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Quantum adiabatic particle transport

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The problem of quantized adiabatic particle transport is studied for three classes of one-dimensional periodic potentials. In cases of periodically modulated potentials, the electron transport (in full bands) induced by the propagating modulation wave is shown to be given by a Diophantine equation. Some analytic results are also obtained for a potential consisting of a moving and a standing part. The results are mainly derived under various approximations, but they are expected to be valid in a wider range of situations due to the topological nature of the problem.

I. INTRODUCTION

Consider a one-dimensional electron system in a periodic potential. If the potential varies slowly and periodically in time, what will be the electron current in response to this variation? According to Thouless,[1] the electron transport, i.e., the time integral of the electron current in a period of time, has to be an integer, if the Fermi energy lies in a gap of the spectrum of the instantaneous Hamiltonian.

A direct generalization of this already quite general result (in respect to the detailed shape of the periodic potential) can be made to higher-dimensional systems, in which the potential is periodic in one direction and the electrons are confined in the perpendicular directions. This result allows one to apply the idea of the quantum adiabatic particle transport (QAPT) to the problem of quantum Hall effect of a two-dimensional electron gas in both a periodic potential and a perpendicular magnetic field.[2] In this application, one evaluates the Hall current in the moving frame in which the electric field is transformed away and and the potential translates at a velocity of $\mathbf{E}\times\mathbf{B}/B^2$.

Yet, there is another important generalization of the result, which makes the idea of QAPT applicable to more realistic systems. It has been shown by the author and Thouless[2] that the electron transport induced by a slow and periodic variation of Hamiltonian is still quantized, in the case that both disorder and many-body interactions are present. One condition needed in order for this to be true is that the ground state of the many-electron system is separated from the other states by an energy gap or a mobility gap, which does not close when the Hamiltonian varies. Another condition is that one can take the thermodynamic limit. This limit is necessary for the quantization, since there are examples of finite systems exhibiting nonintegral particle transport even in the absence of disorder and many-body interactions, as illustrated by Thouless in his original paper. The condition needed in order for a system to be large and close to the thermodynamic limit is that the gap in which the Fermi energy lies does not close up as the limit is taken. The correction to the quantization due to the finiteness of a "large" system is exponentially small, with the exponent being the size of the system divided by the electron-electron correlation length in the ground state.

The notion of QAPT is not restricted to systems described by a nonrelativistic Schrödinger equation. One can consider other quantum Hamiltonian systems in which a continuity equation for the probability density and current can be defined. Some examples in relativistic field theory have been studied by Zee.[3] Amusingly enough, even a discrete Schrödinger equation can be applied with the idea of QAPT.[4] Thus, it is appropriate to say that the quantum numbers of the QAPT should be useful in classifying the spectral structures of a class of quantum-mechanical and mathematical systems.

The present paper is to work out some concrete examples, and to find out the actual values of the integers for the QAPT. Analytic results in the nearly-free-electron (NFE) limit and the tight-binding (TB) limit will be given. For simplicity, many-body interactions and disorder will be ignored, and only the case of one-dimensional electron gas in a periodic potential will be considered. Because of the discrete nature of the QAPT, the results should be valid in a wider domain beyond the limits and the assumptions mentioned above.

In Sec. II, Thouless's theory for the QAPT is reviewed, some of the techniques for evaluating the integers of the QAPT are summarized. In the subsequent sections the following cases are studied: (1) a linear super position of two periodic potentials, one of which stands still, while the other translates in space (Sec. III); (2) an amplitude modulated atomic potential array, with the modulating wave propagating in space (Sec. IV); (3) a propagating sound wave, in which the ions oscillate coherently (Sec. V). Finally, a summary and discussion of the results is given in Sec. VI.

II. THEORETICAL BACKGROUND

Since only the simpler case of 1D periodic potentials will be considered in this article, the original theory of Thouless[1] about the QAPT should be sufficient to provide for a theoretical and calculational basis. Here we give a brief description of his basic results, leaving the details to the reference.

Suppose the electrons are described by the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi=\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi+V(x,t)\psi\ , \tag{1}$$

where the potential varies slowly and periodically in time. In the adiabatic limit, the electronic states can be described in terms of the eigenstates of the instantaneous Hamiltonian $H(t)$. These eigenstates are the Bloch waves, assuming $V(x,t)$ is periodic in x. Suppose the temperature is zero, and the Fermi energy initially lies in a gap (which is hereafter referred as the Fermi gap) between the Bloch bands of $H(0)$. If this gap does not close up as $H(t)$ varies in time, the filled bands will remain filled and the empty bands remain empty, according to the adiabatic theorem.[5] We are interested in the net number of electrons transported across a section, during a period of time that the potential restores back to its initial form. The electron transport is not necessarily zero, because in the case of a slowly sliding potential the electrons simply follow the potential according to the Galilean principle. Also, the electron transport is not always simply determined this way, because one can think of more complicated motion of the potential, in which case the Galilean principle is of no use.

