Stark ladder in a one-dimensional quasiperiodic system

K. Niizeki and A. Matsumura

Department of Physics, Tohoku University, Sendai 980, Japan (Received 27 April 1993)

We have investigated the effect of a uniform field F on the energy spectrum of the Harper model, which includes an irrational ω and the phase variable φ as parameters. The energy levels $E_i(\varphi), i \in \mathbb{Z}$, are periodic on φ , $E_i(\varphi+1)=E_i(\varphi)$, and form a two-dimensional (2D) pattern in the φ -E plane. The pattern which we term a 2D Wannier-Stark ladder (2DWSL) has 2D periodicity because of the equalities $E_i(\varphi)=iF+E_0(\varphi+i\omega), i\in\mathbb{Z}$. The energy spectrum is a vertical section of the 2DWSL through the specified φ and represents a quasiperiodic WSL.

The electronic structure of a quasiperiodic (QP) system is of current interest in connection with quasicrystals.¹ Much progress has been achieved from one-dimensional (1D) models. The simplest of them is the Harper model, whose Hamiltonian is given in the Wannier representation as follows:

$$H_0 = -\sum_n \left(|n\rangle \langle n+1| + |n+1\rangle \langle n| \right) + \sum_n |n\rangle V_n \langle n| ,$$
(1)

$$V_n = V f(n\omega + \varphi) , \qquad (2)$$

where $|n\rangle$ is the Wannier state localized on the site $n, f(x) \equiv 2 \sin(2\pi x)$ is the modulation function, V(>0) is the potential strength, $\omega(0 < \omega < 1)$ is an irrational number, and φ is the phase variable. We adopt the transfer integral and the lattice spacing as the units of energy and length, respectively. The argument $\varphi_n = n\omega + \varphi$ of V_n is called a local phase. The modulation potential breaks the translational symmetry of the system. More precisely, the Hamiltonian $H_0 \equiv H_0(\varphi)$ is transformed by the translation operator $U = \sum_n |n+1\rangle \langle n|$ as follows:

$$U^{-1}H_{0}(\varphi)U = H_{0}(\varphi + \omega) , \qquad (3)$$

which follows from the property $\varphi_{n+1} = \varphi_n + \omega$ of the local phase. The Harper model was originally derived as the equation determining one-electron wave functions on a two-dimensional (2D) rectangular lattice under a uniform magnetic field.² In this view, φ is essentially the wave number along the second axis.

It has been established that the Harper model exhibits a localization-delocalization transition as V is varied.^{1,3} All the eigenstates (wave functions) are extended, critical, or localized for V < 1, V = 1, or V > 1, respectively, and, consequently, the energy spectrum, which is independent of φ , is absolutely continuous, singular continuous, or dense point, respectively.

The energy spectrum will be drastically changed by a uniform electric field F as in the case of a periodic system, where a uniform Wannier-Stark ladder (WSL) takes place.⁴ There exist several works on this subject⁵⁻⁹ but progress is still rudimentary probably because we have not yet identified the proper quantum number which

characterizes the eigenstates. The present work will present an answer to this question. We restrict our considerations to the weak-field regime so that the interband transition from the band included in the model to the other bands omitted can be neglected. The Hamiltonian is given by

$$H = H_0 + F_{op}$$
, (4)

where $F_{op} = \sum_{n} F|n \rangle n \langle n|$. Moreover, we consider only the extended regime, i.e., the case for V < 1. These restrictions will justify Zener's tilted band picture⁴ on the subject. Then the eigenstates are localized and the energy spectrum becomes discrete.⁵ More precisely, the average level spacing is equal to F and the extension of the eigenstates is of the order $l \equiv B/F$, with B being the bandwidth at the zero field. The energy levels form a WSL with nonuniform spacing.⁵

