Phase singularities and quantum dynamics

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We consider Hamiltonians defined on multiply connected domains, which provide models for a great number of physical systems. Their eigenfunctions behave in a characteristic way as a function of enclosed magnetic flux. We establish different possible laws for the change of the phase winding numbers around enclosed flux. These laws provide a common theoretical basis for various quantum effects in orbital magnetism and charged-particle transport. As an illustration we discuss their relevance to particle transport in a constant electric field, emphasizing one-dimensional aspects. We show how the laws of winding-number change directly lead to the equations of quasiclassical dynamics, if the particle is subject to a highly periodic potential, but to completely nonclassical motion if the spatial symmetry is low and the electric field below a threshold value. The nonclassical aspects of quantum transport, particularly Bloch- and Josephson-type oscillations, are due to a periodic appearance of singularities of the phase of the wave function. These singularities are situated at the cores of phase gradient vortices, which periodically move across the physical domain, thereby causing jumps of the phase winding number of each state, associated with a change of the momentum. This picture gives new insight into the microscopic mechanism of momentum change in elastic processes. Further, the speed of motion of the phase singularities determines whether a state is insulating or conducting. We thus obtain a new characterization of such states.

I. INTRODUCTION

An important difference between classical and Schrödinger quantum mechanics is the fact that in the former the initial position and velocity of a particle can be chosen independent of each other (leading to a definite energy), whereas in the latter this is not always the case. Here the position is related to the modulus $R(x)$ and the velocity to the gradient of the phase $\eta(x)$ of a complex wave function $\psi(x)=R(x)\exp[i\eta(x)]$, $x\in\mathbb{R}^p$. This implies an *a priori* relation between position and velocity, since $R(x)$ and $\eta(x)$ are not independent of each other. For stationary wave functions it has been shown[1] that the phase $\eta(x)$ is related in a crucial way to the nodes of $\psi(x)$ [where $R(x)$ vanishes]. Of particular importance are nodal (hyper)surfaces (lines, points) of dimension $p-2$, where $\eta(x)$ is singular, showing jumps of πW, W an integer. These phase singularities lie at the centers of vortices of the gradient of the multivalued phase function $\eta(x)$. The change of phase around a particular nodel (hyper)surface (the phase winding number) is just equal to W, i.e., we have

$$W=\frac{1}{2\pi}\int_P \sum_\alpha \frac{\partial}{\partial x_\alpha}\eta(x)dx_\alpha \ . \tag{1}$$

Here, P is a path, which once encircles the particular $(p-2)$-dimensional nodal surface or line (but no other surface or line of this type). Note that W is integer, since $\psi(x)$ is single-valued.[2,3] These phase gradient vortices are therefore also called quantized vortices.[4]

Relation (1) with W an integer merely follows from the fact that $\psi(x)$ is a regular, complex function. If, in addition, $\psi(x)$ is a solution of a Schrödinger equation describing a system, which can be enclosed in a simply connected domain, such that the quantum-mechanical current density at the boundary of this domain vanishes or is parallel to the boundary, then the following general theorem is true:[1] In the absence of a magnetic field the quantum-mechanical current density is zero unless there exists in the corresponding domain of the configuration space at least one nodal (hyper)surface (line) of dimension $p-2$ with nonzero winding number W. This global result indicates the importance of phase singularities for systems with a nonvanishing current density. Further, a magnetic field $\mathbf{B}(r)=\mathrm{curl}\,\mathbf{A}(r)$ can induce quantized vortices in the system.[1,3,5] The same is true for an electric field, since it can be expressed in terms of a vector potential changing with time. Since phase singularities and quantized vortices have no direct counterpart in classical mechanics, we expect therefore that they are related to quantum effects of orbital magnetism and of particle transport in an electric field.

In this paper we will first investigate some general laws for the evolution of these phase structures as a function of a (changing) vector potential. These laws provide a common theoretical basis for various quantum effects of a wide class of systems, which can be described by a Hamiltonian of the following general type:

$$H=\frac{1}{2m}\sum_\alpha\left[\frac{\hbar}{i}\frac{\partial}{\partial x_\alpha}-\frac{q}{c}\left[b_\alpha(x)+\frac{\partial}{\partial x_\alpha}f(x)\right]\right]^2+V(x)\ , \tag{2}$$

$(x_1,\ldots,x_\alpha,\ldots,x_p)=x\in D\subset\mathbb{R}^p$, where D is a multiply connected domain in $\mathbb{R}^p$ with r holes. We define $f(x)$ as

a regular function of x in D, but it may have singularities (branching points) in the holes, such that, on a closed path P, $f(x)$ may be multivalued, leading to a nonzero flux contribution. If we consider a path P encircling the ith hole once, then

$$\phi_i = \sum_\alpha \int_P \frac{\partial}{\partial x_\alpha} f(x) dx_\alpha \tag{3}$$

denotes the magnetic flux through the ith hole generated by $f(x)$. By definition, we choose $b_\alpha(x)$ to be differentiable in D *and* in the holes. The total vector potential $A_\alpha(x)$ is equal to $b_\alpha(x)+\partial f(x)/\partial x_\alpha$.

The simplest example for a Hamiltonian of type (2) is given by a charged particle on a real loop of circumference L threaded by a total magnetic flux ϕ. Here, H may be expressed in terms of the curvilinear parameter $x_1 = x$ on the loop, and we have

$$f(x) = \phi x / L \ . \tag{4}$$

(The line integral of b_α along the loop is zero in this case, i.e., b_α represents just a gauge term.)

A related example is given by the Bloch theory in solid-state physics. Here, due to periodic boundary conditions in a d-dimension box, D is a torus T^d, and the phase winding number W "around" the ith hole of T^d is just the quasimomentum k in the ith spatial direction (multiplied by $L/2\pi$, where L is the length of the box in the ith direction). Our investigation will therefore give *new insight into the mechanism of momentum change* in elastic-scattering processes.

Other examples are normal and superconducting networks, and, further, particles confined to cylinder or torus geometries. These may either be real geometrical structures or be the result of mathematical idealizations of simply connected systems by means of periodic boundary conditions.

