

Dynamics of an incommensurate charge-density wave*

M. L. Boriack and A. W. Overhauser

Department of Physics, Purdue University, West Lafayette, Indiana 47907

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We present the equation of motion for the drift velocity of a charge-density wave (CDW), the electron drift velocity, and the total electric current in the presence of applied electric and magnetic fields. These equations can be microscopically derived. In this paper, we discuss the electric current and the dynamical effects of an electric field for an incommensurate CDW in a three-dimensional metal. An expression for the effective mass characterizing the CDW acceleration is derived.

I. INTRODUCTION

The discovery of charge-density waves (CDW) in pseudo-one-dimensional conductors and in transition-metal dichalcogenides has stimulated considerable interest in the properties of CDW systems. One of the most fundamental problems is the effect of CDW's on electrical transport properties. Much of the theoretical effort on CDW transport has been directed toward the one-dimensional conductor TTF-TCNQ. The problem of the conductivity associated with fluctuations into the CDW state above the Peierls critical temperature has been addressed by Patton and Sham,¹ Allender, Bray, and Bardeen,² and Fukuyama, Rice, and Varma.³ Lee, Rice, and Anderson⁴ have studied microscopically the problem of a one-dimensional system containing a CDW which is pinned or fixed in space. Rice⁵ has dealt phenomenologically with the problem of a pinned CDW in one dimension.

Although in some systems, the CDW may be pinned, the existence of phason modes⁶ may make it possible to have systems with spatial fluctuations of the CDW's position which are so large that the CDW is not pinned. Thus one of the most fundamental questions which must be answered is that of the electrical transport properties of a system containing an unpinned CDW. It is toward the resolution of this problem that we direct this paper. We begin by presenting a set of equations describing the motion of a CDW and the electron distribution in three-dimensional jellium in the presence of applied electric and magnetic fields. The complete microscopic derivation of these equations will encompass several papers. In this paper we discuss the current and the effects of an applied electric field. The discussion of the magnetic field and scattering processes will be studied in later work.

Because the CDW model has been successful in explaining several of the anomalous properties of potassium, including the Mayer-El Naby optical

absorption⁷ and the conduction-electron spin resonance,⁸ and because spatial fluctuations associated with the phason modes are expected to be large if a CDW is assumed to exist in potassium,⁶ it is of great interest to evaluate the expressions for the current and for the CDW effective mass for values of the various parameters suitable to the CDW model of potassium.

II. EQUATIONS OF MOTION

In this section we write down without motivation a set of equations describing the motion of the CDW and the electron distribution in the presence of an electric field $\vec{\mathcal{E}}$ and a magnetic field \vec{H} . These equations are intended to be used as a reference throughout this and future works in which they shall be motivated and microscopically derived.

For the magnetic field \vec{H} in the \hat{z} direction and the CDW wave vector \vec{Q} in the \hat{x} direction, the equation of motion for the CDW drift velocity \vec{D} can be written

$$\frac{d\vec{D}}{dt} = (1/m^*)(-e\mathcal{E}_x - eHK_y/c) - (D - \beta K_x)/\tau_D, \quad (1)$$

where \vec{D} is along \vec{Q} . (The symbol D was chosen to bring to mind the word "drift." Nowhere in this paper is the electric displacement discussed.) m^* is the effective mass associated with the acceleration of the CDW, and the electronic charge is $-e$. τ_D is the relaxation time for the CDW velocity \vec{D} , and β is another constant which arises due to scattering. \vec{K} is the quasivelocity of the electron distribution and is related to the average electron wave vector $\langle \vec{k} \rangle_{av}$ by

$$\vec{K} \equiv \hbar \langle \vec{k} \rangle_{av} / m, \quad (2)$$

where m is the electron mass. The βK_x term tries to pull the CDW along with the drifting electrons. By $\langle \vec{k} \rangle_{av}$ we mean the average value of the wave-vector label for occupied states.

It may seem somewhat surprising that a magnetic

field can accelerate a CDW. Not only does this arise from a microscopic derivation, but if the electric and magnetic field terms are not as shown in Eq. (1), it is easy to envision an experiment which violates the second law of thermodynamics. This will be shown in a subsequent paper.

