Narrow electronic bands in high electric fields: Static properties

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We present a gauge-invariant formalism for studying the motion of electrons in uniform electric and magnetic fields. This paper treats static properties, mainly the spectral function and density of states. These results will be exploited in a second paper devoted to transport, with the aim of extending the results of Khan, Davies, and Wilkins [Phys. Rev. B **36**, 2578 (1987)] to include periodic bands as well as parabolic bands. In particular, we define a gauge-invariant density of states that can be used in the presence of applied electric and magnetic fields. This density of states can be interpreted as a function of *kinetic* energy in the case of parabolic bands. It reduces smoothly to the usual results in the absence of applied fields and gains a tail into negative kinetic energies when an electric field is applied—a result well known from the theory of electroabsorption. Structure due to Landau levels is seen when a magnetic field is applied. The results are more striking in the case of a periodic energy band. Here the continuous density of states is split into a discrete "Stark ladder" when an electric field is applied, with the levels separated by the energy of Bloch oscillations. It is not necessary to introduce the Stark levels explicitly through the use of a scalar potential; they emerge naturally within the gauge-invariant formalism. Again the density of states shows no unphysical discontinuous behavior as the field goes to zero. The implications of these results for transport are briefly discussed.

I. INTRODUCTION

An exciting result of developments in the fabrication of ultrasmall structures is the ability to perform experiments that probe fundamental problems of quantum mechanics and solid-state physics. An outstanding example is the observation of periodic structure in the magnetoresistance of small loops as the flux through the loop is changed. This is intimately related to the Aharonov-Bohm effect, where a vector potential is used to change the phase of an electron's wave function and modulate the transmission coefficient of a ring-shaped structure. Research is currently under way to exploit this effect in switching devices. A more controversial phenomenon despite its longer history, and one for which there is less clear evidence, is that of Bloch oscillations or Stark ladders in a periodic structure. It may be possible to harness these oscillations directly, or to use negative differential resistance that may arise in the conductance. Again it is hoped to make use of this in practical devices. Artificial "crystals" with a one- or two-dimensional periodic potential may be formed in semiconductors by several methods. Alternating layers of different materials such as GaAs and (Al,Ga)As may be grown to produce a compositional superlattice; the doping of a single material may be changed periodically during growth to produce a doping superlattice; an interdigitated (or otherwise patterned) gate may be used to modulate the potential seen by a two-dimensional electron gas trapped at a heterojunction below the surface. Unfortunately, there is as yet no convincing observation of Bloch oscillations in these devices.

It is perhaps curious that the theory of Bloch oscillations remains controversial nearly 60 years after its inception; a review is given by Krieger and Iafrate.[1] The straightforward theory is well known. Under the influence of an electric field $\mathbf{F}$ that is constant (in time) and uniform (in space), a wave packet centered on crystal momentum $\mathbf{k}$ and with charge e evolves with time according to $\hbar d\mathbf{k}/dt = e\mathbf{F}$. The group velocity is given by $\hbar^{-1}\nabla_k \varepsilon(\mathbf{k})$ in a band with dispersion relation $\varepsilon(\mathbf{k})$, and the motion of the wave packet will therefore be periodic in time if $\varepsilon(\mathbf{k})$ is periodic in $\mathbf{k}$. If $\mathbf{F}$ is applied along a crystal axis of lattice constant a, the period of oscillation is $\tau_0 = 2\pi\hbar/|eFa|$ in time. This oscillatory motion of the electrons will affect their density of states too: one might expect it to be changed from a continuous band to a discrete ladder of states separated in energy by $E_0 = |eFa|$—the Stark ladder.

One objection to the simple theory of Bloch oscillations is that the possibility of (Zener) tunneling from one band to another is neglected. The transition rate has been estimated for a few cases (see Ref. 1) and has been found to be negligible over a wide range of electric fields. It is therefore legitimate to consider effects due to a high electric field within a single isolated band and we shall make that approximation, although the extension to many bands should prove interesting (and challenging). This paper presents the first steps towards a fully-gauge-invariant theory of transport in periodic bands in high

electric fields. It is built upon the earlier results of Khan, Davies, and Wilkins[2] (to be referred to as KDW), who investigated transport in a parabolic band in high electric fields.

We start by showing that it is useful—if not vital—to base the theory on Green functions rather than wave functions, because this permits the use of an entirely-gauge-invariant formalism which cannot be achieved with wave functions. A formalism that is gauge invariant has two important advantages. The first is that it avoids the possibility of making approximations that are intrinsically gauge dependent and therefore physically incorrect. The second is that it emphasizes the physical picture without having this obscured by features due to a particular gauge. The simplest quantity to calculate is the spectral function, from which a density of states can be deduced. The general theory is considered in Sec. II and the applications to electrons in parabolic bands and periodic bands in Secs. III and IV. Both Bloch oscillations and a Stark ladder follow naturally from this theory; moreover, the results reduce clearly to those in the absence of an electric field.

The main aim behind these calculations is to develop further the theory of KDW for transport in high electric fields. They considered only parabolic bands, but a richer variety of results is expected in a periodic band. For example, how is the transport equation modified to include Bloch oscillations? If a "Stark ladder" is formed, do the scattering rates change to reflect the form of jumps between the rungs of the ladders rather than transitions between plane waves? We touch on these questions briefly in the conclusions, but defer a full treatment to a following paper.

We start by considering the general theory of electrons in constant, uniform electric and magnetic fields.

II. THEORY OF ELECTRONS IN AN ELECTRIC FIELD

Since we are restricting attention to electrons in a single band, we may use an effective Hamiltonian of the form

$$H=\varepsilon\left[-i\nabla_r-\frac{e}{\hbar}\mathbf{A}(\mathbf{r},t)\right]+e\phi(\mathbf{r},t)\ , \tag{2.1}$$

which includes both a scalar potential ϕ and a vector potential $\mathbf{A}$; $\varepsilon(\mathbf{k})$ is the dispersion relation of the electrons. We shall set $\hbar=1$ from now on. The applicability and limitations of this effective Hamiltonian are considered in detail by Anderson.[3] It is valid "to all orders of perturbation theory," but is incapable of describing nonperturbative effects such as Zener tunneling or magnetic breakdown. The omission of Zener tunneling is particularly serious, since we are concerned with high electric fields, and future work will be directed towards overcoming the restriction to a single band.

Most work on this subject has been based on wave functions. These have a strong qualitative dependence on the gauge used for the electromagnetic potentials. We shall take two examples to illustrate this, a parabolic band and a co-sinusoidal tight-binding (periodic) band. First, consider free electrons in one dimension with

$$\varepsilon_f(k)=\frac{k^2}{2m}\ , \tag{2.2}$$

where the subscript f denotes a parabolic band, and m is the effective mass.

A. Parabolic band with a scalar potential

If a uniform, constant electric field is introduced through a scalar potential $\phi(x)=-eFx$, the Hamiltonian (2.1) becomes

$$H=-\frac{1}{2m}\frac{\partial^2}{\partial x^2}-eFx\ . \tag{2.3}$$

This has eigenfunctions which are stationary states, Airy integral functions of the first kind (Ref. 4, Sec. 10.4); Airy functions of the second kind cannot be normalized over all space,

$$\psi_\phi(x,t;\omega)\propto \mathrm{Ai}\left[\frac{1}{w}(eFx+\omega)\right]e^{-i\omega t},\quad w=\left[\frac{(eF)^2}{2m}\right]^{1/3}\ . \tag{2.4}$$

The eigenfunctions are standing waves, although it is possible to make current-carrying wave packets from superpositions of Airy functions. Most of their weight, apart from an exponentially small tail that represents tunneling into the classically forbidden region, is in the half-space to one side of $x=\omega/eF$. The energy eigenvalue ω may take any value from $-\infty$ to ∞; in contrast, only positive energies are allowed when no field is applied. The reason is that the Airy function depends on $x+\omega/eF$, so that wave functions with different energies occupy different regions of space—the wave function simply "slides along" as the energy changes. All energies are required in order to fill all space. This means that the density of states averaged over all space, which is the distribution of allowed values of ω, is uniform between $-\infty$ and ∞. This is qualitatively very different from its form in the absence of a field, and it changes discontinuously from one form to the other when an infinitesimal electric field is applied. A *local* density of states can also be defined, with less discontinuous behavior, and will be considered later.

B. Parabolic band with a vector potential

The results are entirely different if a different gauge with a vector potential $\mathbf{A}(t)=-\mathbf{F}t$ is used instead of a scalar potential. The Hamiltonian becomes

$$H=\frac{1}{2m}\left[-i\frac{\partial}{\partial x}+eFt\right]^2\ . \tag{2.5}$$

This is now a function of time and therefore does not yield stationary states, so there are no well-defined energies. However, the time-dependent Schrödinger equation has plane waves as solutions,

$$\psi_A(x,t;p) \propto \exp\left[i \left[px - \frac{1}{2m}[p^2 t + eFpt^2 + \tfrac{1}{3}(eF)^2 t^3] \right] \right] . \quad (2.6)$$

As the electric field is uniform in space, it is physically satisfactory to have a wave function that reflects this, emphasizing that canonical momentum $\mathbf{p}$ is a constant of the motion in this gauge. On the other hand, it is now impossible to construct a density of states at all, since no well-defined energies exist.