The motion of phase gradient vortices (centered by phase singularities) as a function of ϕ_i may change the phase winding number W associated with the ith hole. Recently,[5] phase singularities have been studied for an electron confined to a two-dimensional, doubly connected domain D with asymmetric boundaries, which is threaded by a magnetic flux ϕ (this system was called Aharonov-Bohm "billiard"). Here the phase winding number W along a path encircling once the hole of D has been investigated, and it was found that W of any eigenfunction of H changes with ϕ in the following way:

$$W(\phi+1) = W(\phi)+1 \quad \text{with } \phi \text{ given in units of } hc/e \ . \tag{5}$$

This property has also been found for one-dimensional perturbed loops threaded by a magnetic flux.[3]

In this article we will study the *continuous* evolution of wave functions as a function of a flux parameter ϕ. We will find that in the general case a series of other laws of winding-number changes are possible differing from (5). We will investigate these different cases and their theoretical origin together with the characteristic behavior of the wave functions with which they are associated. We will find that the winding-number changes are connected with various different scenarios of quantized-vortex motion as a function of ϕ. These lie at the origin of seemingly different physical phenomena.

Many different physical systems can be described by a Hamiltonian of type (2). The laws of winding-number and quantized-vortex change therefore provide a general tool for discussing quantum effects of *a priori* different systems from a unified point of view. As a first example we mention the oscillatory magnetic behavior of thin networks[3] and Aharonov-Bohm–type effects.[5,6] In this paper we will illustrate the significance of the general laws by showing their relevance to the dynamics of charged particles in an electric field. Further applications will be discussed in forthcoming papers.

II. DIFFERENT CASES OF WINDING-NUMBER CHANGE

We will investigate various properties as a function of a single flux ϕ (possible other flux variables associated with other holes remaining constant). For the following it is therefore sufficient to consider a Hamiltonian of type (2) describing a particle with charge q on a doubly connected domain D (i.e., containing a single hole) threaded by a flux ϕ. The mathematical properties which are important for the following are best illustrated by the case of one spatial variable ($x_1 = x \in D = [0,L]$; D may be represented as a loop in the plane):

$$H(\phi) = \frac{1}{2m}\left[\frac{\hbar\partial}{i\,\partial x} - \frac{q\phi}{cL}\right]^2 + V(x) \ . \tag{6}$$

In this one-dimensional case $b_\alpha(x)$ of Eq. (2) has been set equal to zero, since its line integral along the loop is zero as we have mentioned, and therefore it has no influence on phase winding numbers.

It is well known[7] that H admits a family of infinitely many (nonequivalent) self-adjoint extensions H_a defined in $L_2([0,L])$, each of which is defined by

$$\int_0^L \frac{\partial \eta(x)}{\partial x} dx = a \pmod{2\pi} \ , \tag{7}$$

where $a \in [0,2\pi)$. Among these Hamiltonians we choose the one with $a=0$, i.e., we choose that self-adjoint extension of H, which is defined by means of functions $\psi(x) = R(x)\exp[\eta(x)]$, which are single-valued on the loop, corresponding to periodic boundary conditions $\psi(0) = \psi(L)$.

Remark: If D describes a *real* loop imbedded in the two- or three-dimensional physical space (i.e., x is the curvilinear parameter along the loop with length L), then this is the only physically correct self-adjoint extension.[2,3] On the other hand, if D represents an open interval (e.g., a rectilinear interval) of length L, then each of these nonequivalent self-adjoint Hamiltonians H_a may be physically possible. However, a definite extension H_a with $a \neq 0$ is unitarily equivalent to a Hamiltonian H_0 (i.e., defined on single-valued functions), where now ϕ is replaced by $\phi - \hbar c a/q$, i.e., to a Hamiltonian with a shifted flux origin. Since for the following discussion the origin of ϕ is

not important, we set $a=0$ also in the case where D is not a closed loop.

The Hamiltonians (6) have the important property that the set of eigenvalues of $H(\phi)$ is identical with the set of eigenvalues of $H(\phi+mhc/q)$ for any given ϕ, where m is any integer. This follows from the fact that the unitary transformation

$$\psi'=\psi\exp[i/\hbar F(x)]\ , \tag{8}$$

where

$$F(x)=-hxm/L,\quad m \text{ an integer}\ , \tag{9}$$

and, hence,

$$\int_0^L \frac{\partial}{\partial x}F(x)dx=-hm\ , \tag{10}$$

transforms $H(\phi+hcm/q)$ into $H'=H(\phi)$, leaving the domain of definition of the operators unchanged provided m is an integer. In other words, the *set* of eigenvalues (the spectrum) $S(\phi)$ of $H(\phi)$ is periodic with ϕ with period hc/q:

$$S(\phi+1)=S(\phi)\ , \tag{11}$$

where ϕ is expressed in units of hc/q, as in the following of this section (hc/q has a sign). The property (11) is independent of the particular form of $V(x)$.

If H depends on more than one spatial variable (e.g., a hollow cylinder or the two-dimensional Aharonov-Bohm "billiard" of Ref. 5), Eq. (11) follows from completely analogous arguments, starting with the fact that there exists a one-parameter family of self-adjoint extensions[7] of H, each of which is characterized by a relation analogous to (7), where now the integral follows any path P which once encircles the hole, and in the same way equation (10) is generalized to

$$\int_P \sum_\alpha \frac{\partial F(x_1,\ldots,x_\alpha,\ldots)}{\partial x_\alpha}dx_\alpha=-hm\ . \tag{10'}$$

For a general Hamiltonian of type (2) with many holes, Eq. (11) is true individually for each of the flux variables ϕ_i.

There exist different forms of $S(\phi)$, which are compatible with (11). Figures 1 and 2 show some examples. These different forms of $S(\phi)$ can be classified according to the behavior of the *individual* energies $E_j(\phi)$ [the union of which composes $S(\phi)$],

$$H(\phi)\psi_j(\phi)=E_j(\phi)\psi_j(\phi)\ , \tag{12}$$

where the labels j are defined such that each $\psi_j(\phi)$ is a *continuous* function of ϕ. This means that across a possible point of degeneracy of the eigenvalue we follow $\psi_j(\phi)$ continuously as a function of ϕ. In the general case an individual $E_j(\phi)$ is not periodic with period 1.