Prior to analyzing the structure of the WSL, we shall note several properties of the Harper model in the absence of the field.¹ The energy spectrum of H_0 in the absence of the modulation potential V_n is composed of a single band. The modulation potential expands the entire bandwidth and, simultaneously, introduces an infinite number of gaps. However, only a finite number of gaps have appreciable magnitudes¹⁰ if V < 1, so that the spectrum is composed virtually of a finite number of minibands, among which the states of the entire band are shared. It can be shown by using the gap labeling theorem 1,11,12 that the fraction of a miniband is written as $\xi = n - m\omega$ with $n, m \in \mathbb{Z}$. We may consider $1/\xi$ to be the "lattice constant" of the miniband, while ξ is that of the "reciprocal lattice." We shall term the symbol [n,m]the index of the miniband. Since $0 < \xi < 1$, m is nonzero and |n|/|m| is a rational approximant to ω ; n and m have the same sign, which is equal to that of $|n|/|m| - \omega$. We can assume that n/m is a best approximant to ω ; otherwise the miniband can be divided into several smaller ones. A sequence of best rational approximants to ω is obtained from the continued fraction expansion of ω . The energy spectrum of the Harper model has the center of the inversion symmetry at the origin of the energy axis and, consequently, the minibands are formed symmetrically. This is because of the inversion symmetry of the modulation potential and the kinetic energy in the real and the reciprocal spaces, respectively.

We see here how the minibands are formed in the case where $\omega = \omega_G \equiv (\sqrt{5}-1)/2$, i.e., the golden mean.^{1,10} The entire band is divided into three subbands by the largest two gaps. Only the central subband is symmetric and has the fraction ω^3 , while the other two are related to each other by the energy inversion and have the fraction $\omega^2:2\omega^2+\omega^3=1$. Each subband branches subsequently into three smaller subbands with the ratio $\omega^2:\omega^3:\omega^2$. This process continues indefinitely, yielding a hierarchical subband structure. If this process is terminated at a finite stage, the resulting minibands have fractions which are powers of ω . We may write $\omega^2=1-\omega$ and $\omega^3=-1+2\omega$, or, more generally, $\omega^k=(-1)^k(F_{k-1}-F_k\omega)$, where F_k are Fibonacci numbers generated by the recursion relation $F_{k+1}=F_k+F_{k-1}$ with the initial conditions $F_0=0$ and $F_1=1$. The ratios F_{k-1}/F_k are best approximants to ω . The successive two approximants F_{k-1}/F_k and F_k/F_{k+1} satisfy $(F_k)^2-F_{k+1}F_{k-1}=(-1)^{k+1}$.

We will consider now what happens when the field is introduced. It is easily conceivable that the field will change each miniband to a nonuniform WSL. The average spacing of the WSL will be F/ξ , where ξ denotes the fraction of the miniband. Since the gap between adjacent minibands is finite, an electron in one of them can move to the other through the Zener tunneling. The tunneling probability is written as $\exp(-F_0/F)$ with $F_0 = c\xi E_g$, where E_g is the band gap.¹³ It follows that the gap is ineffective when $F \gg F_0$. Then the gap is quenched by the field and the two bands merge, forming a larger miniband. A small gap will easily be quenched. Therefore, the effective number of minibands will decrease as the field is increased. On the contrary, if a miniband is separated from others by wide gaps, it will yield an isolated WSL. However, if the level of an almost isolated miniband coincides by chance with the level of a neighboring miniband, resonant Zener tunneling will take place. Therefore, the energy spectrum will vary markedly as the field and/or the potential strength are varied.

The energy levels $E_i, i \in \mathbb{Z}$, in the limit of the vanishing modulation potential (V=0) can be numbered so that $E_i = iF$. If V is switched on adiabatically, they change continuously but the order, $E_i < E_{i+1}, i \in \mathbb{Z}$, cannot change because the energy levels are discrete and never cross as functions of the parameters included in the Hamiltonian; the latter is the general feature of tridiagonal matrices with nonvanishing "transfer integrals." We will consider the dependence of the energy levels $E_i \equiv E_i(\varphi)$ on φ . The corresponding normalized eigenstates $\Psi_i(\varphi)$ satisfy

$$H(\varphi)\Psi_i(\varphi) = E_i(\varphi)\Psi_i(\varphi) .$$
⁽⁵⁾

The quantities $E_i(\varphi)$ and $K_i(\varphi)$ are smooth with respect to φ . We can assume that $\Psi_i(\varphi)$ are real. Then, $\Psi_i(\varphi)$ are determined uniquely by $\Psi_i(0)$. The energy spectrum $\sigma(\varphi) = \{E_i(\varphi) | i \in \mathbb{Z}\}$ with φ being fixed yields a nonuniform WSL. If $i(\in \mathbb{Z})$ is fixed, the relation $E = E_i(\varphi)$ represents a smooth curve on the φ -E plane. It is considered to be a 1D dispersion relation. The dispersion curves for all $i \in \mathbb{Z}$ present a 2D pattern, which we term a 2D Wannier-Stark ladder (2DWSL). Figure 1 shows the 2DWSL for typical values of V, ω , and F.

