LBL-21604 c.2

Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

RECEIVED
LAWRENCE
BERKELEY LABORATORY

JUN 1 8 1986

LIBRARY AND
DOCUMENTS SECTION

Materials & Molecular Research Division

Presented at the Yamada Conference XV on Physics and Chemistry of Quasi One-Dimensional Conductors, Yamanashi, Japan, May 26-30, 1986; and to be published in Physica Scripta

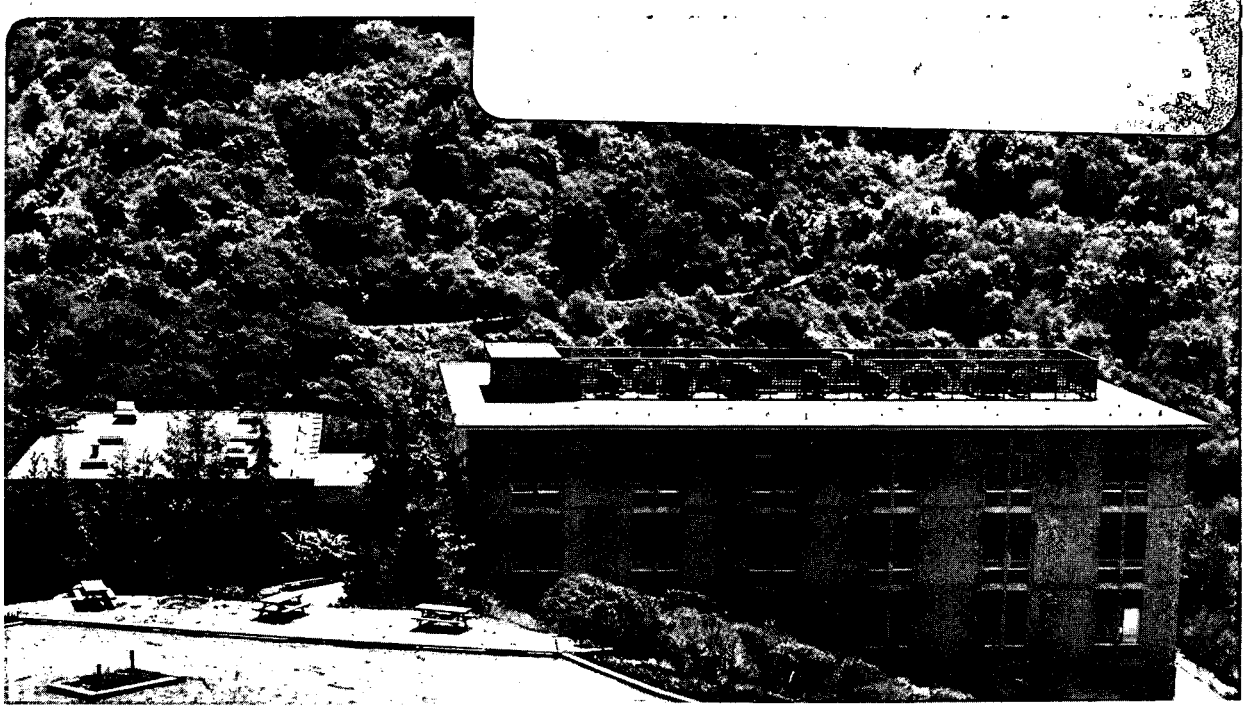
THE EFFECT OF MAGNETIC FIELDS ON THE ELECTRONIC STURCTURE OF DENSITY-WAVE SYSTEMS

L.M. Falicov and C.A. Balseiro

May 1986

TWO-WEEK LOAN COPY

This is a Library Circulating Copy which may be borrowed for two weeks.



LBL-21604 c.2

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.

LBL-21604

THE EFFECT OF MAGNETIC FIELDS ON THE ELECTRONIC STRUCTURE OF DENSITY-WAVE SYSTEMS

L. M. Falicov*

Department of Physics, University of California, and
Materials and Molecular Research Division,
Lawrence Berkeley Laboratory, Berkeley, CA 94720

and

C. A. Balseiro§

Centro Atómico Bariloche, Instituto Balseiro, 8400 Bariloche, Argentina

May 1986

---

*Work supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

§Work performed at the Department of Physics, University of California, Berkeley, under the sponsorship of a J. S. Guggenheim Memorial Foundation Fellowship.

