Superstructure of a spin density wave in a band antiferromagnet with a nonmagnetic impurity

V. N. Men'shov, E. E. Slyadnikov, and V. V. Tugushev

I. V. Kurchatov Institute of Atomic Energy, Moscow

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The formation of a soliton lattice of a spin density wave in a band antiferromagnet with a low concentration of a nonmagnetic impurity is analyzed. Phase diagrams are constructed for the system near the Lifshitz point, both with a variational solution for the envelope of the spin density wave and in an exactly solvable model with an electron reservoir of infinite strength M. A procedure is proposed for finding small corrections which distort the shape of the exact solution for the soliton lattice of the spin density wave in the limit of large values $M \gg 1$ with a weak electron-impurity scattering.

1. INTRODUCTION

In many systems in which electronic phase transitions occur, a modulated long-period structure of the order parameter can be described in the model of an electron soliton lattice.[1] Among these systems are various physical entities, in particular, quasi-one-dimensional superconductors in a magnetic field (the Larkin-Ovchinnikov-Fulde-Ferrell model) and band antiferromagnets with slightly corrugated plane regions on the Fermi surface (the Overhauser-Lomer-Kotani model). In the absence of impurity scattering of electrons, an exact solution can be found for the nonuniform order parameter $\Delta(x)$ on the basis of the mathematical analogy between these models and the Peierls continuum model.[2] It is also possible to construct the thermodynamics of the system in a nonuniform state. Numerical calculations of diagrams for these models, based on the approach of Ref. 1, were carried out in Refs. 3 and 4. Buzdin and Polonskiĭ have recently examined the effect of impurity scattering on the phase diagram of a superconductor in a quasi-one-dimensional model.

Impurities cause several changes in the (T, μ) phase diagram in the model of a band antiferromagnet (T is the temperature, and the parameter μ is a measure of the extent to which the electron and hole Fermi surfaces are not congruent) from that in the "pure" case. Furthermore, the shape of the exact solution $\Delta(x)$ in the model of a spin density wave may be disrupted to a greater or lesser extent, depending on the structure of the electron-impurity scattering matrix elements and the strength of the paramagnetic electron "reservoir" (it is known quite well that this reservoir must be taken into consideration in order to reach an understanding of the properties of real band antiferromagnets). The exact solution may retain its shape only in the limit of an infinitely strong reservoir (a fixed incongruity parameter), in which case the redistribution of the charge density in the modulated antiferromagnetic structure is suppressed.[6]

In the present paper we propose a method for calculating corrections to the solution of Ref. 1 near the Néel point in situations in which the impurity scattering causes only a slight distortion of the structure of the "ideal" soliton lattice of the spin density wave. In addition, we analyze the changes caused in the (T, μ) phase diagram by the impurity scattering. These problems arise from the need to generalize the model of Ref. 1 for dilute alloys of chromium with nonmagnetic impurities[7] and possibly also for quasi-one-dimensional band antiferromagnets.[8]

In pure chromium, a transition to an incommensurable transverse antiferromagnetic structure (AF_1) of a linearly polarized type is known to occur below the Néel point $T_N \approx 312$ K. This structure is modulated along one of the (100) directions of a bcc lattice [here and below, we are discussing only I–Q states with a wave vector $Q = (2\pi/\alpha)(1-\delta, 0, 0)$, where α is the lattice constant]. This structure can be described in the model of a spin density wave with the help of a snoidal solution for the envelope:

$$\Delta(x) = \Delta_2 \operatorname{sn}(\Delta_1 x/v_F, \gamma), \quad \gamma = \Delta_2/\Delta_1,$$

where Δ_1 and Δ_2 are parameters which depend on the temperature T and the incongruity parameter μ. In the rigid-band approximation, which works fairly well for Cr–V and Cr–Mn alloys, the addition of an impurity leads to simply a change in $\mu(\chi)$, where χ is the impurity concentration, so there is the hope that the model of a soliton lattice of a spin density wave[1] will apply to such alloys. The optical,[9] neutron-diffraction,[10] and x-ray[11] data available agree well with the results of numerical calculations on the absorption spectrum and scattering cross sections in the model of Ref. 1 (see Ref. 4).

In most alloys of chromium, however, impurity scattering plays an extremely important role, and the rigid-band approximation is not satisfactory. The situation can be seen particularly clearly in the properties of Cr–Mo and Cr–W alloys (Mo and W are isoelectronic with Cr), which preserve the AF_1 magnetic structure over a wide range of impurity concentrations. From the standpoint of the model which assumes that there are plane regions of the Fermi surface, the incongruity parameter $\mu(\chi)$ remains essentially the same in these systems, and all the changes in the Néel point, the period and amplitude of the envelope of the spin density wave, and other properties result exclusively from the impurity scattering. In alloys of chromium with nonisoelectronic impurities the two factors (the change in the incongruity parameter and the scattering) usually play comparable roles, so it is a fairly complicated matter to analyze their effect on the shape of the density wave and the shape of the phase diagram. In this regard the most convenient entities for a study of the properties of soliton lattices of spin density waves may be ternary Cr–Mo(W)–Me(V) alloys, in which

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these factors can be separated. It is primarily to these alloys that we would apply the results derived below.