From $H(\varphi+1)=H(\varphi)$, we obtain $\sigma(\varphi+1)=\sigma(\varphi)$. On the other hand, Eqs. (3) and (4) yield

$$U^{-1}H(\varphi)U = H(\varphi + \omega) + F .$$
(6)

Therefore, $\sigma(\varphi) = \sigma(\varphi + \omega) + F$, and moreover, the eigenstates of $H(\varphi)$ and $H(\varphi + \omega)$ are transformed to each other by U or U^{-1} . Thus we can conclude that the 2DWSL has 2D periodicity represented by the 2D lattice $L = \{nt_1 + mt_2 | n, m \in \mathbb{Z}\}$ with $t_1 = (1,0)$ and $t_2 = (-\omega, F)$. It follows that there exist integers m and $n \ (\in \mathbb{Z})$ such that $E_i(\varphi + 1) = E_{i+m}(\varphi)$ and $E_i(\varphi) = E_{i-n}(\varphi + \omega) + F$ for all $i \in \mathbb{Z}$. In fact, we obtain m = 0 and n = 1, which have been determined by considering the limit case, V = 0. Consequently, $E_1(\varphi + 1) = E_i(\varphi)$ and



FIG. 1. The 2DWSLs in the case (a) F = 0.05, V = 0.4, and (b) F = 0.05, V = 0.8. The ratio ω is fixed to the golden mean ω_G . The 2D lattice in (a) shows periodicity of the 2DWSL. The vertices, the center, and the edge centers of a unit cell are the centers of the inversion symmetry. The 2DWSLs in (a) and (b) are formed basically of three mini 2DWSLs, one of which is indexed by [-1, -2] and the other two by [1,1]. The former mini 2DWSL is derived from the central miniband of the three to which the entire band is divided, while the latter two are derived from the remaining two. The three kinds of dispersions $E_{\nu}^{*}(\varphi)$ in (b) virtually do not interact with one another. They are superpositions of linear terms and undulatory ones.

 $E_i(\varphi) = E_{i-1}(\varphi + \omega) + F$, for all $i \in \mathbb{Z}$. Similarly, we obtain $\Psi_i(\varphi + 1) = \Psi_i(\varphi)$ and $\Psi_i(\varphi) = U\Psi_{i-1}(\varphi + \omega)$. It turns out that

$$E_i(\varphi) = iF + E_0(\varphi + i\omega) , \qquad (7)$$

$$\Psi_i(\varphi) = U^i \Psi_0(\varphi + i\omega) . \tag{8}$$

Since $E_0(\varphi)$ is a periodic function with the unit period, $E_i(\varphi)$, with φ being fixed, is quasiperiodic on *i* by Eq. (7). The energy spectrum $\sigma(\varphi)$ is a vertical section of the 2DWSL, so that its quasiperiodicity is ascribed to incommensurability of the vertical axis with respect to the lattice *L*. This structure of $\sigma(\varphi)$ is similar to that of an incommensurately modulated system.¹⁴ The 2DWSL is completely specified by the single dispersion relation $E_0(\varphi)$ because $E_i(\varphi)$ are its translations. Figure 2 shows $E_0(\varphi)$ for several values of *V* but with ω and *F* being the same as in Fig. 1.

To take \mathbb{R} (or the torus $T^1 \equiv \mathbb{R}/\mathbb{Z}$) as the domain of φ is nothing but the extended (or reduced) zone scheme. Let us consider the mapping $i \in \mathbb{Z} \to (i\omega \mod \mathbb{Z}) \in T^1$. Then the image of \mathbb{Z} is dense on T^1 . Consequently, the functional form of $E_0(\varphi)$ can be completely retrieved from the data $\{E_i(0)|i\in\mathbb{Z}\}$ via the plot of $E_i(0)$ $-iF[=E_0(i\omega)]$ vs $i\omega \mod \mathbb{Z}(\in T^1)$ because $E_0(\varphi)$ is a continuous function. The dispersion curves in Figs. 1 and 2 have been obtained in this way by a numerical calculation on finite but large samples. However, the energy levels which are situated near both ends have been discarded because they have suffered the boundary effect.

