PHYSICAL REVIEW B VOLUME 17, NUMBER 4 15 FEBRUARY 1978

Tunneling of solitons and charge-density waves through impurities

A. I. Larkin
L. D. Landau Institute for Theoretical Physics, Moscow, Union of Soviet Socialist Republics

Patrick A. Lee
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 14 October 1977)

In the presence of impurity potentials which couple directly to the phase of the charge-density waves the ground state as well as soliton excitations are pinned. The quantum-mechanical tunneling of a sine-Gordon soliton through an impurity potential is calculated. The small tunneling probability for even a moderate impurity potential means that the conductivity due to solitons will be greatly reduced. We also study the electric field and temperature dependence of a charge-density wave pinned by impurities when quasiclassical tunneling is taken into account. The temperature dependence is found to be dominated by simple thermal excitation and the conductivity is activated in both the strong- and weak-pinning limits.

I. INTRODUCTION

There has been considerable interest in the pinning of charge-density waves (CDW) in one dimension by impurities[1-3] or by external sinusoidal potentials.[4] At sufficiently low temperature, amplitude fluctuations may be ignored and the charge density $\rho(x)$ is described by the phase variable $\phi(x)$

$$\rho(x)=\bar{\rho}+\rho_0 \,\mathrm{Re}(e^{iQx+\phi(x)}) . \tag{1.1}$$

The dynamics of the CDW can be described by the Lagrangian[1]

$$\mathcal{L}=\int dt\left\{\int dx\left[\frac{m^*}{2\pi Q}\left(\frac{\partial\phi}{\partial t}\right)^2-\frac{v_F}{4\pi}\left(\frac{\partial\phi}{\partial x}\right)^2\right]-H_1-H_2\right\}, \tag{1.2}$$

where

$$H_1=\int dx\, w[1-\cos\phi(x)] , \tag{1.3}$$

$$H_2=-\sum_i V_i\cos[Qx_i+\phi(x_i)] . \tag{1.4}$$

H_1 describes the coupling of CDW with an external sinusoidal potential. Examples of such a potential are the commensurate energy or the interchain coupling in cases like TTF-TCNQ (tetrathiafulvalene-tetracyanoquinodimethane) which consist of oppositely charged chains. The ground state is clearly pinned by the external potential. However, it has been pointed out by Rice *et al.*[4] that there exist excited states that are the soliton solution to the sine-Gordon equation. Such solitons are able to move freely and contribute to the conductivity. The Hamiltonian H_2 describes the coupling of impurity potentials located at random sites x_i with the CDW. We shall assume for simplicity that the impurity strength V is constant. We note that in our model the impurity couples directly to the phase. Such a model is appropriate for charged impurities as the impurity potential will couple to the oscillatory component of the CDW. This is to be contrasted with the model studied by Fogel *et al.*,[5] where the impurities couple to the gradient of the phase, i.e., the impurity couples to the net charge accumulation upon compression of the CDW. While Fogel *et al.* have shown that soliton propagation is not seriously affected in their model, it is clear that the existence of impurities which couple to the phase directly will inhibit the motion of the solitons. More specifically, we shall consider the interaction of a single soliton with a single impurity. The impurity will pin the phase of the soliton. In order to pass through the impurity and contribute to the conductivity, the soliton must tunnel through the impurity site. In Sec. II we shall study the probability amplitude for such a tunneling process.

The problem of impurity pinning alone in the presence of H_1 is also of great interest.[1-3] Let us suppose that the impurities are on the average $\bar{l}$ apart. In the absence of H_1 there is clearly a competition between the elastic energy term given by $v_F/\bar{l}$ and the impurity pinning energy V. Fukuyama and Lee[1] have introduced the dimensionless parameter

$$\epsilon=V\bar{l}/v_F . \tag{1.5}$$

For $\epsilon\gg 1$, i.e., if V is large or if the impurities are dilute, we have the strong-pinning situation. At every impurity site the phase satisfies $Qx_i+\phi(x_i)=\pi(2n+1)$ to take advantage of the impurity potential. The phase then interpolates linearly between impurity sites in such a way as to minimize the elastic energy. On the other hand, if $\epsilon \ll 1$ we have the weak-pinning situation. The phase is slowly varying over some characteristic length L_0 in such a way to take advantage of the fluctuation in the impurity potential within this length. The length L_0 is determined by minimizing the free energy