The general method of finding the electron transport is to find the current at any giving time. In the zeroth-order adiabatic approximation, the current is zero because the electrons are in full bands. In the first-order approximation, the filled states are coupled to the empty states, giving rise to a current that is of the same order as the changing rate of the potential divided by the size of the energy gap. When this small current is integrated over a period T (which is long), one obtains a transport of order unity. The transport from higher-order approximations should vanish in the adiabatic limit.

Using this approach Thouless[1] derived a very compact formula for the adiabatic electron transport as

$$C=\sum_{\lambda}\int_0^T dt\frac{1}{2\pi i}\int_0^{2\pi/a}dk\left[\left\langle\frac{\partial\psi_\lambda}{\partial k}\middle|\frac{\partial\psi_\lambda}{\partial t}\right\rangle-\left\langle\frac{\partial\psi_\lambda}{\partial t}\middle|\frac{\partial\psi_\lambda}{\partial k}\right\rangle\right], \tag{2}$$

where ψ_λ, as a function of the wave number k and time t, is the normalized Bloch wave function in the λth band of the instantaneous Hamiltonian. In this formula the phase of ψ_λ is chosen such that ψ_λ is a single-valued smooth function of (t,k) in the two-dimensional region $(0\le t<T;\ 0\le k<2\pi/a)$.

Remark 1. As argued by Thouless, the integral in (2) represents the phase change of ψ_λ around the perimeter of the region of integration, giving rise to an integer value of the electron transport. This can be shown by using the Stoke's theorem and by using the fact that ψ_λ is periodic in t and in k up to phase factors that depend on (t,k) but not on x. The phase change of a state due to an adiabatic and periodic variation of the Hamiltonian is known as the Berry phase.[6]

Remark 2. The formula is invariant as ψ_λ is multiplied by a phase factor depending smoothly on (t,k). From the point of view of differential geometry, the formula actually defines the first Chern class of a $U(1)$ principal fiber bundle on a torus.[7] The fibers are the Bloch waves and the torus corresponds to the region $(0\le t<T;\ 0\le k<2\pi/a)$ with the opposite boundary points regarded as the same. For a detailed description, see Ref. 8.

Remark 3. For a periodic potential the number of states per period with energies below a gap is known to be quantized as integers. For an almost periodic potential there is a generalization of this result known as the gap-labeling theorem.[9] The QAPT provides a new set of quantum numbers labeling the gaps. It is, however, the advantage of the QAPT that it is stable against the perturbation of disorder and many-body interactions.[2]

The QAPT as a topological invariant has a very rich physical content. From the Green-function representation as given in the original work of Thouless, the electron transport should be a continuous functional of the potential $V(x,t)$ unless the Fermi gap closes. On the other hand, the QAPT only takes discrete values. Therefore it must stay as a constant for a continuous range of the potential function. This property immediately leads to a powerful way of evaluating the integer of the QAPT for a given Fermi gap. If one can continuously turn off a part of the potential without ever closing the Fermi gap, then one can evaluate the integer just by dealing with the remaining part. This often simplifies the calculation. On the other hand, one can set up theoretical models, the integers found from them should be significant for a wider range of physical situations. The examples studied in this article will be analysed in the NFE and TB limits. Since the energy gaps involved are often infinitesimal, the results seem to be valid only in the formal sense of taking the adiabatic limit first then the other limit second. Yet, from the topological nature of the QAPT, the results found in the limits should be meaningful for a class of finite potentials, for which the gaps are finite and the criterion for the adiabatic approximation can be lower.

For a systematic evaluation of the QAPT for an arbitrary periodic potential, one can use a more transparent formula then (2). Suppose one has a solution of the equation

$$H\psi=E_F\psi,\ \text{where } E_F \text{ is the Fermi energy}\ , \tag{3}$$

with ψ damping to the right. Thouless has shown that the electron transport is equal to the number of node points of ψ that moves to the right of a reference point (say $x=x_0$) as t increases by a period. In other words, the electron transport is simply given by

$$-\sum_i \operatorname{sgn}\left[\frac{\partial\psi}{\partial T}\frac{\partial\psi}{\partial x_0}\right]_{t=t_i}, \tag{4}$$

where the summation is over the zeros of $\psi(x_0)$ as a function of t in a period. This method greatly simplifies the calculation, and will be used for the numerical evaluations in the examples studied in this paper.