C. Periodic bands

New features appear if $\varepsilon(\mathbf{k})$ is periodic rather than parabolic, in which case the band has both upper and lower bounds. A simple one-dimensional example is

$$\varepsilon_t(k) = -C\cos(ka) ; \quad (2.7)$$

the subscript t denotes a periodic ("tight-binding") band. The band has width $2C$ and period $2\pi/a$ in k, corresponding to a lattice of period a in real space. The true wave functions of this model consist of sums over a tight-binding orbital $\chi(x)$ on each site, taking the form

$$\sum_n a_n \chi(x-na) . \quad (2.8)$$

The form of $\chi(x)$ is unknown, however, if the dispersion relation (2.7) alone is given,[5] and only the coefficients a_n can be calculated. This means that the eigenfunctions of a Hamiltonian incorporating (2.7) will appear to be of the form

$$\sum_n a_n \delta(x-na) , \quad (2.9)$$

with the δ functions reflecting the discrete lattice of sites. It is best to think of the coefficients a_n as comprising an envelope function.

D. Tight-binding band with a scalar potential

Introducing an electric field through a scalar potential, we have

$$H = \varepsilon_t\left[-i\frac{\partial}{\partial x} \right] - eFx \quad (2.10)$$

instead of (2.3). The eigenfunctions may be found by making a Fourier transform from x to k and back again; the result for the cosine band is

$$\psi_\phi(x,t;\omega) \propto e^{-i\omega t} \sum_n \delta(x-na-\omega/eF) J_n\left[-\frac{C}{E_0} \right] , \quad (2.11)$$

where $E_0 = eFa$ is the energy of Bloch oscillations. The wave function (2.11) makes sense only if the δ functions occupy the sites of the lattice [compare (2.9)], which places the restriction

$$\omega = NeFa \equiv NE_0 \quad (2.12)$$

on the allowed energies. The wave function is now restricted to a finite region of space, and there is a *ladder* of energies from $-\infty$ to ∞ instead of the continuous spectrum found for the parabolic band; this is the Stark ladder.

E. Tight-binding band with a vector potential

Using a vector potential, the Hamiltonian becomes

$$H = \varepsilon_t\left[-i\frac{\partial}{\partial x} + eFt \right] , \quad (2.13)$$

and the analogue of (2.6) is

$$\psi_A(x,t;p) \propto \exp\left[i \left[px - \int^t d\tau\, \varepsilon_t(p+eF\tau) \right] \right] . \quad (2.14)$$

The periodicity of $\varepsilon_t(k)$ means that this wave function is periodic in time; the period is $\tau_0 = 2\pi/E_0 \equiv 2\pi/eFa$, and is the period of Bloch oscillations. The wave function retains the form of a Bloch state in space, and continues to reflect the translational symmetry of the lattice, but energies can no longer be defined in the usual way.

F. Green functions

It is clear that the wave functions calculated above have very different properties depending on the gauge used to represent the electric field. For example, Bloch oscillations appear through the periodic behavior of $\psi_A(x,t;p)$ in time, but through the "ladder" of allowed energies for $\psi_\phi(x,t;\omega)$. These differences obscure the physics, which must be independent of the choice of gauge. It is, of course, possible to make a gauge transformation to go between the two sets of wave functions like (2.4) and (2.6). An important example is that the eigenfunctions of canonical momentum become the set of Houston functions if transformed to the scalar-potential gauge. On the other hand, one is led to ask whether it would not be better to use a gauge-invariant formalism from the start. This means that it is necessary to go one step beyond wave functions and use (single-particle) Green functions. These can be written in terms of products of two wave functions, between which the gauge dependence can be made to cancel. The most convenient function, and that which follows most naturally from wave functions, is the spectral function A—*not to be confused with the vector potential.* This is defined in terms of an anticommutator of field operators by

$$A(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2) = \langle \{\Psi(\mathbf{r}_1,t_1), \Psi^\dagger(\mathbf{r}_2,t_2)\} \rangle . \quad (2.15)$$

Although it is unusual to define the spectral function directly in this way, the definition is entirely equivalent to that usually given for the retarded and advanced Green functions.[6] The spectral function has an important sum rule that follows from the anticommutation relation of the operators at equal time,

$$A(\mathbf{r}_1,t;\mathbf{r}_2,t) = \langle \{\Psi(\mathbf{r}_1,t), \Psi^\dagger(\mathbf{r}_2,t)\} \rangle = \delta(\mathbf{r}_1-\mathbf{r}_2) . \quad (2.16)$$

The retarded and advanced Green functions G^r and G^a follow immediately from A in the time domain; for example,

$$G^r(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=-i\Theta(t_1-t_2)A(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)\ . \tag{2.17}$$

The combination of (2.15) and (2.17) yields the usual definition of the retarded Green function. If A is a function only of the difference of its time arguments, it may be Fourier transformed to an energy E. The precise definition of E is important, and will be given later. Provided that this may be done, the familiar formula

$$n(E)=-\frac{1}{\pi}\mathrm{Im}\,\mathrm{Tr}G^r(E)=\frac{1}{2\pi}\mathrm{Tr}\,A(E) \tag{2.18}$$

can be used to derive a density of states. The "trace" operation Tr means setting $\mathbf{r}_1=\mathbf{r}_2$ in A. If A is a function of $\mathbf{r}_1-\mathbf{r}_2$ only, it may be Fourier transformed to $\mathbf{k}$ and in this case the trace becomes a sum over all $\mathbf{k}$. This will be clarified later for specific examples.

The equations of motion for the spectral function can be written symbolically as

$$G_U^{-1}(1)A(1,2)=0 \quad \text{and} \quad A(1,2)G_U^{-1}(2)=0\ , \tag{2.19}$$

where

$$G_U^{-1}(1)=i\frac{\partial}{\partial t_1}-\varepsilon\left[-i\frac{\partial}{\partial \mathbf{r}_1}-e\,\mathbf{A}(\mathbf{r}_1,t_1)\right]-e\phi(\mathbf{r}_1,t_1)\ . \tag{2.20}$$

The equations in full are

$$\left[i\frac{\partial}{\partial t_1}-\varepsilon\left[-i\frac{\partial}{\partial \mathbf{r}_1}-e\,\mathbf{A}(\mathbf{r}_1,t_1)\right]-e\phi(\mathbf{r}_1,t_1)\right]A(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=0\ , \tag{2.21a}$$

$$\left[-i\frac{\partial}{\partial t_2}-\varepsilon\left[i\frac{\partial}{\partial \mathbf{r}_2}-e\,\mathbf{A}(\mathbf{r}_2,t_2)\right]-e\phi(\mathbf{r}_2,t_2)\right]A(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)=0\ , \tag{2.21b}$$

with the boundary condition given by (2.16). The equations of motion for the Green functions G^r and G^a have $\delta(\mathbf{r}_1-\mathbf{r}_2)\delta(t_1-t_2)$ instead of zero on the right-hand side, and obey different boundary conditions in time.

There are two routes to finding gauge-invariant spectral functions. One, taken by KDW, is to solve the equations of motion in a particular gauge and then to transform the solution into gauge-invariant form. A second method, which we shall follow here, is to make the equations of motion themselves gauge invariant. The following procedure achieves this for uniform, constant electric and magnetic fields, and is derived from the work of Langreth,[7] Keldysh,[8] and Levinson;[9] similar methods have been used by Mahan and co-workers.[10]

(i) Rather than use Eqs. (2.19) directly, form their sum and difference which can be written symbolically as

$$\{G_U^{-1},A\}=0 \quad \text{and} \quad [G_U^{-1},A]=0\ . \tag{2.22}$$

(ii) Change from the coordinates $(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)$ to sum-and-difference coordinates $(\mathbf{r},t;\mathbf{R},T)$ defined by

$$\begin{aligned}&\mathbf{R}=\tfrac{1}{2}(\mathbf{r}_1+\mathbf{r}_2), \quad \mathbf{r}=(\mathbf{r}_1-\mathbf{r}_2)\\ &T=\tfrac{1}{2}(t_1+t_2), \quad t=(t_1-t_2)\ .\end{aligned} \tag{2.23}$$

(iii) Make a Fourier transform from $(\mathbf{r},t)$ to $(\mathbf{p},\omega)$.
(iv) Replace $(\mathbf{p},\omega)$ by $(\mathbf{k},E)$, defined by

$$\mathbf{k}=\mathbf{p}-e\,\mathbf{A}(\mathbf{R},T), \quad E=\omega-e\phi(\mathbf{R},T)\ . \tag{2.24}$$

It is this last step that ensures gauge invariance. There is a simple classical analogy that illustrates this procedure. The "total" energy ω contains two components: the kinetic energy, and the potential energy due to the scalar potential. Clearly, the latter is gauge dependent, and should be subtracted out in the formula for E. This leaves a gauge-invariant quantity, which could be measured classically by $\frac{1}{2}mv^2$. Similarly, the vector potential $\mathbf{A}$ is subtracted from the canonical momentum $\mathbf{p}$ to leave the gauge-invariant mechanical momentum $\mathbf{k}$, which could be deduced classically from the velocity of the particle.