The equations of motion for the components of the electron quasivelocity parallel (K_x) and perpendicular (K_y, K_z) to \vec{Q} are

$$\begin{aligned}\frac{dK_x}{dt} &= (1/m)(-e\mathcal{E}_x - eHK_y/c) - (K_x - \alpha D)/\tau_x, \\ \frac{dK_y}{dt} &= (1/m)(-e\mathcal{E}_y + eHV_x/c) - K_y/\tau_y, \\ \frac{dK_z}{dt} &= (1/m)(-e\mathcal{E}_z) - K_z/\tau_z.\end{aligned}\quad (3)$$

The relaxation times for electron drift parallel (τ_x) and perpendicular (τ_y, τ_z) to \vec{Q} are different due to the distortion of the Fermi surface caused by the CDW. In the case under consideration $\tau_y = \tau_z$. \vec{V} is the mean group velocity of the electrons, i.e.,

$$\vec{V} \equiv \langle \vec{v}_g \rangle_{av} = \langle \vec{p} \rangle_{av} / m, \quad (4)$$

and is related to \vec{K} and \vec{D} by

$$\begin{aligned}V_x &= (1 - \gamma)K_x + \gamma D, \\ V_y &= K_y, \\ V_z &= K_z.\end{aligned}\quad (5)$$

The current is given by $\vec{J} = -ne\vec{V}$, where n is the number of electrons per unit volume. α is another constant which arises from scattering, and the term $\alpha\vec{D}$ tries to pull the electrons along with the CDW in a manner analogous to the acoustoelectric effect. γ is discussed in Sec. IV.

In this paper we will discuss Eq. (5) and the electric field terms in Eqs. (1) and (3). The terms arising from the magnetic field and from scattering will be dealt with in future work.

III. JELLIUM MODEL FOR A CDW

Our discussion of CDW motion will be given in terms of a three-dimensional jellium model. In the presence of a CDW, the total self-consistent potential in the one-electron Hamiltonian is of the form

$$V(\vec{r}) = G \cos \vec{Q} \cdot \vec{r}. \quad (6)$$

This potential produces a density modulation in the electron gas so that the electron density is given by

$$\rho(\vec{r}) = \rho_0(1 - p \cos \vec{Q} \cdot \vec{r}). \quad (7)$$

The mean density is $\rho_0 = k_F^3/3\pi^2$ and the fractional modulation p is given for an unperturbed free el-

ectron gas by

$$p = (3G/2\epsilon_F)g(Q/2k_F), \quad (8)$$

where

$$g(x) \equiv \frac{1}{2} + [(1 - x^2)/4x] \ln |(1 + x)/(1 - x)| \quad (9)$$

and $\epsilon_F = \hbar^2 k_F^2/2m$.

The density modulation of the electron gas must be compensated by a density modulation of the positively charged background. This requires a local displacement \vec{u} of the background such that

$$\vec{u}(\vec{r}) = (p\vec{Q}/Q^2) \sin \vec{Q} \cdot \vec{r}. \quad (10)$$

Throughout our discussion we will take G in the self-consistent potential, Eq. (6), to be a constant. Since the existence of CDW's depends crucially upon the velocity dependence of G , it is an inconsistent approximation. However, the treatment of velocity dependent effects opens up many intricate questions which would unduly complicate our present discussion and must be postponed to later work.

The one-electron Hamiltonian which incorporates Eq. (6) is

$$\mathcal{H} = p^2/2m + G \cos \vec{Q} \cdot \vec{r}. \quad (11)$$

Compact solutions to this question cannot be written down. However, for our purposes it is sufficiently accurate to divide the potential term into two parts, one which leads to the gap at $\vec{k} = \frac{1}{2}\vec{Q}$ and the other which leads to the gap at $\vec{k} = -\frac{1}{2}\vec{Q}$. Each part must be treated accurately near the gap since the wave functions and energy spectrum are significantly altered there. The simplifying feature of this method is that the effects of the two parts of the potential are additive in many cases.

