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1997 J. Phys.: Condens. Matter 9 L385

(http://iopscience.iop.org/0953-8984/9/27/001)

J. Phys.: Condens. Matter **9** (1997) L385–L390. Printed in the UK PII: S0953-8984(97)82119-4

LETTER TO THE EDITOR

Dynamics of a periodic binary sequence in an ac field

Xian-Geng Zhao

CCAST(World Laboratory) PO Box 8730, Beijing 100080, People's Republic of China, Institute of Applied Physics and Computational Mathematics, PO Box 8009, Beijing 100088, People's Republic of China† and
Institute of Theoretical Physics, Academia Sinica, PO Box 2735, Beijing 100080, People's Republic of China

Received 24 February 1997, in final form 28 May 1997

Abstract. We study the dynamic effect of band electrons in a periodic binary sequence under the action of ac electric fields. Using the technique of the Lie algebra $SU(2)$, we obtain closed-form solutions for the quasienergy and the Floquet states, from which it is found that the evolution behaviour of electrons can be manipulated by the choice of field parameters.

The propagation of particles in a time-dependent potential is a fundamental problem in quantum mechanics. There are many results about this topic, and we can cite only a few [1–7]. Among these previous studies, the particular interest is that of the dynamic effect of band electrons subject to a time-periodic electric field, which reveals unusual fascinating aspects. In the investigation of evolution behaviour of an electron in a laser field, it is found that an initially localized electron will remain localized if the ratio of the field magnitude and the field frequency is a root of the ordinary Bessel function of order zero [8]. This phenomenon involving the dynamic localization of moving carriers was re-examined very recently in a study of quasienergy minibands in superlattices [9]. There it is demonstrated that the occurrence of miniband collapse coincides with the onset of dynamic localization.

In this paper we study another situation for the motion of electrons in a periodic binary sequence under the influence of a high-frequency ac electric field. The character of this model is such that the site energies alternate between the values $\varepsilon \pm 2\Delta$. Such a system is relevant to a variety of fields, including that of exciton states in molecular crystals [10] and electron localization in superlattices [11]. Moreover it may simulate the dimerized systems discussed numerically by Hone and Holthaus [7]. We find that this model can be solved analytically by means of the technique of the Lie algebra $SU(2)$. As a result, we obtained closed-form solutions for the quasienergy bands and Floquet states, from which it is demonstrated that the collapse of quasienergy bands will occur under similar conditions as the single-band case.

The time-dependent Hamiltonian considered here is

$$H(t) = 2\Delta \sum_n (-1)^n |n\rangle\langle n| + V \sum_n |n\rangle\langle n+1| + |n+1\rangle\langle n| - eaE(t) \sum_n n|n\rangle\langle n| \qquad (1)$$

where $|n\rangle$ represents a Wannier state localized on lattice site n, V is the nearest-neighbour intersite hopping matrix element, e is the charge on the electron and a is the periodic structure constant. The ac electric field $E(t)$ can be written explicitly as $E(t) = E\cos\omega t$ with the amplitude E and frequency ω. Obviously, the Hamiltonian (1) is periodic in time

† Mailing address.

with the length $T = 2\pi/\omega$. Therefore Floquet's theorem [12] asserts that the wave function $|\psi(t)\rangle$ can be expressed as the product of a phase factor $\exp(-\mathrm{i}\epsilon t)$ and a Floquet state $|u(t)\rangle$ which is cyclic in time with the period T, where ϵ is the quasienergy.

By expanding the Floquet state $|u(t)\rangle$ as a linear superposition of Wannier states $|n\rangle$, $|u(t)\rangle = \sum_n C_n(t)|n\rangle$, we get the Schrödinger equation for the amplitudes $C_n(t)$ as

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}C_n(t) = \left[2\Delta(-1)^n - \epsilon - neaE\cos\omega t\right]C_n(t) + V\left[C_{n+1}(t) + C_{n-1}(t)\right]. \tag{2}$$

By introducing

$$C_n(t) = \exp\left\{-\mathrm{i}\left[(2\Delta(-1)^n - \epsilon)t - (neaE/\omega)\sin\omega t\right]\right\} f_n(t) \tag{3}$$

we transform equation (2) into

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}f_n(t) = V\mathrm{e}^{\mathrm{i}4\Delta(-1)^n t}\left[f_{n+1}(t)\mathrm{e}^{\mathrm{i}(eaE/\omega)\sin\omega t} + f_{n-1}(t)\mathrm{e}^{-\mathrm{i}(eaE/\omega)\sin\omega t}\right]. \tag{4}$$

