PHYSICAL REVIEW B VOLUME 27, NUMBER 10 15 MAY 1983

Quantization of particle transport

D. J. Thouless
Department of Physics, FM-15, University of Washington, Seattle, Washington 98195
(Received 4 February 1983)

The integrated particle current produced by a slow periodic variation of the potential of a Schrödinger equation is evaluated. It is shown that in a finite torus the integral of the current over a period can vary continuously, but in an infinite periodic system with full bands it must have an integer value. This quantization of particle transport is used to classify the energy gaps in a one-dimensional system with competing or incommensurate periods. It is also used to rederive Prange's results for the fractional charge of a soliton.

I. INTRODUCTION

In this paper the effect of an adiabatic change of the potential on an electron or a system of electrons is considered. The question that is posed is "If the potential is changed slowly in such a way that it returns to its starting value in time T, is the integrated current of electrons across a boundary quantized?" This question, which is formulated in Sec. II, is answered negatively for electrons in a finite torus in Sec. III. In Sec. IV it is shown that for electrons in filled bands in an infinite periodic system the particle transport is quantized. This result is closely related to our earlier work on the quantized Hall effect in a periodic potential.[1] The result may be applicable to problems of sliding charge-density waves in a solid, but that application is not considered here. In Sec. V the result is used to classify the gaps in a system with competing or incommensurate periodicities. In Sec. VI the problem of one-dimensional solitons is considered.[2,3] It is shown how the quantization of charge transport leads to Prange's theorem for soliton charge.[4]

II. ADIABATIC TRANSPORT BY A POTENTIAL

In this paper the motion of particles which satisfy the Schrödinger equation with a slowly varying time-dependent potential $V(\vec{r},t)$ is considered. The potential is taken to be periodic both in time t with period T and in one of the space variables x with period L. For example, we could consider a potential of the form

$$V(\vec{r},t)=V_0(\vec{r})+V_1(x-vt,y,z)\ , \tag{2.1}$$

where V_0 and V_1 have the common period L and v is small. In this case L/v must be a multiple of T. The particle current integrated over the period T gives the total number of particles transported in a period.

Two versions of the problem are examined. In the first case the system is supposed to have periodic boundary conditions in x, so that the solutions satisfy

$$\psi(x+L,y,z)=\psi(x,y,z) \tag{2.2}$$

for all times, while in the second case the system is taken to be infinite in x. In both cases the potential is taken to confine the particles close to the x axis, so the first case is equivalent to a torus of circumference L, while the second case gives an infinite one-dimensional periodic system whose unit cell is of length L.

Since the potential is slowly varying the adiabatic approximation is used for the wave functions—in fact the validity of the adiabatic approximation is the criterion for how slow the potential variation must be. Expansion of the wave functions in terms of the instantaneous normalized eigenfunctions $\psi_j(t)$, with eigenvalues $\epsilon_j(t)$, gives the solution close to $\psi_0(t)$ as[5]

$$|\psi(t)\rangle \approx \exp\left[-(i/\hbar)\int^t \epsilon_0(t')dt'\right]\left[|\psi_0(t)\rangle + i\hbar\sum_{j\neq 0}|\psi_j(t)\rangle(\epsilon_j-\epsilon_0)^{-1}\langle\psi_j(t)|\dot{\psi}_0(t)\rangle\right] \tag{2.3}$$

to first order in the time derivatives, where the phase of $\psi_0(t)$ is chosen in such a way that its time derivative $\dot{\psi}_0$ is orthogonal to ψ_0. To the same order the particle current density produced by the moving potential is

$$\frac{\hbar^2}{2m}\sum_{j\neq 0}\frac{1}{(\epsilon_j-\epsilon_0)}\left[\langle\psi_j\,|\,\dot\psi_0\rangle\left[\psi_0^*\frac{\partial\psi_j}{\partial x}-\frac{\partial\psi_0^*}{\partial x}\psi_j\right]+\langle\dot\psi_0\,|\,\psi_j\rangle\left[-\psi_j^*\frac{\partial\psi_0}{\partial x}+\frac{\partial\psi_j^*}{\partial x}\psi_0\right]\right]. \tag{2.4}$$

