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# AN EFFECTIVE TWO-LEVEL CHANNEL FOR AN IMPURITY IN A SUPERLATTICE*

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The eigenstates and eigenspectrum of a charged particle in a one-dimensional semiconductor superlattice with an impurity under the action of a dc electric field are investigated employing the single-band tight-binding model. We find that the system undergoes a series of avoided crossings, at which resonant oscillations between the impurity and its nearest neighbour occur if appropriate conditions are met, suggesting an effective two-level approximation. This phenomenon shows that introducing an impurity in a perfect lattice provides a promising structure for the observation of terahertz radiation.

**Keywords:** localization, avoided crossing
**PACC:** 7320D, 7215R, 6320K

Semiconductor superlattice models containing different kinds of disorders subjected to external fields have received increasing attention in recent years,[1−8] such as the Kronig-Penney, Aubry, Harper, Fibonacci and Thue-Morse models. Much of the interest has been caused because fabrication is always somewhat imperfect, the individual quantum wells may differ from one another in size, shape and separation. In the present work, we study the dynamics of a one-dimensional system with an impurity under the action of a dc electric field along the single-band tight-binding model, of which the particle is initially in a well-localized state at the impurity site. It is well known that when a dc electric field is applied to a perfect lattice, the particles perform an oscillatory motion with characteristic frequency $\omega_{\rm B} = eaE$ (we take $\hbar = 1$ throughout this paper), i.e. Bloch oscillations,[9] where $e$ is the charge of the particle, $a$ is the lattice constant, and $E$ is the magnitude of the dc electric field. The eigenvalue spectrum is a ladder of discrete, equally spaced levels with spacing $\omega_{\rm B}$, which has become known as the Wannier-Stark (WS) ladder.[10] In this paper, we study the effect of the impurity on the dynamics of this system. By solving numerically the stationary Schrödinger equation we obtain the eigenstates and eigenspectrum. Through a further analysis of the energy spectrum and the probability propagators at relevant sites, we find that avoided crossings in the energy spectrum are related to the resonance condition. If the system parameters are appropriately chosen to be at the point of avoided crossing, the particle oscillates resonantly between the impurity and its nearest-neighbour site as if ignoring the rest of the lattice structure. That is to say, the interaction of the dc electric field and the impurity results in an effective two-level system. Such an effect may have important applications for the generation of strong electromagnetic radiation.

We consider a single-band tight-binding model (SBTB) of a one-dimensional system with an impurity at site 0 in a dc electric field $E$. The corresponding Hamiltonian in the Wannier representation can be written as

$$H = \sum_n V(|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \varepsilon_0 |0\rangle\langle 0| - eaE \sum_n n |n\rangle\langle n| , \qquad (1)$$

where $V$ is the nearest-neighbour intersite hopping matrix element, $\varepsilon_0$ is the impurity potential, and $|n\rangle$ represents a Wannier state localized at the lattice site $n$. In our calculations, we chose $n = 0, \pm 1, ..., \pm 25$, which approximates a realistic model. Therefore, the Hamiltonian (1) can be spanned in terms of the Wannier basis $|n\rangle$ and reduced to a $51 \times 51$ tridiagonal matrix. In the following it is convenient to use $\omega_{\rm B}$ denoting the quantity $eaE$.

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Consider the stationary Schrödinger equation of the Hamiltonian (1)

$$H|\phi_i\rangle = \varepsilon_i|\phi_i\rangle, \tag{2}$$

by diagonalizing $H$ straightforwardly, the energy eigenvalues $\varepsilon_i$ and the energy eigenstates $|\phi_i\rangle$ can be obtained. Figure 1 displays the numerical results of the energy spectrum, where the scaled energies $\varepsilon/\omega_{\rm B}$ are plotted as functions of $\varepsilon_0/\omega_{\rm B}$ with $V/\omega_{\rm B} = 0.05$. An intriguing feature shown in Fig.1 is that on increasing the value of $\varepsilon_0/\omega_{\rm B}$ adiabatically two branches of energies will approach each other virtually. Especially when the value of the impurity potential satisfies

$$\varepsilon_0 = n\omega_{\rm B} \tag{3}$$

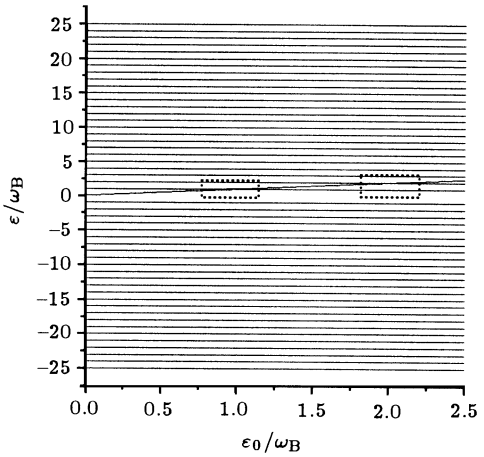



**Fig.1.** The scaled energy spectrum $\varepsilon/\omega_{\rm B}$ as a function of $\varepsilon_0/\omega_{\rm B}$ with $V/\omega_{\rm B} = 0.05$.