THE EFFECT OF MAGNETIC FIELDS ON THE ELECTRONIC STRUCTURE OF DENSITY-WAVE SYSTEMS

L. M. FALICOV*

Department of Physics, University of California, and Materials and Molecular Research Division, Lawrence Berkeley Laboratory, Berkeley, CA 94720, USA

and

C. A. Balseiro§

Centro Atómico Bariloche, Instituto Balseiro, 8400 Bariloche, Argentina

The effect of high magnetic fields on the electronic structure of density-wave systems is examined. Small electron and hole pockets, caused by the density wave, may be obliterated by the magnetic field. The phenomenon is highly anisotropic, changes drastically the energy spectrum and may considerably enhance the density-wave critical temperature in some cases. The theory applies to recent experiments in niobium triselenide and in the TMTSF salts.

1. INTRODUCTION

The behavior of density waves (DW) in high magnetic fields is currently an active subject of investigation.[1-10] In several spin-density wave (SDW) systems,[1-3] in particular $(TMTSF)_2X$ where $X = PF_6$ or ClO_4, the application of pressure destroys the SDW. An applied magnetic field perpendicular to the axis of high conductivity restores the SDW at high pressures.

In $NbSe_3$, a charge-density wave (CDW) system, a magnetic field perpendicular to the high-mobility axis produces[4,5] a large increase in the resistance of the low-temperature phase $T < T_2 \approx 59K$.

Gor'kov and Lebed[6] showed that for a simple anisotropic metal with two open Fermi surface sheets (corrugated planes), the tendency to SDW formation is enhanced by a magnetic field applied in a direction parallel to the sheets. Héritier et al.[7,8] generalized the theory by including a magnetic-field dependence of the SDW q-vector. They found a cascade of first-order transitions that could be observed as the magnetic field is increased.[3] These theoretical contributions focused only on the instabilities of the normal phase, i.e., they studied the divergences of the generalized susceptibilities in the normal phase. Friedel[9] discussed these models in semiclassical terms, which is only valid for weak magnetic fields. He argued that the same effects should be observed in nearly stable CDWs.

In this contribution we analyze the effect of high magnetic fields on the electronic structure of quasi-one-dimensional (Q1D) systems with stable CDWs or SDWs. We also discuss the effect of the magnetic field on the critical temperatures.[10]

2. THE MODEL

The Q1D model used here consists of a tetragonal lattice with constants $a_1 << a_2 = a_3$ in

*Work supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

§Work performed at the Department of Physics, University of California, Berkeley, under the sponsorship of a J. S. Guggenheim Memorial Foundation Fellowship.

which an electronic single s-like tight-binding band exists. The dispersion relation is

$$E_0(\vec{k}) = -2t\cos(k_x a_1) - 2t'[\cos(k_y a) + \cos(k_z a)] - 4t''\cos(k_y a)\cos(k_z a) , \quad (1)$$

where $\vec{k} = (k_x, k_y, k_z)$ and $a = a_2 = a_3$. The parameters are such that $t \gg t', t''$.

If there is one electron per site, the Fermi surface consists of two open sheets centered at $k_x \cong \pm(\pi/2a_1)$. The system shows a tendency to form a DW with a wavevector $\vec{q} = (\pi/a_1, \pi/a, \pi/a)$ which connects (nests) the two sheets of Fermi surface. The stable DW is either a CDW or a SDW, depending on whether the electron-phonon or the repulsive electron-electron interaction dominates.[11] The DW is characterized by a gap order parameter τ. Because of the extra periodicity induced by the DW, the electronic states at $\vec{k}$ and at $(\vec{k}+\vec{q})$ are mixed by a matrix element proportional to τ.

The DW quasi-particle spectrum of the system is given by

$$E_{\pm}(k) = -4t''\cos(k_y a)\cos(k_z a) \pm [\{2t\cos(k_x a_1) + 2t'[\cos(k_y a) + \cos(k_z a)]\}^2 + \tau^2]^{1/2} .$$

For $t'' = 0$ this energy spectrum has a gap 2τ at the center of the band, i.e. at the Fermi level. The DW phase is therefore a semiconductor. This fact is a consequence of the perfect nesting of the normal, $\tau = 0$ Fermi surface.

