift of levels $\sim d_{12}F_1$.

Let us do some estimations of planar 1D quantum dot lattice needed to observe the blockade states. If one bases oneself on the parameters, corresponding to fig. 2, it is reasonable to use parameters $a = b = 20 \text{nm}$, $\Delta = 2 \text{meV}$, $F \sim 10^3 \text{V/cm}$, $\omega \sim 10^{12} \text{Hz}$ conforming with each other, and the Fermi energy should be in the range of 1 meV from the band edge. These values look common to be realized experimentally.

Thus, local probing of the system by electric field with optical frequency is realistic. More careful study demands specifying the experimental situation that goes beyond the topic of the present paper.

**Conclusions.** In conclusions, we have studied electron states and conductance of an open quantum-mechanical system with local vibrating potential, based on a one-dimensional tight-binding model. The computer simulations have been supported by an analytical consideration of the model in the case of narrow allowed band. It was found that this model possesses a couple of distinguished states, namely states which stay local in the presence of vibration, states of ideal transparency and, most unusual, blockade states for which the local vibrating potential in the 1D system plays the role of an ideal mirror, despite the openness of the system. While the local and the reflectionless states are permitted in conservative systems, the blockade states with no transmission occur in the system with vibrating potential only. Our estimations show that the conditions for observation of the blockade states are quite ordinary to be experimentally realized using quantum dot lattices.

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