One important class of $S(\phi)$ (illustrated by Fig. 1) is characterized by the following behavior of all the eigenvalues of a given Hamiltonian:

$$E_j(\phi+n)=E_j(\phi),\quad n\in\{1,2,\ldots\} \tag{13}$$

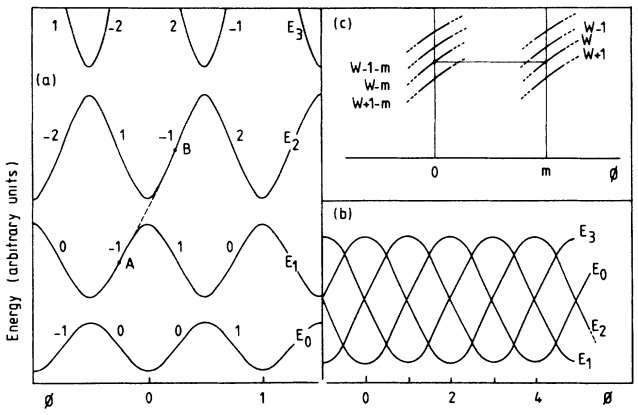

FIG. 1. Schematically shown examples for the periodic ϕ dependence of the eigenvalues, such that in addition to relation (11) also an equation of type (13) is fulfilled. ϕ is given in units of hc/q, where q is the charge of the particle. (a) Energy levels $E_j(\phi)$ periodic with period 1. The numbers shown in the figure are the phase winding numbers $W_j(\phi)$ associated with the corresponding pieces of the energy curve $E_j(\phi)$ in the case where the levels represent eigenvalues of a Hamiltonian of type (6). The dashed line corresponds to a nonadiabatic process (see text). (b) A single band of energy levels $E_j(\phi)$ with ϕ period $n=4$. (c) Energy levels of a single band with ϕ period $n\gg1$, shown in a neighborhood of $\phi=0$ and of $\phi=m$. The levels are labeled by their phase winding numbers which, in the figure, are restricted to a small interval around a given W_j at $\phi=m$ and W_j-m at $\phi=0$.

where n denotes the *smallest integer* for which (13) is satisfied. For the given Hamiltonian, n is the same for all eigenvalues, and the energies may be degenerate only at discrete values of ϕ. The case $n=1$ is illustrated in Fig. 1(a). Note that here no eigenvalue is degenerate (i.e., there is one state per band). An example for the case

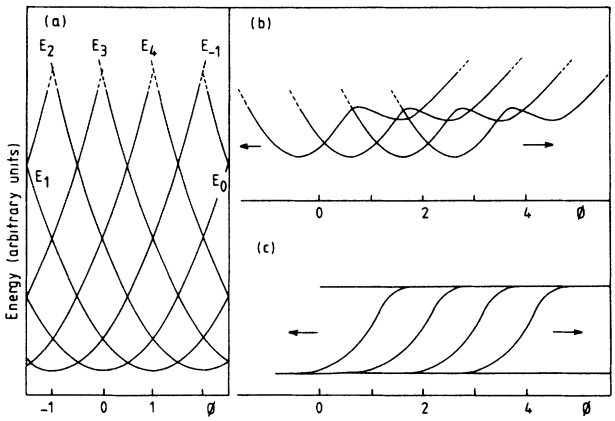

FIG. 2. Schematically shown examples of individual energy levels, which are not periodic with ϕ, i.e., no relation of type (13) holds [but the spectrum still fulfills Eq. (11)]. (a) Parabolic energy levels of a free particle. The level index is equal to its phase winding number (which remains constant for all ϕ). (b) and (c) examples for asymmetric behavior of the individual energy levels.

$n=4$ is shown in Fig. 1(b). The eigenvalues of all one-dimensional Hamiltonians of type (6) with $V(x)$ different from a constant belong to this class. We define the values of the indices j such that, for energies within the same band, we have

$$E_{j+1}(\phi+1)=E_j(\phi), \quad j=0,1,\ldots,n-2 \ . \tag{14}$$

see Fig. 1. For the first energy band $j=0,1,2,\ldots,n-1$, for the second band $j=n,n+1,\ldots,2n-1$, and so on. Within the same band E_{j+n} is identical to E_j.

For Hamiltonians of type (6) the number n in Eq. (13) is related to the periodicity of the spatial potential $V(x)$ on the interval of length L (circumference of the one-dimensional loop): L/n is the spatial period (unit cell) of $V(x)$. The eigenfunctions of (6) (for $\phi=0$) are the usual Bloch functions, and the corresponding eigenvalues $E_j(\phi)$ are the ϕ-dependent Bloch energies forming bands, each containing n energy curves $E_j(\phi)$. Here on a flux interval $0\le\phi\le 1$ each energy curve $E_j(\phi)$ intersects at least two times with each of the other energy curves of the same band, i.e., it intersects at least $2(n-1)$ times in this flux interval. For a potential which is aperiodic (apart from the trivial periodicity) there are no intersections and $n=1$. This illustrates the Wigner–von Neumann anticrossing theorem[8] for eigenvalues depending on one parameter (here ϕ).

Figure 2 illustrates another class of spectra for which no relation of type (13) holds for the individual energies (with the energies being degenerate at most for discrete values of ϕ). A particular example of this class is a Hamiltonian of type (6) with $V(x)=$const. Here the energies are parabolas [Fig. 2(a)]. This may also be considered as the limit $n\to\infty$ of a periodic potential (all energies are in the first band). Figure 2(b) and 2(c) illustrate more general cases of this class, where the individual energy levels are asymmetric as a function of ϕ. Explicit examples will be discussed elsewhere.