For $t'' \neq 0$, there is no longer perfect nesting. As before, the DW induces a direct gap of value 2τ. But the spectrum has now a smaller <u>indirect gap</u> of value $2\Delta g$ given by $2\Delta g = 2\tau - 8t''$ if $\tau/t'' > 4$, and zero otherwise. In this case, depending on the value of τ/t'', the system in the presence of a DW is either a semiconductor or a semimetal.

When a magnetic field is applied, new complications arise. Whereas the DW causes gaps in an otherwise continuous spectrum, the magnetic field quantizes the electronic motion in the two directions perpendicular to it and tends to form either discrete levels and narrow bands if the cyclotron electronic orbits are closed, or complicated continua if they are open.[12-17] The competition between these various effects are the cause of the strange, complex behavior under study here.

3. CALCULATIONS AND RESULTS

The energy spectrum for various values and orientations of the magnetic field were obtained by means of a transfer-matrix method and a formulation similar to that of Harper;[13] the effective-Hamiltonian approximation of Luttinger and Kohn[17] was employed. Results for fields in the z-direction can be summarized as follows.

(i) For low magnetic fields the semiclassical spectra are reproduced.[12]

(ii) For intermediate and high fields there is a substantial broadening of all Landau levels.

(iii) For high magnetic fields electron and hole levels are very broad, and the lowest (highest) boundary of the broadened $n = 0$ electron (hole) level is at an energy very close to τ ($-\tau$). As a consequence, the total three-dimensional spectra for high magnetic fields have a gap for energies $|E| < \tau$ and a continuum of states for $|E| > \tau$. All k_z sections contribute no states for $|E| < \tau$ and continuum states for $|E| > \tau$, just as in the perfect nesting case. In other words, the semimetallic system for high enough fields changes to a semiconductor with $\Delta g = \tau$: there is a semimetal-to-semiconductor transition.

A magnetic field along [011] produces similar but less pronounced effects. A reasonable high magnetic field produces a semiconducting state only for $\tau/t'' > 2$.

Energy spectra for magnetic fields along the high-conductivity [100] x-axis are evaluated in the same fashion. No central gaps are obtained if $\tau/t'' < 4$, i.e., there is essentially no magnetic field effect.

The critical temperature and its magnetic field dependence can also be calculated in a simple way. A linearization of the dispersion relation (1) for k_x in the vicinity of $\pm(\pi/2a_1)$ and the procedure described in Ref. 6 yields an easily solvable integral equation for the critical temperature T_c.

In Fig. 1 the DW critical temperature T_c as a function of a dimensionless coupling constant ξ is shown. Because of the lack of perfect nesting at H = 0, the DW is stable only for $\xi > \xi_c$, a minimum critical value of the interaction. A magnetic field however can induce a DW for $\xi < \xi_c$. This magnetic-field-induced DW was predicted by Gor'kov and Lebed.[6] For $\xi > \xi_c$ the presence of a magnetic field raises the value of T_c. However, if the critical temperature for zero magnetic field is not too low, T_c does not change appreciably with magnetic field.

4. SUMMARY AND DISCUSSION

(a) A magnetic field perpendicular to the axis of high conductivity DW system may induce gaps in the spectrum at the Fermi level, thus transforming a semimetallic structure into a semiconducting one.

(b) The value of the gap Δ_g is a function of the DW strength τ, the cyclotron energy $\hbar\omega_c$ and the "lack of nesting" parameter t", but insensitive to other band-structure parameters.

(c) Although at low magnetic fields the spectrum of the system is well described by the semiclassical quantization scheme, this scheme breaks down for fields such that the cyclotron energy is of the order of, or greater than, the DW mixing parameter τ; in the latter regime band mixing becomes paramount.

(d) The complete spectrum of the system as a function of the various parameters shows two main effects: (d1) in the semiclassical (closed orbit) discrete regime the Landau levels spread into wider and wider bands as the field strength increases; and (d2) in the semiclassical (open orbit) continuum energy gaps appear at high fields.

(e) The semimetal-to-semiconductor transition does not take place for magnetic fields parallel to the axis of high conductivity, the x-axis in this simple model.