2. PHASE DIAGRAM OF A BAND ANTIFERROMAGNETIC NEAR THE LIFSHITZ POINT WITH IMPURITY SCATTERING

In the model of a band antiferromagnet with a spin density wave, electron-impurity scattering is known to lower the transition temperature $T_N(\mu)$ (Ref. 7). Generally speaking, the type of magnetic structure may also change as the impurity concentration χ increases (for example, the long-period modulation of the spin density wave may disappear, if there is such a modulation in the pure system). Concentration related transitions to an AF_0 phase [a linearly polarized transverse commensurable spin density wave with a wave vector $(2\pi/a)(100)$], accompanied by the disappearance of the incommensurable AF_1 structure, occur in many chromium alloys, for example.[7]

In the present paper we are interested in that part of the (T,μ) phase diagram in which the type of antiferromagnetic structure can change even at a low concentration of a nonmagnetic impurity, χ. In other words, we are interested in the neighborhood of the Lifshitz point (T_N^*,μ^*), at which the lines of the transitions from the paramagnetic (P) phase to the uniform (C) and modulated (I) phases converge, along with the line of the I–C transition. The existence of such a point on the phase diagram is a general property of all exactly solvable models of electronic transitions to a soliton-lattice structure.[1] Here and below, the impurity concentration is "low" in the sense that the electron-impurity scattering rate satisfies $\nu \ll (T_N,\mu)$ near the point (T_N^*,μ^*), so that in all the subsequent calculations it will be sufficient to consider only the terms which are linear in ν. We state at the outset that we will understand ν as the total rate of scattering of electrons of the plane regions of the Fermi surface by the impurity both with and without a transition to the reservoir:

$$\nu = 2\pi\chi[\langle V_{nn}^2\rangle N_n(0) + \langle V_{nr}^2\rangle N_r(0)],$$

where $N_n(0)$ and $N_r(0)$ are the state densities of the plane regions and the reservoir, respectively, and V_{nn} and V_{nr} are the matrix elements of the electron-impurity scattering potential respectively without and with a transition to the reservoir. In addition to the rate ν our problem has the rate

$$\nu' = 2\pi\chi\langle V_{nn}^2\rangle N_n(0),$$

which is less than or on the order of ν. As we will see below, the parameter ν'/ν $(0 \leqslant \nu'/\nu \leqslant 1)$ has a strong effect on the shape of the soliton lattice of the spin density wave.

Under these restrictions on the values of ν, T, and μ we can treat the problem of the formation of a nonuniform structure of a spin density wave (a soliton lattice) by a functional approach. In the Ginzburg-Landau expansion for the thermodynamic potential Ω, the effect of impurity scattering is seen in changes in the coefficients, which change the transition temperatures, shift the Lifshitz point, and, generally speaking, distort the shape of $\Delta(x)$ in the I phase from that in the case of a pure system, corresponding to $\nu = \nu' = 0$.

Let us examine the effect of impurity scattering on the (T,μ) phase diagram near the Lifshitz point in the case in which the order parameter $\Delta(x)$ is a slow quantity $(|\Delta'(x)/\Delta(x)| \ll \mu, T/v_F)$ and also a small quantity $(|\Delta(x)| \ll T,\mu)$ (v_F is the velocity at the Fermi surface). We write the thermodynamic potential of the system in the form

$$\Omega(\Delta(x)) = \int\left[\alpha\Delta^2 + \frac{\beta}{2}\Delta^4 + \frac{\gamma_1}{3}\Delta^6 + a_1(\Delta')^2 + a_2(\Delta'')^2 + b(\Delta\Delta')^2\right]dx, \quad (1)$$

where a_2, b, and $\gamma_1 > 0$, and α, β, and a_1 can change sign. These coefficients are given explicitly in the Appendix.

In the absence of impurity scattering we would have $\nu = 0$, and for an infinitely strong reservoir, $M = N_r(0)/N_n(0) \to \infty$, the coefficients of functional (1) are related by

$$\alpha = C_1, \quad \frac{\beta}{2} = \frac{a_1}{v_F^2} = C_2, \quad \frac{\gamma_1}{3} = \frac{2a_2}{5v_F^2} = C_3 = \frac{b}{5}. \quad (2)$$

In the case of a reservoir of finite strength, $M \neq \infty$, corrections $\sim (1+M)^{-1}$ to the terms of fourth and sixth orders in $\Delta(x)$ arise[12]:

$$\frac{\Delta\beta}{2} = \frac{C_4}{1+M}, \quad \frac{\Delta\gamma_1}{3} = \frac{C_5}{1+M}, \quad \frac{\Delta b}{7} = \frac{C_6}{1+M}. \quad (3)$$

In the part of phase diagram in which we are interested here, the coefficients C_2 and C_1 cross zero and change sign, while we have C_6, C_3, C_4, $C_5 > 0$. We do not need explicit expressions for C_3–C_6 in this paper (they are given in Ref. 12); those for C_1–C_3 are given in the Appendix.