For discussion we take the part of the potential which mixes the plane wave state \vec{k} with $\vec{k} - \vec{Q}$ and produces the gap at $\vec{k} = \frac{1}{2}\vec{Q}$. Treating the mixing by degenerate perturbation theory leads to a secular equation which can be solved for the energies of the states above and below the gap,

$$E_{\pm}(\vec{k}) = \frac{1}{2}(\epsilon_{\vec{k}} + \epsilon_{\vec{k}-\vec{Q}}) \pm \frac{1}{2}[(\epsilon_{\vec{k}} - \epsilon_{\vec{k}-\vec{Q}})^2 + G^2]^{1/2}, \quad (12)$$

where $\epsilon_{\vec{k}} = \hbar^2 k^2/2m$. The corresponding eigenfunctions are

$$\begin{aligned}\varphi_{\vec{k}} &= \cos \xi e^{i\vec{k} \cdot \vec{r}} - \sin \xi e^{i(\vec{k}-\vec{Q}) \cdot \vec{r}} \equiv e^{i\vec{k} \cdot \vec{r}} u_{\vec{k}}(\vec{r}), \\ \psi_{\vec{k}} &= \sin \xi e^{i\vec{k} \cdot \vec{r}} + \cos \xi e^{i(\vec{k}-\vec{Q}) \cdot \vec{r}} \equiv e^{i\vec{k} \cdot \vec{r}} w_{\vec{k}}(\vec{r}),\end{aligned}\quad (13)$$

for states below and above the gap, respectively. The coefficients obey the relation

$$\sin 2\xi = G/(E_+ - E_-) \equiv G/W. \quad (14)$$

Away from the gap these wave functions reduce to those found by nondegenerate perturbation theory.

Due to the "softening" of the energy for wave vectors along \vec{Q} , the Fermi surface distorts and takes on a lemon shape.⁶

IV. CURRENT

Equation (5) states that the total momentum or current depends upon the difference in CDW and electron drift velocities. This results because the momentum of an electron in a periodic potential is not simply proportional to the wave vector. To derive Eq. (5) it is most convenient to work in a reference frame in which the CDW is at rest and the electron drift velocity is \vec{K}' . The expectation value of the momentum for an electron in a state $\varphi_{\vec{k}}$ is $\hbar\vec{k}$ plus an additional term which is an odd function of \vec{k} . The total contribution of this term due to all the electrons clearly depends on the position of the electron distribution in \vec{k} space. The expectation value for the momentum operator $\vec{p} = -i\hbar\nabla$ for an electron the state $\varphi_{\vec{k}}$ in Eq. (13) is

$$\langle \varphi_{\vec{k}} | \vec{p} | \varphi_{\vec{k}} \rangle = \hbar\vec{k} - \hbar\vec{Q} \sin^2 \xi. \quad (15)$$

There is similar term due to the part of the potential which causes the other gap. We will consider the case where \vec{Q} and the electron quasi-velocity \vec{k}' are in the x direction. To calculate the net group velocity we add up all the contributions of the occupied states for a distribution centered at mK'_x/\hbar in \vec{k} space. To first order in G/E_F we can approximate the Fermi surface by a sphere, and at zero temperature the net contribution to the group velocity comes from a shell of thickness $mK'_x k_x / \hbar k_F$ at the Fermi surface. Accounting for both gaps the total momentum P'_x in the CDW rest frame is

$$P'_x = nmK'_x (1 - \gamma), \quad (16)$$

with

$$\gamma = \frac{3Q}{k_F} \int_{-1}^1 d(\cos\theta) \cos\theta \sin^2 \xi |_{k=k_F}, \quad (17)$$

where θ is the polar angle measured from the x axis. In the laboratory frame $K_x = K'_x + D$ and the average group velocity is

$$V_x = K_x - \gamma(K_x - D). \quad (18)$$

If \vec{K} is perpendicular to \vec{Q} it is easy to see from Eq. (15) that the periodic potential cannot make the average group velocity unequal to the drift velocity so that we have $V_y = K_y$. Thus the current along \vec{Q} and perpendicular to \vec{Q} should be different for two reasons: different relaxation times and different relationships between the drift velocity and the current.

It is of interest to calculate γ using the values of the proposed CDW model for potassium.^{7,8} Taking $G/E_F \cong 0.35$ from fitting the Mayer-El Naby optical absorption data and $Q/2k_F \cong 1 + G/4E_F$ for \vec{Q} in "critical contact" with the Fermi surface gives a value of $\gamma \cong 0.2$.