After this procedure, it is found that only the electric and magnetic fields $\mathbf{F}$ and $\mathbf{B}$ enter the equations of motion rather than the potentials $\mathbf{A}$ and ϕ, and that $\mathbf{R}$ and T have dropped out. This is to be expected because both the electronic system and the fields are translationally invariant in space and time. It is another advantage of the gauge-invariant formalism that only two variables are needed to describe the Green functions; by contrast, two spatial variables and one temporal variable would be needed in a scalar-potential gauge, or one spatial and two temporal variables if a vector potential were used. The equations of motion for the spectral function become

$$\tfrac{1}{2}\{G_U^{-1},A\}=\left[E-\frac{1}{2}\left\{\varepsilon\left[\mathbf{k}-\tfrac{1}{2}ie\left[\mathbf{F}\frac{\partial}{\partial E}+\mathbf{B}\times\frac{\partial}{\partial \mathbf{k}}\right]\right]+\varepsilon\left[\mathbf{k}+\tfrac{1}{2}ie\left[\mathbf{F}\frac{\partial}{\partial E}+\mathbf{B}\times\frac{\partial}{\partial \mathbf{k}}\right]\right]\right\}\right]A(\mathbf{k},E)=0 \tag{2.25a}$$

and

$$[G_U^{-1},A]=\left[e\mathbf{F}\cdot\frac{\partial}{\partial \mathbf{k}}+i\left\{\varepsilon\left[\mathbf{k}-\tfrac{1}{2}ie\left[\mathbf{F}\frac{\partial}{\partial E}+\mathbf{B}\times\frac{\partial}{\partial \mathbf{k}}\right]\right]-\varepsilon\left[\mathbf{k}+\tfrac{1}{2}ie\left[\mathbf{F}\frac{\partial}{\partial E}+\mathbf{B}\times\frac{\partial}{\partial \mathbf{k}}\right]\right]\right\}\right]A(\mathbf{k},E)=0\ . \tag{2.25b}$$

The solution of these equations for parabolic bands with both electric and magnetic fields will be given at the end of Sec. III, but we shall consider only electric fields in the remainder of the analysis. The first of these equations, (2.25a), can be simplified by making a Fourier transform from E to τ; this means that the time τ is conjugate to the gauge-invariant energy. The result (with $\mathbf{B}=\mathbf{0}$) is

$$\left[i\frac{\partial}{\partial\tau}-\tfrac{1}{2}[\varepsilon(\mathbf{k}+\tfrac{1}{2}e\mathbf{F}\tau)+\varepsilon(\mathbf{k}-\tfrac{1}{2}e\mathbf{F}\tau)]\right]A(\mathbf{k},\tau)=0\ , \tag{2.26}$$

which is of first order in τ and easily integrated to give

$$A(\mathbf{k},\tau)=\exp\left[-i\int_{-\tau/2}^{\tau/2}d\tau'\varepsilon(\mathbf{k}+e\mathbf{F}\tau')\right]\ , \tag{2.27}$$

where the normalization has been chosen to satisfy the boundary condition (2.16), which becomes

$$A(\mathbf{k},\tau=0)=1 \tag{2.28}$$

in terms of $A(\mathbf{k},\tau)$. The result (2.27) was previously derived by KDW [their Eq. (2.30)]. Note that A has the correct symmetry

$$A(\mathbf{k},-\tau)=A^*(\mathbf{k},\tau)\ . \tag{2.29}$$

The second equation, (2.25b), yields no additional information.

G. Sum rules

The ordinary spectral function is subject to a number of sum rules (see, for example, Chap. 3 of Ref. 11). The gauge-invariant quantity $A(\mathbf{k},E)$ also obeys sum rules. The most important of these has already been mentioned:

$$A(\mathbf{k},\tau)\,|_{\tau=0}\equiv\int_{-\infty}^{\infty}\frac{dE}{2\pi}A(\mathbf{k},E)=1 \tag{2.30}$$

[see Eqs. (2.16) and (2.28)]. This follows fundamentally from the anticommutator of the field operators in (2.15). Higher-order sum rules can be obtained by differentiating $A(\mathbf{r}_1,t_1;\mathbf{r}_2,t_2)$ with respect to t_1 and t_2 or, more simply, from the equations of motion (2.25). We find

$$i\frac{\partial}{\partial\tau}A(\mathbf{k},\tau)\bigg|_{\tau=0}\equiv\int_{-\infty}^{\infty}\frac{dE}{2\pi}EA(\mathbf{k},E)=\varepsilon(\mathbf{k}) \tag{2.31}$$

and

$$-\frac{\partial^2}{\partial\tau^2}A(\mathbf{k},\tau)\bigg|_{\tau=0}\equiv\int_{-\infty}^{\infty}\frac{dE}{2\pi}E^2A(\mathbf{k},E)=[\varepsilon(\mathbf{k})]^2 \quad \text{if } \mathbf{B}=\mathbf{0}\ . \tag{2.32}$$

If $\mathbf{B}\neq\mathbf{0}$, the last sum rule gives

$$\frac{1}{2}\left[\varepsilon\left(\mathbf{k}-\tfrac{1}{2}ie\mathbf{B}\times\frac{\partial}{\partial\mathbf{k}}\right)+\varepsilon\left(\mathbf{k}+\tfrac{1}{2}ie\mathbf{B}\times\frac{\partial}{\partial\mathbf{k}}\right)\right]\varepsilon(\mathbf{k})\ , \tag{2.33}$$

although this again reduces to (2.32) for parabolic bands. The spectral functions derived in the following sections can all be verified to obey these sum rules.

H. Comments

Several comments on the gauge-invariant functions can be made at this point.

(1) The equations of motion depend on the *fields*, not on the *potentials*. This removes problems associated with potentials that go to infinity, such as eFx in (2.3). It also avoids the problems associated with boundary conditions at $x=\pm\infty$ pointed out by Churchill and Holmstrom;[12] see also Rabinovitch.[13]

(2) The density of states in a scalar-potential gauge showed an unphysical discontinuous behavior when an electric field was turned on. The gauge-invariant density of states, a function of the energy E defined in (2.24), behaves smoothly in this limit. It is therefore a more physically satisfactory quantity. This will be illustrated in the following sections.

(3) The procedure described above also makes the Green functions and density of states gauge invariant in slowly varying fields, within the lowest order of a "gradient expansion."[14] The fields $\mathbf{F}$ and $\mathbf{B}$ will become functions of the center-of-mass variables $\mathbf{R}$ and T, but the expressions are otherwise unchanged.

(4) It is relatively straightforward to extend these results to an electric field that varies arbitrarily in time, provided that it remains uniform in space. The extension to spatially varying fields is much more complicated.

We shall now examine the spectral function and the density of states in detail for two cases of interest: a parabolic band and a periodic band, taking a one-dimensional cosinusoidal tight-binding band as an example.

III. PARABOLIC BANDS

We shall first derive the spectral function and density of states in an electric field for electrons with a parabolic dispersion relation, denoted by the subscript f:

$$\varepsilon_f(\mathbf{k})=\frac{k^2}{2m}\ . \tag{3.1}$$

The integral in (2.27) for the spectral function is trivial, yielding

$$A_f(\mathbf{k},\tau)=\exp\left[-i\frac{1}{2m}[k^2\tau+\tfrac{1}{12}(eF)^2\tau^2]\right]$$
$$\equiv\exp\left[-i\left[\varepsilon_f(\mathbf{k})\tau+\frac{1}{12}\frac{(eF)^2}{2m}\tau^3\right]\right]\ . \tag{3.2}$$

The Fourier transform of this back to the gauge-invariant energy E is an Airy function,

$$A_f(\mathbf{k},E)=2\pi\frac{2^{2/3}}{w}\mathrm{Ai}\left[-\frac{2^{2/3}}{w}[E-\varepsilon_f(\mathbf{k})]\right]\ , \tag{3.3}$$

where the "width"

$$w=\left[\frac{(eF)^2}{2m}\right]^{1/3}\ . \tag{3.4}$$

These results were used extensively by KDW. It is interesting that A_f does not depend on the direction of $\mathbf{F}$,

even though the field has broken the rotational symmetry of the system; this is true only for parabolic bands. As $\mathbf{F}\to\mathbf{0}$, $w\to 0$ and

$$A_f(\mathbf{k},E)\to 2\pi\delta(E-\varepsilon_f(\mathbf{k}))\ , \tag{3.5}$$

the usual result for a system without scattering. In a translationally invariant system with no applied field, $A(\mathbf{k},E)$ is non-negative even if scattering is included, which allows it to be interpreted as a probability density. This property no longer holds in an electric field, and $A_f(\mathbf{k},E)$ is a smoothly oscillating function taking both signs.

