Electron-phonon interactions and charge-density-wave formations in strong magnetic fields

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(Received 6 December 1985)

An electron gas in a strong magnetic field will attain a one-dimensional energy spectrum due to the quenching of the motion perpendicular to the field into the lowest Landau level. Such a system is then expected to show an instability towards a charge-density-wave formation. In this report, we show that for strongly polar semiconductors, the electron-phonon interactions greatly enhance the critical temperature for an instability and lead to a Peierls instability with a permanent distortion of the electron-phonon system.

It is well known that a (quasi-) one-dimensional (1D) conductor exhibits various kinds of instabilities at low temperatures, such as charge-density wave (CDW) and Peierls instabilities.[1,2] The reason for these two kinds of instabilities in particular is the divergent behavior of the bare electron polarization diagram for wave vectors $q=2k_F$, which is uniquely attributed to the one-dimensional energy spectrum.[2] The divergence of this diagram will cause a formation of a CDW with a wave vector $q=2k_F$ in a 1D electron gas. If there are electron polar-optic phonon interactions, the divergence of the electron polarization diagram means that the frequency of phonons with this wave vector will go to zero, causing a static distortion of the electron-phonon system. This is what we call a Peierls instability.

If a magnetic field is applied to a three-dimensional electron gas, the density-of-states for motions perpendicular to the field will attain a discrete structure, the so-called Landau levels. For strong enough magnetic fields, only one spin direction of the lowest Landau level will be occupied and the energy spectrum will for all practical purposes be 1D, associated with the motion parallel to the field. One would thus expect such a system to display many of the qualities of a 1D system. In particular, Fukuyama[3] has shown that a CDW instability driven by the electron-electron Coulomb interactions is likely to occur. Phenomena that are quite plausibly manifestations of a CDW formation have also been observed experimentally in graphite.[4]

In this paper we calculate the critical temperature for a Peierls instability driven by polar-optic electron-phonon coupling for some strongly polar semiconductors and compare our results with the critical temperature given by Fukuyama's theory,[2] which does seem to predict a critical temperature that agrees fairly well in magnitude with experimental values.[4,5] For strongly polar semiconductors, however, the electron-phonon interactions enhance the critical temperature from that given by Fukuyama's theory[3] and lead to a Peierls instability with a permanent lattice distortion. This distortion should be readily observed by slow neutron scattering or X-ray diffraction. Finally, we also calculate the nature of the phonon dispersion relation near $q=2k_F$ for $T=0$.

We consider an electron-phonon system of dimension L^3 with an applied magnetic field $\mathbf{B}=B\hat{z}$. We assume that the magnetic field is sufficiently strong that only one spin direction of the lowest Landau level is occupied. The system is described by a Hamiltonian $H=H_{\rm el}+H_{\rm ph}+H_{\rm el\text{-}el}+H_{\rm el\text{-}ph}$. The noninteracting electron term is $H_{\rm el}=\sum_\alpha \varepsilon(p)c_\alpha^\dagger c_\alpha$ where $\varepsilon(p)=p^2/2m$ (we take $\hbar=1$) with m the effective mass due to interactions with the static lattice. The kinetic energy $\frac{1}{2}\omega_c$ with $\omega_c=eB/mc$ associated with the motion perpendicular to the field has been subtracted off and p is the z component of the momentum. The operator c_α destroys an electron with the center of its cyclotron motion at $x=X$ and z component of its momentum equal to p; $|\alpha\rangle=|X\rangle\,|p\rangle$. The wave function $\psi_\alpha(\mathbf{r})$ of this state is

$$\psi_\alpha(\mathbf{r})=\frac{1}{\pi^{1/4}l^{1/2}L}\exp[-i(pz+Xy/l^2)-(X-x)^2/2l^2]\,, \tag{1}$$

where $l=(c/eB)^{1/2}$ is the magnetic length.

The noninteracting phonon system is described by $H_{\rm ph}=\sum_{\mathbf{q}}\omega_0(\mathbf{q})a_{\mathbf{q}}^\dagger a_{\mathbf{q}}$ where $a_{\mathbf{q}}$ destroys a longitudinal optical phonon of momentum $\mathbf{q}$ and frequency $\omega_0(\mathbf{q})$.