This equation can be further simplified by using the discrete Fourier transforms $f(k,t) = \sum_n f_{2n}(t)\exp(-\mathrm{i}kn)$, $g(k,t) = \sum_n f_{2n+1}(t)\exp(-ikn)$, $(0 \leqslant k < 2\pi)$. The result is

$$\mathrm{i}\frac{\partial}{\partial t}R(k,t) = H(k,t)R(k,t) \tag{5}$$

where

$$R(k,t) = \begin{pmatrix} f(k,t) \\ g(k,t) \end{pmatrix} \tag{6}$$

and

$$\begin{aligned} H(k,t) &= 2V\cos\left(\frac{k}{2} + \frac{eaE}{\omega}\sin\omega t\right)\left[\cos\left(\frac{k}{2} - 4\Delta t\right)\sigma_x + \sin\left(\frac{k}{2} - 4\Delta t\right)\sigma_y\right] \\ &\equiv X(k,t)\sigma_x + Y(k,t)\sigma_y. \end{aligned} \tag{7}$$

σ_x and σ_y (as well as σ_z used below) are the Pauli matrices. Equation (5) can be solved explicitly by using the Neumann–Liouville expansion [13]

$$R(k,t) = \sum_{m=0}^{\infty} U^{(m)}(k,t,t_0)R(k,t_0) \tag{8}$$

with

$$\begin{aligned} U^{(m)}(k,t,t_0) = (-\mathrm{i})^m &\left(\prod_{l=1}^{m}\int_{t_0}^{t}\mathrm{d}t_l\right)\theta(t_1 - t_2)\theta(t_2 - t_3)\ldots\theta(t_{m-1} - t_m) \\ &\times H(k,t_1)H(k,t_2)\ldots H(k,t_m) \end{aligned} \tag{9}$$

where $\theta(t) = 1$ for $t > 0$ and 0 otherwise. In the following, we will put $t_0 = 0$ without loss of generality. It has been shown that by using the technique of the Lie algebra $SU(2)$, $\sum_{m=0} U^{(m)}(k,t,0)$ can be expressed as [14]

$$\begin{aligned} \sum_{m=0}^{\infty} U^{(m)}(k,t,0) = &\sum_{m=0}^{\infty} U_x^{(2m)}(k,t) + \mathrm{i}\sigma_z\sum_{m=0}^{\infty} U_y^{(2m)}(k,t) + \mathrm{i}\sigma_x\sum_{m=0}^{\infty} U_x^{(2m+1)}(k,t) \\ &+ \mathrm{i}\sigma_y\sum_{m=0}^{\infty} U_y^{(2m+1)}(k,t) \end{aligned} \tag{10}$$

with

$$U_x^{(2m)}(k,t) = (-1)^m \left(\prod_{l=1}^{2m}\int_0^t \mathrm{d}t_l\right)\theta(t_1-t_2)\ldots\theta(t_{2m-1}-t_{2m})X(k,t_1t_2\ldots t_{2m}) \tag{11}$$

$$U_y^{(2m)}(k,t) = (-1)^m \left(\prod_{l=1}^{2m}\int_0^t \mathrm{d}t_l\right)\theta(t_1-t_2)\ldots\theta(t_{2m-1}-t_{2m})Y(k,t_1t_2\ldots t_{2m}) \tag{12}$$

$$U_x^{(2m+1)}(k,t) = (-1)^{m+1} \left(\prod_{l=1}^{2m+1}\int_0^t \mathrm{d}t_l\right)\theta(t_1-t_2)\ldots\theta(t_{2m}-t_{2m+1})X(k,t_1t_2\ldots t_{2m+1}) \tag{13}$$

$$U_y^{(2m+1)}(k,t) = (-1)^{m+1} \left(\prod_{l=1}^{2m+1}\int_0^t \mathrm{d}t_l\right)\theta(t_1-t_2)\ldots\theta(t_{2m}-t_{2m+1})Y(k,t_1t_2\ldots t_{2m+1}) \tag{14}$$

where $X(k,t_1t_2\ldots t_m)$ and $Y(k,t_1t_2\ldots t_m)$ satisfy the following recurrence formulae

$$X(k,t_1t_2\ldots t_m) = X(k,t_1t_2\ldots t_{m-1})X(k,t_m) + Y(k,t_1t_2\ldots t_{m-1})Y(k,t_m) \quad (m \geqslant 2) \tag{15}$$

$$Y(k,t_1t_2\ldots t_m) = X(k,t_1t_2\ldots t_{m-1})Y(k,t_m) - Y(k,t_1t_2\ldots t_{m-1})X(k,t_m) \quad (m \geqslant 2). \tag{16}$$