The density of states (per spin) $n_f(E)$ is given by a special case of (2.18), where the trace means a sum over all $\mathbf{k}$:

$$n_f(E)=\frac{1}{2\pi}\int\frac{d^dk}{(2\pi)^d}A_f(\mathbf{k},E)\ ; \tag{3.6}$$

at this point the dimensionality d enters. This can be interpreted as a density of states in *kinetic* energy, the gauge-independent variable E. The results for electrons in a parabolic band with $d=1,2$ and 3 are, for $d=1$,

$$n_f(E)=\left[\frac{2m}{w}\right]^{1/2}\left[\mathrm{Ai}\left[-\frac{E}{w}\right]\right]^2\ , \tag{3.7a}$$

for $d=2$,

$$n_f(E)=\frac{m}{2\pi}I\left[-\frac{2^{2/3}E}{w}\right]\ , \tag{3.7b}$$

and for $d=3$,

$$n_f(E)=\frac{m}{2\pi}(2mw)^{1/2}\left\{\left[\mathrm{Ai}'\left[-\frac{E}{w}\right]\right]^2+\frac{E}{w}\left\{\mathrm{Ai}\left[-\frac{E}{w}\right]\right\}^2\right\}\ , \tag{3.7c}$$

where

$$I(z)=\int_z^\infty dt\ \mathrm{Ai}(t) \tag{3.8}$$

and $\mathrm{Ai}'(z)$ is the derivative of $\mathrm{Ai}(z)$. The expressions are sketched in Fig. 1. For large energies in two and three dimensions, $n_f(E)$ approaches the form that it would have in the absence of an electric field. The singularity at the edge of the band is destroyed and instead there is a tail of width w to negative (kinetic) energies. This corresponds to the part of the wave function (2.4) with $z>0$ in $\mathrm{Ai}(z)$, representing tunneling into the classically forbidden region. For an effective mass $m^*=0.1$ and $F=1$ MV m^{-1}, $w\approx 7$ meV. These results are well known in the theory of electroabsorption (see Ref. 15), and the gauge-invariant density of states defined here is very closely related to the local density of states $n_\phi(\omega,\mathbf{R})$ calculated in a scalar-potential gauge. The connection is

$$n_\phi(\omega,\mathbf{R})=n_f(\omega+e\mathbf{F}\cdot\mathbf{R})\ . \tag{3.9}$$

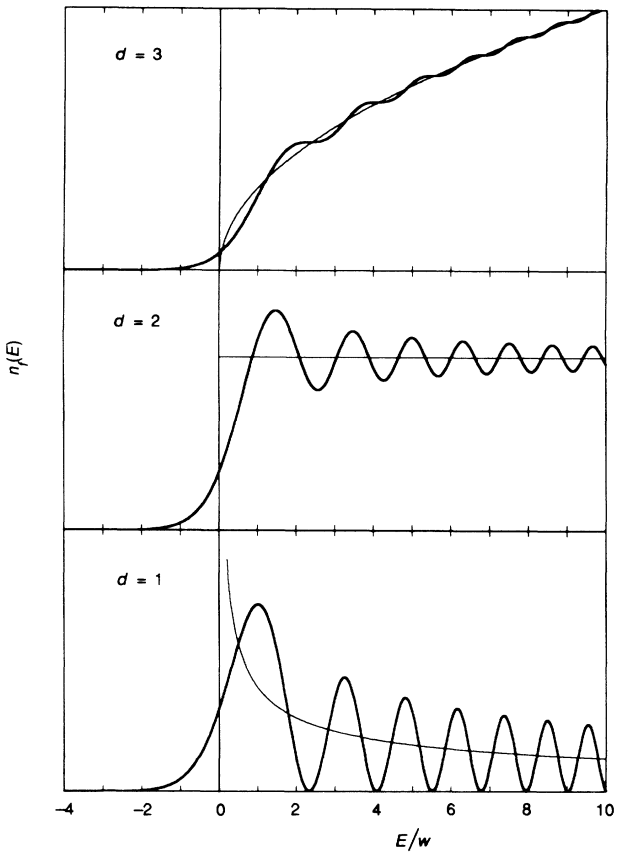

FIG. 1. Gauge-invariant density of states (thick curve) near the bottom of a parabolic band in an electric field in $d=1$, 2, and 3 spatial dimensions. Energies are plotted in units of $w=[(eF)^2/2m]^{1/3}$. The thin curves show the density of states in the absence of a field for comparison.

In one dimension $n_f(E)$ does not approach the density of states in the absence of a field, but continues to oscillate between zero and twice the "$E^{-1/2}$" form. The reason for this can be seen from the wave functions (2.4). Consider a fixed point x. As the energy is raised, the wave functions "slide past" because of their dependence on $x+\omega/eF$. At certain energies there are nodes in the wave function and therefore no contribution to the local density of states. Equation (3.9) shows that these nodes survive in the gauge-invariant density of states $n_f(E)$. This effect is largely washed out in higher dimensions by motion transverse to the field, although the oscillations at small energies in the two-dimensional case do not decrease in amplitude as the strength of the field decreases, but are compressed into an ever smaller range of energies at the bottom of the band.

A. Electric and magnetic fields

It is possible to calculate $A_f(\mathbf{k},E)$ for electrons in uniform electric and magnetic fields, because Eqs. (2.25) simplify considerably in the case of parabolic bands. They become

$$\left[E-\frac{1}{2m}\left\{k^2-\frac{e^2}{4}\left[F^2\frac{\partial^2}{\partial E^2}+B^2\frac{\partial^2}{\partial \mathbf{k}^2}-\left[\mathbf{B}\cdot\frac{\partial}{\partial \mathbf{k}}\right]^2+2\mathbf{F}\times\mathbf{B}\cdot\frac{\partial}{\partial \mathbf{k}}\frac{\partial}{\partial E}\right]\right\}\right]A_f(\mathbf{k},E)=0 \tag{3.10a}$$

and

$$\left[e\mathbf{F}\cdot\frac{\partial}{\partial \mathbf{k}}+2\frac{e}{2m}\left[\mathbf{k}\cdot\mathbf{F}\frac{\partial}{\partial E}+\mathbf{k}\times\mathbf{B}\cdot\frac{\partial}{\partial \mathbf{k}}\right]\right]A_f(\mathbf{k},E)=0\ . \tag{3.10b}$$

The solution of these equations is straightforward but rather tedious, and again it is easier if they are Fourier transformed from E to τ. The result can be written as

$$A_f(\mathbf{k},\tau)=e^{-i\mathbf{v}_d\cdot\mathbf{k}\tau}A_K(\mathbf{k}-m\mathbf{v}_d,\tau)\ , \tag{3.11}$$

where

$$\mathbf{v}_d=\frac{1}{B^2}\mathbf{F}\times\mathbf{B} \tag{3.12}$$

is the drift velocity perpendicular to both $\mathbf{F}$ and $\mathbf{B}$. The "drifted" spectral function A_K obeys the equations of motion

$$\left\{i\frac{\partial}{\partial\tau}-\frac{1}{2m}K^2+\tfrac{1}{2}mv_d^2+\frac{e^2}{8m}\left[-F_\parallel^2\tau^2+B^2\frac{\partial^2}{\partial \mathbf{K}^2}-\left[\mathbf{B}\cdot\frac{\partial}{\partial \mathbf{K}}\right]^2\right]\right\}A_K(\mathbf{K},\tau)=0 \tag{3.13a}$$

and

$$\frac{e}{m}\left[\mathbf{K}\times\mathbf{B}\cdot\frac{\partial}{\partial \mathbf{K}}+mF_\parallel\hat{\mathbf{B}}\cdot\frac{\partial}{\partial \mathbf{K}}+iF_\parallel\tau\hat{\mathbf{B}}\cdot\mathbf{K}\right]A_K(\mathbf{K},\tau)=0\ , \tag{3.13b}$$

where

$$F_\parallel=\hat{\mathbf{B}}\cdot\mathbf{F} \tag{3.14}$$

is the component of the electric field parallel to the magnetic field, and $\hat{\mathbf{B}}$ is a unit vector parallel to $\mathbf{B}$. These equations are to be solved subject to the boundary condition (2.28). This is most easily done in cylindrical polar coordinates, where K_ρ is the radial component and K_z is the z component parallel to $\mathbf{B}$. Equations (3.13) then take the form

$$\left[i\frac{\partial}{\partial\tau}-\frac{1}{2m}(K_\rho^2+K_z^2)+\tfrac{1}{2}mv_d^2-\frac{e^2}{8m}F_\parallel^2\tau^2+\frac{e^2}{8m}B^2\left[\frac{\partial^2}{\partial K_\rho^2}+\frac{\partial}{K_\rho\partial K_\rho}+\frac{\partial^2}{K_\rho^2\partial K_\phi^2}\right]\right]A_K(K_\rho,K_\phi,K_z,\tau)=0 \tag{3.15a}$$

and

$$\frac{e}{m}\left[-B\frac{\partial}{\partial K_\phi}+mF_\parallel\frac{\partial}{\partial K_z}+iF_\parallel\tau K_z\right]A_K(K_\rho,K_\phi,K_z,\tau)=0\ . \tag{3.15b}$$