A graphical technique is convenient for seeing the effect of impurity scattering on the coefficients of functional (1) and the change in relations (2) among them. Figure 1, a and b, illustrates the situation with some terms of fourth order in $\Delta(x)$ in functional (1). The solid lines are the temperature Green's functions in the paramagnetic phase (for the electrons of the plane regions, we use the index n; for the electrons of the reservoir we use r); the circles represent the order parameter $\Delta(x)$; and the dashed lines represent the electron-impurity scattering potential.

In the standard diagram technique,[13] the scattering by a nonmagnetic impurity gives rise to corrections of two types. First, a damping appears in the Green's functions (Fig. 1a), which is seen in the shift in the imaginary frequencies:

$$i\omega_k \to i\tilde{\omega}_k = i\omega_k(1+\nu/|\omega_k|), \quad \omega_k = \pi T(2k+1), \quad k = 0, \pm 1 \ldots$$

By itself, this procedure does not violate the relations (2) among the coefficients of functional (1) in the limit $M \to \infty$, and in place of C_1, C_2, and C_3 in the corresponding equations we will simply have their renormalized values $\tilde{C}_1$, $\tilde{C}_2$, $\tilde{C}_3$ (see the Appendix). Second, it is necessary to "dress" with impu-

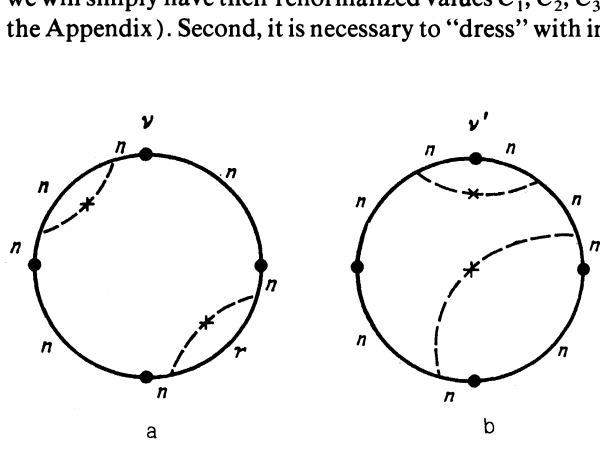

FIG. 1.

rity lines the vertices which contain single circles and pairs of circles. It is not difficult to see that the contributions of such diagrams are proportional to $\nu' \sim \nu(1+M)^{-1}$ under the assumption that the matrix elements $\langle V_{nn}^2 \rangle$ and $\langle V_{nr}^2 \rangle$ are of the same order of magnitude. In this case we have $\nu'/\nu \sim (1+M)^{-1} \to 0$ at $M \gg 1$. One could also imagine a situation in which, because of some special factors (e.g., the particular symmetry properties of the wave function), the scattering accompanied by a transition to the reservoir (i.e., actually to another band) is suppressed. In such a case we would have $\nu'/\nu \sim 1$ even in the case $M \gg 1$.

Specific calculations will be carried out for two limiting cases: $\nu'/\nu = 0$ and $\nu'/\nu = 1$. In the limit $\nu'/\nu = 0$ the restriction that ν be small in comparison with (T, μ) is not fundamental in the sense that a soliton solution of the type in Ref. 1 does not change shape, even far from the Lifshitz point, where the expansion which was used, (1) is not applicable. Unfortunately, we cannot make a similar statement for the case $\nu'/\nu \sim 1$.

We will show that functional (1) with the coefficient

$$\alpha = C_1, \quad \frac{\beta}{2} = \frac{a_1}{v_F^2} = C_2, \quad \frac{\gamma_1}{3} = \frac{2a_2}{5v_F^2} = C_3$$

(i.e., with $\nu' = 0$) allows an exact solution in the class of Jacobi elliptic functions which has the form of a single-period soliton lattice. For this purpose we vary (1) with respect to $\Delta(x)$, and we find an Euler-Lagrange equation of the following type:

$$\tfrac{1}{2} v_F^4 C_3 \Delta^{IV} - v_F^2 C_2 \Delta'' + C_1 \Delta + 2C_2 \Delta^3 + 3C_3 \Delta^5$$
$$-5v_F^2 C_3 [\Delta (\Delta')^2 + \Delta^2 \Delta''] = 0. \tag{4}$$

According to Ref. 1, a single-period solution of the modified Korteweg-de Vries equation

$$\Delta''' - 6A\Delta^2\Delta' + B\Delta' = 0, \tag{5}$$

with constants A and B and second integral C of Eq. (5) all chosen appropriately, is also a solution of (4). The first and second integrals of (5) are of the known form

$$\Delta'' - 2A\Delta^3 + B\Delta = 0, \quad (\Delta')^2 - A\Delta^4 + B\Delta^2 = 0. \tag{6}$$

The vanishing of the first integral in (6) ensures that periodic solutions will be chosen; we restrict the discussion below to periodic solutions. Now differentiating (5) and then combining the resulting expression with (6), we find (4) with the following conditions on the coefficients:

$$\frac{C_1}{C_3} + B\frac{C_2}{C_3} + \frac{B^2}{2} + C = 0, \tag{7}$$
$$A = 1, \quad B = \Delta_1^2 + \Delta_2^2, \quad \Delta_1^2 \Delta_2^2 = C;$$

$$\Delta_0(x) = \Delta_2 \operatorname{sn}\left(\frac{\Delta_1 x}{v_F}, \gamma\right), \quad \gamma = \frac{\Delta_2}{\Delta_1}, \tag{8}$$

where $\operatorname{sn}(y, \gamma)$ is the elliptic sine with a modulus and period of $4K(\gamma)$.