In this paper we are interested in the behavior of the eigenfunctions $\psi_j(x)$ as a function of ϕ. We will see how this is related to the ϕ dependence of the energies $E_j(\phi)$. First, we consider the case where a relation of type (13) holds, and we seek the relation between $\psi_j(\phi+n)$ and $\psi_j(\phi)$ for all ϕ. To this end we consider the equation

$$H(\phi+n)\psi_j(\phi+n)=E_j(\phi+n)\psi_j(\phi+n) \ . \tag{15}$$

Due to the unitary transformation

$$\psi'_j=\psi_j(\phi+n)\exp[(i/\hbar)F(x)] \ , \tag{16}$$

where $F(x)$ fulfills Eq. (10′) with m equal to n, and relation (13), Eq. (15) is equivalent to

$$H(\phi)\psi'_j=E_j(\phi)\psi'_j \ . \tag{17}$$

Hence,

$$\psi'_j=\psi_j(\phi) \ , \tag{18}$$

From (16) and (18) we obtain

$$\psi_j(\phi+n)=\psi_j(\phi)\exp[(-i/\hbar)F(x)] \ . \tag{19}$$

This means, in particular,

$$|\psi_j(\phi+n)|=|\psi_j(\phi)| \tag{20}$$

and using (10′),

$$W_j(\phi+n)=W_j(\phi)+n \ . \tag{21}$$

Remark: At first, Eq. (18) in the above derivation only holds for all ϕ, where the energy is not degenerate. But it is also valid for a value ϕ', where E_j is degenerate, since at such a point we have defined ψ_j as the continuous limit $\phi\to\phi'$ of $\psi_j(\phi)$. If we omit the index j in the above derivation [i.e., we do not make use of an equation of type (13)], then, as a consequence of (11), for any two nondegenerate values ϕ and $\phi+m$ (m any integer), for which $E(\phi)=E(\phi+m)$, we have

$$W(\phi+m)=W(\phi)+m \tag{21'}$$

for the corresponding eigenfunctions at ϕ and $\phi+m$. But these two energies and winding numbers do not have the same label j, if m is different from an integer multiple of n, see Fig. 1(b), or if no relation of type (13) holds (Fig. 2).

Summarizing, we emphasize that the spectrum $S(\phi)$ of any Hamiltonian $H(\phi)$ of type (2), which depends on one or several flux variables ϕ, is periodic with respect to each flux variable ϕ separately with period 1 [Eq. (11)]. The phase winding number associated with two nondegenerate eigenvalues $E(\phi)=E(\phi+m)$, m *any* integer, obeys Eq. (21′). If a relation of type (13) holds, the phase winding number of an eigenfunction $\psi_j(\phi)$ of $H(\phi)$ obeys the law (21) [$\psi_j(\phi)$ is defined as a *continuous* function of ϕ, and n is fixed for all eigenfunctions of the same Hamiltonian]. If $H(\phi)$ depends only on one spatial variable x, then L/n is just the spatial period of the potential $V(x)$. Further, in all cases of aperiodic energy levels $E_j(\phi)$ [i.e., where no relation of type (13) holds] known to the author, the winding numbers W_j do not change with ϕ [e.g., Fig. 2(a)].

It is important to note that as soon as a symmetry which causes degeneracy of the energy (crossing of levels) at certain values of ϕ is destroyed by a perturbation with reduced symmetry, a definite number of formerly intersecting levels now anticross at these ϕ values. For instance, the free-particle parabolas of Fig. 2(a) are modified by a potential $V(x)$ with spatial period L/n such that the perturbed levels anticross at the Bloch band edges, leading to energy levels $E_j(\phi)$, which obey Eq. (13). The presence of a totally asymmetric potential destroys all degeneracy (in accordance with the Wigner–von Neumann theorem[8]) and, as a consequence, leads to Eq. (21) with $n=1$.

If relation (13) holds, Eq. (21) gives the difference of W_j for discrete ϕ values lying $\Delta\phi=n$ apart. It means that over a long ϕ interval much larger than n the average W_j change per flux unity is always equal to 1 for a given function $\psi_j(\phi)$. On the other hand, Eq. (21) says nothing about the effective ϕ dependence of W_j for flux values within an interval $\Delta\phi=n$. Here various scenarios for the change of W_j as a function of ϕ, which are compatible with (21), are possible. If $n=1$, the simplest case of a W_j change is an increase (decrease) by unity in each consecutive flux interval of length 1, occurring for *all* eigenstates

$\psi_j(\phi)$ of the Hamiltonian. Such a behavior has been found[6] for the wave functions of the Aharonov-Bohm effect and the two-dimensional Aharonov-Bohm "billiard."[5] Here phase singularities [nodal points of $\psi(x,y)$], each forming the center of a phase gradient vortex with individual winding-number unity, migrate across the two-dimensional domain from its external boundary into its hole, where one vortex center enters per flux interval $\Delta\phi=1$.

An important system for the following is a charged particle on a one-dimensional domain [Eq. (6)]. Here the possible *scenarios of W_j change* are determined by the numbers n of Eq. (13) [i.e., by the periodicity of the spatial potential $V(x)$] together with the energy index j. At the flux values, where the levels anticross, W_j jumps. In the intervals between the energy anticrossing point the phase winding number $W_j(\phi)$ of a solution can be derived from the corresponding *free*-particle spectrum by following the parabolas $E_j(\phi)$ of Fig. 2(a) piecewise as a function of ϕ, such that, instead of level intersections, one observes level anticrossing after each flux interval $\Delta\phi=n/2$ (except for the ground state, where $\Delta\phi=n$).[3] Here, n is the periodicity number of the potential $V(x)$ in the Hamiltonian under consideration. Between adjacent anticrossings the winding number W_j is then identical to that of the corresponding free-particle curve.