the two branches appear to cross. Figures 2(a) and 2(b) shows the enlargement of the two regions bounded by the rectangles in Fig.1. We can see that the crossings are avoided. We expect fundamental changes of the dynamic behaviour of the system occur at these avoided crossings.

To elucidate the effects of the avoided crossings displayed in Fig.2 on the quantum mechanical behaviour of the system we examine the dynamic evolution of an initial state. Given that the electron is initially localized at the impurity site $|0\rangle$, we therefore investigate its subsequent dynamic evolution. By expressing the particle state $|\phi(t)\rangle$ as a linear combination of Wannier states $|n\rangle$,

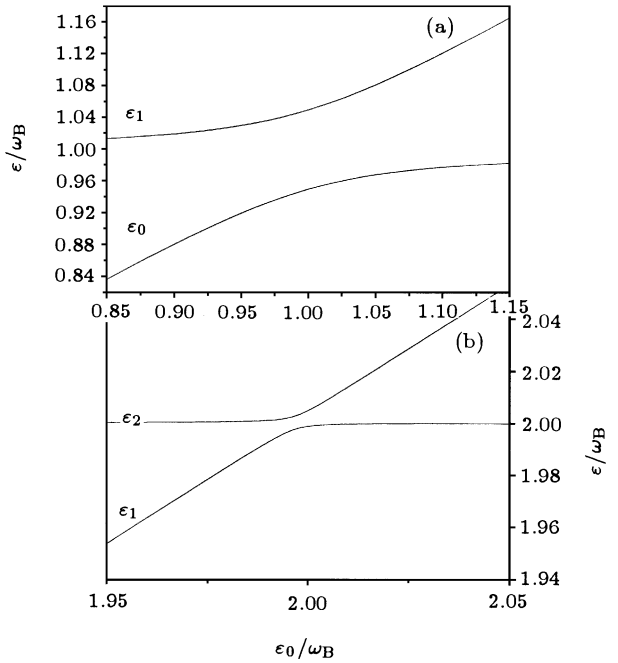



**Fig.2.** Magnification of the two regions bounded by the rectangles in Fig.1.

$$|\phi(t)\rangle = \sum_n c_n(t)|n\rangle, \tag{4}$$

where $c_n(t)$ are the time-dependent amplitudes $\langle n|\phi(t)\rangle$, one obtains from Eq.(1) the following evolution equation for the amplitudes $c_n(t)$:

$$\begin{aligned} {\rm i}\frac{d}{dt}c_n(t) =& V(c_{n+1}(t) + c_{n-1}(t)) \\ &+ \varepsilon_0 c_0(t)\delta_{n,0} - n\omega_{\rm B}c_n(t), \end{aligned} \tag{5}$$

with the initial condition

$$c_n(0) = \delta_{n,0}. \tag{6}$$

In the absence of any scheme for solving these equations analytically, we resort to numerical calculations. By solving Eqs.(5) and (6) with a fourth order Runge-Kutta integration, we can obtain the probability propagator $\psi_n(t)(= |c_n(t)|^2)$ for any site $n$ at time $t$. We present in Figs.3(a)–3(e) the time evolution of the probability propagators for sites 0 and $-1$ (represented respectively by $\psi_0(t)$ and $\psi_{-1}(t)$), where the five values of $\varepsilon_0/\omega_{\rm B}$ are respectively 0.88, 0.94, 1.00, 1.06 and 1.12. It is shown in these figures that when we change the value of the impurity potential $\varepsilon_0$ towards the avoided crossing, the oscillation amplitude of $\psi_0(t)$ and $\psi_{-1}(t)$ increases little by little. Until, at the avoided crossing point where $\varepsilon_0/\omega_{\rm B} = 1$, both $\psi_0(t)$ and $\psi_{-1}(t)$ oscillate between 0 and 1, meaning that a complete resonance (Rabi oscillation) takes place between the impurity and its nearest-neighbour

