Localized states on defects in electronic transitions into a soliton-lattice state

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We consider the properties and structure of the localized states produced on defects in systems that undergo transitions into a disordered phase. It is shown that the local rise of the transition temperature always leads in this case to the appearance of localized states. Singly and doubly period solutions are analyzed for the order parameter in the one-dimensional model of a soliton lattice. The nonlinear superposition principle is used to obtain, in the same model, a solution that describes the localized state, and also to consider the problem of formation of deep impurity levels in a forbidden band of the electron spectrum. The applicability of the results to specific systems with electronic and magnetic transitions into an inhomogeneous state is discussed.

INTRODUCTION

The presence of defects in crystals with electronic phase transitions can lead to the onset of localized states (LS)—"local phase transitions"—above the homogeneous transition point. This situation is realized, for example, if the transition temperature rises locally near the defect. Many examples of systems with LS are known by now: surface magnetism,[1] local structural transitions,[2] localized superconductivity,[3] localized spin-density wave (SDW),[4] and others. Whereas the different transitions into a homogeneous phase have been considered in sufficient detail, much less has been learned about the behavior of defects in transitions into an inhomogeneous phase. Yet this question is of considerable interest, since there are many known systems that undergo electronic and magnetic phase transitions into inhomogeneous states, including quasi-one-dimensional Peierls[5] and spin-Peierls[6,7] systems, quasi-one-dimensional superconductors in an exchange field,[8] band antiferromagnets,[6,7] and modulated long-period magnets.[10]

The temperature T_d at which localized states appear at a defect above the point of transition into an inhomogeneous phase, the subject of the present paper, can be solved by analyzing the corresponding free-energy functional, in which account must be taken of higher terms in the gradients of the order parameters. The linearized equations for the order parameters can always be solved (see §§2,3), but in many cases of practical interest it is possible also to solve the nonlinear equation, by using their integrability property and the close analogy with the higher Korteweg–de Vries (KdV) equations.

Let us list the main results of the paper. In §2 we determine the onset temperature and structure of the LS near a planar defect in the three-dimensional model of the inhomogeneous transition. In §3 we consider, for the same model, the formation of LS near a point defect. In §4 are analyzed singly and doubly periodic solutions of the nonlinear equations for the order parameter in the one-dimensional model of a soliton lattice. Using the principle of nonlinear superposition we obtain in §5, in the same one-dimensional model, an exact solution for the LS. The problem of formation of deep levels connected with the LS in the forbidden band of the electron spectrum is solved in §6 for a one-dimensional soliton lattice.

§2. LOCALIZED SOLUTION NEAR A PLANAR DEFECT IN THE THREE-DIMENSIONAL MODEL

We determine in this section how the presence of a planar defect, capable of enhancing the tendency to a phase transition, influences the temperature of the inhomogenous transition and the structure of the resultant LS. Assuming a short-range transition potential (falling off at distances shorter than the correlation length ζ), we can describe the system by adding to the free-energy functional the term $-\gamma\delta(x)\psi^2(\mathbf{r})$, where $\sigma(x)$ is a one-dimensional δ function, and the coordinate axis $\mathbf{x}$ is perpendicular to the plane of the defect. The generalized order parameter ψ can describe, for example, a magnetic Peierls or a superconducting transition. Note that the defects considered in this and following sections represent local rises of the transition temperature. In principle, defects can add to the functional also terms that are linear in ψ, viz., defects of the "local field" type.

We assume that in the absence of a defect the transition is of second order, and that the system can be described by the functional

$$\mathcal{F} \sim \int \{\alpha\psi^2 - |\beta|\zeta_0^2(\nabla\psi)^2 + \zeta_0^4(\nabla^2\psi)^2 - \gamma\delta(x)\psi^2\}\,d\mathbf{r}, \qquad (1)$$

where ζ_0 is the correlation length at $T=0$. As usual, we assume that only the coefficient $\alpha = (T-T_0)/T_0$, is temperature-dependent; here T_0 is the temperature of the transition into a homogeneous state, and at a temperature $T_c > T_0$ we actually have a transition into an inhomogeneous state with wave vector $q_0^2 = \beta\zeta_0^{-2}/2$ and $\alpha_c = (T_c - T_0)/T_0 = B^2/4$ and $\alpha_c = (T_c/T_0)/T_0 = \beta^2/4$. Clearly, the condition for the functional (1) to be able to describe the inhomogeneous phase is the inequality $|\beta| \ll 1$. We have confined ourselves in (1) only to terms quadratic in ψ, since the temperature of the transition and the form of the LS are determined by a linear equation obtained by variation of (1) with respect to ψ:

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$$\psi+\Delta^2\psi+\frac{|\beta|}{\alpha^{1/2}}\Delta\psi=\frac{\gamma\delta(x)}{\alpha\xi(T)}\psi(x=0), \tag{2}$$

where we have used the dimensionless coordinates $x\to x/\zeta(T)$ and $\zeta^2=\zeta_0^2/\alpha^{1/2}$ and similarly $y\to y/\zeta, z\to z/\zeta$. In the absence of a defect, the transition is to a state with a dimensionless wave vector $q_0^2=1$, corresponding to the maximum transition temperature T_c.

In the presence of planar defects, near which the tendency to a phase transition becomes stronger, the LS is produced somewhat above the temperature of the volume inhomogeneous transition. We can expect in our case $\psi^{(r)}$ to decrease in oscillatory fashion with increasing distance from the defect plane $x=0$. It is curious, however, that the most favorable (see below) is a solution with "fast" modulation over the plane $x=0$, with a wave vector close to q_0. Thus, a planar defect causes the appearance of a solution that is inhomogeneous in two coordinates (in the $x=0$ plane and in a perpendicular direction).