For a spatial potential with $n=1$, the values of $W_j(\phi)$ in the intervals between the energy anticrossing points $\phi=p/2$, p an integer, are indicated in Fig. 1(a). Here, W_2 is equal to 1 for $-\frac{1}{2}<\phi<0$, then it jumps to -1 at $\phi=0$, then it jumps to 2 at $\phi=\frac{1}{2}$, and so on. If $n>1$, the W_j of a Bloch function $\psi_j(\phi)$ jumps only after a flux interval $\Delta\phi=n/2$, except in the lowest band, where $\Delta\phi=n$. The jumps occur at the band edges (except for the ground state). For instance, $W_0=0$ for $-n/2<\phi<n/2$, then at $\phi=n/2$ it jumps to n, at $\phi=3n/2$ it jumps to $2n$, etc. $W_1=1$ for $-n/2+1<\phi<n/2+1$, at $\phi=n/2+1$ it jumps to $n+1$, at $\phi=3n/2+1$ it jumps to $2n+1$, etc. W_{-1} (which is identical with W_n-1) $=-1$ for $-n/2-1<\phi<n/2-1$, at $\phi=n/2-1$ it jumps to $n-1$, at $\phi=3n/2-1$ it jumps to $2n-1$, and so on.

In the case of a one-dimensional system the behavior of the phase $\eta_j(x)$ with the periodic jumps of its winding number W_j can be visualized[3] by extrapolating the phase function $\eta_j(x)$ of a given state $\psi_j(x)$ into the plane, into which the one-dimensional domain of length L (represented as a circle) can be embedded, see Fig. 3: Here, by drawing the lines of constant phase one obtains a picture of vortices, whose cores (the phase singularities) lie inside, outside or on the perimeter (e.g., a plane-wave state shows a single, symmetric vortex whose core is in the center of the circle). These vortices move in the plane as a function of ϕ. At a ϕ value, where the energy levels anticross, one or several vortex centers (phase singularities) cross the perimeter, which causes a jump of the phase winding number W_j (defined along the perimeter). (If the dimension of the domain of the system is greater than 1, the phase gradient vortex structure is usually visible without extrapolation.) Figure 3 illustrates a typical vortex structure of the ground state of a Hamiltonian of type (6) where the potential has spatial period $L/2$ (i.e., $n=2$). We remark that, for given ϕ, the relevant topology of the vortex structure of an eigenstate with a given index j is the same for all Hamiltonians of type (6), whose potentials $V(x)$ have the same periodicity n (cf. Ref. 3).

III. APPLICATION TO QUANTUM TRANSPORT

The general behavior of W as a function of ϕ discussed in the preceding section is important since it constitutes the common theoretical origin of various *quantum* effects occurring in different areas of physics. As a first example, we mention the oscillatory properties of normal and superconducting loops and micronetworks as a function of magnetic flux. These are due to the periodic passage of phase gradient vortex centers across the branches of a network.[3] In the present paper we will emphasize the relevance of phase singularities and vortex motion to quantum effects in charged-particle dynamics. We will discuss here mainly one-dimensional systems. Applications to other systems will be treated in forthcoming papers.

In the presence of an electric field E_x along the one-dimensional domain, the vector potential $A_1=A_x$ depends on time, i.e.,

$$A_x=\phi/L\ , \tag{22}$$

with

$$\phi=-cE_xLt\quad(\phi\text{ in cgs units})\ . \tag{23}$$

The knowledge of $W_j(\phi)$ represents then the *adiabatic* time evolution of the phase winding number of the function $\psi_j(x,t)$ in the presence of an electric field E_x. Adiabatic functions are very useful for the description of particle dynamics, even in the nonadiabatic limit (see below). Let us first discuss the physical properties of the adiabatic solutions.

First, we consider a free particle. The energies $E_W(\phi)$ are given by the parabolas of Fig. 2(a):

$$E_W=(h^2/2mL^2)(q\phi/hc-W)^2\ . \tag{24}$$

Here the energies are labeled according to their phase

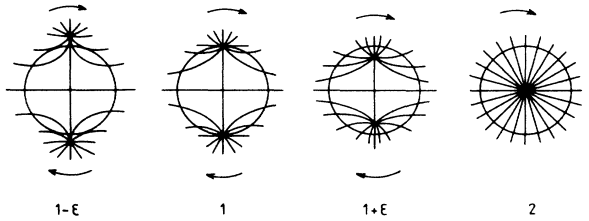

FIG. 3. Typical vortex structure for the ground state of a Hamiltonian of type (6) with a potential $V(x)$ with periodicity $n=2$, shown for different flux values ϕ (given in units of hc/q). The one-dimensional periodic system is represented by the circle. Shown are the lines of constant phase η in the extrapolation plane, with a difference of $\pi/6$ between neighboring lines. η increases in the direction of the arrows.

winding number W, which is related to the wave vector by

$$k=2\pi W/L \ . \tag{25}$$

The center of a wave packet formed of free-particle functions $(1/\sqrt{L})\exp(ikx)$ moves with the velocity[9]

$$v_k=\frac{1}{\hbar}\frac{dE_k}{dk}=(h/mL)(kLW/2\pi-q\phi/hc) \tag{26}$$

$$=(\hbar/m)k+(q/m)E_x t \ . \tag{27}$$

As usual, in Eq. (27) k is understood as the mean k value of a narrow wave packet in k space; further, L is supposed to be sufficiently large, such that the energy levels are closely spaced. In the absence of inelastic processes the numbers k (or W) are *constant* with ϕ, i.e., according to (23), constant for all times. Equation (27) is the classical law of motion of a charged particle in the presence of an electric field E_x (Newton's law), which is thus obtained from quantum mechanics by following the *continuous* adiabatic solutions. (The generalization to three dimensions is obvious by considering the energy hyperparaboloids depending on three flux variables.)