Note that the second equation shows no dependence on K_ρ at all. The drifted spectral function is finally found to be

$$A_K(\mathbf{K},\tau)=2e^{-K_\rho^2/eB}\sum_{n=0}^{\infty}(-1)^nL_n\left[\frac{2}{eB}K_\rho^2\right]\exp\left[-i\left[\frac{1}{2m}K_z^2\tau+\frac{1}{12}\frac{e^2}{2m}F_\parallel^2\tau^3\right]\right]\exp\{-i[(n+\tfrac{1}{2})\omega_c-\tfrac{1}{2}mv_d^2]\tau\}\ , \tag{3.16}$$

where

$$\omega_c=\frac{eB}{m} \tag{3.17}$$

is the cyclotron frequency. The sum over n with Laguerre polynomials L_n reflects the Landau levels induced by the magnetic field. Motion parallel to $\mathbf{B}$ is unaffected by this and the terms with $K_z^2\tau$ and $F_\parallel^2\tau^3$ are exactly as for a one-dimensional system in an electric field $F_\parallel$. The final feature is the uniform drift velocity $\mathbf{v}_d$ in crossed electric and magnetic fields. Mahan[10] has given a similar result. The Fourier transform to real space is given by

$$A_f(\mathbf{r},\tau)=e^{im\mathbf{v}_d\cdot(\mathbf{r}-\mathbf{v}_d\tau)}A_s(\mathbf{r}-\mathbf{v}_d\tau,\tau)\ , \tag{3.18}$$

with

$$A_s(\mathbf{s},\tau)=\frac{eB}{2\pi}e^{-eBs_\rho^2/4}\sum_{n=0}^{\infty}L_n\left[\frac{eB}{2}s_\rho^2\right]\exp\{-i[(n+\tfrac{1}{2})\omega_c-\tfrac{1}{2}mv_d^2]\tau\}\left[\frac{m}{2\pi i\tau}\right]^{1/2}\exp\left\{-i\left[\frac{1}{12}\frac{e^2}{2m}F_\parallel^2\tau^3-\frac{m}{2\tau}s_z^2\right]\right\}\ , \tag{3.19}$$

which is again expressed in cylindrical polar coordinates and exhibits the same features as (3.16). The drift motion is shown particularly clearly by (3.18).

The gauge-invariant density of states can be obtained by setting $\mathbf{r}=\mathbf{0}$ in (3.18), which performs the trace required in (2.18), and taking the Fourier transform from τ to E. The result is best written as a convolution,

$$n_f(E)=\int_{-\infty}^{\infty} d\bar{E}\, n_{\parallel}(\bar{E})n_{\perp}(E-\bar{E})\ . \tag{3.20}$$

The first part, $n_{\parallel}(E)$, is due to the motion parallel to $\mathbf{B}$ and is the density of states for a one-dimensional system in an electric field $F_{\parallel}$:

$$n_{\parallel}(E)=\left[\frac{2m}{w}\right]^{1/2}\left[\mathrm{Ai}\left[-\frac{E}{w_{\parallel}}\right]\right]^2, \tag{3.21}$$

with

$$w_{\parallel}=\left[\frac{(eF)^2}{2m}\right]^{1/3}. \tag{3.22}$$

This reduces to

$$\frac{1}{\pi}\left[\frac{m}{2E}\right]^{1/2}\Theta(E) \tag{3.23}$$

if $F_{\parallel}=0$, where $\Theta(E)$ is a step function. The "transverse" part $n_{\perp}(E)$ is influenced by the Landau levels and drift motion in the plane normal to $\mathbf{B}$:

$$n_{\perp}(E)=\frac{eB}{2\pi}\sum_{n=0}^{\infty}\frac{1}{(\pi eBv_d^2)^{1/2}}\exp\left[-\frac{[E-\frac{1}{2}mv_d^2-(n+\frac{1}{2})\omega_c]^2}{eBv_d^2}\right]H_n^2\left[\frac{E-\frac{1}{2}mv_d^2-(n+\frac{1}{2})\omega_c}{(eBv_d^2)^{1/2}}\right], \tag{3.24}$$

where $H_n(z)$ is a Hermite polynomial (following the notation of Abramowitz and Stegun[4]). If there is no component of $\mathbf{F}$ perpendicular to $\mathbf{B}$, in which case $\mathbf{v}_d=\mathbf{0}$, this reduces to the well-known set of Landau levels,

$$n_{\perp}(E)=\frac{eB}{2\pi}\sum_{n=0}^{\infty}\delta(E-(n+\tfrac{1}{2})\omega_c)\ . \tag{3.25}$$

The δ functions are broadened by the drift motion if $\mathbf{v}_d\neq\mathbf{0}$; their functional forms are those of the probability density of the levels of a harmonic oscillator.

These results should be useful in analyzing transport in strong electric and magnetic fields. An example of an interesting process is "quasi-elastic inter-Landau level scattering" (QUILLS) proposed by Eaves *et al.*,[16] where transport occurs by hopping from one Landau level to another with the energy provided by the electric field.

We shall now abandon magnetic fields and investigate the behavior of a periodic energy band in an electric field.

IV. PERIODIC BANDS

We shall consider only a one-dimensional model for simplicity and because this emphasizes the properties induced by the electric field. The lattice constant is a, so the dispersion relation $\varepsilon_t(k)$ has period $2\pi/a$ in k; the subscript t denotes a periodic ("tight-binding") band. The energy now has an upper bound as well as a lower bound (the parabolic band has only a lower bound). The spectral function is given [using (2.27)] by

$$A_t(k,\tau)=\exp\left[-i\int_{-\tau/2}^{\tau/2}d\tau'\varepsilon_t(k+eF\tau')\right]. \tag{4.1}$$

One might expect $A_t(k,\tau)$ to be periodic in τ with the period of Bloch oscillations, given by

$$\tau_0=\frac{2\pi}{E_0},\quad E_0=|eFa| \tag{4.2}$$

(A_t is, of course, periodic in k). Surprisingly, this is not the case. Consider instead $A_t(k,\tau+2\tau_0)$:

$$A_t(k,\tau+2\tau_0)=\exp\left[-i\int_{-\tau/2-\tau_0}^{\tau/2+\tau_0}d\tau'\varepsilon_t(k+eF\tau')\right]. \tag{4.3}$$

The integral can be reduced as follows:

$$\int_{\tau/2}^{\tau/2+\tau_0}d\tau'\varepsilon_t(k+eF\tau')=\frac{1}{|eF|}\int_{eF\tau/2+k}^{eF\tau/2+k+2\pi/a}d\kappa\,\varepsilon_t(\kappa)=\frac{I_0}{|eF|}, \tag{4.4}$$

where I_0 is a constant independent of τ and k because the integral is over a full cycle of a periodic function:

$$I_0=\int_0^{2\pi/a}d\kappa\,\varepsilon_t(\kappa)\ . \tag{4.5}$$

The part of the integral from $-\tau/2-\tau_0$ to $-\tau/2$ can be treated likewise. Therefore,

$$A_t(k,\tau+2\tau_0)=e^{-2iI_0/|eF|}A_t(k,\tau)\ . \tag{4.6}$$

Equation (4.5) shows that I_0 is the average energy in the band. It may therefore be made to vanish by choosing the reference of energy judiciously [i.e., by adding a constant to $\varepsilon_t(k)$]. Equation (4.6) then shows that $A_t(k,\tau)$ has period $2\tau_0$ in τ, and it can be verified that there is no period of τ_0. If we make a Fourier transform from τ to the gauge-invariant energy E, the resulting function $A_t(k,E)$ will be a sum of δ functions with spacing $\frac{1}{2}E_0$, not E_0, which is expected to be the spacing of the Stark ladder.

This periodic behavior of A_t is very different from that in the absence of an applied field. In that case the spectral function is given by

$$A_t(k,\tau)=e^{-i\varepsilon_t(k)\tau}, \tag{4.7}$$

which shows that A_t has a *different* period in τ for each value of k. By contrast, we see from Eq. (4.6) that A_t has the *same* period $2\tau_0$ for *all* k when a field is applied. This qualitative difference is blurred by scattering, which causes $A_t(k,\tau)$ to decay for large $|\tau|$. The fact that A_t has the same period in τ for all k is essentially a manifestation of Bloch oscillations, showing that the motion of electrons is periodic; in fact, the period of $|A_t(k,\tau)|^2$ is τ_0, the period expected for Bloch oscillations.