We solve Eq. (2) by taking Fourier transforms, and seek the solution in the form $\psi=\exp(iky)f(x)$, where the y axis lies in the plane $x=0$. Substituting this form of the funciton ψ in (2), we obtain for the Fourier component

$$f_q=\tilde{\gamma}f(x=0)/[1+(k^2+q^2)^2-\tilde{\beta}(k^2+q^2)], \tag{3}$$

where $\tilde{\gamma}=\gamma/(\xi_0\alpha^{3/4}), \tilde{\beta}=|\beta|/\alpha^{1/2}$. Using the "self-consistency" condition

$$f(x=0)=\sum_q f_q,$$

we write the equation for the local transition temperature T_d:

$$1=\tilde{\gamma}\int\frac{1}{2\pi}[1+(k^2+q^2)^2-\tilde{\beta}(k^2+q^2)]^{-1}\,dq. \tag{4}$$

The vector **k**, which describes the modulation over the plane $x=0$, should be chosen to maximize T_d. Integration yields

$$1=\frac{\tilde{\gamma}\{(\tilde{\beta}/2-k^2)+[(\tilde{\beta}/2-k^2)^2+\beta_1^2]^{1/2}\}^{1/2}}{\beta_1\{2[(\tilde{\beta}/2-k^2)^2+\beta_1^2]\}^{1/2}}, \tag{5}$$

where $\beta_1=[1-\tilde{\beta}^2/4]^{1/2}$. It is easy to verify that the maximum value of T_d corresponds to the condition $(\tilde{\beta}/2-k^2)^2=\beta_1^2/3$; it follows then from (5) that

$$\alpha_d-\alpha_c=(T_d-T_c)/T_0=3/4(\gamma/\xi_0)^{4/3}. \tag{6}$$

The excess of the LS temperature (T_d) above the corresponding critical temperature (T_c) of the volume transition into the inhomogeneous state $(T_d-T_c)/T_0\propto(\gamma/\xi_0)^{4/3}$, is stronger in terms of the parameter $\gamma/\xi_0\ll 1$ than in the case of an LS in a system that undergoes a homogeneous transition (where $(T_d-T_0)/T_0\propto(\gamma/\xi_0)^2$

If only solutions homogeneous over the $x=0$ plane are considered, meaning that $k=0$ is chosen, we obtain a much smaller increase of T_d compared with T_c viz., $(T_d-T_c/T_0\propto(\gamma/\xi_0)^2$, as in the homogeneous case. Note that the solution with $k=0$ appears precisely in the case of a planar effect of the "local field" type [the term $-\gamma\delta(x)\psi(\mathbf{r})$ in the functional (1)], and can be easily obtained by the method used above.

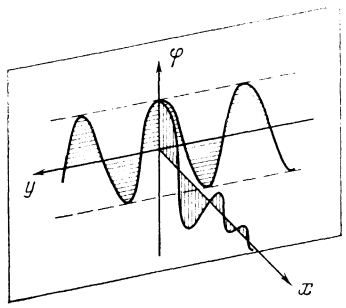

FIG. 1.

The distinguishing feature of the considered localized solution is that the wave vector of its modulation over the plane $x=0$ is $k\sim 1$ and practically coincides with the optimal period of the inhomogeneous state. In the direction perpendicular to the plane, the solution changes much more slowly and oscillates downward as $|x|$ increases, with a characteristic wave vector $q\propto\tilde{\gamma}^{1/3}\ll 1$ (see Fig. 1).

A defect of the type considered is, for example, a domain wall in a ferromagnetic superconductor. It is known[11] that an inhomogeneous superconducting state can arise in a uniform exchange field at a temperature $T<T^*$ (tricritical point). The effective exchange field becomes weaker near the domain wall, and the Ginzburg-Landau expansion (1) is applicable near the tricritical point.

The model considered can also be used to describe surface ordering in ferromagnets with inhomogeneous (long-period) structure.[10]

§3. LOCALIZED SOLUTION NEAR A POINT DEFECT IN A THREE-DIMENSIONAL MODEL

We consider in this section the influence of point defects on the properties of systems that undergo a transition into an inhomogeneous phase. Assuming a short-range defect potential, we can describe it by adding to the functional a term $-\gamma\delta(\mathbf{r})\,\psi^2(\mathbf{r})$, where $\delta(\mathbf{r})$ is a three-dimensional δ function (the generalization to the case of a "local field" defect is trivial). The linear equation that describes the LS structure and determines the temperature T_d of the onset of the LS takes in dimensionless coordinates the form

$$\psi+\Delta^2\psi+\frac{|\beta|}{\alpha^{1/2}}\Delta\psi=\frac{\gamma}{\alpha\zeta^3(T)}\delta(\mathbf{r})\psi(\mathbf{r}=0). \tag{7}$$

Note that the presence of the term $\Delta^2\psi$ in (7) of a term leads to a substantial difference between our problem and the situation in which a defect is present in a system that undergoes a transition to a homogeneous state. In the latter case, since the term $\beta(\nabla\psi)^2$ in the free-energy functional is positive, there is no need to include in (7) the term $\sim\Delta^2\psi$ (provided that there are no grounds for assuming β to be anomalously small). The problem of the temperature at which the LS occurs becomes equivalent to the problem of finding the lower energy level in the "potential" produced by the defect $-\gamma\delta(\mathbf{r})$. The role of the energy is assumed in this case by the quantity $\sim(T_0-T)$. In the one-dimensional

case (on a planar defect) an LS is always produced and $T_d > T_0$, meaning that there is always a bound state in a one-dimensional potential well.[12] The situation is different for a three-dimensional well: there is no bound state in a shallow potential well.[12] This means that the point defects, generally speaking, may also not lead to formation of LS, i.e., $T_d = T_0$.