For the problem of a torus (periodic boundary conditions) this can be integrated over all space to get the current as

$$J_0=\frac{\hbar^2}{mL}\sum_{j\neq 0}\frac{1}{(\epsilon_j-\epsilon_0)}\left[-\langle\psi_j\,|\,\dot\psi_0\rangle\left\langle\frac{\partial\psi_0}{\partial x}\middle|\psi_j\right\rangle-\langle\dot\psi_0\,|\,\psi_j\rangle\langle\psi_j\left|\frac{\partial\psi_0}{\partial x}\right\rangle\right]$$

$$=\frac{\hbar^2}{mL}\left[\left\langle\frac{\partial\psi_0}{\partial x}\middle|(\epsilon_0-H)^{-1}\,|\,\dot\psi_0\right\rangle+\langle\dot\psi_0\,|\,(\epsilon_0-H)^{-1}\left|\frac{\partial\psi_0}{\partial x}\right\rangle\right]. \tag{2.5}$$

After some manipulation this can be written in terms of the Green function as

$$J=-\frac{\hbar^2}{2\pi imL}\oint dE\int dx\int dx'\frac{\partial}{\partial x}G(x,x';E)\frac{\partial}{\partial t}G(x',x;E)\,, \tag{2.6}$$

where the contour goes round the eigenvalue ϵ_0.

For an infinite periodic system with filled bands Eq. (2.6) remains valid if the integration over x is restricted to one period and if the integration over E surrounds the energies of the filled bands only. Equation (2.5) can be replaced by

$$J=\frac{\hbar^2}{2\pi m}\sum_{\lambda\mu}\int dk\,\frac{f_\lambda(1-f_\mu)}{\epsilon_\lambda(k)-\epsilon_\mu(k)}\left[\left\langle\frac{\partial\psi_{\lambda k}}{\partial x}\middle|\psi_{\mu k}\rangle\langle\psi_{\mu k}\,|\,\dot\psi_{\lambda k}\right\rangle+\langle\dot\psi_{\lambda k}\,|\,\psi_{\mu k}\rangle\langle\psi_{\mu k}\left|\frac{\partial\psi_{\lambda k}}{\partial x}\right\rangle\right], \tag{2.7}$$

where k is the Bloch wave number, λ and μ are band indices, f_λ is unity for full bands and zero for empty bands, and the Bloch wave functions $\psi_{\lambda k}$ are normalized in a unit cell.

III. TRANSFER AROUND A TORUS

If the wave functions in Eq. (2.5) satisfy the periodic boundary conditions (2.2) the integral of the current is a continuously variable quantity. This can be shown by evaluation of the integral for special cases. For example, in a pure one-dimensional problem with a potential of the form

$$V(x,t)=-A\delta(x-vt)\quad\text{for } 0<t<L/v \tag{3.1}$$

an explicit expression for the Green function can be obtained. The qualitative nature of the result can be studied by taking A to be sufficiently small that perturbation theory is applicable. The eigenfunctions can be written as $\phi_n(x-vt)$, where, for the ground state,

$$\phi_0(x)\approx L^{-1/2}[1+mA(x-\tfrac{1}{2}L)^2/\hbar^2L] \tag{3.2}$$

up to first order in A. The overlap of $\partial\phi_0/\partial x$ with ϕ_n is given by

$$(\sqrt{2}/L)(2mA/\hbar^2L)\int_0^L(x-\tfrac{1}{2}L)\sin(2\pi nx/L)dx$$

$$=-mA\sqrt{2}/\pi\hbar^2n\,. \tag{3.3}$$

The integral of the current J_0 over the period L/v gives the particle transfer as