V. EFFECTS OF AN APPLIED ELECTRIC FIELD

It is well known that electrons in a periodic potential (i.e., Bloch electrons) obey the equation of motion

$$\frac{d\vec{k}}{dt} = -e\vec{\mathcal{E}}/\hbar \quad (19)$$

in an applied electric field $\vec{\mathcal{E}}$. However, the electric field has the additional effect of "polarizing" the electron density in a manner analogous to the way an atomic wave function is perturbed by an electric field.⁹ This polarization should not be confused with interband transitions which are negligible for our purpose. This effect is present for electrons in any periodic potential and results in an electron density which is out of phase with the original periodicity of the potential. This results in a net force on the lattice and is the microscopic origin of the so-called "Bragg reflection force."¹⁰ Whereas in many problems the ions are fixed in the lattice, in jellium the ions are free to adjust to the new charge density and thus the CDW can be accelerated by the electric field.

The Hamiltonian of an electron in a periodic potential $V(\vec{r})$ and an applied uniform electric field $\vec{\mathcal{E}}$ is

$$\mathcal{H} = p^2/2m + V(\vec{r}) + e\vec{\mathcal{E}} \cdot \vec{r}. \quad (20)$$

The spacial periodicity of $V(\vec{r})$ allows the solution in zero electric field to have the Bloch form,

$$\varphi_{n\vec{k}}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{n\vec{k}}(\vec{r}), \quad (21)$$

where $u_{n\vec{k}}(\vec{r})$ is periodic in \vec{r} and n is the band index.

In dealing with the term containing the applied electric field, mathematical difficulties arise due to the fact that the coordinate operator \vec{r} is not square integrable with the wave functions in Eq. (21) over infinite space. To avoid these problems we will use the Bloch or crystal momentum representation. If a general wave function ψ is

$$\psi(\vec{r}) = \frac{1}{8\pi^3} \sum_n \int d^3k a_n(\vec{k}) e^{i\vec{k} \cdot \vec{r}} u_{n\vec{k}}(\vec{r}) \quad (22)$$

in the coordinate representation, then ψ is

$$\psi(\vec{k}) = [a_0(\vec{k}) a_1(\vec{k}) a_2(\vec{k}) \dots] \quad (23)$$

in the Bloch representation. $\psi(\vec{k})$ is an (infinite) column vector. In this representation the x component of \vec{r} , for example, is¹¹

$$x = iI \partial/\partial k_x + X_{nn'}(\vec{k}), \quad (24)$$

where I is an (infinite) unit matrix and

$$X_{nn'}(\vec{k}) \equiv i \int d^3r u_{n\vec{k}}^\dagger(\vec{r}) \partial [u_{n'\vec{k}}(\vec{r})] / \partial k_x. \quad (25)$$

The Hamiltonian (20) with $\vec{\mathcal{E}} = 0$ is, of course,

diagonal in this representation with diagonal elements

$$\mathcal{H}_{nn}(\vec{k}) \equiv E_n(\vec{k}), \quad (26)$$

which are the energy bands.

From Eq. (24) for the x operator in the Bloch representation, the two effects of the electric field can be seen. If we consider an electron described by a wave packet confined to one band, say $E_0(\vec{k})$, then

$$\psi(\vec{k}) = [a_0(\vec{k}) 0 0 \dots]. \quad (27)$$

We assume that $a_0(\vec{k})$ is nonzero only in a small region of \vec{k} space. The first term on the right in Eq. (24) leads to an equation of motion for $|a_0(\vec{k})|^2$ which is solved by some general function of the form $F(\vec{k} + e\vec{\mathcal{E}}t/\hbar)$. Thus the wave packet moves in \vec{k} space according to the equation $d\vec{k}/dt = -e\vec{\mathcal{E}}/\hbar$. For a distribution of electrons, this leads to the electric field term in Eq. (3).