The picture is entirely different if the transition is to an inhomogeneous phase. In this case the equation for the order parameter is not longer analogous to the Schrödinger equation and, as will be shown, a localized state on a point defect is always produced at a temperature $T_d > T_c$.

Transforming to the solution (7), we note that the spherically symmetric solution of the Laplace equation $\nabla^2\psi + k^2\psi = 0$ satisfies (7) provided that

$$k^4 - \frac{|\beta|}{\alpha^{1/2}} k^2 + 1 = 0, \qquad k^2 = (k_1 \pm ik_2)^2 = \frac{|\beta| \pm i(4\alpha - \beta^2)^{1/2}}{2\alpha^{1/2}}. \tag{8}$$

Since the wave vector $\mathbf{k}$ is complex, the solution of interest to us takes the form

$$\psi(\mathbf{r}) = \psi(0) \frac{\sin k_1 r}{k_1 r} \exp(-k_2 r). \tag{9}$$

Thus, the decrease of the order parameter with increasing distance from the defect is oscillatory. The temperature at which the LS sets in can be easily found by substituting the solution (9) in the free-energy functional (1). This temperature corresponds to vanishing of the coefficient of $\psi^2(0)$. Using the fact that $\psi(\mathbf{r})$ satisfies Eq. (7), and integrating in (1) in succession by parts, we write the condition for the onset of the LS in the form

$$\alpha\zeta^3(T) 8\pi\psi(0)\psi'(0) - \gamma\psi^2(0) = 0, \tag{10}$$

from which we find the temperature of the local transition

$$\frac{T_d - T_c}{T_0} = \frac{|\beta|}{32\pi^2} \left(\frac{\gamma}{\zeta_0^3}\right)^2. \tag{11}$$

A point defect leads thus always to the appearance of an LS at a temperature somewhat higher than the temperature of the volume transition into an inhomogeneous state. The fact that such LS exist can have interesting physical consequences. Thus, for example, in the case of an inhomogeneous magnetic transition (long-period ferro-magnets[10]) at a temperature $T_d > T_c$ (T_c is the temperature at which the magnetization wave appears), when the LS is produced the defect acquires a magnetic moment

$$M = \psi(0)\zeta^3 \int_0^\infty \frac{\sin k_1 r}{k_1 r} \exp(-k_2 r) 4\pi r^2 \, dr \approx \psi(0) \frac{4\gamma}{k_1 \beta^2}. \tag{12}$$

The appearance in the paramagnetic phase of such local moments should increase drastically the susceptibility below the temperature T_d, and the system considered is similar in this sense to a superparamagnet. In the case of inhomogeneous superconductivity in an exchange field, the spatial fluctuations of the pairing constant or of the exchange field should lead to a strong smearing of the superconducting transition.

As applied to band antiferromagnets with spin density waves (SDW), the question of formation of LS was considered in Ref. 4. in the framework of the three-dimensional model of the electron spectrum.

§4. PROPERTIES OF THE NONLINEAR SELF-CONSISTENCY EQUATIONS IN EXACTLY SOLVABLE ONE-DIMENSIONAL MODELS OF ELECTRON SOLITON LATTICES

In the preceding sections we considered only linearized solutions of three-dimensional equations for the order parameter. Unfortunately, there is no known general procedure for obtaining for nonlinear equations three-dimensional solutions that minimize functionals of type (1), with allowance for terms ψ^4, $(\psi\psi')^2$, ψ^6 etc., given the boundary conditions at the defect. The situation is different for one-dimensional systems, where there are many exactly solvable models that describe physical situations of importance for actual applications (the continual model of the Peierls structural transition,[5,13] the model of a band ferromagnet with SDW,[8,9] the model of a superconductor in an exchange field,[8] and others). It is very important that the exact soliton solutions, obtained by microscopic analysis of these models by the inverse-scattering-theory problem, can be relatively simply constructed by minimizing the corresponding functionals (naturally, in the parameter range in which these functionals are valid). Since the construction of soliton solutions, in terms of functionals, has been previously discussed for the indicated one-dimensional systems very briefly[8,13] even in the absence of defects, we shall discuss this interesting question in greater detail.

In the absence of defects, the initial functional with order parameter ψ (as already mentioned, ψ is generalized here and can describe all the aforementioned types of phase transitions) is conveniently written in the form

$$\mathcal{F} \sim \int \left\{ \alpha\psi^2 + \frac{b}{2\psi_0^2}\psi^4 + \frac{c}{3\psi_0^4}\psi^6 + \zeta_0^4(\psi'')^2 + \beta\zeta_0^2\psi'^2 + g\frac{\zeta_0^2}{\psi_0^2}(\psi\psi')^2 \right\} dx, \tag{13}$$

where ψ_0 is the characteristic value of the order parameter at $T = 0$. When a transition to a homogeneous state ($\psi = \text{const}$) is considered, it usually suffices to retain in (13), besides the term quadratic in ψ, the contributions $\propto \psi^4$. In our case, when the transition is to an inhomogeneous phase ($\beta < 0$), it is necessary to retain the term $\propto (\psi'')^2$. The characteristic value of the wave vector of the inhomogeneous structure is $q_0^2 \sim |\beta|/\zeta_0^2$, and for an approach based on a functional to be valid it is necessary, first, to stipulate $|\beta| \ll 1$, i.e., restrict the analysis to the vicinity of the Lifshitz point. Second, analysis of the coefficients of the functional (13) for the aforementioned models shows (see, e.g., Ref. 13 for the Peierls model) that the coefficient of the term ψ^4 vanishes simultaneously with β. This requires that the terms $(\psi\psi')^2$ and ψ^6, whose coefficients have no anomalies near the Lifshitz point, be taken into account in (13). Thus, the expansion (13) is valid because of the specific be-

havior of the coefficients β and b in the investigated model systems.