Next, consider the density of states as a function of the gauge-invariant energy E. In a periodic band the trace in Eq. (2.18) becomes

$$n_t(E)=\frac{1}{2\pi}\int_{-\pi/a}^{\pi/a}\frac{dk}{2\pi}A_t(k,E)=\frac{1}{2\pi}\int_{-\pi/a}^{\pi/a}\frac{dk}{2\pi}\int_{-\infty}^{\infty}d\tau\exp\left[i\left[E\tau-\int_{-\tau/2}^{\tau/2}d\tau'\varepsilon_t(k+eF\tau')\right]\right], \tag{4.8}$$

which has an integral only over the Brillouin zone, not over all k. If the integral over k is performed before the Fourier transform from τ to E, the resulting function of τ has period τ_0 rather than $2\tau_0$, thus ensuring that $n_t(E)$ is a set of δ functions with spacing E_0 as one would physically expect. The density of states appears to consist of δ functions even for infinitesimal fields, while it is a continuous function if the field is strictly zero. This anomaly disappears if one considers the spectral function in the presence of scattering. Roughly speaking, the δ functions are broadened by the scattering to a width Γ given by the scattering rate. The peaks in $n_t(E)$ are well separated if $\Gamma \ll E_0$, and the approximation of using δ functions is accurate. In the opposite limit of small electric fields, where $E_0 \ll \Gamma$, the peaks merge together to form a continuous function and all trace of periodicity is lost. The physical picture is that an electron is scattered before it has had time to complete more than a small fraction of a Bloch oscillation.

The density of states given by (4.8) can usefully be termed a "Stark ladder," but it is important to distinguish between this and the Stark ladder defined in Sec. II, which had "rungs" of equal weight and extended from $-\infty$ to ∞. The ladder defined by (4.8) has rungs of varying weight, and does not extend far beyond the unperturbed bandwidth unless the applied field is very strong. This will be made clear by an example.

A. One-dimensional cosinusoidal band

Consider a cosinusoidal band of the form

$$\varepsilon_t(k)=-C\cos(ka)\ ; \tag{4.9}$$

the bandwidth is $2C$ and the effective mass near the extrema is $m^*=1/a^2C$. The spectral function for this band is

$$A_t(k,\tau)=\exp\left[iC\int_{-\tau/2}^{\tau/2}d\tau'\cos[(k+eF\tau')a]\right]$$
$$=\exp\left[-i\varepsilon_t(k)\frac{\sin(\frac{1}{2}E_0\tau)}{\frac{1}{2}E_0}\right]. \tag{4.10}$$

This correctly reduces to

$$\exp[-i\varepsilon_t(k)\tau] \tag{4.11}$$

as $F\to 0$, with period $2\pi/\varepsilon_t(k)$ in τ, while its period is $4\pi/E_0\equiv 2\tau_0$ when $F\neq 0$ as shown for the general case above. Next take the Fourier transform, which returns us to the gauge-invariant energy E,

$$A_t(k,E)=\int_{-\infty}^{\infty}d\tau\exp\left[i\left[E\tau-\varepsilon_t(k)\frac{\sin(\frac{1}{2}E_0\tau)}{\frac{1}{2}E_0}\right]\right]. \tag{4.12}$$

Set $u=\frac{1}{2}E_0\tau$, and exploit the periodicity by splitting the integral into pieces 2π long,

$$A_t(k,E)=\frac{2}{E_0}\sum_{n=-\infty}^{\infty}\exp\left[2\pi i n\frac{E}{\frac{1}{2}E_0}\right]\int_{-\pi}^{\pi}du\exp\left[i\left[\frac{E}{\frac{1}{2}E_0}u-\frac{\varepsilon_t(k)}{\frac{1}{2}E_0}\sin u\right]\right]. \tag{4.13}$$

The summation can be treated separately, and the Poisson summation formula yields

$$\sum_n\exp\left[2\pi i n\frac{E}{\frac{1}{2}E_0}\right]=\sum_n\delta\left[n-\frac{E}{\frac{1}{2}E_0}\right]$$
$$=\tfrac{1}{2}E_0\sum_n\delta\left[E-n\frac{E_0}{2}\right], \tag{4.14}$$

while the remaining integral is

$$\int_{-\pi}^{\pi}du\exp\left[i\left[nu-\frac{\varepsilon_t(k)}{\frac{1}{2}E_0}\sin u\right]\right]=2\pi J_n\left[\frac{\varepsilon_t(k)}{\frac{1}{2}E_0}\right], \tag{4.15}$$

where J_n is a Bessel function of the first kind. Thus,

$$A_t(k,E)=2\pi\sum_{n=-\infty}^{\infty}J_n\left[\frac{\varepsilon_t(k)}{\frac{1}{2}E_0}\right]\delta\left[E-n\frac{E_0}{2}\right]. \tag{4.16}$$

The spectral function is a set of δ functions of spacing $\frac{1}{2}E_0$, as asserted before. The Bessel functions $J_n(z)$ decay rapidly for $|n|>|z|$, or $|E|>|\varepsilon_t(k)|$. This means that $A_t(k,E)$ is mainly confined within the bandwidth $|E|<C$, but has exponentially decaying tails outside. An interesting special case is $k=\pm\pi/2a$, the middle of the band in energy, where $\varepsilon_t(k)=0$. Using the identity $J_n(0)=0$ for $n\neq 0$, we see that

$$A_t(k=\pm\pi/2a, E)=2\pi\delta(E) . \tag{4.17}$$

$A_t(k,E)$ can be divided into two sets of peaks using the relation for Bessel functions,

$$J_n(-z)=(-1)^n J_n(z) . \tag{4.18}$$

This shows that the series of peaks with $n=0,\pm2,\pm4,\ldots$ contributes an even function of E, while the series with $n=\pm1,\pm3,\ldots$ is odd in E. This further implies that $A_t(k,E)$ is generally two-signed; this is like $A_f(k,E)$, but is unlike the spectral function in the absence of a field. The peaks with odd n are vital to satisfy the sum rules of Sec. II.

The density of states $n_t(E)$ is found from (4.8) and (4.16) to be

$$n_t(E)=\frac{1}{a}\sum_{n=-\infty}^{\infty}\left[J_n\left[\frac{C}{E_0}\right]\right]^2\delta(E-nE_0) , \tag{4.19}$$

which is a ladder with the expected spacing E_0. It must be stressed again that the energy argument E is the gauge-invariant energy, not the "total" energy. It seems to be difficult to give a precise physical description of E because there is no classical analogue like the kinetic energy of a free particle, as there is for a parabolic band. The concept of kinetic energy is generalized in quantum mechanics to allow negative values during tunneling, as shown by the densities of states in Fig. 1. The concept of "band energy" needs to be generalized in the same way to include the energies outside the original band shown in the density of states (4.19). These correspond to electrons tunneling into "classically forbidden regions" under the influence of the applied electric field, and are illustrated by the tails of the wave functions (2.11).

The density of states given by (4.19) is plotted against energy in Fig. 2, using the dimensionless variables $aCn_t(E)$ and E/C. The heights of the bars representing the δ functions are

$$\frac{C}{E_0}\left[J_n\left[\frac{C}{E_0}\right]\right]^2 , \tag{4.20}$$

which are the values that would be obtained if the density of states were broadened into a smooth curve. This allows a direct comparison with the density of states in the absence of an electric field, but this way of plotting the data unfortunately tends to give the misleading impression that the number of states in the band decreases at large electric fields. The densities of states are symmetric in E and, like A_t, exhibit tunneling beyond the edges of the band. Note that the "Stark ladders" shown in Fig. 2 are largely confined within the original band ($|E|<C$) and do not extend to $\pm\infty$ as they would if "total" energy rather than the gauge-invariant energy were used [compare Eq. (2.12)]. The envelope of the δ functions approaches the density of states in the absence of a field as $E_0/C\to0$, except for the oscillations due to the one-dimensional nature of the system, discussed in Sec. III in connection with $n_f(E)$.

The behavior near the edges of the band can be estimated using the asymptotic expansion for Bessel functions in terms of Airy functions:

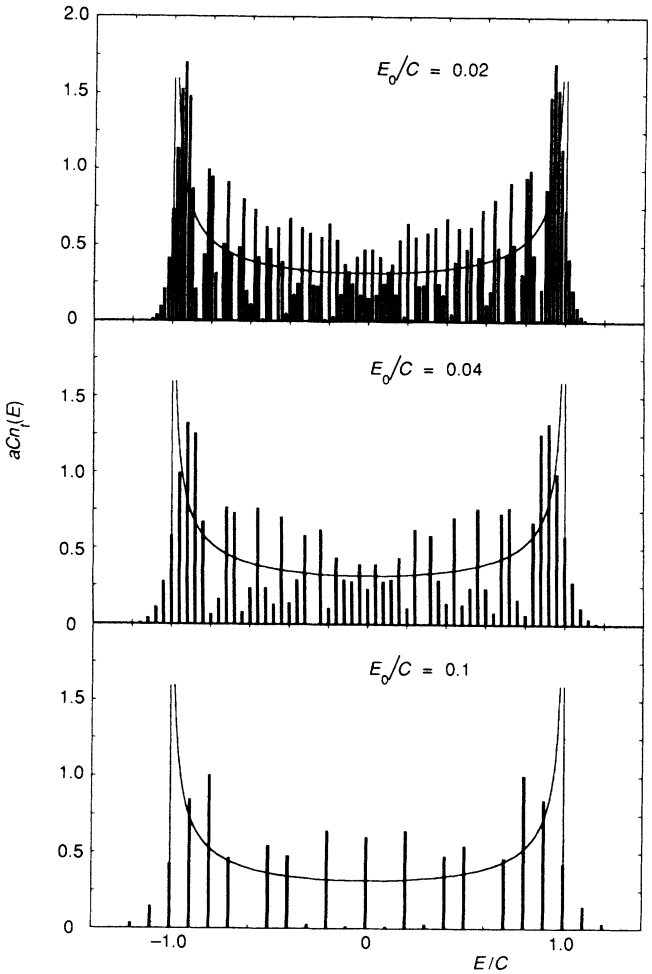

FIG. 2. Gauge-invariant density of states (bars) for a one-dimensional periodic (cosine) band, for three ratios of the Stark energy $E_0=eFa$ to the half-bandwidth C. The thin continuous curve shows the density of states in the absence of a field for comparison.