The field term F_{op} preserves the inversion symmetry of the modulation potential. We can conclude from this that the space group of the 2DWSL is represented by p2and also that the dispersion relation $E_0(\varphi)$ has the centers of the inversion symmetry at $\varphi=0$ and 1/2.

If the dispersion curves belonging to two different minibands cross, they must interact and, consequently, reconnect so that the crossing is lifted. However, the reconnection virtually cannot be observed in the case where the interaction is very weak. This is usually the case if the two minibands do not immediately neighbor. This effect is similar to the magnetic breakdown in the de Haas-Van Alphen effect.¹⁵ A miniband may be almost isolated on account of the breakdown. We shall consider below the contribution of such a miniband to the 2DWSL.

We assume that the energy levels $E_{\nu}^{*}(\varphi), \nu \in \mathbb{Z}$, derived from an almost isolated miniband, are virtually continuous functions of φ and $E_{\nu}^{*}(\varphi) < E_{\nu+1}^{*}(\varphi)$ for all ν . Then they form a subpattern of the 2DWSL, which is termed a mini 2DWSL. It has the same translational symmetry as that of the original 2DWSL but has not the inversion symmetry, except in the case of a symmetric miniband. Consequently, there exist integers *m* and *n* such that

$$E_{v}^{*}(\varphi+1) = E_{v+m}^{*}(\varphi) , \qquad (9)$$

$$E_{\nu}^{*}(\varphi) = E_{\nu-n}^{*}(\varphi + \omega) + F .$$
 (10)

It follows that

$$E_{\nu}^{*}(\varphi+n-m\omega)=E_{\nu}^{*}(\varphi)+mF. \qquad (11)$$



FIG. 2. The dispersion relation $E_0(\varphi)$ for V=0.1, 0.2, 0.4, 0.6, 0.8, and 1.0, while $\omega = \omega_G$ and F=0.05. It exhibits a number of oscillations in one period and the number increases with V. It has many cusps for large Vs on account of "crossing and reconnection."

Equations (9) and (11) must be consistent with the fact that the average level spacing is equal to $F' \equiv F/\xi$ with ξ being the fraction of the miniband. We can easily show, by using the irrationality of ω and ξ , that this condition is satisfied only when [n,m] indexes the miniband, i.e., $\xi = n - m\omega$. It is interesting that the index of the miniband determines completely the transformation property of $E_{\nu}^{*}(\varphi)$ with respect to the additive group L.

Equation (11) shows that $E_{\nu}^{*}(\varphi)$ is divided into a linear term and the bounded one, $E_{\nu}'(\varphi)$, with respect to the variable φ :

$$E_{\nu}^{*}(\varphi) = m\varphi F' + E_{\nu}'(\varphi) . \qquad (12)$$

The bounded term satisfies $E'_{\nu}(\varphi+\xi)=E'_{\nu}(\varphi)$ and $E'_{\nu}(\varphi)=E'_{\nu-1}(\varphi+\eta)+F'$ with $\eta=p-q\omega$, where p and q are integers satisfying pm-qn=1. We can assume that p/q(=|p|/|q|) is the rational approximant situated next to n/m in the sequence of best approximants to ω . It follows that

$$E'_{\nu}(\varphi) = \nu F' + E'_{0}(\varphi + \nu n) .$$
(13)

The dispersions $E'_{\nu}(\varphi)$ have the same translational symmetry as those of the Harper model with the lattice constant $1/\xi$ and the ratio $\omega' = \eta/\xi [=(p-q\omega)/(n-m\omega)]$, which is a modular transformation of ω . The appearance of a hierarchical structure like this is characteristic of 1D QP systems.^{1,16}

Since the dispersion relation $E = E_v^*(\varphi)$ includes the bias term $m\varphi F'(=m\varphi F/\xi)$ by Eq. (12), it exhibits several crossings (i.e., breakdowns) with those from other mini-

bands when φ is increased by ξ . We may assign the positive (or negative) sign to each crossing if it is down to up (or up to down). Then we can conclude from Eq. (11) that $m = n_{+} - n_{-}$, with n_{+} (or n_{-}) being the number of positive (or negative) crossings.