There is another method of deriving a dynamical equation which directly uses the periodicity (11) of the spectrum together with the law (21′) for the change of the winding number W with ϕ [or with t by virtue of (23)]. This method is applicable whenever there are many closely spaced energy levels, as in the case of a Bloch band of a particle in a periodic potential $V(x)$ with periodicity number $n\gg 1$. Consider the fixed flux value $\phi_m=nhc/q$ and a small interval of winding numbers $W(\phi_m)$, see Fig. 1(c). Within this interval the energy levels at $\phi=\phi_m$ can be labeled by their winding numbers $W(\phi_m)$, i.e., we have $E(W,\phi_m)$. Due to the periodicity (11) of $S(\phi)$ these energy curves at $\phi=\phi_m$ can be mapped to other energy curves $E(W',0)$ at $\phi=0$, which have the same energies, i.e.,

$$E(W',0)=E(W,\phi_m) \ , \tag{28}$$

and whose winding numbers W' are shifted according to (21′):

$$W'=W-m \ . \tag{29}$$

The translated levels have the same functional dependence on ϕ. We therefore have (in the limit $n\to\infty$)

$$\frac{1}{\hbar}\frac{\partial E(W,\phi)}{\partial W}\bigg|_{(W-m,\,0)}=\frac{1}{\hbar}\frac{\partial E(W,\phi)}{\partial W}\bigg|_{(W,\,mhc/q)} \ . \tag{30}$$

Since $W=kL/2\pi$ and according to (23) the right-hand side of (30) is the velocity $v(t)$ at the time

$$t=-mh/qE_x L \ . \tag{31}$$

From the left-hand side of (30) we obtain

$$v(t)=\frac{1}{\hbar}\frac{\partial E(k)}{\partial k} \ , \tag{32}$$

where the derivative is taken at

$$k(t)=2\pi[W-m(t)]/L=2\pi(W+tqE_x L/h)/L \ . \tag{33}$$

Equation (33) reads, in differential form,

$$\frac{dk}{dt}=\frac{qE_x}{\hbar} \ . \tag{34}$$

Equation (34) is the continuous limit of $\Delta k/\Delta t$, where $\Delta k=2\pi/L$, and Δt is defined with (23) by

$$\Delta\phi=hc/q=-cE_x L\,\Delta t$$

$$\text{whence } \Delta t=-h/qE_x L=\tau\,\mathrm{sgn}(\Delta t) \ . \tag{35}$$

Equations (32) and (34) are the well known equations of quasiclassical dynamics.[9] They describe the velocity of a Bloch wave packet (following the evolution of the Bloch functions adiabatically as a function of t) by the velocity of *another* wave packet made of Bloch functions at $t=0$, which has the same velocity. We have shown that (for large periodicity n) these equations follow immediately from the general ϕ periodicity (11) of the spectrum of a Hamiltonian of type (6) together with its corresponding law of winding-number change (21′).

From (32), expressing k as a function of ϕ, using (23) and (33) one obtains

$$I=qv/L=-c\frac{\partial E}{\partial\phi} \ . \tag{36}$$

The last expression is just the expectation value I of the current operator in a state $\psi(\phi)$ of the one-dimensional system of length L, which is valid for any ϕ and any potential $V(x)$ (i.e., also if $n=1$), whereas Eqs. (32) and (34), which describe the time evolution of the velocity of the center of a wave packet composed of Bloch functions, are only meaningful if $n\gg 1$, such that there are sufficiently many states per band, allowing the limit towards a continuous variable k. In the presence of disorder, $n=1$ and the k vector at $\phi=0$ is no longer a meaningful time-dependent variable (in the strict adiabatic limit). Here there is only one state per band; hence dk/dt would vanish, in contradiction to (34). In this case the average velocity of a wave packet (case of weak disorder, where one can still speak of wave packets) or, more generally, the current density in the system, is given by the more general equation (36).

As a consequence of (13), due to Eqs. (32) and (34) [or (36)] [see Figs. 1(a) and 1(b)] the particle velocity $v(t)$ (or the current I) oscillates in time with period $n\tau=n\,|\,h/qE_x L\,|$ (Zener-Bloch oscillations). (This means that, *in the adiabatic limit,* in our one-dimensional system, only a free particle can be accelerated indefinitely according to Newton's law.) According to a current textbook statement this is due to reflection of the wave vector at the boundary of the first Brillouin zone. This is a statement in the framework of the equivalent picture of quasiclassical dynamics [Eqs. (32) and (34)], where the velocity of the true wave packet at $\phi(t)\neq 0$ (with k fixed) is expressed in terms of Bloch functions ψ_k (of the same band) at $\phi(t)=0$, but with a time-dependent k. In this picture the wave function changes within the first Brillouin zone [defined for $\phi(t)=0$] and never gets out of it (with "small" discontinuous changes between Bloch func-

tions of neighboring k values and with periodic "big" discontinuous changes whenever the k vector is "reflected" at the zone boundary, i.e., when the k vector jumps from a Brillouin-zone boundary to the opposite one).

However, in reality, as we have seen, each wave function $\psi_j(\phi(t))$ changes *continuously* with time in a *nonperiodic* way, and it never comes back to the initial function. The modulus of a wave function $\psi_j(x;\phi)$ is periodic with ϕ, but its phase function $\eta(x)$ is not [see Eq. (19)]. The subspace spanned by the $\psi_j(x)$ of a single band is continuously changed with $\phi(t)$ in a nonperiodic way. We have seen that the *true* k vector, which is proportional to the phase winding number W_j, changes in accordance with Eq. (21). This equation says that, on the average, on a time interval which is much larger than $n\tau$, there is a *constant* increase (or decrease) of W_j with ϕ (time).

The true microscopic mechanism responsible for the velocity oscillations is the periodic energy-level anticrossing at the band edge (the upper edge for the lowest band) with time period equal to $n\,|\,h/qE_xL\,|$, causing the phase winding numbers W_j $(=k_jL/2\pi)$ to jump in integer multiples of n at these values. As we have mentioned, these jumps are caused by singularities of the phase function $\eta(x)$ (each being the center of a phase gradient vortex), which cross the loop of length L, as can be visualized in the plane embedding the loop.

If $V(x)$ is asymmetric, n is equal to 1. Hence the velocity oscillations are extremely fast, with time period $\tau=|\,h/qE_xL\,|$, which tends to zero for L tending to infinity. This means that the particle stays at the same spot indefinitely. This result is true for any asymmetric potential $V(x)$ whatever small. (We remark again that L must be smaller than the distance a wave packet can move before inelastic scattering occurs.)