$$J_v(v+v^{1/3}z)\sim\left[\frac{2}{v}\right]^{1/3}\mathrm{Ai}(-2^{1/3}z) \tag{4.21}$$

(Ref. 4, Eq. 9.3.23). Using this near the bottom of the band, $E\approx-C$, we find that (4.19) can be approximated by

$$n_t(E)\approx\left[\frac{2m^*}{w^*}\right]^{1/2}\left[\mathrm{Ai}\left[-\frac{E-(-C)}{w^*}\right]\right]^2 \times\sum_n\delta\left[\frac{E}{E_0}-n\right] , \tag{4.22}$$

where

$$w^*=\left[\frac{(eF)^2}{2m^*}\right]^{1/3}=(\tfrac{1}{2}E_0^2C)^{1/3} \tag{4.23}$$

sets the scale on which the density of states decays outside the original band, and $m^*=1/a^2C$ is the effective mass at the bottom of the cosine band. The envelope of (4.22) is exactly the density of states at the bottom of a

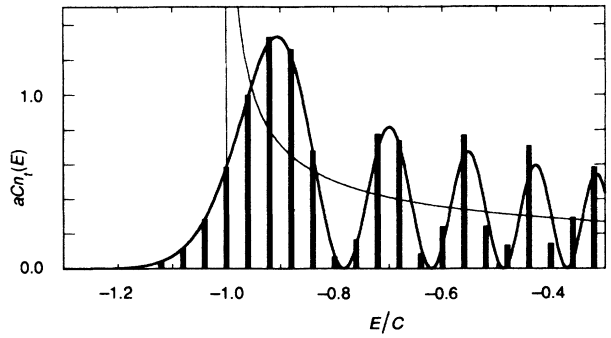

FIG. 3. Comparison of the density of states near the lower edge of a cosinusoidal band (bars) with that of a parabolic band with the same effective mass (thick curve). The strength of the electric field gives $E_0/C=0.04$, and the thin curve shows the density of states for the cosine band in the absence of a field.

one-dimensional band with effective mass m^*, given by (3.7a). This is illustrated in Fig. 3.

B. Modified spectral functions

Our main purpose in calculating the spectral functions, apart from obtaining the density of states, is to use them in calculating scattering rates in a quantum-mechanical transport equation (see KDW, Sec. II D). The peaks in $A_t(k,E)$ at half-integral spacings of E_0 may therefore present something of an embarrassment, as we would expect scattering to be between rungs of the Stark ladder and that the energies of the initial and final states should differ by integral multiples of E_0. This anomaly can be removed by the introduction of modified spectral functions, which KDW found to be more appropriate in the construction of scattering rates. These modified functions $A_\pm(\mathbf{k},\tau)$ are defined in general (not just for periodic bands) by

$$\begin{aligned} A_\pm(\mathbf{k},\tau) &= A(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}\tau,\tau) \\ &= \exp\left[-i\int_{-\tau/2}^{\tau/2} d\tau'\varepsilon(\mathbf{k}\pm\tfrac{1}{2}e\mathbf{F}\tau+e\mathbf{F}\tau')\right] \\ &= \exp\left[-i\int_0^{\tau} d\tau'\varepsilon(\mathbf{k}\pm e\mathbf{F}\tau')\right] . \end{aligned} \tag{4.24}$$

For a periodic energy band, in which case $\varepsilon(k)=\varepsilon_t(k)$, the resulting functions $A_\pm(k,\tau)$ have period τ_0 in τ, in contrast to the unmodified functions $A(k,\tau)$ which had period $2\tau_0$. This is clear since if τ is replaced by $\tau+\tau_0$ in (4.24) this just adds one complete cycle of $\varepsilon_t(k)$ to the integral. In turn, the modified Fourier transforms $A_{t\pm}(k,E)$ are sets of δ functions separated by E_0. For the cosinusoidal band,

$$A_{t\pm}(k,\tau)=\exp\left[i\frac{C}{E_0}[\sin(ka\pm E_0\tau)\mp\sin(ka)]\right] . \tag{4.25}$$

Note that the modified spectral functions obey

$$A_\pm(\mathbf{k},-\tau)=A^*_\mp(\mathbf{k},\tau) \tag{4.26}$$

rather than the usual relation (2.29). This means that the modified Fourier transforms $A_\pm(\mathbf{k},E)$ will not be purely real as is the case for conventional spectral functions; the pair are related by

$$A_\pm(\mathbf{k},E)=A^*_\mp(\mathbf{k},E) . \tag{4.27}$$

In the case of the cosinusoidal band,

$$\begin{aligned} A_{t\pm}(k,E)=2\pi\sum_{n=-\infty}^{\infty}&\exp\left[\pm i\left[\frac{C}{E_0}\sin(ka)+nka\right]\right] \\ &\times J_n\left[\frac{C}{E_0}\right]\delta(E-nE_0) , \end{aligned} \tag{4.28}$$

which shows the expected spacing E_0 of the δ functions.

C. Spectral functions in real space

It is sometimes useful to have expressions for the spectral functions in real space rather than $\mathbf{k}$ space. Consider first

$$A(\mathbf{r},\tau)=\int\frac{d\mathbf{k}}{(2\pi)^d}e^{i\mathbf{k}\cdot\mathbf{r}}A(\mathbf{k},\tau)=\int\frac{d\mathbf{k}}{(2\pi)^d}\exp\left[i\left[\mathbf{k}\cdot\mathbf{r}-\int_{-\tau/2}^{\tau/2}d\tau'\varepsilon(\mathbf{k}+e\mathbf{F}\tau')\right]\right] . \tag{4.29}$$

Note that $\mathbf{r}$ is a *relative* coordinate; there is no "center-of-mass" coordinate because of the translational symmetry. Restrict attention to one-dimensional periodic systems. The periodicity of $\varepsilon_t(k)$ means that the integral over k may be split into segments of length $2\pi/a$ in the same way as the integral over τ in (4.12). The result is again a sum over δ functions:

$$A_t(x,\tau)=\sum_n\delta(x-na)\frac{a}{2\pi}\int_0^{2\pi/a}dk\exp\left[i\left[nka-\int_{-\tau/2}^{\tau/2}d\tau'\varepsilon_t(k+eF\tau')\right]\right] . \tag{4.30}$$

This contains a sum over δ functions for the same reason as the wave function (2.9) of the tight-binding model, and should be regarded as an envelope function.

In the limit of large electric fields, $A_t(x,\tau)$ becomes localized in space. Consider the integral over τ' in (4.30). This can be written as

$$\frac{1}{eF}\int_{k-eF/2}^{k+eF/2} d\kappa\, \varepsilon_t(\kappa) \tag{4.31}$$

by making the substitution $\kappa = k + eF\tau'$. Now $\varepsilon_t(\kappa)$ is a periodic function, and its integral over one period is given by I_0 [Eq. (4.5)], which has been chosen to be zero. Therefore the part of the integral in (4.31) that covers full periods of $\varepsilon_t(\kappa)$ vanishes. This means that the integral does not grow monotonically as F (and therefore the range of the integral) increases, but remains bounded. The prefactor then forces the overall value of (4.31) to decay as $1/eF$ at large fields. In the limit of very large fields this term may be dropped completely and we find from (4.29) the limit

$$\lim_{F\to\infty} A_t(k,\tau) = \int \frac{d\mathbf{k}}{(2\pi)^d}\exp(i\mathbf{k}\cdot\mathbf{r}) = \delta(\mathbf{r}) \ . \tag{4.32}$$

This result shows that the spectral function becomes localized onto one site in very strong fields, and the Stark states must do the same. The reason is best seen by taking a scalar potential. This induces a difference in energy of $E_0 = |eFa|$ between adjacent sites. The amplitude for tunneling between the sites falls drastically if this difference in energy exceeds the bandwidth $2C$. The Stark states and spectral function then become localized mainly onto single sites, and the sites are effectively isolated from one another. The condition for this localization to occur is

$$E_0 \gg C \ . \tag{4.33}$$

In an ordinary crystal, where $a \approx 0.3$ nm and $C \approx 2$ eV, this requires colossal fields of order 10^{10} V m^{-1}. Superlattices in semiconductors have much larger values of a, around 10 nm, and smaller values of C, around 10 meV. In this case fields need only exceed about 10^6 V m^{-1} to fulfill condition (4.33) and achieve isolation of the "sites." Zener tunneling between bands is likely to be significant under these conditions, however, and should be included.