(f) There is also considerable anisotropy for fields perpendicular to the high-

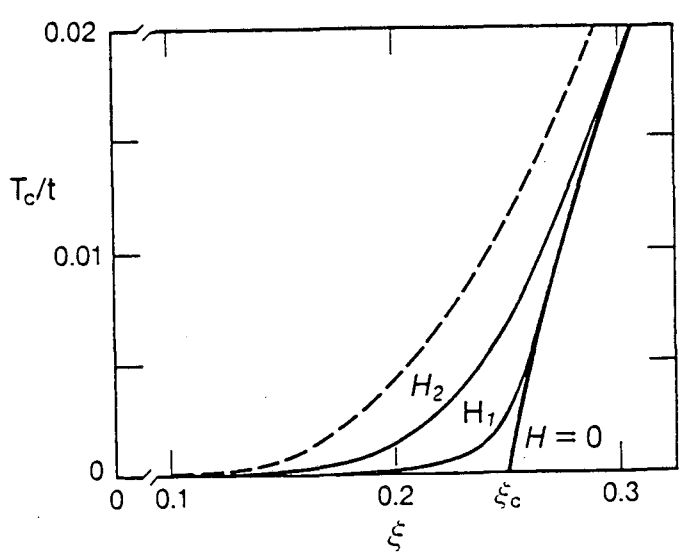


FIGURE 1

The critical temperature T_c as a function of interaction strength ξ for (a) the perfect nesting case t" = 0 and H = 0 (dashed line); (b) a semimetallic case t" = 0.01 t and H = 0 (observe the critical value ξ_c); (c) and (d) the case shown in (b) for magnetic fields parallel to [001], and strengths H_1 and $H_2 = 2H_1$ where $H_1 = (hc/200\,ea_1a)^2$. It should be noted that T_c changes appreciably with magnetic-field strength only for ξ in the vicinity of ξ_c. For the lattice parameters of $NbSe_3$, H_1 = 250 kG.

conductivity axis [the (y,z) plane].

(g) The DW transition temperature T_c is enhanced by the magnetic field. The enhancement, however, is only appreciable if the situation is such that the interaction strength ξ is just below or just above the critical value ξ_c, i.e. for marginally stable or marginally unstable,[6] semimetallic DWs. For well established, stable DWs the enhancement effect is small.

(h) All effects encountered in this tetragonal model can be directly applied to interpret the experiments in the more anisotropic, real systems such as $NbSe_3$ (a CDW system) or the TMTSF salts (SDWs). The complexity of the spectra and electronic effects found here are complicated even more by the complexity of the real band structure in these materials, where several sheets of Fermi surface (of various topologies) contribute to the conduction process.

REFERENCES

1. R. Brusetti, P. Garoche, and K. Bechgaard, J. Physique Colloq. C 3 (1983) 1051.

2. T. Takahashi, D. Jérome, and K. Bechgaard, J. Phys. (Paris), Lett. 43 (1982) 565.

3. F. Pesty, P. Garoche, and K. Bechgaard, Phys. Rev. Lett. 55 (1985) 2495.

4. R. V. Coleman, G. Eiserman, M. P. Everson, A. Johnson, and L. M. Falicov, Phys. Rev. Lett. 55 (1985) 863.

5. R. V. Coleman, M. P. Everson, G. Eiserman, and A. Johnson, this volume.

6. L. P. Gor'kov and A. G. Lebed, J. Phys. (Paris), Lett. 45 (1984) 433.

7. M. Héritier, G. Mantambaux, and P. Lederer, J. Phys. (Paris), Lett. 45 (1984) 943.

8. G. Montambaux, M. Héritier, and P. Lederer, Phys. Rev. Lett. 55 (1985) 2078.

9. J. Friedel, Phil. Trans. Roy. Soc. London, Ser. A 314 (1985) 189.

10. C. A. Balseiro and L. M. Falicov, Phys. Rev. Lett. 55 (1985) 2336.

11. C. A. Balseiro, P. Schlottmann, and F. Yndurain, Phys. Rev. B 21 (1980) 5267.

12. L. Onsager, Philos. Mag. 43 (1952) 1006.

13. P. G. Harper, Proc. Roy. Soc. London, Sect. A 68 (1955) 874.

14. J. Zak, Solid State Phys. 27 (1972) 1.

15. W. Y. Hsu and L. M. Falicov, Phys. Rev. B 13 (1976) 1595.

16. D. R. Hofstadter, Phys. Rev. B 14 (1976) 2239.

17. J. M. Luttinger and W. Kohn, Phys. Rev. 97 (1955) 869.

This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720