Applying the periodicity of the Floquet state $|u(t)\rangle$ to equation (3) yields

$$f_n(t+T) = f_n(t)\exp\{\mathrm{i}[2\Delta(-1)^n - \epsilon]T\} \tag{17}$$

which leads to

$$R(k,t+T) = \mathrm{e}^{-\mathrm{i}\epsilon T}\left[\cos(2\Delta T) + \mathrm{i}\sigma_z\sin(2\Delta T)\right]R(k,t). \tag{18}$$

Note that $\sum_m U^{(m)}(k,t,0)$ is actually the evolution operator $U(t,0)$ in k space. Therefore, by employing the properties of the evolution operator, $U(t,0) = U(t,t')U(t',0)$ and $U(t,0) = U^\dagger(0,t)$, to equations (8) and (18) we get the eigenvalue equation

$$\det\left\{\sum_{m=0}^{\infty} U^{(m)}(k,T,0) - \mathrm{e}^{-\mathrm{i}\epsilon T}[\cos(2\Delta T) + \mathrm{i}\sigma_z\sin(2\Delta T)]\right\} = 0. \tag{19}$$

Substituting equation (10) into this equation and through a long but straightforward calculation, we obtain the quasienergies

$$\epsilon_\pm(k) = \pm\frac{\phi(k,T)}{2\pi}\omega \quad \mathrm{mod}(\omega) \tag{20}$$

where

$$\phi(k,T) = \cos^{-1}\left\{\cos(2\Delta T)\sum_{m=0}^{\infty}U_x^{(2m)}(k,T) + \sin(2\Delta T)\sum_{m=0}^{\infty}U_y^{(2m)}(k,T)\right\}. \tag{21}$$

The corresponding wave functions have also been obtained which we have not presented here.

From equation (20) it is clearly seen that the quasienergy spectrum is that of two separated bands. Note that from equation (21) we have always $|\phi(k,T)| \leqslant \pi$. Therefore the quasienergies must be in the range $-\omega/2 \leqslant \epsilon(k) < \omega/2$. This means that the length of a 'Brillouin zone' in the quasienergy space is ω. We call the range $-\omega/2 \leqslant \epsilon(k) < \omega/2$ the first Brillouin zone. Other Brillouin zones can be obtained by adding integral multiples of ω to the quasienergy.

In principle, equation (21) can hold exactly. This however requires us to calculate infinite integrals, which, obviously, is impossible. Therefore, to obtain an explicit expression for the quasienergy we need to make some approximation. Here, as an example, we consider the high-frequency limit of the ac electric field. In that case, we can cut off the series in (21) to do practical calculations.

As the lowest-order approximation of $1/\omega$, we have

$$\cos\phi(k,T) \simeq \cos(2\Delta T)\left[1+U_x^{(2)}(k,T)\right]+\sin(2\Delta T)U_y^{(2)}(k,T). \tag{22}$$

By the use of equations (7), (11), (12), (15) and (16) for $U_x^{(2)}(k,T)$ and $U_y^{(2)}(k,T)$, and through a long but straightforward calculation we obtain

$$\cos\phi(k,T) = 1-2\left(\frac{2\pi}{\omega}\right)^2\left[\Delta^2+(VJ_0(eaE/\omega)\cos(k/2))^2\right] \tag{23}$$

where J_0 is the ordinary Bessel function of order zero. This gives

$$\phi(k,T) \simeq \frac{4\pi}{\omega}\left[\Delta^2+(VJ_0(eaE/\omega)\cos(k/2))^2\right]^{1/2}. \tag{24}$$

Therefore we have

$$\epsilon_\pm(k) = \pm 2\left[\Delta^2+(VJ_0(eaE/\omega)\cos(k/2))^2\right]^{1/2}\,\mathrm{mod}(\omega). \tag{25}$$

It has been shown that the energy bands of the undriven system are [15]

$$\epsilon_\pm^0(k) = \pm 2\left[\Delta^2+V^2\cos^2\frac{k}{2}\right]^{1/2}. \tag{26}$$