$$v_F/L_0 + V(L_0/\bar{l})^{1/2}. \qquad (1.6)$$

The dynamics of the problem have been studied by Fukuyama and Lee[1] who concluded that there is a finite restoring force in both the strong- and weak-pinning cases. The conductivity therefore has a peak at finite frequency and the dc conductivity is zero. Similar conclusions are also reached by Gor'kov[3] in the strong-pinning case starting from a microscopic Hamiltonian and by Efetov and Larkin[2] in the weak-pinning case. Three-dimensional and Coulomb effects are also included in the latter work. So far, the discussion has been restricted to zero temperature. In this paper we shall study the dc conductivity at finite temperature and in finite electric field.

Phenomenologically the current is given by

$$j = (e/\pi)\dot{\phi}. \qquad (1.7)$$

In order to carry a current the phase must increase as a function of time. In particular, some mechanism must be available for the phase to increase at the impurity sites. The mechanism might be thermally activated hopping or quantum-mechanical tunneling. In Sec. III we consider the tunneling probability in both the strong- and weak-pinning limits. In Sec. IV we discuss the implication for the temperature and electric field dependence of the dc conductivity.

II. TUNNELING OF A SOLITON THROUGH AN IMPURITY

In this section we consider the interaction of a single soliton with a single impurity potential located at the origin. There are two separate regimes, depending on whether the impurity potential V is large or small compared with the soliton energy E_S, and we shall study these two cases separately.

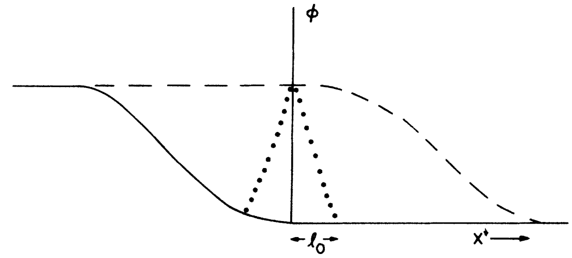

FIG. 1. Tunneling of a soliton through an impurity located at the origin. Solid line and dashed line are the initial and final states, respectively. Dotted line depicts the rapid tunneling at the impurity site.

Recently, Maki[6] has considered the tunneling problem in the presence of an electric field for the H_1 only problem. He uses a method in imaginary time proposed by t'Hooft[7] which we also find convenient to use here. The probability amplitude is given by e^A, where the action A is obtained by minimizing the function $\int d\tau \mathcal{L}(\tau)$, where the Lagrangian $\mathcal{L}$ is the same as that given in Eq. (1.2), except that $(\partial\Phi/\partial t)^2$ is replaced by $-(\partial\phi/\partial\tau)^2$. The justification is clear in the case of a single-particle tunneling through a potential barrier. The probability amplitude for semiclassical tunneling is given by $\exp(-\int dr\, q(r))$, where $q(r)=\{2m[V(r)-E]\}^{1/2}$. We can interpret $q(r)$ as the momentum for a particle of negative mass (or moving in imaginary time). In this case, we have $\int d\tau[\mathcal{L}(\tau)+E]=\int dr\, q(r)$, where $\mathcal{L}(\tau)=-\frac{1}{2}m(\partial r/\partial\tau)^2 - V(r)$ and E is the energy of the system. This argument can clearly be generalized to the case of tunneling of a field variable $\phi(x)$.

We first consider the case $V \gg E_S$. Our problem is to find $\phi(x,\tau)$ which changes from the initial to the final state illustrated in Fig. 1 while minimizing the action. It is convenient to change variables to $\tau_0' = v\tau$, where v is the phase mode velocity given by $v = v_F(m/m^*)^{1/2}$ and m^*/m is the ratio of the effective mass to the electron band mass, and rewrite the action in the form

$$A = -\frac{1}{4\pi}\left(\frac{m^*}{m}\right)^{1/2}\int d\tau'\, dx\left[\left(\frac{\partial\phi}{\partial\tau'}\right)^2 + \left(\frac{\partial\phi}{\partial x}\right)^2 - \frac{4\pi w}{v_F}(\cos\phi - 1) - \frac{4\pi V}{v_F}\delta(x)\cos(\phi)\right]. \qquad (2.1)$$

