# Acceleration of Electrons by an External Force Field

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The usual proof that an electron in an energy band reacts to an external force as though it had an effective mass is shown to be invalid. It is shown, however, that for static externally applied fields, modified (field-dependent) energy bands can be found for which the acceleration theorem is rigorously correct.

## INTRODUCTION

A FUNDAMENTAL theorem in the band theory of metals states that for an electron in a Bloch state the rate of change of mean velocity proceeds as though the electron were a free carrier with an effective mass

$$m_{\text{eff}}^{-1}=\partial^2 E/\partial p^2.$$

The proofs usually given for this theorem,[1–3] however, can be shown to be invalid. As Kretschmann[4] has shown, the true value of $dv/dt$ for an electron in a Bloch state of any periodic potential is the same as though the carrier were a free electron.

Kretschmann at first thought that the failure of the effective-mass theorem meant that the free mass rather than the effective mass should be used in making theories of the conductivity of metals. However, Peierls[5] pointed out and, later, Pfirsch and Spenke[6] discussed in detail the reason that the free mass does not replace the effective mass in the theory of conduction. In brief, the explanation is that acceleration with free mass takes place for only a short time, after which the acceleration oscillates about its effective-mass value.

The work of Pfirsch and Spenke shows clearly that the failure of the effective-mass theorem at short times can be traced directly to a field-induced mixing together of wave functions from different energy bands. We wish to show that if one modifies the Bloch wave functions so as to eliminate interband couplings which lead to high-frequency fluctuations, the resulting modified Bloch states will be such that the acceleration theorem is rigorously true.

### 1.

We will begin by showing in detail how the failure of the acceleration theorem comes about. The unperturbed Hamiltonian $H_0$ can be that for any periodic potential and the perturbation will be simply $-Fx$, in which $F$ is the force field and $x$ a Cartesian component of position.

Let $\psi_{nk}$ be a wave function of the $n$th energy band, and let an electron be initially in that state. The change in the wave function which takes place during a small interval of time $\delta t$ can then be written

$$i\hbar\delta\psi/\delta t=E_n(k)\psi_{nk}+iF\partial\psi_{nk}/\partial k_x -F\textstyle\sum_{n'}\psi_{n'k}X_{n'n}(k). \quad (1.1)$$

In Eq. (1.1), $E_n(k)$ is the energy eigenvalue for the state $k$ in the $n$th band and $X_{n'n}(k)$ is the interband matrix element of the coordinate at wave number $k$. Equation (1.1) may be obtained directly from the paper of Houston.[7] Thus, for short times and to first order in $F$, the wave function may be written

$$\psi(\delta t)=[\psi_{nK}-F\delta t\textstyle\sum_{n'}\psi_{n'K}X_{n'n}(K)]_{K=k+F\delta t/\hbar}. \quad (1.2)$$

We can calculate the mean velocity using $\psi$ as given by Eq. (1.2) and from it we find, to first order in $F$,

$$\langle\psi(\delta t)|v_x|\psi(\delta t)\rangle=\{v_n(K)+(iF\delta t/m\hbar)\textstyle\sum_{n'} \times[P_{nn'}X_{n'n}-X_{nn'}P_{n'n}]\}_{K=k+F\delta t/\hbar}. \quad (1.3)$$

The $f$-sum rule[8] may be used to simplify the bracketed expression to give

$$\langle v(\delta t)\rangle=v_n(k+F\delta t/\hbar)+F\delta t[(1/m)-(1/m_{\text{eff}})]. \quad (1.4)$$

The usual derivations of the effective mass theorem drop the second term of Eq. (1.4) on the assumption that for sufficiently short times interband processes can be ignored. If, however, we develop $v_n(k+F\delta t/\hbar)$ to first order in $F$, we see that the effective-mass acceleration is exactly cancelled by the second term in brackets on the right-hand side of (1.4), and acceleration with the free mass results as Kretschmann[4] has shown by use of the Ehrenfest theorem.

### 2.

Pfirsch and Spenke[5] have shown that for finite times the second term on the right-hand side of (1.4) oscillates at an atomic frequency, so that the acceleration consists of a large, rapidly oscillating part superposed on a steady acceleration corresponding to the effective mass rather than the free mass. They note that by choosing a momentum wave packet for initial state rather than a sharp Bloch state, they can arrange for the oscillatory term to rapidly die out, and from this they argue that

[1] H. Jones and C. Zener, Proc. Roy. Soc. (London) **A144**, 101 (1934).
[2] A. H. Wilson, *The Theory of Metals* (Cambridge University Press, London, 1953), p. 50.
[3] F. Seitz, *The Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), p. 316.
[4] E. Kretschmann, Z. Physik **87**, 518 (1934).
[5] R. Peierls, Z. Physik **88**, 786 (1934).
[6] D. Pfirsch and E. Spenke, Z. Physik **137**, 309 (1954).
[7] W. V. Houston, Phys. Rev. **57**, 184 (1940).
[8] Reference 2, p. 47.

only the effective mass part of the acceleration should be used in conduction.