III. TWO COMPONENT POTENTIALS

The periodic potentials considered in this section are of the form

$$V_1(x)+V_2\left[x-\frac{t}{T}l\right], \tag{5}$$

where V_1 and V_2 have a spatial periodicity l. A particular simple case is

$$A_1\cos\left[\frac{2\pi}{l}x+\theta_1\right]+A_2\cos\left[\frac{2\pi}{l}x-\frac{2\pi t}{T}+\theta_2\right], \tag{6}$$

where A_i,θ_i $(i=1,2)$ are independent of t. We can also write (6) as

$$R(t)\cos\left[\frac{2\pi}{l}x-\Phi(t)\right] \tag{7}$$

with

$$R(t)e^{-i\Phi(t)}=A_1e^{i\theta_1}+A_2e^{-i\theta_2}e^{-2i\pi t/T}. \tag{8}$$

The eigenvalue equation with (7) as the potential is the so-called Matheiu's equation. A necessary and sufficient condition for all the energy gaps to be open is that $R(t)>0$.[10] This is guaranteed if $|A_1|\neq|A_2|$. Now if $|A_1|>|A_2|$, we can continuously turn off A_2 without closing the energy gaps. The QAPT in case of $|A_1|>|A_2|>0$ must be identical to that in case of $A_2=0$, according to the topological property of the QAPT. On the other hand, if $|A_1|<|A_2|$, the QAPT can be identically determined in the limit $A_1=0$. In brief, the electrons in filled bands are locked into the stronger part of the potential.

Another simple case of (5) is the potential

$$A_1\sum_n\delta(x-nl)+A_2\sum_n\delta\left[x-nl-\frac{t}{T}l\right]. \tag{9}$$

In a transfer matrix approach, the energy spectrum can be found from the function

$$\begin{aligned}\mathrm{tr}M=&2\cos(kl)\\&+\frac{2m(A_1+A_2)}{\hbar^2K}\sin(kl)\\&+\left[\frac{2m}{\hbar^2k}\right]^2A_1A_2\sin\left[k\frac{t}{T}l\right]\sin\left[kl\left[1-\frac{t}{T}\right]\right],\end{aligned} \tag{10}$$

where $k=(2mE/\hbar^2)^{1/2}$, and M is the transfer matrix through a period. The energy gaps are given for those values of k for which $|\mathrm{tr}M|>2$. At $kl=n\pi>0$, we have

$$\mathrm{tr}M=(-1)^n\left[2-\left[\frac{2m}{\hbar^2k}\right]^2A_1A_2\sin^2\left[kl\frac{t}{T}\right]\right]. \tag{11}$$

For $A_1A_2<0$, $k=n\pi/l>0$ lies in a gap if $t/T\neq m/n$ ($m=$integer). When $t/T=m/n$, $k=n\pi/l$ is at a band edge. The gap bounded by this edge is closed only when

$$\left.\frac{\partial(\mathrm{tr}M)}{\partial k}\right|_{kl=n\pi,t/T=m/n}=(-1)^nl\left[\frac{2m(A_1+A_2)}{\hbar^2k}\right]=0 \tag{12}$$

which is impossible if $A_1+A_2\neq0$. Thus, for $A_1A_2<0$ and $|A_1|\neq|A_2|$, the energy gap close to $k=n\pi/l>0$ is open for all time t. The QAPT in this case can be simply obtained in the limit $A_1=0$ ($A_2=0$) if $|A_1|<|A_2|$ ($|A_2|<|A_1|$).

For other cases of the parameters, exact analytical results are difficult to obtain, and numerical methods are necessary.

In the limit of a weak potential of the form in (5), we can use the NFE approximation. To the first order of the perturbation, the size of the nth gap in the spectrum is determined by

$$\begin{aligned}&\Delta_n(t)\equiv A_n+B_ne^{-2i\pi nt/T},\\&A_n\equiv\int_0^l dx\,V_1(x)e^{-2i\pi nx/l},\\&B_n\equiv\int_0^l dx\,V_2(x)e^{-2i\pi nx/l}.\end{aligned} \tag{13}$$