It is apparent that there are two separate regimes in the tunneling process. The phase at the impurity site will tunnel through in a short time τ_0' to minimize the impurity potential energy while the change in phase of the soliton away from the impurity site will proceed more slowly. To describe the tunneling at the impurity site, let us write the following trial solution:

$$\phi(x,\tau') = \frac{2\pi\tau'}{\tau_0'}\left(1 - \frac{|x|}{l_0}\right),$$

$$\text{for } 0<\tau'<\tau_0' \text{ and } |x|<l_0. \qquad (2.2)$$

Since $V \ll E_S$ the contribution from $w\cos\phi$ in Eq. (2.1) may be ignored and we obtain a contribution to the action for this time interval equal to

$$A_1 = -\left(\frac{m^*}{m}\right)^{1/2}\left[\frac{2\pi}{3}\left(\frac{l_0}{\tau_0'} + \frac{\tau_0'}{l_0}\right) + \tau_0'\frac{V}{v_F}\right]. \quad (2.3)$$

Minimizing with respect to l_0, it is clear that $l_0 = \tau_0'$ and

$$A_1 = -(m^*/m)^{1/2}(\tfrac{4}{3}\pi + l_0 V/v_F). \quad (2.4)$$

The next tunneling regime we consider takes place away from the impurity site when the phase changes from the solid curve shown in Fig. 1 to the dashed curve. Now the impurity potential no longer plays a role. The phase then obeys the equation

$$\frac{\partial^2\phi}{\partial\tau'^2} + \frac{\partial^2\phi}{\partial x^2} = -2\pi\frac{w}{v_F}\sin\phi \quad \text{for } x, \tau' > l_0. \quad (2.5)$$

This equation is now isotropic in (x, τ') space. The right-hand side of Eq. (2.5) may be ignored if w/v_F is less than $1/x^2$, where x is the characteristic size of the spatial variation. Since this size is less than the soliton size $l_s \sim (w/v_F)^{-1/2}$, the condition is marginally satisfied. Equation (2.5) is then approximated by the two-dimensional Poisson equation

$$\frac{\partial^2}{\partial\tau'^2}\phi + \frac{\partial^2}{\partial x^2}\phi = 0 \quad \text{for } x, \tau' > l_0, \quad (2.6)$$

subject to certain boundary conditions. Under the condition $l_s \gg l_0$ (which can be verified *a posteriori*) we can solve Eq. (2.6) in cylindrical coordinates r and θ. A simple solution is given by $\phi = 2\theta$. The interpretation of this solution is as follows. For $\tau' \to -\infty$, $\phi = -\pi$ for all x. Let us restrict our attention to $x > 0$. As τ' increases toward zero, the phase ϕ changes from $-\pi$ at the origin to being zero at infinity over a shorter and shorter distance. As τ' passes through zero the phase at $x = 0$ suddenly jumps to π and eventually for $\tau' \to \infty$, $\phi = \pi$ everywhere. In the region in time and space near the origin where the phase jumps from $-\pi$ to π, the impurity potential needs to be taken into account. However, this is precisely the first tunneling regime we treated earlier in arriving at Eq. (2.4). Thus we remove a circle of radius l_0 at the origin from our present consideration. Putting this solution into the action

$$A_2 = -\frac{1}{4\pi}\left(\frac{m^*}{m}\right)^{1/2}\int dx\, d\tau'\left[\left(\frac{\partial\phi}{\partial\tau'}\right)^2 + \left(\frac{\partial\phi}{\partial x}\right)^2\right], \quad (2.7)$$

the integral is clearly logarithmically divergent, in analogy to the energy of a vortex in two dimensions. The natural cutoffs for the radial integration are l_0 and l_s. We obtain

$$A_2 = -2(m^*/m)^{1/2}\ln(l_s/l_0). \quad (2.8)$$

The numerical factor in this expression is accurate, the only correction will appear inside the logarithmic term.

It remains to determine the cutoff l_0. This is done by minimizing the sum $A_1 + A_2$. The result is

$$A_1 + A_2 = -2(m^*/m)^{1/2}[c + \ln(V/E_S)], \quad (2.9)$$

where c is a number of order unity ($c = \frac{1}{2} + \frac{2}{3}\pi$ within our approximation). It is interesting that the action depends only logarithmically on the impurity potential. The large action means that the conductivity by solitons will be greatly reduced.