The one equation which we still need in order to unambiguously determine the coefficients Δ_1 and Δ_2 (or, equivalently, B and C), should be found from the condition that thermodynamic potential (1) reaches a minimum when exact solution (8) is substituted into it:

$$\Omega(T, \mu) = C_1 I_2 \Delta_2^2 + C_2 I_4 \Delta_2^4 + C_3 I_6 \Delta_2^6. \tag{9}$$

The quantities $I_2(\gamma)$, $I_4(\gamma)$, and $I_6(\gamma)$ are given explicitly in the Appendix. It is convenient to vary (9) with respect to Δ_2 and find the other equation which we need:

$$C_1 I_2 + 2C_2 I_4 \Delta_2^2 + 3C_3 I_6 \Delta_2^4 = 0. \tag{10}$$

We would like to discuss the shape of the (T, μ) phase diagram near the Lifshitz point, which is specified by the system of equations

$$\alpha(T^*, \mu^*) = C_1(T^*, \mu^*, \nu) = 0, \quad a_1(T^*, \mu^*) = C_2(T^*, \mu^*, \nu) = 0. \tag{11}$$

The line of the second-order transition from the paramagnetic phase to the commensurable phase of the spin density wave (the P–C transition) in the region $\mu < \mu^*$ is determined by the condition

$$C_1(T_C, \mu, \nu) = \alpha(T_C, \mu, \nu) = 0, \tag{12}$$

while that of the transition to the incommensurable phase of the spin density wave (the P–I transition) in the region $\mu > \mu^*$ is determined by the condition

$$C_1(T_I, \mu, \nu) - C_2^2(T_I, \mu, \nu)/2C_3(T_I, \mu, \nu) = 0. \tag{13}$$

Relation (13) is found from (10) and (7) in the limit γ, $\Delta_2 \to 0$. Analysis shows that both of the transitions (P–C and P–I) are indeed of second order and that the difference between the thermodynamic potentials of the P and C or P and I phases vanishes on lines (12) and (13), respectively.

We can now discuss the question of the line of the I–C transition near the point (T^*, μ^*). Expanding (1) in powers of Δ_2, and using (8) and (2) in the limit $\gamma \to 1$, we find, in leading order in the logarithm, $L = (\ln(4/\gamma'))^{-1}$,

$$\Omega(T, \mu) = C_1 \Delta_2^2 + C_2 \Delta_2^4 + C_3 \Delta_2^6 - L(C_1 \Delta_2^2 + {}^2/_3 C_2 \Delta_2^4 + C_3 \Delta_2^6),$$
$$\gamma' = (1-\gamma^2)^{1/2}. \tag{14}$$

Condition (7) and the vanishing of the coefficient of L determine the line of the second-order I–C transition,

$$C_1 C_3 = {}^5/_{27} C_2^2, \quad C_1 > 0, \quad C_2 < 0, \tag{15}$$

and the value of $\Delta_2^2 = \Delta_1^2$ on this line

$$\Delta_2^2 = \Delta_1^2 = \frac{5}{9}\frac{|C_2|}{C_3}, \quad C_2 < 0, \quad C_1 > 0. \tag{16}$$

Calculating the potential of the I and C phases on line (15), we find

$$\Delta\Omega_I(T, \mu) = \Delta\Omega_C(T, \mu) = -\frac{5^2}{9^3}\frac{|C_2|^3}{C_3^2}$$

with respect to the paramagnetic phase. In other words, the I–C transition occurs as a second-order transition, as do the P–C and I–C transitions.

Figure 2a shows the change in the (T, μ) phase diagram during the Lifshitz point when the parameter ν varies. For all transition temperatures $T(\mu, \nu)$ the condition $\Delta T = T(\mu, \nu) - T(\mu, 0) \ll T(\mu, 0)$ holds, and we can use the approximations

$$\Delta T^* \approx -0.3\nu, \quad \Delta\mu^* \approx -0.2\nu,$$
$$\Delta T_I(\mu) \approx -\nu[0.3 + 2.4(\mu - \mu^*)], \quad \mu > \mu^*,$$