The second term on the right in Eq. (24) leads to off-diagonal terms in the Hamiltonian matrix \mathcal{H}_{mn} . These off-diagonal terms can be eliminated to first order in $\vec{\mathcal{E}}$ by using a new set of basis functions given by first-order perturbation theory⁹

$$u_{n\vec{k}}^{(1)} = u_{n\vec{k}} + \sum_{n'} u_{n'\vec{k}} \frac{\langle u_{n'\vec{k}} | ie\vec{\mathcal{E}} \cdot \vec{\nabla}_{\vec{k}} | u_{n\vec{k}} \rangle}{E_n(\vec{k}) - E_{n'}(\vec{k})}, \quad (28)$$

where $\vec{\nabla}_{\vec{k}}$ is the gradient operator in \vec{k} space. Thus it is clear that the electric field polarizes the electron wave functions (as soon as it is turned on) by mixing states with the same \vec{k} in different energy bands. This is analogous to atomic physics where the electric field polarizes the atomic wave functions by mixing the wave functions belonging to various states.

We can now evaluate the change in electron probability density due to the electric field for the CDW state, Eq. (13). The perturbed wave functions $\phi_{\vec{k}}^{(1)}$ are

$$\phi_{\vec{k}}^{(1)} = \varphi_{\vec{k}} - \psi_{\vec{k}} \langle w_{\vec{k}} | ie\vec{\mathcal{E}} \cdot \vec{\nabla}_{\vec{k}} | u_{\vec{k}} \rangle / W. \quad (29)$$

The change in probability density is given by

$$|\phi_{\vec{k}}^{(1)}|^2 - |\varphi_{\vec{k}}|^2 = (\hbar^2 Ge\vec{\mathcal{E}} \cdot \vec{Q} / mW^3) \sin \vec{Q} \cdot \vec{r}. \quad (30)$$

The corresponding change for a state $\psi_{\vec{k}}$ above the gap is opposite in sign. Note that the part of electron density induced by the electric field is 90° out of phase with that produced by the self-consistent potential $G \cos \vec{Q} \cdot \vec{r}$. It is only the component of $\vec{\mathcal{E}}$ along with \vec{Q} which gives rise to this out-of-phase part of the electron density.

The total electron density induced by the electric field is found by summing the contributions

from all states $\varphi_{\vec{k}}$ and $\psi_{\vec{k}}$ weighted by the appropriate Fermi-Dirac occupation probability. For zero temperature only states up to the Fermi energy are filled and the total electron probability density induced by the electric field is

$$\Delta N_g = \frac{2\hbar^2 Ge\vec{\mathcal{E}} \cdot \vec{Q}}{m} \int \frac{d^3k}{4\pi^3} \frac{1}{W^3}, \quad (31)$$

where a factor of 4 has been included to account for spin degeneracy and for both parts of the potential. The volume of integration is that enclosed by the Fermi surface. Note that ΔN_g does not depend on the electron drift or CDW velocities.

VI. CDW ACCELERATION AND EFFECTIVE MASS

In an applied electric field and the absence of scattering processes, the total electron density will be phase shifted, i.e., moved in space, with respect to the density of the positive ion background. This phase shift is proportional to the magnitude of the electric field. With the electron and ion densities out of phase, there will be nonzero net forces on the ions; and they will move in such a manner that the local displacement \vec{u} of the background can be described by an accelerating running wave,

$$\vec{u}(\vec{r}) = (p\vec{Q}/Q^2) \sin[\vec{Q} \cdot (\vec{r} - \vec{D}t - \frac{1}{2}\vec{A}t^2)], \quad (32)$$

where \vec{D} and \vec{A} are the CDW velocity and acceleration respectively. Thus the periodic ion density tries to catch up to that of the electrons only to find the periodic part of the electron density pulled ahead by the electric field like the carrot before the nose of the proverbial donkey. Note that the acceleration \vec{A} of the CDW, i.e., that of the periodic part of the electron and ion densities, is not the same quantity as the rate of change of the electron drift velocity given by Eq. (19).

The acceleration of the CDW can be determined by making the ions obey Newton's second law of motion, $\vec{F} = M\vec{a}$, where M is the ion mass. Alternatively, the same result can be obtained by requiring that the rate at which the total energy in the system is changing is equal to the rate at which the applied electric field does work on the system. Both methods, of course, give equivalent results; but since the first is tidier, only it will be given here.