We next consider the opposite case when $V \ll E_S$. In this case, the impurity potential is a small perturbation and the soliton will maintain its integrity in the tunneling process. The phase can be described by $\phi_s(x - x_0(t))$, where ϕ_s is the soliton solution and x_0 describes the location of the soliton. We then have the effective Lagrangian

$$\mathcal{L} = \tfrac{1}{2}m_s(\dot{x}_0)^2 - V\{1 - \cos[\phi_s(-x_0(t))]\}, \quad (2.10)$$

where $m_s = E_S/v^2$ and we have a single particle problem described by the parameter x_0. The tunneling amplitude is given by e^A where

$$A = -\int [2m_s V(1 - \cos\phi_s)]^{1/2}\, dx_0. \quad (2.11)$$

This can be simplified by noting that

$$\frac{d\phi_s}{dx} = \left(\frac{4\pi w}{v_F}\right)^{1/2}(1 - \cos\phi_s)^{1/2}. \quad (2.12)$$

Changing the integration variable to ϕ_s, Eq. (2.11) becomes

$$A = -2\pi(2m_s(v_F V/4\pi w)^{1/2}$$
$$= -8[(m^*/m)V/E_S]^{1/2}. \quad (2.13)$$

Our quasiclassical treatment is valid only if $|A| \gg 1$. If this is not obeyed, a full quantum-mechanical treatment of Eq. (2.10) is required. We simply note here that if the soliton momentum p is sufficiently small the scattering of the soliton by the impurity is described by an effective Hamiltonian

$$H_{eff} = \frac{p^2}{2m_s} + \int V[1 - \cos\phi_s(x')]\, dx'\, \delta(x)$$
$$= \frac{p^2}{2m_s} + \frac{VE_S}{2w}\delta(x). \quad (2.14)$$

The soliton-impurity problem becomes identical to the usual electron-impurity problem. There is an extensive literature dealing with the localization in one dimension of this problem.[8]

III. TUNNELING THROUGH RANDOM IMPURITIES

In this section we study the problem of tunneling through impurities in the absence of the external potential H_1. First we treat the strong-pinning case $\epsilon \gg 1$. In this case, the phase must change from the initial to a final state in which the phase has jumped by 2π between two impurity states. This problem is similar to the soliton-impurity problem discussed in Sec. II. The tunneling problem is again divided into two parts, the rapid tunneling at the impurity site and the slow change of the phase from 0 to 2π in between impurity sites. The result is the same as Eq. (2.9) except that we must replace the soliton size l_s by the impurity spacing $|x_1 - x_2|$. If we set $|x_1 - x_2| = \bar{l}$, we obtain

$$A = -2(m^*/m)^{1/2}\ln\epsilon\,, \tag{3.1}$$

where ϵ is defined in Eq. (1.2).

We next consider the weak-pinning case. Let us suppose that a section of length L_0 [defined in Eq. (1.3)] tunnels from one state to another of similar energy in the time τ_0'. In general, such states are well separated in $\phi(x)$ space. Unlike the strong-pinning case, the phase will go smoothly from the initial to the final state and the action is roughly given by

$$A = -\left(\frac{m^*}{m}\right)^{1/2}\left[\frac{L_0}{\tau_0'} + \frac{\tau_0'}{L_0} + \frac{4\pi V}{v_F}\left(\frac{L_0}{l}\right)^{1/2}\tau_0'\right]. \tag{3.2}$$

The last term is an estimate of the fluctuation in the impurity potential. Minimizing with respect to τ_0' and using the expression for L_0, we obtain

$$A = -c(m^*/m)^{1/2}\,, \tag{3.3}$$

where c is a numerical constant of order unity.

IV. RESISTIVITY

In this section we discuss the resistivity in the presence of random impurities in the absence of external potential H_1. We begin with the strong-pinning case. Let us first discuss a very artificial model in which the impurity spacings are all equal to $\bar{l}$ while the pinned phases are random. The nonlinear conductivity can be discussed very simply in this model. The phase will tunnel from the initial state shown in Fig. 2 to the final state. The energy gained from the electric field equals eEl, where l is the size of the tunneling segment. The elastic energy is different in the initial and final state only in the first and last impurity sections. In the one-dimensional problem we should add the resistance from different segments in the chain. The resistivity will be dominated by those segments with the largest resistance. In the present case, this means segments in which the impurity phases are almost equal so that the elastic energy difference is given by $2v_F(2\pi)^2/4\pi\bar{l}$. The number of impurity sites we have to tunnel through is given by balancing the electrical energy gained with the elastic energy $eEl = v_F(2\pi)/\bar{l}$, and the resistance is given by