If $|A_n|\neq|B_n|$, the gap remains open for all t. Suppose the Fermi energy lies in this gap, then we can continuously turn off the other Fourier components of the potential (5) without changing the value of the electron transport. The remaining part has the form

$$(A_n+B_ne^{-2i\pi nt/T})e^{2i\pi nx/l}+\text{c.c.} \tag{14}$$

Using the arguments for the case of the potential (6), we can conclude that the electrons filling the bands below the nth gap are locked into the potential V_1 (or V_2) if $|A_n|>|B_n|$ ($|A_n|<|B_n|$). This conclusion should be valid if we are not very far from the weak-potential limit. Far beyond this limit, the conclusion has to be modified. We have worked out an example in which V_1 is a square wave and V_2 an array of δ potentials. The result indicates that the sharper potential appears stronger than its Fourier components suggest, at least for the lower-order gaps. But the discrepancy vanishes quickly as the potentials get weaker.

A particularly interesting question is the following. Will all the electrons follow the stronger potential, if $V_1(x)$ and $V_2(x)$ have the same functional form but with different amplitudes? Here the "strengths" are measured in terms of the absolute values of the amplitudes. We suspect that this is true in the generic case, according to the Wigner–von Neuman theorem.[11] The theorem says that in general we need to vary three parameters in the potential in order to close a gap. Now, we have only two relevant parameters: the relative amplitude and position of the two potentials. Thus we expect a gap not to be closed as we vary the two parameters, except when the relative amplitude becomes ±1, where the total potential can double its period or vanish altogether at certain relative positions.

IV. AMPLITUDE MODULATED POTENTIAL

The potential considered in this section is of the form

$$\sum_n \left[A + B\cos\left[\frac{2\pi q}{p} n - \frac{t}{T} 2\pi \right] \right] V(x - na) , \tag{15}$$

where $V(x)$ is the atomic potential centered at the origin. The total potential has a periodicity of Pa.

Let us consider the weak potential limit first. In the NFE approximation, the gaps are determined by the Fourier components of (15):

$$U_m = \int_0^{pa} dx \sum_n \left[A + B\cos\left[\frac{2\pi q}{p} n - \frac{t}{T} 2\pi \right] \right] \times V(x - na) e^{-2\pi i m x/pa}$$

$$= pV_m \sum_l \left[A\delta_{m,lp} + \frac{B}{2} e^{-2\pi i t/T} \delta_{m,lp+q} + \frac{B}{2} e^{2\pi i t/T} \delta_{m,lp-q} \right] , \tag{16}$$

where

$$V_m = \int_{-\infty}^{\infty} dx\, V(x) e^{-2\pi i m x/pa} . \tag{17}$$

Energy gaps are opened up by the coupling between the degenerate states $k = r\pi/pa$ and $k = -r\pi/pa$, with r being a positive integer. For $r = lp$, $lp + q$, or $lp - q$, the pair of degenerate states are coupled directly by AV_r, $(B/2)V_r e^{-2\pi i t/T}$, or $(B/2)V_r e^{2\pi i t/T}$, respectively. For other values of r, they are coupled indirectly through the intermediate states. The gap size is predominantly determined by the couplings which involve a minimum number of intermediate states.

It is proved in Appendix A that the dominant coupling between the states $k = r\pi/pa$ and $k = -r\pi/pa$, with $r \neq lp$, involves totally $|S_r|$ steps of the lengths $[lp + \mathrm{sgn}(S_r)q,\ l = \text{integer}]$ measured in units of $2\pi/pa$ in the Fourier space, where S_r is the solution of the Diophantian equation

$$S_r q + t_r p = r , \tag{18}$$

with $|S_r|$ as small as possible.

In the $|S_r|$th degenerate perturbation theory, the effective Hamiltonian (see Appendix B) in the space of the states $k = r\pi/pa$ and $k = -r\pi/pa$ has the form

$$\begin{bmatrix} U_r & \Delta_r \\ \Delta_r^* & U_r \end{bmatrix} , \tag{19}$$

where Δ_r has a time-dependent phase factor of $e^{-i2\pi S_r t/T}$. Then it can be shown that as we increase k by $2\pi/pa$, the wave function of the rth band will pick up a phase $2\pi S_r t/T$ from the rth gap, and a phase $-2\pi S_{r-1} t/T$ from the $(r-1)$ the gap. The total phase change of the wave function around the perimeter of tk space ($0 \le t < T$, $0 < k < 2\pi/pa$) is given by $(S_r - S_{r-1})2\pi$, yielding an electron transport

$$C_r = S_r - S_{r-1} . \tag{20}$$

When $r = lp$, the states $k = r\pi/pa$ and $k = -r\pi/pa$ are coupled directly by the time-independent term AV_r. The final result (20) is still valid, with S_r given by (18). Another comment for the case of $p =$ even is the following. In this case, with $r = p/2$, the equation (18) does not have a unique solution by demanding $|S_r|$ as small as possible. In fact, the energy gap closes at $t = T/2$.