The electron-electron interaction is

$$H_{\rm el\text{-}el}=\tfrac{1}{2}\int d\mathbf{r}\int d\mathbf{r}_1\,\psi^\dagger(\mathbf{r}_1)\psi^\dagger(\mathbf{r})v(\mathbf{r}-\mathbf{r}_1)\psi(\mathbf{r})\psi(\mathbf{r}_1) \tag{2}$$

with $\psi(\mathbf{r})=\sum_\alpha\psi_\alpha(\mathbf{r})c_\alpha$. Here $v(\mathbf{r})=e^2/\epsilon_0 r$ is the Coulomb interaction where ϵ_0 is the dielectric constant of the background medium. Our only concern with $H_{\rm el\text{-}el}$ is that it contains information on how the mobile conduction electrons screen a charge-density fluctuation.[6] This screening is expressed by a dielectric constant $\epsilon(\mathbf{q},\omega)$ that will effect the renormalization of the phonon frequencies. We will assume that $\epsilon(\mathbf{q},\omega)$ has been calculated by some suitable approximation, such as the Thomas-Fermi or the random-phase approximation (RPA).

The electron-phonon interaction is of the form

$$H_{\rm el\text{-}ph}=\sum_{\mathbf{q}}M(\mathbf{q})(a_{-\mathbf{q}}^\dagger+a_{\mathbf{q}})\rho_{\mathbf{q}}^\dagger \tag{3}$$

which describes the creation of an electron-hole pair of momentum $\mathbf{q}$ and the creation or annihilation of a phonon. The matrix element $M(\mathbf{q})$ for polar-optic phonons is

given by

$$|M(\mathbf{q})|^2=\frac{2\pi e^2\omega_{\mathrm{LO}}(1/\epsilon_\infty-1/\epsilon_0)}{q^2L^3}\ . \tag{4}$$

Here ω_{LO} is the longitudinal optical frequency, assumed to be constant, and ϵ_∞ is the high-frequency dielectric constant, given by the square-root of the refractive index.

For the basis given by Eq. (1), the density-operator $\rho_{\mathbf{q}}$ is

$$\rho_{\mathbf{q}}=\sum_\alpha \exp[-iq_x(X+\tfrac{1}{2}l^2q_y)-\tfrac{1}{4}(q_\perp l)^2]c^\dagger_{\alpha+}c_\alpha\ , \tag{5}$$

where $|\alpha^+\rangle=|X+l^2q_y\rangle|p+q_z\rangle$ and $q_\perp^2=q_x^2+q_y^2$. Hence the electron-phonon interaction can be written

$$H_{\text{el-ph}}=\sum_{\mathbf{q},\alpha}\tilde{M}(\mathbf{q})\exp(iq_xX)(a^\dagger_{-\mathbf{q}}+a_{\mathbf{q}})c^\dagger_{\alpha+}c_\alpha\ , \tag{6}$$

where $\tilde{M}(\mathbf{q})=M(\mathbf{q})\exp[iq_xq_yl^2-\frac{1}{4}(q_\perp l)^2]$.

As the ions vibrate, they will couple to the electron density by $H_{\text{el-ph}}$ and thus induce a fluctuation in the electron density, which will tend to screen the motion of the ions. The effect of this screening will be to reduce the phonon frequencies, since the fluctuation in the electron density will reduce the ion-ion coupling. This is expressed by the fact that the new, screened phonon frequencies $\omega_{\mathbf{q}}$ are given by the poles of the renormalized phonon propagator, which is

$$D(\mathbf{q},\omega)=\frac{2\omega_0(\mathbf{q})}{\omega^2(\mathbf{q})-\omega_0^2(\mathbf{q})-2\omega_0(\mathbf{q})\dfrac{|\tilde{M}|^2P(\mathbf{q},\omega)}{\epsilon(\mathbf{q},\omega)}}\ , \tag{7}$$

where $P(\mathbf{q},\omega)$ is the real part of the retarded electron polarization graph. Since $\omega_{\mathrm{LO}}\ll\omega_p$, the electron plasma frequency, we can replace $P(\mathbf{q},\omega)$ and $\epsilon(\mathbf{q},\omega)$ by their static limits $P(\mathbf{q})$ and $\epsilon(\mathbf{q})$. For $q_z=2k_F$ the polarization graph is then[2,3]

$$P(q_z=2k_F)=-\frac{L^3m}{(2\pi l)^2k_F}\ln\left[\frac{1.14\varepsilon_F}{k_BT}\right]\ , \tag{8}$$

where k_F is the Fermi momentum in the z direction and ε_F the Fermi energy. The prefactor is just the total density of states in the z direction and reflects the high degeneracy caused by the magnetic field.