Using the subsitutions $\psi \to \varphi = \psi/\psi_0$, $x \to x/\zeta_0$, we obtain an equation for the order parameter:

$$\varphi^{IV} - \beta\varphi'' + \alpha\varphi + \beta\varphi^3 + c\varphi^5 - g(\varphi\varphi'^2 + \varphi^2\varphi'') = 0. \quad (14)$$

A general analysis of (14) is difficult, but some of its solutions can be indicated.

Let us show that the single-period solution of the first modified KdV (mKdV) equation

$$\varphi''' - 6A\varphi^2\varphi' + B\varphi' = 0 \quad (15)$$

is also a solution of (14) if the constants A and B and the second integral C are suitably chosen. The periodic solution (15) is known to take the form of the soliton lattice $\varphi \propto \operatorname{sn} x$. The solution (15) can be easily expressed in quadratures, since the first and second integrals of (15) are known:

$$\varphi'' - 2A\varphi^3 + B\varphi = 0, \quad (16)$$

$$\varphi'^2 - A\varphi^4 + B\varphi^2 = C. \quad (17)$$

The equality of the first integral of (15) to zero ensures separation of the periodic solutions. Differentiating (15) and combining the result with (16) multiplied by λ_1 ad $\lambda_2\varphi^2$, and also with (17) multiplied by $\lambda_3\varphi$, where λ_1, λ_2, and λ_3 are numerical factors, we obtain an equation of type (14). From the conditions that the coefficients in the equations be equal, we obtain the connection of the constants A, B, and C with the parameters of the functional:

$$A = [g \pm (g^2 - 32c/3)^{1/2}]/16, \quad B = (b - 2A\beta)/(20A - 2g),$$
$$C = [\alpha + (B+\beta)B]/(g - 12A). \quad (18)$$

It can be seen that $A \sim g \sim 1$, but for the approach itself to be valid the characteristic period $\sim B^{-1/2}$ of the solution must be large compared with ζ_0, as is possible when $|b, \beta| \ll 1$. This condition is indeed met in the models considered. Note, however, that simultaneous vanishing of β and b is not mandatory for the solution to be valid, provided only that $|b, \beta| \ll 1$. Therefore when the soliton-lattice models are generalized to the case when the coefficients b and β do not vanish simultaneously (but nevertheless at nearby points on the phase diagram), the foregoing analysis remains correct.

It was noted in Ref. 14 that for the microscopic model of a Peierls transition near the doubling there exists a singly as well as doubly periodic solution. The functional approach, as will be demonstrated, also leads to this result. However, whereas the coefficients c and g in (13) were previously regarded as arbitrary, they must now be subject to a number of constraints. Namely, for the indicated microscopic models $\beta = b/2$, $c = 6$, $g = 10$:

$$\mathcal{F} \sim \int \{\alpha\varphi^2 + \beta(\varphi^4 + \varphi'^2) + \varphi''^2 + 10(\varphi\varphi')^2 + 2\varphi^6\}\, dx, \quad (19)$$

and the equation for φ takes the form

$$\varphi^{IV} - 10\varphi\varphi'^2 - 10\varphi^2\varphi'' + 6\varphi^5 - \beta(\varphi'' - 2\varphi^3) + \alpha\varphi = 0. \quad (20)$$

Using the Miura transformation[15] we introduce the function $u = \varphi^2 + \varphi'$ and show that it satisfies the second KdV equation, whose solution yields in fact the doubly periodic function $\varphi(x)$. We write the second KdV equation in the form

$$c_i \delta I_i/\delta u = 0, \quad i = -1, 0, 1, 2, \quad (21)$$

where I_i are integrals of the KdV equation[16]

$$I_{-1} = \int u\, dx, \quad I_0 = \int u^2\, dx, \quad I_1 = \int [u'^2/2 + u^3]\, dx,$$
$$I_2 = 1/2 \int [u''^2 - 5u^2u'' + 5u^4]\, dx. \quad (22)$$

We rewrite (21) in the form

$$(c_2J_2 + c_1J_1 + c_0\varphi)' + 2\varphi(c_2J_2 + c_1J_1 + c_0\varphi)$$
$$+ c_2[\varphi''^2 + 10\varphi^2\varphi'^2 - 2\varphi^6 - 2\varphi'\varphi^3] + c_1(\varphi^4 - \varphi'^2) - c_0\varphi^2 + c_{-1} = 0, \quad (23)$$

$$J_1 = \varphi'' - 2\varphi^3, \quad J_2 = \varphi^{IV} - 10\varphi^2\varphi'' - 10\varphi\varphi'^2 + 6\varphi^5. \quad (24)$$

At the same time, multiplying (10) by φ', we can represent it by

$$[\alpha\varphi^2 + \beta(\varphi^4 - \varphi'^2) - (\varphi''^2 - 2\varphi'\varphi^3 - 2\varphi^6 + 10\varphi^3\varphi'^2)]' = 0. \quad (25)$$

Comparison shows that (25) and (23) are equal if $c_2 = 1$, $c_1 = -\beta$, $c_0 = \alpha$. We conclude thus that the solution $\varphi(x)$ of (20) indeed leads to the second KdV equation for $u = \varphi^2 + \varphi'$, i.e., $\varphi(x)$ is in the general case a doubly periodic function.