$$C_0=(\hbar^2/m)\sum_{n=1}^{\infty}4(mA/\pi\hbar^2n)^2 2m(L/2\pi n\hbar)^2$$

$$=(mAL/\hbar^2)^2/45\,. \tag{3.4}$$

For the other states the degeneracy is broken by the potential, so that they come in pairs separated by an energy $2A/L$. The integral of the gradient of one function multiplied by the other is

$$-(4\pi n/L^2)\int_0^1\sin^2(2\pi nx/L)dx=-2\pi n/L\,, \tag{3.5}$$

so the leading term in the integral of the current is

$$C_n=\pm 4\pi^2\hbar^2n/mAL\,, \tag{3.6}$$

with the plus sign for the lower state and the minus sign for the upper state. This also depends continuously on the strength A of the potential, but diverges as A goes to zero whereas (3.4) tends to zero.

IV. FILLED BANDS IN A PERIODIC SYSTEM

In Eq. (2.7) it is possible to replace

$$[\epsilon_\lambda(k)-\epsilon_\mu(k)]^{-1}\partial/\partial x$$

by $(im/\hbar^2)\partial/\partial k$, as might be expected from the for-

mal relations between x and $i\partial/\partial k$, and between the commutator of x with the Hamiltonian and $\partial/\partial x$. To show this explicitly one can write

$$\psi_k = u_k e^{ikx}, \tag{4.1}$$

where u_k satisfies periodic boundary conditions and the equation

$$\left[\frac{1}{2m}\left[-i\hbar\frac{\partial}{\partial x}+\hbar k\right]^2-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right] + V-\epsilon(k)\right] u_k = 0 . \tag{4.2}$$

From this it follows that

$$\frac{\partial u_{\lambda k}}{\partial k} = ig(k)u_{\lambda k} + \sum_{\mu\neq\lambda} u_{\mu k}\frac{1}{\epsilon_\lambda(k)-\epsilon_\mu(k)} \times\frac{\hbar^2}{m}\left\langle u_{\mu k}\left|\left[-i\frac{\partial}{\partial x}+k\right]\right|u_{\lambda k}\right\rangle , \tag{4.3}$$

where $g(k)$ is an arbitrary real function. With Eq. (4.1) this gives

$$\frac{\partial \psi_{\lambda k}}{\partial k} = i[g(k)+x]\psi_{\lambda k} + \sum_{\mu\neq\lambda}\psi_{\mu k}\frac{1}{\epsilon_\lambda(k)-\epsilon_\mu(k)} \times -\frac{i\hbar^2}{m}\left\langle\psi_{\mu k}\left|\frac{\partial\psi_{\lambda k}}{\partial x}\right\rangle\right. . \tag{4.4}$$

Substitution into Eq. (2.7) and integration over t (which eliminates the term involving the matrix element of x) give the particle transfer as

$$C=\frac{i}{2\pi}\sum_\lambda f_\lambda\int_0^T dt\int_0^{2\pi/L} dk\left[\left\langle\frac{\partial\psi_{\lambda k}}{\partial t}\left|\frac{\partial\psi_{\lambda k}}{\partial k}\right\rangle\right. -\left\langle\frac{\partial\psi_{\lambda k}}{\partial k}\left|\frac{\partial\psi_{\lambda k}}{\partial t}\right\rangle\right.\right] . \tag{4.5}$$

In the paper of Thouless *et al.*[1] it was argued that such an integral over two parameters in which the Hamiltonian is periodic should give $2\pi i$ times an integer, since the integral is equal to i times the change of phase of the wave function round the perimeter of the region of integration. The integral defines the first Chern class of the mapping of the torus in tk space on the complex projective space of normalized wave functions.[6]

There is a slightly different way of understanding the integral. Rather than allowing ψ_k to be analytic, but possibly multiple-valued functions of t and k on the torus, one can make them single-valued by demanding that the functions at one particular reference point in space be real and positive. This definition introduces singularities at those values of t,k for which ψ is zero at the chosen point. The integral then reduces to a sum of contributions from these singularities, and it can be shown that the contribution of a singularity is $\pm 2\pi i$, with a sign that depends on the sign of $\mathrm{Im}(\psi^*\partial\psi/\partial k)$ at the reference point.