It is convenient to work in the laboratory frame of reference and to take $\vec{D} = 0$ at time $t = 0$. The instantaneously accelerating wave of Eq. (32) becomes

$$u(\vec{r}) \cong (p\vec{Q}/Q^2) [\sin \vec{Q} \cdot \vec{r} - (\vec{Q} \cdot \vec{A} t^2 / 2) \cos \vec{Q} \cdot \vec{r}]. \quad (33)$$

The $\sin \vec{Q} \cdot \vec{r}$ term leads to a term in the one-electron Hamiltonian which is proportional to

$\cos\vec{Q}\cdot\vec{r}$. We put this together with the $\cos\vec{Q}\cdot\vec{r}$ parts from the Hartree, exchange and correlation terms to get the static CDW potential in Eq. (6).

Due to the out-of-phase electron density induced by the electric field [Eq. (31)], there will be a force \vec{F}_1 on a unit volume of the background which is easily found using Poisson's equation. The result is

$$\vec{F}_1 = (4\pi e^2 \rho_0 \vec{Q} / \epsilon_1 Q^2) \Delta N_g \cos\vec{Q}\cdot\vec{r}, \quad (34)$$

where ϵ_1 is the electron-gas dielectric function for wave vector \vec{Q} which results from including electron-electron interactions self-consistently. ϵ_1 is discussed in the Appendix.

The other term in Eq. (33) is present only when the acceleration of the CDW is nonzero and gives rise to an additional Coulomb term \mathcal{K}' in the one-electron Hamiltonian where

$$\mathcal{K}' = (2\pi e^2 \rho_0 \vec{A}\cdot\vec{Q} / Q^2) t^2 \sin\vec{Q}\cdot\vec{r}. \quad (35)$$

\mathcal{K}' is explicitly time dependent, and time-dependent perturbation theory can be used to find the perturbed wave functions and the expectation value of the Hamiltonian. This leads to a force \vec{F}_2 on a unit volume of the background where

$$\vec{F}_2 = (8\pi e^2 \rho_0 \vec{Q} G / \epsilon_1 Q^2) (\vec{A}\cdot\vec{Q}) \sum_{\vec{k}} \frac{1}{W^3} \cos\vec{Q}\cdot\vec{r}, \quad (36)$$

where ϵ_1 is discussed in the Appendix.

From Eq. (32) the acceleration of a unit volume of the background at time $t=0$ is

$$\frac{d^2 \vec{u}}{dt^2} = -(p\vec{Q} / Q^2) (\vec{A}\cdot\vec{Q}) \cos\vec{Q}\cdot\vec{r}. \quad (37)$$

Writing Newton's second law using Eqs. (34), (36), and (37) results in an equation for the acceleration of the CDW,

$$\vec{F}_1 + \vec{F}_2 = -\rho_0 p M \vec{A}\cdot\vec{Q} / Q^2 \cos\vec{Q}\cdot\vec{r}. \quad (38)$$

Solving for $\vec{A}\cdot\vec{Q}$ we have,

$$\vec{A}\cdot\vec{Q} = -e \vec{\mathcal{E}}\cdot\vec{Q} / m^*, \quad (39)$$

where

$$m^*/m = 1 + M p \epsilon_1 / 8\pi e^2 \hbar^2 G \sum_{\vec{k}} \frac{1}{W^3}, \quad (40)$$

and m^* is the zero-temperature effective mass characterizing the acceleration of the CDW in an electric field. Note that near the gaps $W \sim 1/G$. The volume in \vec{k} space where $W \sim 1/G$ is of order G^2 . Thus $\sum_{\vec{k}} (1/W^3) \sim 1/G$ plus higher-order terms in G . For this reason the second term Eq. (40) goes to zero linearly with G for small G and m^* approaches m as the CDW amplitude vanishes. Thus the CDW acceleration is the same as that of the electron distribution in this limit.