Now consider the tight-binding limit of the potential (15), for which the level spacing in the atomic potential $V(x)$ is much larger than the coupling between the states in neighboring atomic potentials. For simplicity, we assume $A = 1$ and $B \ll 1$. The wave function in the periodic potential (15) can be written as

$$\psi(x) = \sum_n f_n \phi(x - nl) , \tag{21}$$

where $\phi(x)$ is an eigenenergy state (say, with energy ϵ_0) in the atomic potential $V(x)$. The coefficients f_n are determined by

$$\Delta(f_{n+1} + f_{n-1}) + \epsilon_0 \left[1 + B\cos\left[\frac{2\pi q}{p} n - \frac{2\pi t}{T} \right] \right] f_n = E f_n . \tag{22}$$

This is the Harper's equation, extensively studied in the context of a 2D-electron gas in a periodic potential and a uniform perpendicular magnetic field. The union $U_{0<t<T}\sigma(t)$ of the energy spectrum $\sigma(t)$ of the equation (22) has been calculated by Hofstadte[12] for $\Delta = \epsilon_0 B$, and for every fraction q/p with p less than or equal to 50. The union spectrum consists of p bands separated by energy gaps, except for p even where the central two bands touch each other at the center. As q/p approaches a irrational number, the spectrum becomes as a Cantor set.[13]

The equation (22) is invariant under the translation $n \to n + p$, so we can write f_n as Bloch waves:

$$g_n(k,t) e^{ikan},\quad 0 \le k < \frac{2\pi}{pa} . \tag{23}$$

The electron transport of the rth band is given by the phase change of $\psi(x)$ in (21), or equivalently $g_n(k,t)$ in (23), when (t,k) travels around the perimeter of the region $0 \le t < T$, $0 \le k < 2\pi/pa$. According to the work of Thouless *et al.*,[14] the phase change of $g_n(k,t)$ in the rth band is given by $2\pi(S_r - S_{r-1})$, where

$$S_r q + t_r p = r \tag{24}$$

taking the solution of smallest $|S_r|$.

Thus, the electron transport for filled bands in the tight-binding limit is exactly the same as in the near-free electron limit. It is likely that the energy gaps keep open, as the system varies continuously from one limit to the other.

Equation (22) can also be understood as the instantaneous eigenvalue problem corresponding to the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}f_n=\Delta(f_{n+1}+f_{n-1})+\varepsilon_0\left[1+B\cos\left[\frac{2\pi q}{p}n-\frac{t}{T}2\pi\right]\right]f_n\ . \tag{25}$$

If one defines $|f_n|^2$ as the probability for a particle to be at the site n, then the operator for the jumping rate from site n to site $n+1$, is given by

$$\frac{1}{i\hbar}[n,H]=-\frac{2\Delta}{i\hbar}\sin\left[-i\frac{\partial}{\partial n}\right]\ . \tag{26}$$

One can then ask what will be the particle transport for a filled band when t adiabatically increases by a period T. Following an argument parallel to that of Thouless,[1] one can show that the transport is exactly given by the phase change (divided by 2π) of the Bloch function around the perimeter of the (t,k) unit cell. This is an example of a general quantum-mechanical Hamiltonian system, to which the notion of the QAPT is applicable.

V. SOUND WAVE

In this section, we consider an array of atomic potentials, whose centers oscillate coherently as in a propagating sound wave.

$$U(x)=\sum_n V(x-x_n)\ ,\qquad X_n=na+b\cos\left[\frac{2\pi q}{p}n-\frac{t}{T}2\pi\right]\ . \tag{27}$$

If $b=0$, the potential has a periodicity of "a," and the spectrum consists of Bloch bands. When $b\neq 0$, the period becomes pa, and each Bloch band splits into p subbands.