It is then evident that the renormalized phonon frequencies $\omega(q_\perp,2k_F)$ will tend to zero as the temperature is lowered; a so-called giant[7] Kohn anomaly.[8] When $\omega(q_\perp,2k_F)$ goes to zero, there is a static distortion of the electron-phonon system which will open up a gap in the electron energy spectrum. The critical temperature at which this occurs can be written, by combining Eqs. (4), (7), and (8),

$$T_c=\frac{1.14\varepsilon_F}{k_B}\exp\left[-\frac{1}{\dfrac{mL^3}{(2\pi l)^2k_F}\dfrac{2|\tilde{M}(\mathbf{q}_0)|^2}{\omega_0(\mathbf{q}_0)\epsilon(\mathbf{q}_0)}}\right]\ , \tag{9}$$

where $q_0=(q_\perp,2k_F)$. This expression is clearly of the same form as the BCS formula for the critical temperature of the superconducting state.[9] With[10] $\epsilon(q_0)=1+\kappa^2/q_0^2$, where $(\kappa l)^2=(2me^2/\pi\epsilon_0k_F)\exp[-\frac{1}{2}(q_\perp l)^2]$, Eq. (9) becomes

$$T_c=\frac{1.14\varepsilon_F}{k_B}\exp\left[-\frac{4(k_Fl)^2+Q^2+\dfrac{2me^2}{\pi\epsilon_0k_F}e^{-Q^2/2}}{\dfrac{m}{\pi k_f}\left[\dfrac{1}{\epsilon_\infty}-\dfrac{1}{\epsilon_0}\right]e^{-Q^2/2}}\right]\ . \tag{10}$$

Here $Q\equiv q_\perp l$. The observable transition will be the one with Q maximizing T_c. This evidently occurs for $Q=0$ which gives

$$T_c=\frac{1.14\varepsilon_F}{k_B}\exp\left[-\frac{4(k_Fl)^2+\dfrac{2me^2}{\pi\epsilon_0k_F}}{\dfrac{m}{\pi k_F}\left[\dfrac{1}{\epsilon_\infty}-\dfrac{1}{\epsilon_0}\right]}\right]\ . \tag{11}$$

We have compared the critical temperature given by Eq. (11) with the one given by Fukuyama's theory,[3] which is a Hartree-Fock calculation for a CDW formation of an electron gas in a magnetic field, without electron-phonon coupling. In this theory, the vertex of the electron density-density correlation function is approximated by an RPA term and a ladder term. The momentum transfer in the z direction in the ladder term is then averaged over $(-k_F,k_F)$ to obtain a Dyson equation for the vertex. One can show[11] that this theory is correct to order k_Fl. The critical temperature is then the temperature at which the expression for the vertex diverges, which occurs for

$$T_c=\frac{1.14\varepsilon_F}{k_B}\exp\left[-\frac{1}{\dfrac{me^2}{\pi\epsilon_0k_F}\Phi_0(Q,k_Fl)}\right]\ , \tag{12}$$

where

$$\Phi_0(Q,k_Fl)=\frac{1}{k_Fl}\int_0^\infty dx\,e^{-x^2/2}J_0(xQ)\frac{x}{[x^2+(\kappa l)^2]^{1/2}}\times\tan^{-1}\frac{k_Fl}{[x^2+(\kappa l)^2]^{1/2}}-\frac{e^{-Q^2/2}}{Q^2+4(k_Fl)^2}\ . \tag{13}$$

Here we have modified Fukuyama's theory[3] by allowing screening of the Coulomb line in the ladder diagram. This can be rigorously justified[11] diagrammatically, and it was taken into account by Yoshioka and Fukuyama[5] when they applied Fukuyama's theory[3] to graphite, but was neglected in Fukuyama's original paper.[3] In Eq. (13), the integral comes from the ladder term and drives the instability, whereas the second term is the RPA term and counteracts the instability. The transition occurs for the value of Q that maximizes the integral $\Phi_0(Q,k_Fl)$. This value is $Q=Q_0$, where Q_0 is between 1 and 2. Naturally, one does not expect the electron-phonon coupling to have any significant effect on T_c until the coupling is sufficiently strong. Hence for nonpolar or weakly polar semiconductors one would expect formation of an electron CDW with a negligible ion displacement. For strongly polar semiconductors, however, the strength of the