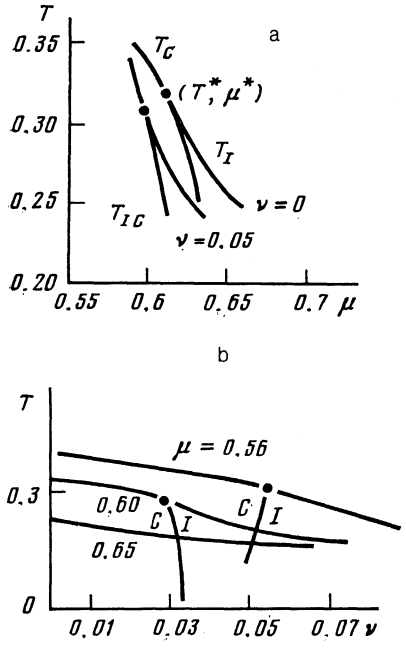

FIG. 2.

$$\Delta T_c(\mu)\approx -\nu[0.3+3.5(\mu-\mu^*)], \quad \mu<\mu^*,$$
$$\Delta T_{IC}(\mu)\approx -\nu[0.3+40(\mu-\mu^*)], \quad \mu>\mu^*, \tag{17}$$

If $\nu'/\nu\sim 1$, relations (2) are violated even if contribution (3) is ignored, and there is no exact solution (8) which minimizes functional (1). There is the hope, however, that this solution will remain applicable as a variational solution, at least under the condition $\nu' \ll (T^*, \mu^*)$, in which case the corrections to the coefficients $\{C_i\}$ of the exactly solvable model without impurity scattering are small. An advantage of choosing a snoidal solution as the variational solution instead of the sinusoidal solution which is conventionally used (Ref. 14, for example) for the model of a spin density wave is that an infinite number of harmonics can be taken into account in a compact way. This advantage is particularly important near the line of the *I–C* transition. Calculations show that for any $\nu \ll (T, \mu)$ the thermodynamic potential $\Omega_{sn}(T, \mu, \nu)$ in the class of snoidal solutions (8) is smaller than in the class of sinusoidal solutions $\Delta(x) = \Delta_2 \sin(\Delta_1 x/v_F)$. Figure 2b shows phase diagrams for the case $\nu' = \nu$. As before, with $\nu' = 0$, all of the transitions (*P–I*, *P–C*, and *I–C*) are of second order. This point was verified through a direct calculation of the thermodynamic potential $\Omega_{sn}(T, \mu, \nu)$, found by substituting variational solution (8) into (1) and minimizing Ω_{sn} with respect to the parameters Δ_1 and Δ_2 of the soliton lattice.

3. CHANGE CAUSED IN THE SHAPE OF THE SOLITON LATTICE OF THE SPIN DENSITY WAVE BY IMPURITY SCATTERING AND BY A FINITE RESERVOIR STRENGTH

We turn now to a more correct derivation of the form of the function $\Delta(x)$ in the case in which relations (2) among the coefficients of functional (1) do not hold. An equation of the general form

$$a_2\Delta^{IV}-a_1\Delta''+\alpha\Delta+\beta\Delta^3+\gamma\Delta^5-b(\Delta(\Delta')^2+\Delta^2\Delta'')=0 \tag{18}$$

has solutions in the class of two-period functions.[15] We are interested in those solutions which satisfy the conditions of slowness and smallness which we used in constructing the functional (1).

We assume that the corrections to relations (2) are small, on the order of the parameter $(1+M)^{-1} \ll 1$; correspondingly, the corrections of the type in (3) are small, and we have the relation $\nu'/\nu\sim(1+M)^{-1}$. It is convenient to include all of the impurity contributions at once in the coefficients α, a_1, and a_2 at low powers of $\Delta(x)$. The other corrections for impurity scattering and for a finite reservoir strength lead to a violation of relations (2), and we now have

$$b=(10a_2+b')/v_F^2, \quad \gamma_1=(6a_2+\gamma_1')/v_F^4,$$
$$\beta=(2a_1+\beta')/v_F^2, \quad b', \gamma' \ll a_2, \quad |\beta'| \ll 2|a_1|. \tag{19}$$

The explicit expressions for γ_1', b', and β' are not important here. The only point which is of importance is that all of these corrections are $\sim(1+M)^{-1}$ and are small in the limit of large reservoir strength M. The most serious restriction on this smallness comes from the requirement $|\beta'| \ll 2|a_1|$, since a_1 may itself vanish at the Lifshitz point. Accordingly, in the immediate vicinity of this point, relation (2) between β and a_1 is markedly violated, and the method constructed below for calculating the corrections to solution (8) cannot be used. As M increases, the region in which the relation $|\beta'| \ll 2|a_1|$ is violated becomes progressively narrower, while the region of applicability of the calculation method becomes wider. Introducing the dimensionless variables $\Delta \to \Delta(|a_1|/a_2)^{1/2}$, $x \to x(a_2/|a_1|)^{1/2} v_F^{-1}$ we can rewrite (18) in the form

$$\Delta^{IV}-2\,\mathrm{sign}(a_1)\Delta''+z\Delta+[2\,\mathrm{sign}(a_1)+\beta'/|a_1|]\Delta^3+(6+\gamma'/a_2)\Delta^5$$
$$-(10+b'/a_2)[\Delta(\Delta')^2+\Delta^2\Delta'']=0, \tag{20}$$
$$z=\bar{C}_1C_3/|C_2|^2.$$

In the region in which nonuniform solution (20) exists we have $a_1<0$.