In the NFE approximation, the size of the gaps are determined by the Fourier components of $U(x)$,

$$U_m=\frac{1}{pa}\int_0^{pa}dx\,U(x)e^{-2\pi imx/pa}=V_m\sum_{n=1}^{p}\exp\left\{-i\frac{2\pi m}{pa}\left[na-b\cos\left[\frac{2\pi q}{p}n-\frac{t}{T}2\pi\right]\right]\right\}, \tag{28}$$

$$V_m=\frac{1}{pa}\int_{-\infty}^{\infty}dx\,V(x)e^{-2\pi imx/pa}\ . \tag{29}$$

The potential responsible to the rth gap is given by

$$R_r(t)\cos\left[\frac{2\pi r}{pa}x-\Phi_r(t)\right], \tag{30}$$

where

$$R_r(t)e^{-i\Phi_r(t)}=V_r\sum_{n=1}^{P}\exp\left\{-i\frac{2\pi r}{Pa}\left[na+b\cos\left[\frac{2\pi q}{P}n-\frac{2\pi t}{T}\right]\right]\right\}. \tag{31a}$$

Using Poisson's summation formula and the integral representation of Bessel's function, the last expression can be written as

$$R_r(t)e^{-i\Phi_r(t)}=V_r\sum_{S_r}e^{-2\pi iS_rt/T}(-i)^{S_r}J_{S_r}(2\pi rb/pa)\ , \tag{31b}$$

where S_r satisfies the Diophantine equation

$$S_rq+Ip=r\ . \tag{32}$$

For $|2\pi rb/pa|$ small, the summation on the right-hand side of (31b) is dominated by the term with smallest possible $|S_r|$. Therefore the electron transport carried by the lowest r bands should be the solution S_r of (32) with smallest possible absolute value. This result is confirmed by a number of numerical evaluations of (31a), with $|b/a|\leq 0.2$ and $r\leq p$.

The tight-binding limit is investigated for

$$V(x)=\gamma\delta(x)\ . \tag{33}$$

The energy spectrum in the potential (27) with this form of the atomic potential has been studied by Azbel,[15] and de Lange and Janssen.[16]

In the limit $2m\gamma a/\hbar^2=+\infty$, the states are localized in the intervals bounded by neighboring δ potentials. In the interval between X_n and X_{n+1}, the energy levels are given by

$$E_{n,l}=\frac{\hbar^2}{2m}\left[\frac{\pi l}{d_n}\right]^2,\quad l=1,2\ldots, \tag{34}$$

where

$$d_n=X_{n+1}-X_n=a-2b\sin\frac{\pi q}{p}\sin\left[\frac{\pi q}{P}(2n+1)-\frac{2\pi t}{T}\right]. \tag{35}$$

The levels $\{E_{n+Np,l},\ N=0,\pm1,\ldots\}$ are degenerate. If $2m\gamma a/\hbar^2$ is finite but $\gg 1$, these levels (for a given n and l) are broadened into a narrow band. The width of the band is of order $(2m\gamma a/\hbar^2)^{-p}$, since the degenerate levels are coupled through p successive δ barriers. The wave functions in this band are strongly peaked in the intervals $\{n+Np,\ N=0,\pm1,\ldots\}$. This picture is of course correct only when $E_{n,l}$ is far from all the other levels $E_{n',l'}$ with $n'\neq n$ (mod p) compared with the coupling strength a/γ through a δ potential. As t varies, level crossing can happen. As a result of resonant tunneling, an energy gap is generated at the crossing point. Suppose the level $E_{n,l}$ crosses with the level $E_{n'+N'p,l}$ with $n'\neq n$ (mod p). The energy gap generated at the crossing point is of order $(2m\gamma a/\hbar^2)^{-S}$, where

$$S=\min_{N'=0,\pm1,\ldots}\{|n'+N'p-n|\}\ . \tag{36}$$

This rule comes from the fact that the dominant tunneling takes place through the least possible number of barriers. Clearly $s<p$, so the states originally in the narrow band centered at $E_{n,l}$ go into the narrow band centered at $E_{n',l'}$ after the crossing. The electrons originally in the in-

tervals $\{n+Np,\ N=0,\pm1,\ldots\}$ then jumps into the intervals $\{n'+N'p,\ N'=0,\pm1,\ldots\}$. The number of intervals that an electron jumps is given by

$$n'+N'p-n\ , \tag{37}$$

where N' is determined by the minimizing condition (36). The sign of this number tells the direction of jumping: positive for the right, negative for the left.

Suppose one wants to know the electron transport carried by the narrow band centered at $E_{n,l}$ at $t=0$. When t increases by a period T, several level crossings may happen in succession. Through each crossing point, one can determine a number as in (37). The net number of intervals that an electron jumps is the sum of these numbers. The sum should be of the form $C\cdot p$ ($C=$integer), since the energy levels vary periodically with t; an electron eventually must be in the same level as it was originally in. The number C is the electron transport carried by the narrow band one concerns.