The choice of some particular solution of the self-consistency equation (20) (singly or doubly periodic) is dictated by energy considerations. Unfortunately, it is difficult to calculate the free energy (19) for the doubly periodic solution, and the question of the regions where singly and doubly periodic solutions exist remains moot.

Thus, in the region were the Landau expansion is valid, the functional language is fully adequate when is comes to obtaining nonlinear periodic one-dimensional solutions.

§5. FORMATION OF IMPURITY LS, AND LOCAL PHASE TRANSITION IN THE ONE-DIMENSIONAL MODEL OF AN ELECTRONIC SOLITON LATTICE

It was shown previously[6,8] that an exact solution of the type of soliton lattice exists for a number of models of electronic phase transitions at arbitrary temperature T and arbitrary values of the noncongruence parameter μ. We recall that μ describes the deviation of band occupation from one-half in the Peierls-transition model, the separation between the electron and hole Fermi surfaces in the SDW and CDW models, and the spin splitting of the electronic states in an exchange field in superconductors. The phase diagram of the investigated models in the coordinates (T, μ) contains a region of homogeneous (C) and inhomogeneous (IC) structures). On the (T, μ) diagram there are transition lines $T_1(\mu)$ $T_2(\mu)$ and $T_3(\mu)$ between the symmetric, homogeneous, and inhomogeneous phases (Fig. 2). These three lines intersect at the Lifshitz point $\Theta(T^* \approx 0.31\psi_0, \psi^* \approx 0.604\psi_0$, where ψ_0 is the order parameter at $T = 0$ in the model with ideal congruence $\mu = 0$), near which the Landau expansion is valid. The parameter ψ can be regarded here as small ($|\psi| \ll T, \mu$) and slowly varying ($|\psi'/\psi| \ll \zeta_0^{-1}$). The potential

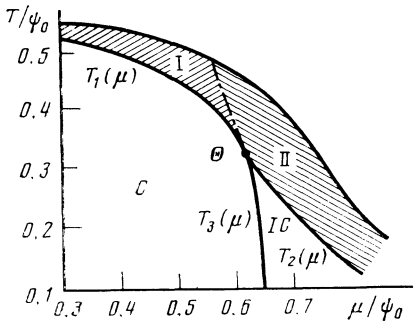

FIG. 2.

of the defect is assumed, as before, to be short-range, and the origin is taken to be the location of the defect.

To describe LS on a defect above a volume transition, we use a functional of type (19) with account taken of the contribution of the energy defect, whose variation yields the equation

$$C_3(\varphi^{IV}-10\varphi\varphi'^2-10\varphi^2\varphi''+6\varphi^5)-2C_2(\varphi''-2\varphi^3)+2C_1\varphi = D(\varphi)\delta(x). \quad (26)$$

The coefficients C_1, C_2, and C_3 and the dimensionless variables φ and x are defined in Appendix 1, where the form of the source function $D(\varphi)$ ($D=\delta T/\delta\varphi$) is also discussed for some specific situations.

We begin with the region I on the phase diagram (Fig. 2), where $2C_1/C_3<(C_2/C_3)^2$. Far from the point Θ, at $C_2>0$, we can neglect in the functional (A.1) the contribution of the terms $\sim C_3$. Equation (26) is then simplified and takes the form of the first integral of the mKdV equation with a point source:

$$\varphi''-2\varphi^3-\tilde{A}\varphi=-\frac{D(\varphi)}{2C_2}\delta(x), \qquad \tilde{A}=\frac{C_1}{C_2}. \quad (27)$$

The boundary conditions for φ far from the defects are $\varphi(\pm\infty)=0$, $\varphi'(\pm\infty)=0$, so that integration of (27) yields

$$\varphi(x)=\tilde{A}^{1/2}/\mathrm{sh}(\tilde{A}^{1/2}|x|+\Phi), \quad (28)$$

Φ is an arbitrary constant that determines the boundary condition on the defect:

$$\tilde{B}=\exp(-2\Phi)=\frac{[\varphi^2(0)+\tilde{A}]^{1/2}-\tilde{A}^{1/2}}{[\varphi^2(0)+\tilde{A}]^{1/2}+\tilde{A}^{1/2}}. \quad (29)$$

Matching the solutions (28) and (29) at the origin, we get

$$4\tilde{A}(1+\tilde{B})\tilde{B}^{1/2}/(1-\tilde{B})^2=D(\varphi)/2C_2. \quad (30)$$

For systems with a defect of the "local field" type, $D(\varphi)=D$, this solves the problem completely. As for systems with local phase transitions, where $D(\varphi)\sim\varphi$, Eq. (30) determines for them the line on which the LS arise. Specifically, if we choose $D(\varphi)=F_1\varphi$, Eq. (30) yields in the linear approximation the condition for absolute instability with respect to formation of LS:

$$4(C_1C_2)^{1/2}=F_1>0. \quad (31)$$

In the region $4(C_1C_2)^{1/2}<F_1$ the amplitude $\varphi(0)$ at the defect is given by

$$\varphi^2(0)\approx C_1^{1/2}[F_1-4(C_1C_2)^{1/2}]/2C_2^{3/2}. \quad (32)$$

In the immediate vicinity of the Lifshitz point, where $C_2\to 0$ (but is still in region I), the terms $\sim C_3$ must be retained. We have then near the absolute-instability line (31)

$$\varphi^2(0)=8aC_1^{1/2}(4a^2-b^2)[F_1-4a(C_1C_3)^{1/2}]/DC_3^{3/2}, \quad (33)$$

$$D=81a^6-45a^4b^2+10a^2b^4-b^6, \quad a,\ b=[C_2/C_3\pm(2C_1/C_3)^{1/2}]^{1/2}. \quad (34)$$