We seek a correction to solution (8) which is linear in β', γ_1', b' in the form $\Delta(x)-\Delta_0(x)=\Phi(x)\Delta_0'(x)$. The linearized equation for the function $\Phi(x)$ is[16,17]

$$\Delta_0'\Phi^{IV}+4\Delta_0''\Phi'''+2[3\Delta_0'''+\Delta_0'(1-5\Delta_0^2)]\Phi'' \tag{21}$$
$$+4[\Delta_0^{IV}+\Delta_0''(1-5\Delta_0^2)-5(\Delta_0')^2\Delta_0]\Phi'=f(x),$$

where $\Delta_0(x)$ is given by (8), and

$$f(x)=-\frac{\beta'\Delta_0^3}{|a_1|}-\frac{\gamma_1'\Delta_0^5}{a_2}+\frac{b'}{a_2}[\Delta_0(\Delta_0')^2+\Delta_0^2\Delta_0''] \tag{22}$$

is an odd periodic function with a period of $4K(\gamma)$. The substitution $\Phi'(x)=h(x)/\Delta_0'(x)$ lowers the order of the differential equation (21):

$$h'''+\frac{\Delta_0''}{\Delta_0'}h''+\left[3\frac{\Delta_0'''}{\Delta_0'}-2\left(\frac{\Delta_0''}{\Delta_0'}\right)^2+2-10\Delta_0^2\right]h'$$
$$+\left[3\frac{\Delta_0^{IV}}{\Delta_0'}-4\frac{\Delta_0''\Delta_0'''}{\Delta_0^2}+2\left(\frac{\Delta_0''}{\Delta_0'}\right)^3\right.$$
$$\left.+(2-10\Delta_0^2)\frac{\Delta_0''}{\Delta_0'}-20\Delta_0'\Delta_0\right]h=f(x). \tag{23}$$

It is not difficult to see that under the condition $f(x)=0$ the latter equation is satisfied by the solutions of the equation

$$h''+\left[3\frac{\Delta_0'''}{\Delta_0'}-2\left(\frac{\Delta_0''}{\Delta_0'}\right)^2+2-10\Delta_0^2\right]h=\frac{C}{\Delta_0'} \tag{24}$$

with an arbitrary constant C. We denote by $h_1(x)$ and $h_2(x)$ the solutions of the homogeneous version of Eq. (24) ($C=0$), and we denote its Wronskian by $W=h_1h_2'-h_1'h_2$. A particular solution of the inhomogeneous version of Eq. (24) with $C=W$ is then

$$h_3(x)=h_2(x)\int^x\frac{h_1(x')}{\Delta_0'(x')}dx'-h_1(x)\int^x\frac{h_2(x')}{\Delta_0'(x')}dx'. \tag{25}$$

The triad of functions h_1, h_2, h_3 is the basis for an arbitrary solution of Eq. (23) with $f(x)=0$. A particular solution of the same equation with its right side is of the standard form

$$h_4(x)=\frac{1}{W}\left[h_2(x)\int^x\frac{h_1(x')}{\Delta_0'(x')}-h_1(x)\int^x\frac{h_2(x')}{\Delta_0'(x')}\right]\int^{x'}\Delta_0'(x'')f(x'')\,dx''\,dx'. \tag{26}$$

We can now write a general solution of the inhomogeneous version of equation (23),

$$h(x)=\sum_{i=1}^3A_ih_i(x)+h_4(x), \tag{27}$$

and we can find the functions h_1 and h_2 explicitly. We first use (6) and (7) to rewrite the "potential" in (24):

$$3\frac{\Delta_0'''}{\Delta_2'}-2\left(\frac{\Delta_0''}{\Delta_0'}\right)^2+2-10\Delta_0^2$$

$$=2-3(\Delta_1^2+\Delta_2^2)+2\left(\frac{\Delta_0}{\Delta_0'}\right)^2(\Delta_1^2+\Delta_2^2)^2. \tag{28}$$

Using transformations of the elliptic functions,[18] we see that we have

$$\frac{\Delta_0(x)}{\Delta_0'(x)}=-\frac{1}{\Delta_1(1-\gamma^2)}\frac{\mathrm{cn}(\Delta_1x+K(\gamma))}{\mathrm{sn}(\Delta_1x+K(\gamma))\,\mathrm{dn}(\Delta_1x+K(\gamma))}. \tag{29}$$

Second, combining (28) and (29), and introducing the new variables

$$y=(1+\gamma)(\Delta_1x+K(\gamma)),\quad k=2\gamma^{1/2}(1+\gamma)^{-1},\quad k^2+k_1^2=1,$$

we can rewrite (24) with $C=0$ in the form of a Lamé equation of first degree:

$$h''(y)+2\left[1+\frac{1-3B/2}{4\Delta_1^2}(1+k_1)^2-k^2\,\mathrm{sn}^2(y+K(k)+iK'(k),k)\right]h(y)=0. \tag{30}$$