In the strict adiabatic limit, if an acceleration of a particle during a time much bigger than τ is possible, this is a consequence of the fact that each energy curve $E_j(\phi)$ as a function of the parameter ϕ consecutively intersects with many other energy curves [Figs. 1(b) and 2(a)], leading to a monotonic increase or decrease of the energies $E_j(\phi)$ as a function of ϕ, with long pieces of similar curvature. This happens for sufficiently high periodicity of $V(x)$, i.e., $n\gg1$. If this symmetry is destroyed, energy-level intersections are excluded according to the Wigner–von Neumann theorem,[8] and the energies behave as in Fig. 1(a) $(n=1)$. In two dimensions, where the domain is a 2-torus, the eigenvalues depend on the two flux parameters $\phi_x=-cE_xL_xt$, $\phi_y=-cE_yL_yt$. Here, again, in the absence of symmetry, energy-surface intersections are excluded by the same theorem. The eigenvalues as a function of the two flux variables are then intersection-free, rippled, and, on the average, horizontal surfaces which are periodic in each of the two flux variables separately. Therefore the motion of the center of a wave packet can be decomposed into two perpendicular, periodic one-dimensional oscillations with time periods $\tau_x=|\,h/qE_xL_x\,|$ and $\tau_y=|\,h/qE_yL_y\,|$. This leads to a highly localized (in general, aperiodic) motion around the same spot in the (x,y) plane. This means that macroscopically the particle does not move despite the electric field, in complete analogy to the one-dimensional situation.

In three dimensions, however, where the eigenvalues depend on *three* parameters ϕ_x, ϕ_y, ϕ_z, degeneracy of the energy levels is possible according to the Wigner–von Neumann theorem, even in the absence of spatial symmetry. This means qualitatively that in three dimensions, in the presence of disorder, we cannot exclude the possibility of wave-packet centers being accelerated over noninfinitesimal times much larger than τ_x, τ_y, or τ_z, even in the adiabatic limit, in contrast to one and two dimensions. This behavior is reminiscent of the situation in localization theory, according to which in one and two dimensions, in the presence of any disorder, all states are localized (hence nonconducting), while in three dimensions both localized and delocalized (conducting) states exist.

So far we have discussed the *adiabatic* limit of solutions of the time-dependent Schrödinger equation. In the presence of low symmetry this limit is realized only under special conditions. Consider $V(x)=V^n(x)+V^1(x)$, where V^n is periodic with period L/n, $n\gg1$, and V^1 (the disorder potential) with period L. Here, in general, a state which at an initial time is equal to the adiabatic wave function develops at later times into a linear combination of all adiabatic solutions. Since $n=1$ we have pairwise anticrossing adiabatic energy levels [Fig. 1(a)]. Here two simple limiting processes are possible: one is the adiabatic limit, which we have discussed. The other is the Zener tunneling limit, where the time-dependent solution develops as if the energy levels would intersect, following the unperturbed adiabatic solution [the dashed line in Fig. 1(a)], which leads again to quasiclassical behavior. For this to happen the matrix element $|\,\langle\psi_s\,|\,V^1\,|\,\psi_t\rangle\,|$ must be much smaller than $|\,E_{s+1}(\phi')-E_s(\phi')\,|$, where $E_s(\phi)$ and $E_t(\phi)$ are the unperturbed levels (corresponding to $V^1=0$) assumed to intersect at $\phi=\phi'$. This guarantees that the adiabatic wave function is sufficiently close to the unperturbed function outside the level-crossing zone. Under this condition, we can use the Zener formula[10] for a rough estimation of the conditions under which these two limiting situations occur. According to this formula the probability P for passing from point A to point B of the upper branch in Fig. 1(a), instead of adiabatic anticrossing, is given by

$$P=\exp(-\pi G^2)\,, \tag{37}$$

where G is proportional to the square of the matrix element $|\,V^1_{s,t}\,|$. This means that for vanishing perturbation V^1 we always have Zener tunneling and, hence, free-particle $(V^n=0)$ or quasiclassical $(V^n\neq0)$ behavior. As an example, let us consider the case of a free particle $(V^n=0)$ slightly perturbed by V^1. For the levels in the neighborhood of $\phi=0$, we obtain, from the general formula,[10]

$$\pi G^2=mL\,|\,V^1_{s,-s}\,|^2/(\hbar^2s\,|\,qE_x\,|)\,. \tag{38}$$

Equation (38) tells us that for a given system with finite L and $V_{s,-s}$ there is always a threshold field $E_c(s)$, such that for $E_x\gg E_c(s)$ one has Zener tunneling and, hence,

classical dynamic behavior. On the other hand, for $E_x \ll E_c(s)$ the time evolution is adiabatic, leading to, as we have seen, completely nonclassical oscillatory behavior.[11]

As an example, for a spin-$\frac{1}{2}$ particle at the Fermi level in a weak-disorder potential $V^1(x)$, we obtain (setting $\pi G \simeq 1$)

$$E_c = \pi^2 h^2 b^2 d / 4qmL^2 , \tag{39}$$

where d is the one-dimensional particle density and b is defined by

$$| V^1_{s,-s} | = b(E_{s+1}(\phi=0) - E_s(\phi=0)) \simeq bh^2 d / 4mL . \tag{40}$$

Here, s labels the free-particle state at the Fermi level before the perturbation $V^1(x)$ is present. We only consider weak perturbation corresponding to $b \lesssim 0.1$. for an electron, with $b=0.1$, $d=10^7$ cm^{-1}, and $L=10^{-4}$ cm, Eq. (39) gives $E_c L \simeq 10^{-4}$, where $E_c L$ is the potential difference along L expressed in volts. This means that for $E_x L \ll 10^{-4}$ V a wave packet at the Fermi level behaves in an adiabatic oscillatory manner, whereas for $E_x L \gg 10^{-4}$ V it behaves according to classical dynamics. In the intermediate region, where E_x is of the order of E_c, successive "branching" between adiabatic and nonadiabatic orbits occurs, leading to a superposition of many different adiabatic functions $\psi_j(x,t)$ after a time interval much larger then τ. Such an intermediate situation has recently been investigated numerically.[12]

In principle, these different types of dynamical behavior could be experimentally investigated on a suitable microphysical loop[13] at sufficiently low temperatures, such that the average time between two inelastic-scattering events is much larger than τ. (Note, however, that self-consistency effects and many-particle interactions have been neglected in our estimate.)