For the example of the cosine band, the spectral function in real space becomes

$$A_t(x,\tau) = \sum_n \delta(x-na) i^n J_n\left[\frac{2C}{E_0}\sin(\tfrac{1}{2}E_0\tau)\right] \ . \tag{4.34}$$

This has the usual period of $2\tau_0$ [although $|A_t(r,\tau)|^2$ has period τ_0]; one could instead use the modified function $A_{t\pm}(x,\tau)$ which has period τ_0. The Bessel functions $J_n(z)$ vanish at $z=0$, except for J_0, demonstrating that the property (4.32) holds. We can also make the Fourier transform to $A_t(x,E)$:

$$A_t(x,E) = 2\pi \sum_{m,n=-\infty}^{\infty} \delta(x-a(m-n)) \times \delta\left[E - \frac{E_0}{2}(m+n)\right] J_m\left[-\frac{C}{E_0}\right] \times J_n\left[-\frac{C}{E_0}\right] \ . \tag{4.35}$$

The density of states can be obtained from this using (2.18), but the definition of the trace needs to be treated with care in a periodic system. We must set x to zero as usual, but must also replace the δ function by a Kronecker δ, making this step the equivalent of the finite integral over k restricted to the first Brillouin zone in (4.8):

$$\delta(a(m-n)) \to \frac{1}{a}\delta_{m,n} \ . \tag{4.36}$$

The result reproduces the previous one [Eq. (4.19)].

D. Generalization to higher dimensions

It is trivial to generalize the above results for the density of states to certain simple higher-dimensional systems. An example is a superlattice grown in a semiconductor where the periodic potential is in one direction only. The energy band might be modeled with the form

$$\varepsilon(\mathbf{k}) = \varepsilon_t(k_x) + \frac{1}{2m}(k_y^2 + k_z^2) \ , \tag{4.37}$$

with a cosine band for $\varepsilon_t(k_x)$. If an electric field is applied only along the x axis, the resulting density of states is a convolution of that for $\varepsilon_t(k_x)$ in a field with that of free electrons in the yz plane; in this case each δ function of the one-dimensional density of states becomes a step function of height $m/2\pi\hbar^2$. A similar result would be obtained if the y and z motion were also governed by cosine bands, provided that $\mathbf{F}$ were still aligned with x.

The analysis is more complicated if $\mathbf{F}$ is not along a principal axis. Consider a two-dimensional "square" system with cosine bands:

$$\varepsilon_t(\mathbf{k}) = -C[\cos(k_x a) + \cos(k_y a)] \ . \tag{4.38}$$

The spectral function becomes

$$A_t(\mathbf{k},\tau) = \exp\left[iC\int_{-\tau/2}^{\tau/2} d\tau' \{\cos[(k_x + eF\tau')a] + \cos[(k_y + eF\tau')a]\}\right] \tag{4.39}$$

$$= \exp\left[-i[-C\cos(k_x a)]\frac{\sin(\frac{1}{2}eF_x a\tau)}{\frac{1}{2}eF_x a}\right] \times \cdots \ , \tag{4.40}$$

where F_x and F_y are components of $\mathbf{F}$ and the ellipses represent similar terms for y. We see that $A_t(\mathbf{k},\tau)$ is a product of two functions; each of these has the same form as the spectral function in one dimension (4.10), but the two have different frequencies in τ. The Fourier transform $A_t(\mathbf{k},E)$ will therefore be a convolution of two functions like (4.16), and the result is

$$A_t(\mathbf{k},E)=2\pi\sum_{m,n=-\infty}^{\infty}J_m\left[\frac{-C\cos(k_xa)}{\frac{1}{2}eF_xa}\right]J_n\left[\frac{-C\cos(k_ya)}{\frac{1}{2}eF_ya}\right]\delta(E-m(\tfrac{1}{2}eF_xa)-n(\tfrac{1}{2}eF_ya))\ . \tag{4.41}$$

If F_x/F_y is rational, we can write

$$F_x=pF_r,\quad F_y=qF_r\ , \tag{4.42}$$

where p and q are integers, and p/q is in its lowest terms. Setting $E_r=eF_ra$, the δ function in (4.41) becomes

$$\delta(E-\tfrac{1}{2}(mp+nq)E_r)\ . \tag{4.43}$$

In this case the spectral function consists of a discrete set of δ function in energy, although the δ functions may be very close together if E_r is small.

If, instead, F_x/F_y is irrational, the δ functions in (4.41) cover all real values of E densely and the periodic structure is lost; there are no Bloch oscillations or Stark ladders, and no gaps in the density of states. As with the limit of the electric field tending to zero, the mathematical distinction between rational and irrational values of F_x/F_y will be blurred by scattering.

A severe limitation of this work, mentioned earlier, is the restriction to a single band within the framework of the effective Hamiltonian (2.1). This implies particularly the omission of Zener tunneling, which is expected to be of great importance in high electric fields. There have been several studies of electrons in rings subject to an electric field, a simple example of an effectively periodic system. The complexity introduced by Zener tunneling is amazing, illustrated by the work of Blatter and Browne.[17] The effect of Zener tunneling in more conventional systems has recently been studied by Krieger and Iafrate.[1,18]

We shall now consider briefly the implications of these results for transport in high electric fields.

V. CONCLUSIONS

We have presented a gauge-invariant formalism for studying electrons in uniform electric and magnetic fields. The gauge invariance is gained by basing the theory on Green functions rather than on wave functions. In particular, we have defined a gauge-invariant density of states by choosing it to be a function of *kinetic* energy. This density of states reduces smoothly to the usual result as the electric field vanishes; it does not show the unphysical discontinuous behavior that is seen when the ordinary density of states and a scalar potential are used. Perhaps the most important results are those concerning the Stark ladder in a system with a periodic energy band, which has an upper bound as well as a lower bound. We have demonstrated the existence of this ladder—a density of states that breaks up into a series of δ functions—without having to construct it explicitly by introducing the electric field through a scalar potential.

Although we have concentrated on the spectral function and density of states in this paper, our main thrust is towards the theory of transport in high electric fields. KDW developed gauge-invariant transport equations, but considered only parabolic bands. The band structure enters the scattering rates of the transport equation through the spectral function, so we now have the ingredients to extend the theory of KDW to periodic energy bands. This is planned to be described in a further paper, but some general remarks can be made now.

The transport equation should reduce to the Boltzmann equation at low electric fields. This has scattering rates that contain δ functions to conserve energy of the form

$$\delta(\varepsilon(\mathbf{k}+\mathbf{q})-\varepsilon(\mathbf{k})-\Omega_{\mathbf{q}})\ , \tag{5.1}$$

which is for scattering from $\mathbf{k}$ to $\mathbf{k}+\mathbf{q}$ by absorption of a phonon of wave vector $\mathbf{q}$ and energy $\Omega_{\mathbf{q}}$. The form of (5.1) reflects the fact that $\mathbf{k}$ states form the natural basis at low electric fields. There is no sign of periodic motion of the electrons—it does not matter whether $\varepsilon(\mathbf{k})$ is periodic or parabolic—which implies that the discrete nature of $A_t(\mathbf{k},E)$ must be blurred away by scattering in the same way as for $n_t(E)$ at low electric fields, discussed in Sec. IV. The scattering rates must therefore be calculated using spectral functions that themselves contain scattering; in other words, it is vital to calculate the scattering rates *self-consistently*.

In high electric fields the discrete nature of $A_t(\mathbf{k},E)$ should be manifested in the scattering rates. These would therefore be expected to contain δ functions of the form

$$\delta(nE_0-\Omega_{\mathbf{q}}) \tag{5.2}$$

instead of (5.1), and correspond to an electron jumping between rungs of the Stark ladder. Electrons make many Bloch oscillations between scattering events in such strong fields, so $\mathbf{k}$ states are no longer an appropriate basis set. Localized Stark states, like those derived for the cosine band [Eq. (2.11)], provide a better description, and it may be clearer to use a transport equation in real space than $\mathbf{k}$ space.

There is an important difference between these two regimes of transport. In low fields, the "natural" basis is of $\mathbf{k}$ states which are current carrying, and scattering *impedes* transport. The Stark states that are appropriate in high electric fields are localized in space and in this case scattering between levels *promotes* transport. Saitoh[19] introduced a theory of transport based on a Stark ladder explicitly constructed in a scalar potential, and his work has been extended by Sawaki and Nishinaga,[20] Sawaki,[21] Holden and Debney,[22] and Movaghar.[23] It is extremely difficult to treat the limit of low electric fields in this formalism, because huge numbers of Stark states then overlap strongly in space. Krieger and Iafrate[18] have recently taken the opposite point of view and explicitly used a vector potential throughout, extending the work of Levinson[9] and Calecki and Pottier[24] to many bands; this has the advantage that it is straightforward to extend the theory to fields that vary in time (*but not space*).

We plane to show in a further paper how the gauge-invariant transport theory of KDW and the present work can be combined to provide a framework for describing transport in periodic bands that works over the whole range of electric fields, from linear response to the behavior dominated by Bloch oscillations in very high fields.

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