The two linearly independent solutions of this equation are expressed in terms of the Jacobi eta and theta functions[18]:

$$h_\pm(y)=\frac{\theta_1(y+y_0,k)}{H_1(y,k)}\exp[\mp yZ(y_0,k)]. \tag{31}$$

Here $Z(y_0,k)$ is the zeta function of argument y_0, which can be found from the equation

$$k^2\,\mathrm{cn}^2(y_0,k)=1+\frac{(1+k_1)^2(1-3B/2)}{2\Delta_1^2}. \tag{32}$$

Since we have $\Phi'=h/\Delta_0'$, we must impose the boundary conditions $h(x=\pm K(\gamma)/\Delta_1)=0$ on the solutions of Eq. (23). These boundary conditions are satisfied by linear combinations of functions (31):

$$h_1=h_+-h_-, \tag{33}$$

$$h_2=h_+\exp(2K(k)Z(y_0,k))-h_-\exp(-2K(k)Z(y_0,k)).$$

Here we have $h_1(x)=h_2(-x)$.

Using the functions $h_{1,2}(x)$ in (33), we can write a solution of (26), (27) which satisfies the specified boundary conditions:

$$\Phi'(x)=\frac{1}{W}\left\{\frac{h_2(x)}{\Delta_0'(x)}\int_{-x_0}^x\frac{h_1(x')}{\Delta_0'(x')}\times\left[A_3+\int_{-x_0}^{x'}\Delta_0'(x'')f(x'')\,dx''\right]dx'-\frac{h_1(x)}{\Delta_0'(x)}\int_{x_0}^x\frac{h_2(x')}{\Delta_0'(x')}\left[A_3+\int_{-x_0}^{x'}\Delta_0'(x'')f(x'')\,dx''\right]dx'\right\},$$

$$x_0=\frac{K(\gamma)}{\Delta_1}. \tag{34}$$

Through an appropriate choice of integration limits in (34), we can normalize with $A_1=A_2=0$. We also require that the unknown function

$$\Phi(x)=\Phi(0)+\int_0^x\Phi'(x')\,dx' \tag{35}$$

and its derivative (34), satisfy the quasiperiodic boundary conditions

$$\Phi\left(\frac{K(\gamma)}{\Delta_1}\right)=\exp\left(\frac{2iqK(\gamma)}{\Delta_1}\right)\Phi\left(-\frac{K(\gamma)}{\Delta_1}\right), \tag{36}$$

$$\Phi'\left(\frac{K(\gamma)}{\Delta_1}\right)=\exp\left(\frac{2iqK(\gamma)}{\Delta_1}\right)\Phi'\left(-\frac{K(\gamma)}{\Delta_1}\right), \tag{37}$$

where q is the wave number. The last equation can be rewritten as follows with the help of (34):

$$A_3W[\exp(2iqK(\gamma)/\Delta_1)-1]=\int_{-x_0}^{x_0}\Delta_0'(x)f(x)\,dx. \tag{38}$$

Equation (38) thus determines the constant A_3. The perturbation-theory algorithm formulated above is applicable under the condition $|\Phi(x)\Delta_0'(x)|\ll|\Delta_0(x)|$, which is satisfied by the choice $\Phi(0)=0$. Condition (36), along with the relation $h_1(x)=h_2(-x)$, yields the value $q=\pi\Delta_1(2n+1)/2K(\gamma)$, where n is an integer. Using this circumstance and the fact that we have $f(x)=-f(-x)$, we immediately find $A_3=0$ from (38). We thus finally find

$$\Delta(x)=\Delta_0(x)+\Delta_0'\int_0^x\frac{h_4(x')}{\Delta_0'(x')}dx', \tag{39}$$

where $h_4(x)$ is given by (26). Figure 3 shows a sketch of the function (39) for one period of the soliton lattice [the origin of coordinates has been chosen in such a way that we have $\Delta'(x=0)>0$; the dashed line shows the function $\Delta_0(x)$].

We thus see that a finite reservoir strength M and impu-

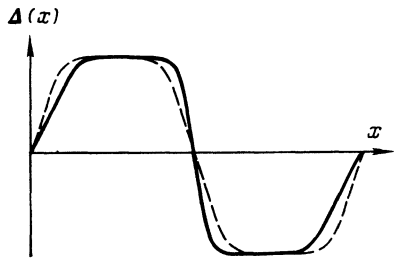

FIG. 3.

rity scattering give rise not only to changes in the amplitude and period of the soliton lattice of the spin density wave [this effect is incorporated in $\Delta_0(x)$ through the change in the parameters Δ_1 and Δ_2] but also to an asymmetric distortion of the shape of the spin density wave at the scale of the new period.