We proceed to consider region II, where $2C_1/C_3>(C_2/C_3)^2$ and retention of the terms $\sim C_3$ in (26) is necessary in principle. We are interested now only in real solutions that are even in x and tend to zero as $x\to\pm\infty$. In the absence of a source, Eq. (26) is satisfied by the solution of the first mKdV equation:

$$\varphi'''-6\varphi^2\varphi'+\tilde{A}_j\varphi'=0 \quad (35)$$

for

$$\tilde{A}_j^{1/2}=b'\pm ia', \quad j=1,\ 2, \qquad a',\ b'=[(2C_1/C_3)^{1/2}\pm C_2/C_3]^{1/2}. \quad (36)$$

Solutions of (35) that decrease as $x\to\pm\infty$ are two complex-conjugate functions:

$$\varphi_j(x)=i\tilde{A}_j^{1/2}/\mathrm{sh}(i\tilde{A}_j^{1/2}|x|+\Phi_j), \qquad \varphi_2=\varphi_1. \quad (37)$$

We introduce the functions $p_j(x)$ and $q_j(x)$, which are connected with $\varphi_j(x)$ by the Miura transformation:

$$p_j,\ q_j=\varphi_j^2\pm\varphi_j' \quad (38)$$

and thus satisfy the first KdV solution that is conjugate to (35). The method of constructing an exact real solution of Eq. (26) from the complex auxiliary solutions (37) is based on the principle of nonlinear superposition,[15] which yields, in particular, in explicit form a new solution of the second KdV equation, expressed in terms of three other solutions of the same equation: the arbitrary solution (p_0,q_0) and two solutions $(p_j,q_j,j=1,2)$, that are connected with (p_0,q_0) by the Backlund transformation [see (A.2)]. We choose for (p_0,q_0) the trivial solution of (26) $p_0=q_0=0$, and then the Bäcklund-transformations parameters must be chosen to be in the form $-i\tilde{A}_1^{1/2}/2$ for p_1, q_1 and $i\tilde{A}_2^{1/2}/2$ for p_2, q_2. Using Eq. (A.2), we write the solution of interest to us in the form

$$\varphi(x)=1/2[Q(x)-P(x)], \quad (39)$$

$$P,\ Q=(\tilde{A}_2^{1/2}-\tilde{A}_1^{1/2})/[(\tilde{A}_1^{1/2}+\tilde{A}_2^{1/2})L(p,\ q)-i], \quad (40)$$

$$L(p,q)=\left[\int_{|x|}^{\infty}[(p,q)_1-(p,q)_2]dz\right]^{-1}. \quad (41)$$

We turn now to the question of the boundary conditions at the origin ($x\to 0$). The solution of interest to us should be continuous and have continuous derivatives up to second order, inclusive. This follows from the condition for the applicability of the functional (19). The third derivative φ''' has at $x=0$ a discontinuity of first order. The system of equations

$$\varphi''(+0)=\varphi''(-0), \quad \varphi'''(+0)-\varphi'''(-0)=D[\varphi(0)]/C_3 \quad (42)$$

determines thus a pair of arbitrary constants $\Phi_{1,2}$.

Linearization of (39) with allowance for (42) yields the LS absolute-instability line for systems with local phase transitions ($D\varphi$) = $F_1\varphi$):

$$4\{C_1[C_2+(2C_1C_3)^{1/2}]\}^{1/2}=F_1. \tag{43}$$

Near this line we have for $\varphi(x)$ the result (39), which coincides with the solution of the linearized equation (26):

$$\varphi(x)=\varphi(0)\exp(-a'|x|)\{\cos b'|x|+(a'/b')\sin b'|x|\}, \tag{44}$$

where $\varphi(0)$ is given by relation (33) with the substitutions $a\to a', b\to ib'$.

We point out the characteristic features of the spatial variation of $\varphi(x)$: In region I, $\varphi(x)$ falls off exponentially far from the defect, while in region II periodic oscillations are superimposed on the exponential decrease. The local-transition line $T_d(\mu)$ given by relation (43) is shown in Fig. 2.

We examine now in greater detail some physical consequences of the existence of LS in the model of a band antiferromagnet with congruent sections of the Fermi surface. Specific examples of such systems can be dilute alloys of chromium.[17] In these systems $\varphi(x)$ describes the distribution of a linearly polarized SDW, therefore the one-dimensional source conjugate to $\varphi(x)$ can be the local magnetization in the direction of the SDW polarization. This can be, in particular, a chromium surface oriented perpendicular to the (100) direction, near which ferromagnetic order sets in below the Curie point $T_C\approx 800$ K. Near the Neel temperature ($T_n\approx 312\ K\ll T_C$) we have thus a magnetic moment frozen on the surface; this moment plays the role of the "local field" for the SDW, forming an LS on a scale $\zeta(T)$ at any temperature $T<T_C$. A source function of the "local field" type for a microscopic model of a planar spin-polarized defect in a system with SDW is calculate (A4).