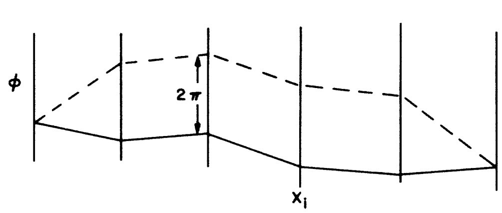

FIG. 2. Vertical lines denote impurity sites. Solid line is the initial ground state and dashed line is the final state.

$$\rho = \exp[(2\pi v_F/eE\bar{l}^2)(m^*/m)^{1/2}\ln\epsilon]\,. \tag{4.1}$$

By averaging the resistance of different types of segments weighted by their probability, we can show that the result given in Eq. (4.1) is unchanged.

Next, we consider the resistivity at finite T. The energy can be supplied by a thermal bath instead of an electric field. The density of such excitation is given by $\exp(-2\pi v_F/\bar{l}kT)$. Such an excitation will diffuse by tunneling through one impurity at a time and the tunneling rate is what we calculated earlier. The resistivity is then given by

$$\rho = \exp(\pi v_F/\bar{l}kT)\exp[(m^*/m)^{1/2}\ln\epsilon]\,. \tag{4.2}$$

We note that the activation energy can be written $\pi V/\epsilon$ and is thus smaller than the impurity potential for $\epsilon \gg 1$.

Unfortunately in reality the impurity spacing is not uniform. The distribution of impurity spacing is Poisson, i.e., $P(l) = \bar{l}^{-1}\exp(-l/\bar{l})$. The resistance will be dominated by segments in which the impurity spacing is short. The shortest spacing allowed without going over to the weak-pinning regime is given by $l_m = \bar{l}/\epsilon$. In Eq. (3.2) for the temperature-dependent conductivity, $\bar{l}$ should be replaced by $\bar{l}/\epsilon$ and $\ln\epsilon$ replaced by unity. Thus, the activation energy is given by the impurity potential V. In this case, the thermal bath supplies an energy V and tunneling is in fact unnecessary. The resistivity is simply $\rho = \exp(-V/kT)$. Similar consideration applies toward the electric field dependence. The probability of having n short impurity spacings, each of length l_m, is of order ϵ^{-n}. As long as $(m^*/m)^{1/2} > \ln\epsilon$, the small probability for the existence of this segment is overcome by the large action and Eq. (4.1) for the nonlinear conductivity must be modified by replacing $\bar{l}$ by $\bar{l}/\epsilon$ and $\ln\epsilon$ by unity. The dependence on E remains the same but the characteristic field becomes much larger.

Recently nonlinear resistivity of the form $\exp(E_0/E)$ has been observed in $NbSe_3$.[9] However, putting numerical estimates into Eq. (4.1) indicates that an extremely large value of $\bar{l}$ is required to produce the observed characteristic field of the order of 1 eV/cm. Furthermore, there is the difficulty already noted by Maki[6] that the energy supplied by the electric field can also be supplied by the thermal energy kT. Thus, the observation of such a small characteristic field at a relatively high temperature (~100 K) cannot be explained by the present model.

The resistivity in the weak-pinning case is much more complicated and we can present here only a qualitative discussion. The physical picutre for the ground state consists of regions of size L_0 inside which the phase is slowly varying. There may be other metastable states with similar energy. However, the phase will be very different from the ground state and generally speaking, the smaller the energy difference, the longer is the segment l over which the phase function is different. The only way to make transition to these low-lying states is by tunneling, and from Sec. III we know that the probability is very small, being given by $\exp[-n(m^*/m)^{1/2}]$, where $n = l/L_0$. Without knowing the dependence of the typical excitation energy on n, we cannot study the temperature dependence of this mechanism. However, at very low temperature the situation actually becomes more simple in one dimension, the reason being that it is the segments with the largest resistance that dominate the resistivity. Such a segment may consist of impurities that happen to have the same phase within $\Delta\phi$. The probability of having such a segment is given by $(\Delta\phi/2\pi)^{l/\bar{l}}$, where l is the length of the segment. Inside this segment we have basically the case studied by Maki and Rice *et al.*, with the impurities playing the role of an external sinusoidal potential. Conduction is by thermal activation and propagation of solitons. The soliton energy E_S' and size l_s' are roughly estimated by minimizing

$$V(l_s'/\bar{l}) + v_F/l_s' ,$$

from which we obtain $l_s' = \epsilon^{-1/2}\bar{l}$ and $E_S' = \epsilon^{-1/2}V$. Combining with the probability of having a segment of length l_s, we obtain the resistivity from such a segment,

$$\rho = \exp[\epsilon^{-1/2}V/kT - \epsilon^{-1/2}\ln(2\pi/\Delta\phi)] . \qquad (4.3)$$