4. CONCLUSION

This analysis of the model of a soliton lattice of a spin density wave with electron scattering by nonmagnetic impurities makes it possible to predict the shape of the phase diagram of a doped band antiferromagnet near the Lifshitz point. There are some qualitatively new effects which are not seen in the case of the rigid-band approximation. First, the Lifshitz point itself shifts when the impurity concentration changes. Second, the slopes of the temperatures $T_N(\chi)$ of the transitions from the P phase to the C and I phases change, as does the temperature $T_{IC}(\chi)$ of the transition between the I and C phases. The change in the temperature $T_{IC}(\chi)$ is particularly large; in fact, $\partial T_{IC}(\chi)/\partial\chi$ may acquire the sign opposite that in the rigid-band case (Fig. 2, for example). The phase diagrams in terms of the temperature-(impurity concentration) variables may as a result acquire a rather unusual slope, depending on the particular relation between the parameters $\mu(\chi)$ and $\nu(\chi)$ (e.g., of the type shown in Fig. 4, where $\mu = 0.63$). We know quite well[7] that this diversity cannot be explained, even qualitatively, by the simple model which incorporates only a change in $\mu(\chi)$. This deficiency is remedied in the method proposed here.

Some serious restrictions, which rule out a direct application of the results of this study to other models with electron soliton lattices, are the requirement that the reservoir strength M be large and that the impurity scattering of the electrons of singular regions of the Fermi surface be small, $\nu' \ll \nu$ (in the model of a quasi-one-dimensional superconductor, for example, we would have $M = \infty$ but $\nu' = \nu$, while in the Peierls model we would have $M = 0$ and $\nu' = \nu$). In this connection we note that Machida and Fujita's generalization[4] of the model of a soliton lattice of a spin density wave to the case of a low reservoir strength can be regarded only as a variational model, since terms of the form (3) violate relations (2) and thus the exact integrability of the functional (1).

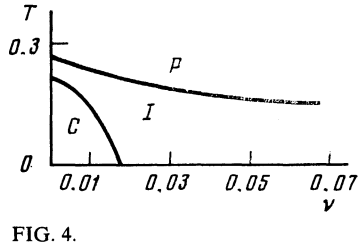

FIG. 4.

APPENDIX

The coefficients of functional (1) calculated by the standard technique[13] are

$$\alpha = C_1 + 2\nu' \frac{\psi_2}{\pi T}, \tag{A1}$$

$$a_1 = C_2 v_F^2 + \frac{5}{4}\nu' \frac{\psi_4 v_F^2}{(\pi T)^3}, \tag{A2}$$

$$a_2 = \frac{1}{2} C_3 v_F^4 + \frac{4}{2}\nu' \frac{\psi_6 v_F^4}{(\pi T)^5}, \tag{A3}$$

$$\beta = 2C_2 + 4\nu' \frac{\psi_4}{(\pi T)^3}, \tag{A4}$$

$$b = 5C_3 + 8\nu' \frac{\psi_6 v_F^2}{(\pi T)^5}, \tag{A5}$$

$$\gamma_1 = 3C_3 + 6\nu' \frac{\psi_6}{(\pi T)^5}, \tag{A6}$$

$$\bar{C}_1 = C_1 + \nu \frac{\psi_2}{\pi T}, \tag{A7}$$

$$\bar{C}_2 = C_2 + \frac{3}{4}\nu \frac{\psi_4}{(\pi T)^3}, \tag{A8}$$

$$\bar{C}_3 = C_3 + \frac{5}{8}\nu \frac{\psi_6}{(\pi T)^5}, \tag{A9}$$

$$C_1 = \ln\frac{T}{T_0} - \psi\left(\frac{1}{2}\right) + \operatorname{Re}\psi\left(\frac{1}{2} + i\eta\right), \tag{A10}$$

where $\psi(z)$ is the digamma function, $\eta = \mu/2\pi T$, $z = 1/2 + i\eta$,

$$C_2 = \varphi_2/2(\pi T)^2, \quad C_3 = \varphi_4/4(\pi T)^4,$$

$$\psi_2 = \frac{1}{4}\operatorname{Im}\frac{\partial\psi}{\partial\eta}, \quad \psi_4 = \frac{1}{96}\operatorname{Im}\frac{\partial^3\psi}{\partial\eta^3}, \quad \psi_6 = \frac{1}{7680}\operatorname{Im}\frac{\partial^5\psi}{\partial\eta^5}; \tag{A11}$$

$$\varphi_2 = \frac{1}{16}\operatorname{Re}\frac{\partial^2\psi}{\partial\eta^2}, \quad \varphi_4 = \frac{1}{768}\operatorname{Re}\frac{\partial^4\psi}{\partial\eta^4}. \tag{A12}$$

The coefficient of functional (9) are

$$I_2 = J_2, \quad I_4 = 2J_4 + \gamma^{-2} - (1+\gamma^{-2})J_2, \tag{A13}$$

$$I_6 = 8J_6 + \left(\frac{1}{2} + 6\gamma^{-2} + \frac{1}{2}\gamma^{-4}\right)J_2 - 7(1+\gamma^{-2})J_4;$$

$$J_2 = \gamma^{-2}\left[1 - \frac{E(\gamma)}{K(\gamma)}\right], \quad J_4 = \frac{1}{3}\gamma^{-2}[2(\gamma^2+1)J_2 - 1],$$

$$J_6 = \frac{1}{5}\gamma^{-2}[4(\gamma^2+1)J_4 - 2J_2]. \tag{A14}$$

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