A nonmagnetic defect in a system with SDW plays the role of a self-consistent source for $f(0)$. An LS is produced in this case below the local-transition temperature $T_d(\mu)$ and an uncompensated magnetic moment appears on the defect.[4] Calculating the coefficient F_1 for the model of a nonmagnetic point defect [see (A.5)], we find from the condition for the LS existence ($F_1>0$) that at $|\overline{U}|\ll 1$ (where $\overline{U}$ is the dimensionless constant of the electron-impurity interaction) the moment at the defect is equal to

$$M_i\approx 16\mu_B\psi_0\varphi(0)|\overline{U}\bar{\varphi}_1|/\pi T, \tag{45}$$

$\varphi(0)$ is given by relation (33) in region I or by its analog in region II, and μ_B is the Bohr magneton. The condition for the existence of an LS above T_c at $|\overline{U}|\ll 1$ reduces to the requirement $\overline{U}_\mu>0$. Note that in our microscopic calculation for a substitutional impurity [see Eq. (A.5)] we have assumed for simplicity that the maximum of the spin-density distribution $S(x)\sim\varphi(x)$ is centered exactly on the defect, i.e., we assumed that the phase of the SDW to be fixed. Otherwise it would be necessary to introduce a complex order parameter $\varphi=\varphi_{\mathrm{Re}}+i\varphi_{\mathrm{Im}}$, that describes the SDW phase collapse, and the problem would become much more complicated. This is possibly just what occurs in case of an interstitial impurity.

The presence of localized moments M_d leads to a Curie-Weiss behavior of $\chi(T)$ at $T_N<T<T_d$. Such a behavior was experimentally observed in chromium alloys (see the bibliography in Ref. 17).

§6. FORMATION OF IMPURITY LEVELS IN CRYSTALS WITH ELECTRONIC SOLITON LATTICES

So far we have investigated the question of penetration of LS near the point of transition into the inhomogeneous phase. We now consider LS considerably below the transition point, in the region of a modified phase having the structure of a soliton lattice. The functional approach used above is no longer valid, since the order parameter ψ is neither small nor slowly varying. We turn therefore to the usual Green's function method. In the entire analysis that follows we use a two-band model of a metal with a quasi-one-dimensional (corrugated) spectrum that is unstable to formation of a charge density wave (CDW). The corresponding order parameter will be traditionally designated by the symbol $\Delta(\mathbf{r})$. The Hamiltonian of the model takes in the mean-field approximation the form

$$H=\begin{pmatrix}\varepsilon_1(-i\nabla) & -\Delta(\mathbf{r})\\ -\Delta^*(\mathbf{r}) & \varepsilon_2(-i\nabla)\end{pmatrix}+\frac{|\Delta|^2}{g},$$
$$\varepsilon_1(\mathbf{k})=\xi(k_x)+\eta(\mathbf{k}_\perp),\quad \varepsilon_2(\mathbf{k}+\mathbf{Q})=-\xi(k_x)+\eta(\mathbf{k}_\perp), \tag{46}$$

where $\xi(kx)=v_Fkx$, v_F is the velocity on the Fermi surface in the direction of the vector $\mathbf{Q}=\mathbf{Q}\mathbf{e}_x$ that combines the electron and hole sections of the Fermi surface, $\eta(k_\perp)$ is the transverse corrugation of the spectrum, while $|\eta|\ll W$ (W is the width of bands (1) and (2) in the x direction). Generally speaking, however, $|\eta|$ can be larger than or of the order of $|\Delta|$; g is the effective potential of the interaction that forms the CDW.

It is convenient to write the single-particle Green's functions of the Hamiltonian (46) in a mixed representation, taking the Fourier transform with respect to time:

$$\mathcal{G}_{ij}^0(\mathbf{r},\mathbf{r}',\omega)=\tilde{\mathcal{G}}_{ij}^0(x,x',\boldsymbol{\rho}_\perp-\boldsymbol{\rho}_\perp',\omega)$$
$$\times\exp\left[\pm\left(\frac{iQ(x-x')}{2}+\frac{i\mathbf{Q}_\perp(\boldsymbol{\rho}_\perp-\boldsymbol{\rho}_\perp')}{2}\right)\right], \tag{47}$$

where the plus sign is used for the components $\mathcal{G}_{11}^0$ and $\mathcal{G}_{12}^0$, and the minus sign for $\mathcal{G}_{21}^0$ and $\mathcal{G}_{22}^0$. We write the order parameter $|\Delta|$ in the form

$$\Delta(\mathbf{r})=\bar{\Delta}(x)\exp[iQx+i\mathbf{Q}_\perp\boldsymbol{\rho}_\perp], \tag{48}$$

where the vector $\mathbf{Q}_\perp$ determines the modulation of the CDW in the transverse direction. The actual choice of $\mathbf{Q}_\perp$ depends on the possible anisotropy of the interaction constant $g(\mathbf{Q}_\perp)$ and also on the form of the corrugation of the electron spectrum $\eta(\mathbf{k}_\perp)$.