Equations (12) and (13) show that the average change of $E_v^*(\varphi)$ as a function of φ and v is given by the linear function $\overline{E}_v(\varphi) \equiv (m\varphi + v)F' + C$, with C being the average of $E'_0(\varphi)$. The resulting averaged mini 2DWSL is a linear grid with equal spacings; each grid line is specified by v. The index [n,m] of the miniband agrees with that of the direction $nt_1 + mt_2$ of the grid lines, whose slopes have the same sign as that of m. The grid yields a single closed curve on the 2D torus $T^2 \equiv \mathbb{R}^2/L$. The homology class to which the curve belongs is indexed by n and m. The appearance of such topological numbers may be related to the gauge-field nature of the magnetic field but their physical origin is, as yet, an open question.

The various features described above are identified in the 2DWSLs shown in Fig. 1. Equations (7) and (8) show that the *i*th eigenstate has its own phase, $\phi + i\omega$, which is the local phase of a representative site of the region where the state is localized. That is, the phase variable is a good quantum number to characterize the eigenstates. Most properties of the Harper model under the field do not depend on the choice of φ but they are well understood by considering the 2DWSL which shows the dependence of the energy levels on φ . This is because 2D periodicity is latent in a 1D QP structure.¹⁴

The basic theory developed in the arguments between Eqs. (5) and (8) does not assume V < 1, and applies to the case $V \ge 1$ as well. For the latter case, however, the physical picture behind F and/or V dependence of the 2DWSL awaits further investigation because the miniband picture is not justified.

The Fibonacci lattice is representative of 1D QP systems whose modulation functions take only discrete values.¹ Our preliminary calculation revealed that the dispersion relation $E_0(\varphi)$ of this model has many discontinuities. Therefore, analyticity of $E_0(\varphi)$ depends critically on the modulation potential. This model awaits extensive investigation.

It has recently become known that QP superlattices¹⁷ as well as periodic ones can be manufactured and the WSL has been observed in the case of a periodic superlattice.¹⁸ An observation of the WSL of a QP system may stimulate the search for a novel device because it not only has fascinating features but also a high nonlinearity on the field because of the tunneling effect.

We acknowledge helpful conversations with S. Takagi and K. Satoh. This work was supported by a Grant-in-Aid for Scientific Research on Priority Areas, from the Ministry of Education, Science, and Culture.

- ¹See, for example, J. B. Sokoloff, Phys. Rep. **126**, 189 (1985); H. Hiramoto and M. Kohmoto, Int. J. Mod. Phys. **6**, 281 (1992).
- ²P. G. Harper, Proc. Phys. Soc. London Sect. A 68, 874 (1955).
- ³S. Aubry and G. Andre, Ann. Isr. Phys. Soc. 3, 133 (1980).
- ⁴G. H. Wannier, Rev. Mod. Phys. **34**, 645 (1962).
- ⁵M. Luban and J. H. Luscombe, Phys. Rev. B 34, 3674 (1986).
- ⁶J. F. Weisz and C. Slutzky, Phys. Rev. B **34**, 4162 (1986).
- ⁷J. F. Weisz, Phys. Rev. B **37**, 4781 (1988).
- ⁸Y. J. Kim, J. Phys. A 24, L1339 (1991).
- ⁹C. S. Ryu, G. Y. Oh, and M. H. Lee, J. Phys. Condens. Matter **4**, 6811 (1992).
- ¹⁰M. Fujita and K. Machida, J. Phys. Soc. Jpn. 56, 1470 (1987).
 ¹¹F. H. Claro and G. H. Wannier, Phys. Rev. B 19, 6068 (1979).

- ¹²J. Bellissard, A. Bovier, and J.-M. Ghez, Rev. Math. Phys. 4, 1 (1992).
- ¹³P. N. Argyres, Phys. Rev. **126**, 1386 (1962).
- ¹⁴T. Janssen and A. Janner, Adv. Phys. 36, 519 (1987).
- ¹⁵M. H. Cohen and L. M. Falicov, Phys. Rev. Lett. 7, 231 (1961).
- ¹⁶D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976).
- ¹⁷R. Merlin, K. Bajema, R. Clarke, F.-Y. Juang, and P. K. Bhattacharya, Phys. Rev. Lett. 55, 1768 (1985).
- ¹⁸E. E. Mendez, in *Proceedings of the Twentieth International Conference on the Physics of Semiconductors* (World Scientific, Singapore, 1992), p. 1206 and references therein.