It is also possible to change from the variable k to the variable $E=\epsilon_\lambda(k)$. The integral over a period of k becomes a contour integral over E which surrounds the energy band. This integral can be continued into the complex plane by restricting $|\psi_E\rangle$ to those solutions that satisfy the Floquet condition with a negative real part of the exponent; $\langle\psi_E|$ is then the adjoint solution with a positive real part of the exponent. The particle transfer is

$$C=\frac{i}{2\pi}\int_0^T dt\oint dE\left[\left\langle\frac{\partial\psi}{\partial t}\left|\frac{\partial\psi}{\partial E}\right\rangle\right. -\left\langle\frac{\partial\psi}{\partial E}\left|\frac{\partial\psi}{\partial t}\right\rangle\right.\right] . \tag{4.6}$$

For the one-dimensional Schrödinger problem this topological invariant can be expressed in a form that is more transparent. Firstly, ψ_E can only have zeros for E on the real axis, since, from the Floquet condition, a zero at one point implies zeros at any multiple of L from that point, and so implies a solution of the homogeneous eigenvalue problem in a system of length L. Secondly, since $|\psi_E\rangle$ can be constructed by integrating the Schrödinger equation from an arbitrarily large value X of x to small values of x and taking the limit $X\to\infty$, the nodes of $|\psi_E\rangle$ move monotonically toward larger values of x as E is increased. This implies that $\partial\psi/\partial x$ and $\partial\psi/\partial E$ have opposite signs at the nodes, so that if $\partial\psi/\partial t$ and $\partial\psi/\partial E$ have the same sign the node is moving to the right, while if they have opposite signs at a node it is moving to the left. If the contour in Eq. (4.6) crosses the real axis at E_F and at some point below all the bands, then the integral is just the sum of contributions from all those values of t for which there is a node at the reference point of the wave function at E_F; the contribution is $-2\pi i$ for a node moving right and $+2\pi i$ for a node moving left. The particle transfer C is just the net flux of nodes moving through a given point at energy E_F during a period T.

V. COMPETING AND INCOMMENSURATE PERIODS

This method can be used to classify the energy gaps of a one-dimensional Schrödinger equation with competing periods. The potential is taken to have the form

$$V(x)=\sum_i V_i(x/\xi_i-\eta_i) \quad \text{with } V_i(x+1)=V_i(x) \tag{5.1}$$

so that ξ_i is the period of the component i and η_i gives its phase. In the general case, according to the Wigner–von Neumann theorem,[7] an energy gap will not close when a single parameter η_i is varied continuously, so, if the contour of integration crosses the real axis at E_F in an energy gap, then the gap is characterized by an integer t_i which gives the particle transfer when η_i is increased adiabatically by unity; this integer is given by

$$t_i=\frac{1}{2\pi i}\oint dE\int_0^1 d\eta_i\left[\left\langle\frac{\partial\psi}{\partial\eta_i}\middle|\frac{\partial\psi}{\partial E}\right\rangle-\left\langle\frac{\partial\psi}{\partial E}\middle|\frac{\partial\psi}{\partial\eta_i}\right\rangle\right]. \tag{5.2}$$

The path of integration may have to be shifted as η_i is varied to keep it within an energy gap.

If the gap remains open for all values of the phases and if there is a lowest common multiple $\xi=p_i\xi_i$ of the periods, then a uniform translation of the whole potential by a distance ξ is equivalent to successive translations of the η_i by p_i. This gives

$$\sum_i p_i t_i=m\ , \tag{5.3}$$

where m is the total number of particles in the length ξ; all the numbers in this equation are integers. This is a generalization of Eq. (5) of Ref. 1.

If the gap closes for some values of the η_j, the values of t_i may depend on the other η_j. A closed path that goes through a single-level crossing leads to a half-integer value of C, since the wave function changes sign round such a path.[8]

For incommensurate potentials continuity suggests that these relations should still hold. If the gap remains open for all values of the phases, then the generalization of Eq. (5.3) is

$$\sum_i t_i/\xi_i=\rho\ , \tag{5.4}$$

where ρ is the average particle density.