A simple and clean result can be obtained if $|b|$ is smaller than $a/2$ such that the coupling between states with different l can be neglected. Consider the rth band in the lth cluster of subbands. One can show that the electron transport carried by this band is S_r-S_{r-1}, where S_r is given by

$$S_r q+t_r p=r \tag{38}$$

demanding $|S_r|$ as small as possible.

Exact numerical calculations based on the formula (4) have been carried out for the case $b/a=0.2$ and $2mVa/\hbar^2=1.5$, with $r\le p$ and with $p\le 7$. The results agree with the theoretical predictions (32) or (38). Several numerical calculations are also made for the case with $b/a=0.5$ and $2mVa/\hbar^2=4.7$. The Diophantine equation (38) is still satisfied by the electron transports, but the minimizing condition on $|S_r|$ is sometimes violated. For instance, when $q=1$ and $p=3$, we found that $S_2=2$ instead of -1.

VI. CONCLUSION AND DISCUSSION

The quantum adiabatic particle transport originally proposed and formulated by Thouless[1] is studied for three classes of 1D periodic potentials. In the two component potential case, the electrons in full bands tend to be locked in the part of the potential whose Fourier component corresponding to the Fermi gap is larger in absolute value. This conclusion is obtained in the NFE approximation, and is shown to be exact for the sinusoidal potential and for the potential consisting of two δ potential arrays with different signs of the amplitudes. Possible deviations from this simple result have also been pointed out.

In the cases of periodically modulated (in amplitude or position) potentials, analytical results are obtained in both the NFE approximation and in the TB approximation. The electron transports are quantized and are simply determined by a Diophantine equation under suitable constraint. Such a Diophantine equation was first found by Wannier[17] who used it to classify the energy gaps of the Harper's equation. In the context of quantum Hall effect on a two-dimensional periodic potential, the integer of the Hall conductance is found to be described by such an equation.[14,18,19] Since the Hall conductance can be evaluated in the moving frame in which the electric field becomes zero, it is intimately related to the electron transport induced by the moving potential in this frame. In fact, both the Hall conductance and the electron transport enter into the Diophantine equation, and are dual to each other in some sense.[4,19]

From the topological nature of the QAPT, the results obtained in various approximations should be valid in wider situations, where the energy gaps are finite, and the condition for the adiabatic approximation can be relatively easily fulfilled. Again, from the topological nature of the QAPT, the results should be significant for other systems which are close to the models studied here. Also, the presence of weak disorder and weak electron-electron interactions should not worry us very much, according to the work of Niu and Thouless.[2]

Can the process of adiabatic electron transport be realized in physical experiments? This may be possible but is difficult. One method that immediately came to mind is to send a coherent sound wave in a quasi-one-dimensional system and to measure the induced electron current. For this to be observable, the wavelength has to be as short as the Fermi wavelength of the electrons. Also, the amplitude should be large enough to generate a gap at the Fermi energy, and the size of the gap should be large compared with the wave frequency, in order for the adiabatic approximations to be valid.

For most quasi-one-dimensional metals, a Peierls gap already exists at low enough temperatures.[20] One may try to send in a sound wave to drive the CDW in motion. If this can be realized, then one has a nonelectrical means to obtain electron currents.

In CDW transport experiments, the driving force is usually an external electric field. One may observe the phonon spectrum in company with the CDW motion. The relation between the phonon spectrum and the electron current might be akin to that in an imaginary process in which the traveling coherent phonon wave drives the electron current.

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APPENDIX A: FORM OF THE DOMINANT COUPLING

Suppose the coupling between the degenerate states $k=r\pi/pa$ and $k=-r\pi/pa$ is achieved by a_l steps of length $lp+q$, b_l steps of length $lp-q$, and c_l steps of length lp. The lengths here are measured in units of $2\pi/pa$ in the Fourier space. The set of numbers $\{a_l,b_l,c_l\}$

has to satisfy the equation

$$\sum_{l=-\infty}^{\infty}[a_l(lp+q)+b_l(lp-q)+c_l lp]=r\ , \tag{A1}$$

and the requirements

$$a_l\geq 0,\quad b_l\geq 0,\quad \text{and } c_l\geq 0\ . \tag{A2}$$

We want to minimize the total number of steps

$$\sum_l (a_l+b_l+c_l)\ , \tag{A3}$$

in order to find the dominant couplings.