IV. ON THE NATURE OF CONDUCTING AND INSULATING STATES

The conducting or insulating nature of a state $\psi_j(\phi)$ of the one-dimensional systems described by Eq. (6) depends on the form of its energy $E_j(\phi)$. Since the current $I_j(\phi)$ is equal to $-c\partial E_j(\phi)/\partial\phi$, we define a state *conducting (insulating)* if $(I_j)_{\rm av} \gg 0$ ($\ll 0$), where $(I_j)_{\rm av}$ is the average value of $I_j(\phi)$ between two band edges. In other words, insulating states have flat energy curves. For monotonic curves as in Fig. 1, this means that the current of an insulating state is almost zero (or zero) for *all* times, i.e., a particle which at $t=0$ is at a band edge and, hence with velocity zero, cannot be accelerated sensibly for future times, in contrast to a conducting state.

It is interesting to note that the criterion[14] for localized (delocalized) states corresponding to weak (strong) dependence of the eigenvalues on the phase-boundary condition is consistent with our definitions, since changing the phase at the boundary in Ref. 14 is unitarily equivalent to a change of the flux origin in our Hamiltonians, as we have mentioned earlier.

We found that the functional dependence of $E_j(\phi)$ on ϕ is related to the mathematical structure of the wave functions $\psi_j(\phi)$ as follows: First, we repeat that for ϕ values, where $E_j(\phi)$ reaches a band edge [where $\partial E_j(\phi)/\partial\phi$ changes sign], one or several phase gradient centers (phase-singularity points being nodes of the wave function) lie on the one-dimensional domain D (except at the lowest band edge). Visualized in the extrapolation plane, this means that they cross the perimeter for these ϕ values (except in the lowest band edge). Further, from numerical calculations of a series of different examples (see also Refs. 3 and 15) we have found the following general behavior: *conducting* states are characterized by a *rapid* passage of the vortex centers across the perimeter. This means that this passage takes place during a time interval much smaller than $n\tau$ (corresponding to a flux interval much smaller than nhc/q). The vortex centers are then far away from the perimeter, except for this short flux interval in the neighborhood of the band-edge values. Further, outside this short flux interval, i.e., in the large ϕ intervals between adjacent band-edge values, the wave functions are appreciably different from zero for *all* spatial points of D and, in addition, are far from being real functions.

On the other hand, for *insulating* states the vortex centers pass across the perimeter *slowly*. They are situated close to their crossing points on the perimeter during most of the interval between neighboring band-edge values. (One can speak here of pinning or localization of the vortex centers at the perimeter.) As a consequence, the wave functions are nearly zero at these spatial points for *all* values of ϕ. We also found that insulating states are almost real functions for all ϕ. Our findings provide new insight into the *phase* structure of insulating and conducting states. In particular, the speed of motion of the phase vortex centers (phase singularities) in the extrapolation plane determines whether a state is insulating or conducting. This is a new characterization of these states.

We found further that for *insulating* states the following qualitative relation holds for *all* ϕ,

$$\frac{\hbar c}{q}\frac{\partial}{\partial x}\eta_j(x) - A_x \simeq 0 . \tag{41}$$

For these states Eq. (41) is valid at all points x, where the modulus $R(x)$ is appreciably different from zero. These are the points which lie outside the neighborhood of the nodes of $\psi_j(x;\phi=0)$, since these nodes are just the points where the phase singularities (i.e., the vortex centers) cross the perimeter periodically (see also Ref. 3). At the spatial points, where Eq. (41) holds, the effect of the vector potential is thus compensated for by the phase gradient and, hence, the current vanishes. In particular, Eq. (41) means that if the vector potential increases linearly with time [Eqs. (22) and (23)], the gradient of the phase also increases almost linearly with time at these points. We emphasize that such a relation, holding for times $t > n\tau$, is only possible because of the periodic appearance of phase singularities on points between the spatial intervals, where (41) holds, corresponding to the passage of phase gradient vortex centers across the perime-

ter. In addition, this passage must be slow. In the limit of a very strongly perturbing potential $V^1(x)$, expression (41) exactly tends to zero for states with sufficiently low energy. For example, in the ground state, in the presence of a thin but infinitely high barrier, this is true for all x outside the barrier.[15] Together with (23), Eq. (41) then becomes a relation of Josephson type, leading to *monochromatic* oscillations of the current with frequency $1/\tau = |qE_xL/h|$. (However, in this limit the amplitude of the current tends to zero.)

On the other hand, for a *conducting state the wave functions are similar to plane waves,* with modulus and phase nearly independent of ϕ for each flux period between two consecutive vortex-crossing intervals. But inside the small crossing intervals, $R_j(x)$ and $\eta_j(x)$ qualitatively change in the same manner as for an insulating state, only here this change is very *fast.*

The phase structure alone also gives information about the modulus $R(x)$ of the wave function due to the fact that the phase singularities are located at zeros of $R(x)$. Whenever phase singularities are close to the perimeter, the modulus $R(x)$ is almost zero at these spatial points on the perimeter. For an insulating state this situation occurs for all values of ϕ. This means that *the modulus of an insulating state is localized in disconnected regions* (situated between the vortex-crossing points) for *all* values of ϕ. For a conducting state this happens only in a short ϕ interval each time $E_j(\phi)$ reaches a band edge (except the lowest band edge). This characterizes insulating and conducting states of our periodic system *in terms of the modulus.* We believe that, together with the characteristic phase structure discussed in this paper, in particular with the nature of its time evolution in the presence of an electric field, it provides a rather complete description of insulating and conducting states, at least for the one-dimensional periodic systems discussed in this paper, where the potential $V(x)$ is fixed (i.e., where no averaging over a distribution of disorder is considered).

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