site in the left. Such oscillations should result in emission of electromagnetic radiation with a frequency in the terahertz range. After the value of the impurity potential exceeds $\omega_B$, the oscillation amplitude for both sites decreases little by little. This presents a localization-resonance-localization process. The most important feature revealed in Fig.3 is that when the system parameters are chosen near the avoided crossing $\varepsilon_0 = \omega_B$, the system can be approximated by an effective two-level system (TLS), in which the impurity site $|0\rangle$ and its left nearest-neighbour $|-1\rangle$ are the two localized basis functions. To illustrate this point, by neglecting the amplitudes other than $c_0$ and $c_{-1}$, we have calculated the time evolution of the reduced system with the same parameters used in Fig.3(c). We find that the result is exactly identical to that shown in Fig.3(c), suggesting the validity of the TLS consideration.

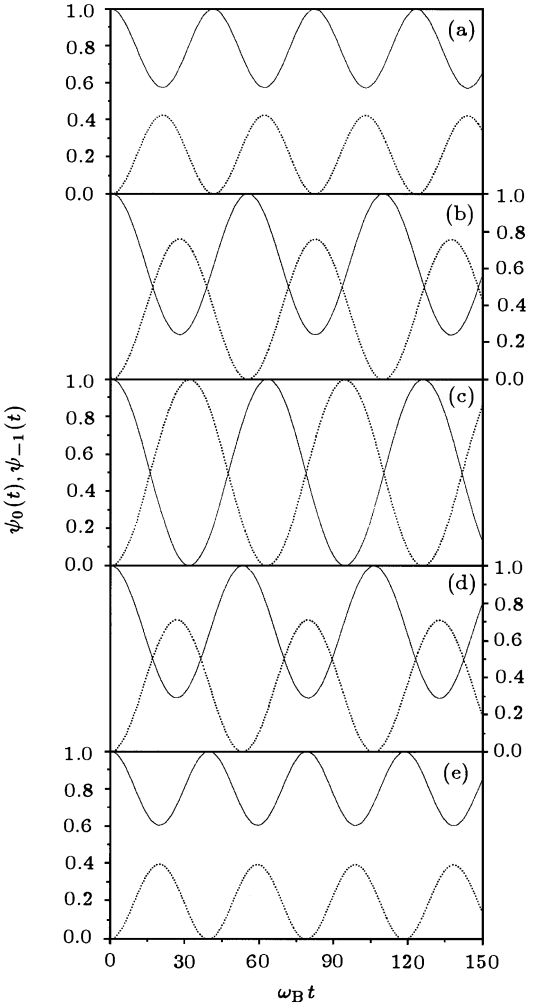



**Fig.3.** $\psi_0(t)$ and $\psi_{-1}(t)$ are plotted as functions of dimensionless time $\omega_B t$ for five different values of the ratio $\varepsilon_0/\omega_B$, (a) $\varepsilon_0/\omega_B = 0.88$, (b) $\varepsilon_0/\omega_B = 0.94$, (c) $\varepsilon_0/\omega_B = 1.00$, (d) $\varepsilon_0/\omega_B = 1.06$, and (e) $\varepsilon_0/\omega_B = 1.12$. The solid line corresponds to site 0 and the dotted line corresponds to site $-1$.

To understand the underlying physics of this transition from localization to resonance we investigate the shapes of the eigenstates $|\phi_0\rangle$ and $|\phi_1\rangle$ corresponding to the two energy levels shown in Fig.2(a). We present in Figs.4(a) and (b) the occupation probability of the two eigenstates $|\phi_0\rangle$ and $|\phi_1\rangle$ on the Wannier basis $|0\rangle$ and $|-1\rangle$ respectively. The reduced values of $\varepsilon_0$ are the same as those used in Fig.3. Fig.4 shows that the two eigenstates are dominated by the site states $|0\rangle$ and $|-1\rangle$ and the components of other site states are negligible. For different values of $\varepsilon_0$, the weights of the site states $|0\rangle$ and $|-1\rangle$ are also different. We notice that, at the avoided crossing $\varepsilon_0 = \omega_B$, the components of two site states are both about 0.5 in the two relevant eigenstates. In this case, the energy state is a superposition of the two eigenstates with equal amplitudes, thus leading to the complete resonance between the impurity and its nearest-neighbour in the left.