VI. SOLITON CHARGES

There are two types of discrete solitons in one-dimensional systems:

(a) solitons such that each soliton must be succeeded by some sort of antisoliton. An example of this is a domain wall in a ferroelectric polarized along the chain. In this example the soliton charge is just twice the component of the dipole moment along the chain divided by the spacing between dipoles. There is no constraint on the value of such a soliton charge.

(b) solitons which can occur in succession without any intervening antisoliton. The solitons in polyacetylene [$(CH)_x$] discussed by Su, Schrieffer, and Heeger[2] are of this sort—they are breaks in the alternating sequence of double and single bonds along the chain of carbon atoms.

Polyacetylene does not have fractionally charged solitons because the molecular orbital states are occupied by two electrons. A model in which the magnetic field is so strong that only one spin state is occupied for the valence electron can be considered. For example, a regular chain of alternating B and Be atoms joined by alternating double and single bonds has solitons of type (a), as is shown in Fig. 1(a), since the soliton illustrated, with two double bonds on a B atom, must be succeeded either by two single bonds on a B atom or by two double bonds on a Be atom. The B-Be pairs carry a dipole moment, so movement of the soliton one unit cell (two atoms) to the right, as shown in Fig. 1(b), involves a charge transfer which is not just one electron going half a unit cell to the right, as the figure suggests; but also there is an additional amount which depends on the polarization of the bonds.

B—Be=B—Be=B=Be—B=Be—B
(a)

B—Be=B—Be=B—Be=B=Be—B
(b)

B—B=B—B=B=B—B=B—B=B
(c)

FIG. 1. Possible configurations for polymers with alternating single and double bonds when the magnetic field is so strong that only one spin state of the valence electron is allowed. In (a) and (b) the bonds have an electric dipole moment that is reversed on the two sides of the soliton. In (c) there is no dipole moment, but the units carry a net charge of one unit for each pair of atoms.

In the polyboron shown in Fig. 1(c) there is no polarization of the bonds, but there is a net charge of one proton on each pair of boron atoms. This soliton can be succeeded either by a similar soliton or by the antisoliton with two single bonds. The results of Sec. IV can be applied to such a soliton.

The potentials in which the electrons move are, of course, associated with ionic charges, so movement of the potentials involves also movement of these ionic charges, which are multiples of the proton charge and treated classically. A periodic system is constructed which has a large number N unit cells, each of length a (except near the soliton) and charge m units, with a soliton at the end of each group of N unit cells. The period of the system is

$$L = Na + d \ , \tag{6.1}$$

so that d is the length taken up by the soliton, and the net charge per period is $Nm + m'$ units, so that m' is the extra charge associated with the soliton. From the theorem of Sec. IV translation of the whole system by a distance L produces transport of an integer number of electrons (and certainly involves transport of an integer number of ionic charges), provided the Fermi energy lies in a band gap, so that m and m' are integers.

A second type of periodic motion of the system that can be considered consists of adiabatic displacement of the soliton one unit cell to the right, followed by uniform displacement of the whole system one unit cell to the left. If q_s is the soliton charge, this process involves the displacement of a charge $q_s - mN - m'$ in each length L a distance a, so the total charge transport, which again must be an integer, is

$$(q_s - mN - m')a/(Na + d) = -m \ . \tag{6.2}$$

The value of this integer must, of course, be $-m$ since N is large. This leads to the result

$$q_s = m' - md/a \ . \tag{6.3}$$

For the type (b) solitons fractional charge is only possible if there is a net charge on the chain, and if the fractional part of the charge is equal to minus the charge per unit cell multiplied by the ratio of the length taken by the soliton to the length of a unit cell. These results are identical to those originally derived by Prange.[4]

ACKNOWLEDGMENT

This work was supported in part by the National Science Foundation under Grant No. DMR-79-20785.

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