It is interesting to evaluate m^*/m for the proposed CDW model of potassium.^{7,8} Figure 1 shows

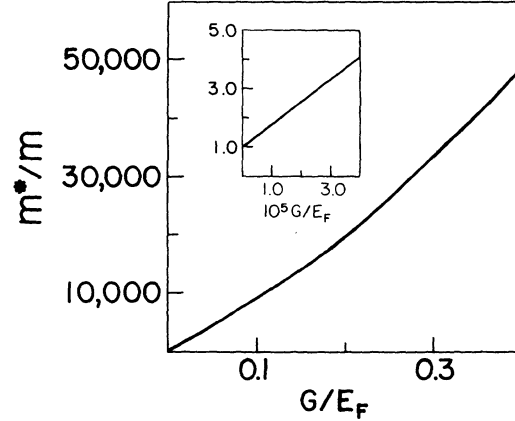


FIG. 1. Charge-density-wave effective mass m^* versus energy gap G for a jellium model with electron density and ion mass suitable for potassium. m is the free-electron mass and E_F is the Fermi energy. See text for details.

a plot of m^*/m versus the normalized energy gap G/E_F for a jellium model with M equal to the mass of a potassium ion and ϵ_1 suitable for an electron gas with the density of that in potassium. Using the value $G/E_F \approx 0.35$, the effective mass m^* would be about 40 000 times the electron mass.

For the large value of m^* which would be required for a CDW in potassium and assuming that the CDW terminal velocity is of the same order of magnitude as the electron drift velocity, Eq. (5) implies that a transient effect should be seen in the current since the CDW should accelerate about 40 000 times slower than the electrons. For any materials in which the CDW is unpinned, this effect should exist. Since the results derived in this paper assume a spherical Fermi surface, it would be necessary to take account of the actual Fermi surface to derive quantitative expressions for anisotropic materials.

VII. CONCLUSION

We have presented a set of equations describing the CDW velocity, the electron drift velocity, and the current in the presence of applied electric and magnetic fields for a three-dimensional jellium model of a system with an unpinned CDW. These equations can be microscopically derived. In this paper we discussed the current and the rates of change of the CDW and the electron drift velocities in an applied electric field. We derived an expression for the CDW effective mass in terms of the CDW energy gap G and found that as G goes to zero, the CDW effective mass goes to the electron mass.

APPENDIX

The out-of-phase electron density induced by an applied electric field was found in Eq. (31) to be

$$\Delta N_{\delta} = \frac{2\hbar^2 G e \vec{\mathcal{E}} \cdot \vec{Q}}{m} \int \frac{d^3 k}{4\pi^3} \frac{1}{W^3}. \quad (A1)$$

To calculate the total induced electron density self-consistency it is necessary to include electron-electron interactions. There will be an additional Hartree term due to the change in the electron charge density. Exchange and correlation effects can be accounted for by the observation that to first order in $\vec{\mathcal{E}}$, the effect of the electric field is to change the phase (or spatial position) of the periodic part of the electron density but not to change its amplitude. For a CDW to exist the exchange and correlation potential V_{xc} would of necessity be highly nonlocal or velocity dependent. However, since we have ignored this velocity dependence throughout, for the discussion here we approximate V_{xc} by the Slater potential,

$$V_{xc} = - (e^2 k_F / 2\pi\rho_0) \Delta N. \quad (A2)$$

We can then write the total self-consistent per-

turbation due to the electric field as

$$\mathcal{H}'_{xc} = e \vec{\mathcal{E}} \cdot \vec{r} + \left(\frac{4\pi e^2}{Q^2} - \frac{e^2 k_F}{2\pi\rho_0} \right) \Delta N_{\delta}^{sc} \sin \vec{Q} \cdot \vec{r} \quad (A3)$$

where ΔN_{δ}^{sc} is the magnitude of the $\sin \vec{Q} \cdot \vec{r}$ part of the self-consistent electron density. The second term in (A3) contains the Hartree and exchange-correlation effects. It follows that

$$\Delta N_{\delta}^{sc} = \Delta N_{\delta} / \epsilon_1 \quad (A4)$$

with

$$\epsilon_1 = 1 + \frac{m e^2}{\pi \hbar^2 k_F} \frac{g(x)}{x^2} (1 - 3x^2/2), \quad (A5)$$

where $g(x)$ is given in Eq. (9) and $x = Q/2k_F$.

A similar treatment of the perturbation (35) due to the acceleration of the ions leads to Eq. (36).

In order that m^*/m can be calculated for the proposed CDW model of potassium,^{7,8} we evaluate ϵ_1 for an electron gas with the density of that in potassium. ϵ_1 is a function of G through its dependence on $Q/2k_F$. For $G/E_F \cong 0.35$ we find $\epsilon_1 \cong 0.81$.

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