First, consider the case

$$\sum_l a_l>\sum_l b_l\ . \tag{A4}$$

If $\sum_l b_l>0$, we can pick up a pair of integers (i,j), such that $a_i>0$, and $b_j>0$. We can reduce (A3) by the replacements

$$\begin{aligned} &a_i\rightarrow a_i-1\ ,\\ &b_j\rightarrow b_j-1\ ,\\ &c_{i+j}\rightarrow c_{i+j}+1\ , \end{aligned} \tag{A5}$$

without dissatisfying (A1) and (A2). We can continue this process until all the b_l's become zero. In all the processes (A3) are reduced, so the minimizing solutions must be contained in the following equations:

$$\begin{aligned} &b_l=0\ ,\\ &\sum_l[a_l(lp+q)+c_l(lp)]=r\ , \end{aligned} \tag{A6}$$

where $\sum_l a_l>0$ because of (A4). Suppose $\sum_l c_l>0$, we can again pick up a pair of integers (i,j), such that $a_i>0$, $c_j>0$. (A3) is reduced under the replacements

$$\begin{aligned} &a_i\rightarrow a_i-1\ ,\\ &c_j\rightarrow c_j-1\ ,\\ &a_{i+j}\rightarrow a_{i+j}+1\ . \end{aligned} \tag{A7}$$

Since $\sum_l a_l$ is not changed in the above modifications, we can continue the process until all the c_l's become zero. Thus, the minimizing solutions must be in the form

$$\begin{aligned} &b_l=0\ ,\\ &c_l=0\ ,\\ &\sum_l a_l(lp+q)=r\ . \end{aligned} \tag{A8}$$

The quantity (A3) can be further reduced if we set

$$\sum_l a_l=S_r,\quad \sum_l l a_l=t_r\ , \tag{A9}$$

where S_r is the smallest positive integer of the solution of the equation

$$S_r q+t_r p=r\ . \tag{A10}$$

The equations in (A9) can be satisfied for any S_r and t_r; one solution is

$$a_0=S_r-1,\quad a_t=1\ . \tag{A11}$$

It should be clear now that the best solutions under the constraint (A4) are given by (A8)–(A10).

The best solutions in the other case, i.e.,

$$\sum_l b_l>\sum_l a_l \tag{A12}$$

can also be found in a similar way. The result is

$$\begin{aligned} &a_l=c_l=0\ ,\\ &\sum_l b_l=S_r',\quad \sum_l l b_l=t_l'\ ,\\ &-S_r' q+t_r' p=r\ , \end{aligned} \tag{A13}$$

where S_r' takes the smallest positive integer value.

For $r\neq lp$, (A4) and (A12) include all the possible cases. Summarizing the results, we obtain the conclusion in the text [see Eq. (18) and the statements above and below it].

APPENDIX B: DEGENERATE PERTURBATIONS

Because the states which couple to the degenerate pair $(k=r\pi/pa,-r\pi/pa)$ are separated from them by at least an energy $(\hbar^2/2m)(2\pi/ap)^2$, degenerate perturbation theory is applicable if the couplings are small compared with this energy.

Consider the eigenvalue equation

$$(E-H_0)\,|\psi\rangle=H_1\,|\psi\rangle\ , \tag{B1}$$

where H_1 is the perturbation to H_0. Define Q as the projection operator onto the manifold of the degenerate levels, and $P=1-Q$ as the projection off these levels. From (B1), we have

$$P\,|\psi\rangle=\frac{1}{E-H_0}PH_1\,|\psi\rangle\equiv M\,|\psi\rangle\ . \tag{B2}$$

If we write

$$|\psi\rangle=|\psi_0\rangle+P\,|\psi\rangle\ . \tag{B3}$$

where $|\psi_0\rangle$ is in the degenerate space, then

$$|\psi\rangle=|\psi_0\rangle+M\,|\psi_0\rangle+M^2\,|\psi_0\rangle+\cdots\ . \tag{B4}$$

Also from (2) we have

$$(E-H_0)\,|\psi\rangle=H_1\,|\psi_0\rangle+H_1M\,|\psi_0\rangle+H_1M^2\,|\psi_0\rangle+\cdots\ . \tag{B5}$$

Acting Q on both sides, we obtain

$$(E-H_0)\,|\psi_0\rangle=(QH_1+QH_1M+QH_1M^2+\cdots)\,|\psi_0\rangle\ . \tag{B6}$$

The effective Hamiltonian in the space of degenerate levels is given by

$$H_{\text{eff}}=H_0+QH_1Q+QH_1MQ+QH_1M^2Q+\cdots\ . \tag{B7}$$

This is a generalized version of the Brillouin-Wigner perturbation expansion. If the term after the $(n+1)$th are cut off, one is taking an nth-order degenerate perturbation.

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