Note that this makes a large contribution to the total resistivity if $kT \ll V$, since $\Delta\phi$ can be such that $\ln(2\pi/\Delta\phi)$ is a number of the order of unity.

Still another contribution to the resistivity is by thermal excitation. In this case, the typical excitation involves a segment of size L_0 and an energy of $\epsilon^{-1/3}V$ as shown in Eq. (1.3). Thus, there will be a contribution to the resistivity of the form $\exp(\epsilon^{-1/3}V/kT)$. However, we see that the activation energy in this case is smaller than that given in Eq. (4.3) and we expect Eq. (4.3) to dominate the very low-temperature dependence of the resistivity.

V. CONCLUSION

We have studied the temperature and electric field dependence of the resistivity for pinned CDW in one dimension. In a system like TTF-TCNQ, where chains of opposite charge present to each other an external potential, it has been suggested that solitons may provide conductivity with low activation energy. If impurities are also present we show that in order to conduct, the solitons must tunnel through each impurity. As a result, its conductivity is reduced by the tunneling probability $\exp[-4(m^*/m)^{1/2}\ln(V/E_S)]$ if $V \gg E_S$. On the other hand, for very weak impurity potential the problem reduces to the electron-impurity problem in one dimension. In the case of random impurities alone, we have studied the tunneling probability through the impurity potential and the contribution of tunneling to conductivity. However, we find that in the strong-pinning case the resistivity is dominated by regions where the impurities are close together and the resistivity is simply that of classical thermal activation, $\exp(V/kT)$. The weak-pinning region is more complicated, but the low-temperature resistivity is still activated, with an activation energy given by $\epsilon^{-1/2}V$.

Finally, we should discuss the validity of the quasiclassical approximation to the tunneling probability. The criterion for small quantum-mechanical corrections is that $m^*/m \gg 1$, so that the tunneling probability is small. We recall the formula $m^*/m = 1 + 4\Delta^2/\lambda\omega_0^2$, where Δ and ω_0 are the energy gap and the phonon frequency, respectively. The condition $m^*/m \gg 1$ is satisfied if $\Delta \gg \sqrt{\lambda}\omega_0$. On the other hand, if $\Delta \ll \sqrt{\lambda}\,\omega_0$, the problem is much more complicated since the possibility of superconducting fluctuations will have to be considered.[10]

ACKNOWLEDGMENT

This work has been carried out at the Aspen Center for Physics while the authors were participants in the Joint Research Group in Condensed Matter Physics of the Joint US-USSR Commission on Scientific and Technological Cooperation. The authors would like to thank the Aspen Center for Physics for its hospitality.

[1]H. Fukuyama and P. A. Lee, Phys. Rev. B (to be published).
[2]K. B. Efetov and A. I. Larkin, Sov. Phys.-JETP (to be published).
[3]L. P. Gor'kov, Sov. Phys.-JETP (to be published).
[4]M. J. Rice, A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Phys. Rev. Lett. 36, 432 (1976).
[5]M. B. Fogel, S. E. Trullinger, A. R. Bishop, and J. A. Krumhansl, Phys. Rev. B 15, 1578 (1977).
[6]K. Maki, Phys. Rev. Lett. 39, 46 (1977).
[7]G. t'Hooft, Phys. Rev. Lett. 37, 8 (1976).
[8]V. L. Bereshinskii, Zh. Eksp. Teor. Fiz. 65, 1251 (1974) [Sov. Phys.-JETP 38, 620 (1974)].
[9]P. Monceau, N. P. Ong, A. M. Portis, A. Murschant, and J. Rouxel, Phys. Rev. Lett. 37, 602 (1976).
[10]Yu. A. Bychkov, L. P. Gor'kov and I. E. Dzyaloshinskii, Zh. Eksp. Teor. Fiz. 50, 738 (1966) [Sov. Phys.-JETP 23, 489 (1966)].