We believe that Pfirsch and Spenke have given an essentially correct resolution of the Kretschmann pseudo-paradox. However, we find it objectionable from the formal point of view to base the theory of conduction on wave packet theorems, since we do not see how to actually carry out such a theory when degenerate statistics must be used. Accordingly, we will present a different treatment which we believe is capable of providing a more satisfactory basis for transport theory.

Our first step is to construct a set of Bloch states which to first order in $F$ are "decoupled" in the energy bands in the manner of Adams.[9] These wave functions are not eigenfunctions of the unperturbed Hamiltonian, but instead are eigenstates of a partial Hamiltonian $H_F$ which, in the representation by the states of the unperturbed Hamiltonian has the matrix elements

$$\langle nk|H_F|n'k'\rangle=\delta(k-k')[E_n(k)\delta_{nn'}-FX_{nn'}(k)]. \quad (2.1)$$

We need diagonalize $H_F$ to only first order in $F$, and this may be done by means of perturbation theory. The result is

$$\langle nk|H_F|n'k'\rangle=\delta(k-k')[E_n(k)-FX_{nn}(k)]\delta_{nn'}. \quad (2.2)$$

The wave functions $\varphi_{nk}$ which diagonalize $H_F$ are

$$\varphi_{nk}=\psi_{nk}+\textstyle\sum_{n'}\psi_{n'k}FX_{n'n}/E_{n'n}, \quad (2.3)$$

and by using the full Hamiltonian it is readily shown that to first order in $F$

$$i\hbar\partial\varphi_{nk}/\partial t=[E_n-FX_{nn}(k)]\varphi_{nk}+iF\partial\varphi_{nk}/\partial k. \quad (2.4)$$

Thus if initially an electron is in the state $\varphi_{nk}$, after a short time $\delta t$ it will be in the state $\varphi_{nK}$, where

$$K=k+F\delta t/\hbar.$$

It remains to calculate the mean velocity for an electron in a state $\varphi_{nk}$. From Eq. (2.3)

$$(\varphi_{nk},v_x\varphi_{nk})=v_{nk}+\textstyle\sum_{n'}F(P_{nn'}X_{n'n}-X_{nn'}P_{n'n})/E_{n'n}. \quad (2.5)$$

From the fact that $(p/m)$ is the time derivative of $x$, it follows[8] that

$$X_{nn'}=\hbar P_{nn'}/miE_{nn'}, \quad (2.6)$$

so the last term on the right-hand side of (2.5) vanishes. Thus to first order in the field $F$, the mean velocity of an electron in the state $\varphi_{nk}$ is exactly the same as the mean velocity in the state $\psi_{nk}$. Since the states $\varphi_{nk}$ accelerate without interband mixing, it follows that they constitute a set of states for which the effective mass theorem is rigorously true. That is to say, if an electron is initially in the state $\varphi_{nk}$ of the $n$th modified band, it will remain in that band while its momentum changes at the rate $F$ and its mean velocity changes at the rate $(F/m_{\text{eff}})$.

[9] E. N. Adams, Phys. Rev. **85**, 41 (1952).

### 3.

We have seen that the acceleration theorem with the effective mass is not valid for the Bloch states $\psi_{nk}$ of the unperturbed Hamiltonian, but that there exists a set of field Bloch states $\varphi_{nk}$ which are very closely related to the $\psi_{nk}$ and for which the acceleration theorem is rigorously true. In addition, we have seen that each of the states $\varphi_{nk}$ carries exactly the same mean current as the state $\psi_{nk}$. It is natural to surmise that the band theory of transport phenomena depends for whatever validity it has on the existence of the states $\varphi_{nk}$.

In the representation by the $\varphi_{nk}$, the equation

$$\partial f_n/\partial t|_{\text{electric field}}=(eF/\hbar)\partial f_n/\partial k \quad (3.1)$$

for the probability $f_n(k)$ that the state $\varphi_{nk}$ is occupied, is strictly valid. Thus if the collisions had no other effect than to cause scattering within the modified individual bands, a Boltzmann treatment could be used to get the current contributions of each of the bands. For example, if we assume a phenomenological collision time we can immediately obtain the formula for current obtained by Karplus and Luttinger[10] by a density matrix treatment, a formula which they have used to discuss the anomalous Hall effect in ferromagnets.

A careful examination of the fundamental theory of scattering or of the theory of conduction in time-dependent fields shows that there can exist complications that are not resolved by introducing the $\varphi_{nk}$. While we will omit a detailed discussion here, we note that in the first case there exist effects of collision which involve interband matrix elements in such a way that a Boltzmann description of transport is inadequate and the more elaborate density-matrix description must be used.

We conclude that the well-known effective-mass equation for the acceleration by a force field is strictly valid to first order in the applied field, although the usual proofs attain the correct result through a compensation of errors.

### ACKNOWLEDGMENTS

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[10] R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).