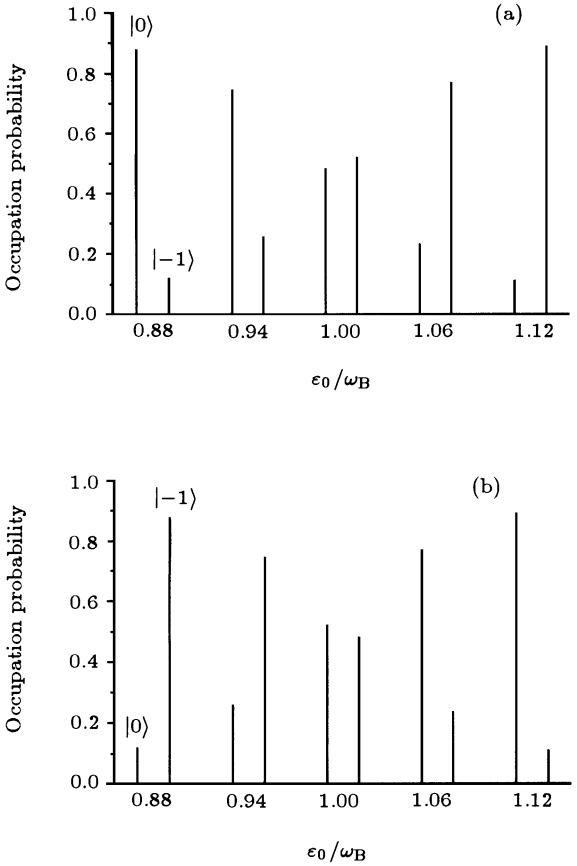



**Fig.4.** The occupation probability of two eigenstates $|\phi_0\rangle$ (depicted in Fig.4(a)) and $|\phi_1\rangle$ (depicted in Fig.4(b)) in terms of the Wannier basis $|0\rangle$ and $|-1\rangle$ for five values of $\varepsilon_0/\omega_B$ used in Fig.3.

Another feature, i.e. exchange of the state structure at the avoided crossing, displayed in Fig.4, should be stressed. We can see in Fig.4 that with increasing impurity potential around the avoided crossing, the

occupation probability flows from the state $\phi_0$ to $\phi_1$, and vice versa. After exchanging their state structure, the two states turn into each other. So now the state $\phi_1$, instead of $\phi_0$, has a large component of the impurity site state $|0\rangle$. On further increasing the impurity potential, another avoided crossing occurs at $\varepsilon_0 = 2\omega_{\rm B}$. In this case, we expect that there will be a resonance between the impurity site and its next-nearest-neighbour in the left. This is verified in Fig.5, where $\psi_0(t)$ and $\psi_{-2}(t)$ are plotted as functions of dimensionless time $\omega_{\rm B}t$. We can see a similar trend for the particle oscillating between the impurity and site $-2$ as that shown in Fig.3(c), but with decreasing amplitude and a long period. It is reasonable that the resonance is not complete. With increasing impurity potential, i.e. the value of $n$, the particle is more and more localized at its original site because the barriers strongly inhibit the hopping.

In conclusion, proceeding with the energy spectrum of the system, we have numerically studied the dynamics of a superlattice with an impurity under the action of a dc electric field. We find that the avoided crossings in the energy spectrum occur at the points where the impurity potential is integral multiples of Bloch oscillation frequency, which corresponds to the resonance condition $\varepsilon_0 = n\ \omega_{\rm B}$. In particular for $n = 1$, the particle oscillates resonantly between the impurity and its nearest-neighbour site and the system can be considered as an effective two-level system. We believe such an effect can be useful in detecting the coherent electromagnetic radiation in a semiconductor superlattice structure.

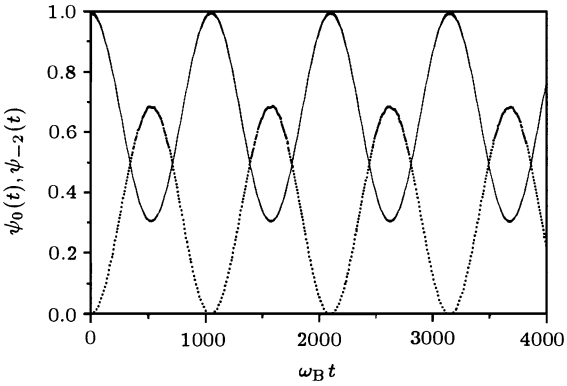



**Fig.5.** $\psi_0(t)$ and $\psi_{-2}(t)$ are plotted as functions of dimensionless time $\omega_{\rm B}t$. The solid line corresponds to site 0 and the dotted line corresponds to site $-2$.

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