Therefore by comparing equations (25) and (26) we find that the doublet of quasienergy bands can be rewritten as

$$\epsilon_\pm(k) = \pm 2\left[\Delta^2+V_{\mathrm{eff}}^2\cos^2\frac{k}{2}\right]^{1/2}\,\mathrm{mod}(\omega) \tag{27}$$

with

$$V_{\mathrm{eff}} = VJ_0(eaE/\omega) \tag{28}$$

which indicates that the influence of the high-frequency driving laser field on the quasienergy bands is to suppress the band widths through the effective hopping V_{eff} because of the decay of Bessel function J_0 when increasing its argument. A remarkable feature equation (28) shows is that the effective hopping V_{eff} vanishes entirely whenever the ratio of the Bloch frequency $\Omega = eaE$ and the laser frequency ω is a root of J_0. When this happens, the band widths of the doublet will shrink into zero, and the quasienergies will turn into exactly the alternating site energies $\pm 2\Delta$. This phenomenon of band collapse can be clearly seen from figure 1, where the scaled quasienergies $\epsilon_\pm/\omega$ are plotted as a function of eaE/ω. The other parameters in the figure are fixed as $\Delta/\omega = 0.03$ and $V/\omega = 0.22$. Since at the collapse points, for example $eaE/\omega = 2.4$, the bands are flattened, the electron will have an infinite effective mass, and hence its motion becomes localized. Keeping this in mind, we can conclude that the band collapse is the manifestation of the dynamic localization. Such observations agree with the numerical findings in two dimerized systems where the corresponding well width and barrier width of superlattices alternate between certain regions [7] and are consistent with the evolution behaviour of moving carriers in ac fields [8, 16].

It is interesting to extend the above analysis to the case when the chain becomes quasiperiodic or random. There are some discussions on this topic for the tight-binding single-band case in [17, 18] where it was found that the effect of the electric field on localization is much stronger than disorder is and one could manipulate the degree of disorder-induced localization, e.g. Anderson localization [19], by tuning the field parameters.

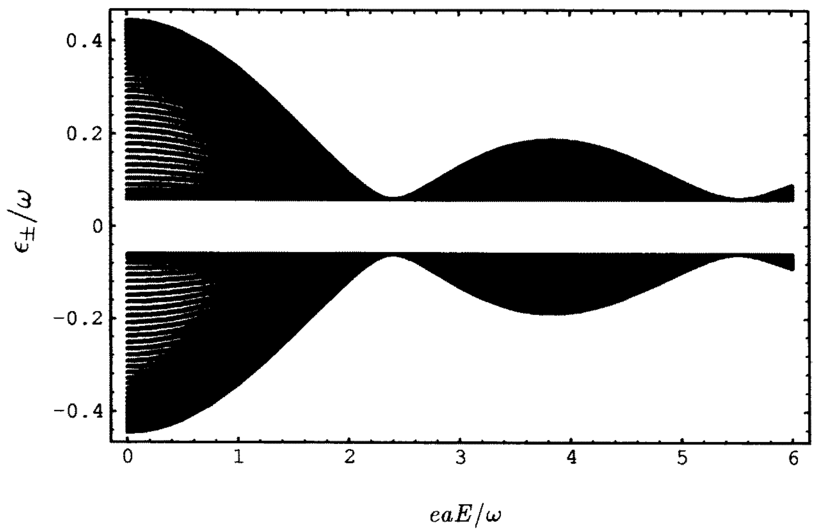

Figure 1. The scaled quasienergies $\epsilon_\pm/\omega$ as a function of eaE/ω. The other parameters are $\Delta/\omega = 0.03$ and $V/\omega = 0.22$.

However, the investigation on the influence of disorder to the Rabi oscillations between Bloch bands [20] which is generated by the Zener tunnelling under the action of dc–ac fields, is still absent. We will study this elsewhere.

In summary, we have solved the problem of electrons moving in a periodic binary sequence under the action of ac electric fields. Using the technique of the Lie algebra $SU(2)$, we obtained analytical solutions for the quasienergy bands and Floquet states. The evolution behaviour of electrons was found to be dominantly controlled by the field parameters. This means that we can manipulate the motion of electrons by adjustment of the electric field.

This work was supported in part by the National Natural Science Foundation of China and the grant of the China Academy of Engineering and Physics.

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