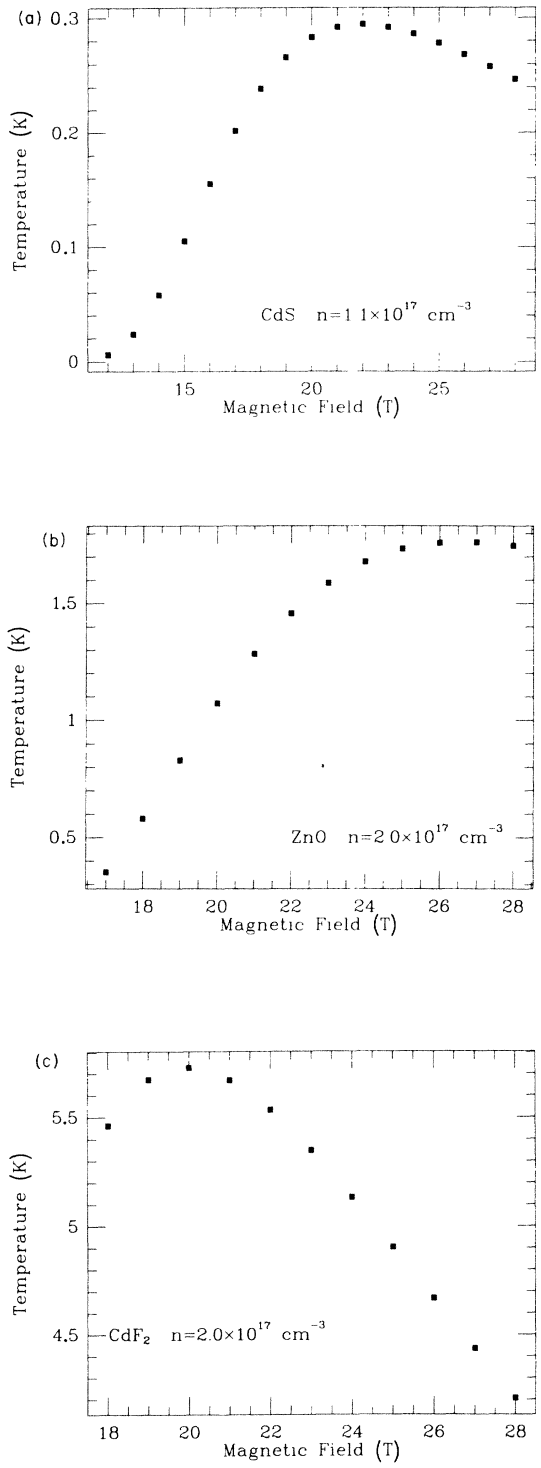

FIG. 1. (a) Critical temperature for a Peierls instability for CdS from Eq. (11). For the same range of magnetic field, T_c as given by Fukuyama's theory [Eq. (12)] is less than 2×10^{-3} K. (b) Critical temperature for ZnO. The CDW temperature is less than 2×10^{-3} K. (c) Critical temperature for CdF_2. Here the CDW temperature is $\ll 10^{-6}$ K.

electron-phonon interaction will increase the transition temperature given by Fukuyama's theory[3] resulting in a large static lattice displacement. The dependence of T_c on the magnetic field and the electron density n will also be different from that of the electron CDW. Equation (12) gives approximately (neglecting the dependence of the screening length on the magnetic field) $T_c \sim n^2 B^{-2} \exp(-n^2 B^{-5/2})$, whereas Eq. (11) gives $T_c \sim n^2 B^{-2} \exp(-n^3 B^{-4})$.

Numerical calculations show that for $\alpha \geq 0.5$ the electron-phonon interactions give rise to a critical temperature much higher than that given by Fukuyama's theory[3] for certain electron densities. In particular, we have calculated T_c as given by Eq. (12) and Eq. (11) for CdS, ZnO, and CdF_2, which have polaron coupling constants[12] $\alpha=0.527$, $\alpha=0.849$, and $\alpha=3.2$. The results are shown in Fig. 1.

It is also interesting to study how the phonon dispersion relation $d\omega(\mathbf{q})/d\mathbf{q}$ for the optical phonons behaves near the instability for $T=0$. In this case, the electron polarization graph is easily calculated with the result

$$P(\mathbf{q}) = -\frac{L^3}{(2\pi l)^2}\frac{2m}{p}\ln\left|\frac{pk_F+p^2/2}{p^2/2-pk_F}\right| . \tag{14}$$

For $p \approx 2k_F$, this implies that the phonon dispersion relation diverges as

$$\ln\left|\frac{pk_F+p^2/2}{pk_F-p^2/2}\right| + \frac{1}{pk_F-p^2/2} , \tag{15}$$

similar to the strong divergence displayed by a planar Fermi surface.[7]

In conclusion, an electron gas in a strong magnetic field has a one-dimensional energy spectrum and should thus show a tendency towards CDW formations, similar to that of a 1D electron gas. For strongly polar semiconductors, the electron-phonon coupling tends to enhance the transition temperature and give rise to a permanent distortion with a wave vector $\mathbf{q}=(0,0,2k_F)$ of both the lattice and the electron gas. This distortion should be readily observable by conventional experimental techniques. In the calculations presented here, we have assumed an isotropic system, whereas for a real system one would expect the transition to occur in a direction determined by the symmetry of the crystal.

Note added in proof. The possibility of a phase transition in similar systems was first considered in a paper by H. Fröhlich and C. Torreaux.[13] The authors would like to thank Dr. M. J. Rice for making us aware of the existence of this paper.

ACKNOWLEDGMENTS

The authors would like to thank Professor P. L. Taylor for fruitful discussions and valuable comments on the manuscript. This work was supported by National Science Foundation (NSF) Grant No. DMR-83-04244.

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