We take the Fourier transforms of the functions $\tilde{\mathcal{G}}_{ij}^0$ with respect to the transverse coordinate $(\rho_\perp-\rho_\perp')$, after substituting

$$\tilde{\mathcal{G}}_{ij}^0(x,x',\mathbf{q}_\perp,\omega)=G_{ij}^0(x,x',\tilde{\omega})\exp[i\eta_+(\mathbf{q}_\perp)(x-x')/v_F], \tag{49}$$
$$\tilde{\omega}=\omega-\eta_+(\mathbf{q}_\perp),\quad \eta_\pm(\mathbf{q}_\perp)=\tfrac{1}{2}[\eta(\mathbf{q}_\perp+\mathbf{Q}_\perp/2)\pm\eta(\mathbf{q}_\perp-\mathbf{Q}_\perp/2)]$$

we arrive at the following one-dimensional equation

$$[\hat{I}\tilde{\omega}-\hat{H}]\hat{G}^0=\hat{I}\delta(x-x'), \tag{50}$$

where $\hat{I}$ is a unit matrix in the band-index space

$$\hat{H}=\begin{pmatrix} iv_F d/dx & -\Delta(x) \\ -\Delta(x) & -iv_F d/dx \end{pmatrix}. \tag{51}$$

The Green's functions G_{ij}^0 are of the form (see, e.g., Ref. 18)

$$G_{11}^0(x,x',\tilde{\omega})=\sum_n \frac{u_n(x)u_n^*(x')}{\tilde{\omega}-E_n}, \tag{52}$$

$$G_{21}^0(x,x',\tilde{\omega})=\sum_n \frac{u_n(x)v_n^*(x')}{\tilde{\omega}-E_n}, \tag{53}$$

while G_{22}^0 and G_{12}^0 are obtained by making the substitutions $u_n \to v_n$, $E_n \to -E_n$ in (52) and (53). It is convenient to write the functions u_n and v_n in the form u_n $v_n = 2^{-1/2}(f_n^{(1)} \pm if_n^{(2)})$, where $f_n^{(1)} f_n^{(2)}$ are solutions of the Lame equation[18]

$$\left[E_n^2+v_F^2\frac{d^2}{dx^2}-\Delta^2 \mp v_F\frac{d\Delta}{dx}\right]f_n^{(1,2)}=0, \tag{54}$$

$$\Delta(x)=\Delta_\gamma \operatorname{sn}(x\Delta_\gamma/v_F\gamma,\gamma), \tag{55}$$

$\operatorname{sn}(y,\gamma)$ is the Jacobi elliptic function, and $E_n=\varepsilon_n\Delta_\gamma$ are the eigenvalues of Eq. (53). We make next the substitution $x \to x\Delta_\gamma/v_F\gamma$.

It is easy to verify that the self-consistency equation for the order parameter $\Delta(x)$

$$\tilde{\Delta}(x)=g\sum_{\tilde{\omega}} G_{21}(x,x,\tilde{\omega}) \tag{56}$$

is identically satisfied upon substitution of G_{21} from (53).

We consider now the problem of a single point defect with identical potential matrix elements in the band indices ($U_{ij}=U$), although the last restriction is immaterial and is included only as part of the method. The Green's function of the system with the impurity can be expressed in the known method in terms of the Green's function $\mathcal{G}^0$ of an ideal system and the total vertex of the electron-impurity scattering:

$$\mathcal{G}_{ij}(\mathbf{r},\mathbf{r}')=\mathcal{G}_{ij}^0(\mathbf{r},\mathbf{r}')+\mathcal{G}_{il}^0(\mathbf{r},\mathbf{r}_0)\Gamma_{lm}(\mathbf{r}_0)\mathcal{G}_{mj}^0(\mathbf{r}_0,\mathbf{r}'), \tag{57}$$

where $\mathbf{r}_0$ is the coordinate of the impurity center,

$$\Gamma_{lm}=\Gamma=U\Big/\Big[1-U\sum_{i,j}\mathcal{G}_{ij}^0(\mathbf{r}_0,r_0,\omega)\Big]. \tag{58}$$

The energy of the localized impurity state is determined by the pole of the vertex (58):

$$1=U\sum_{i,j}\mathcal{G}_{ij}^0(\mathbf{r}_0,\mathbf{r}_0,\omega)=U\sum_{i,j}\int G_{ij}^0(x_0,x_0,\tilde{\omega})\frac{d\mathbf{q}_\perp}{(2\pi)^2}. \tag{59}$$

We consider the simplest case $\eta_+ \equiv 0$, which can hold, for example, if $\mathbf{Q}_\perp=(\pi/a_y,\pi/a_z)$ in the tight-binding approximation for transverse corrugation of a quasi-one-dimensional center

$$\eta(\mathbf{q}_\perp)=W_y\cos(q_y a_y)+W_z\cos(q_z a_z)$$

(a_y and a_z are the periods of the lattice in the transverse directions, while W_y and W_z are the overlap integrals. It is easy to verify that at $\eta_+=0$ the problems of calculating the energy of the local level for the corrugated and purely one-dimensional models of the electron spectrum are perfectly similar and the summation over the transverse quasimomentum $\mathbf{q}_\perp$ reduces to renormalization of the density of states in the one-dimensional model. Substituting the Green's functions (52) and (53) in explicit form in (61) and introducing the state density with allowance for the spin degeneracy[5]

$$\sum_{\omega}\to\frac{L\Delta_\gamma}{\pi\gamma v_F}\int\frac{(\varepsilon^2-\Omega^2)\theta[(\varepsilon^2-\varepsilon_-^2)(\varepsilon^2-\varepsilon_-^2)]}{[(\varepsilon^2-\varepsilon_+^2)(\varepsilon^2-\varepsilon_-^2)]^{1/2}}d\varepsilon, \tag{60}$$

$$\Omega^2=\varepsilon_+^2 E\left(\frac{2\gamma'}{1+\gamma}\right)\Big/K\left(\frac{2\gamma'^{1/2}}{1+\gamma}\right), \quad \varepsilon_\pm=\frac{1}{2}\left(\frac{1}{\gamma}\pm 1\right), \tag{61}$$

where E and K are complete elliptic integrals of the first and second kind, and L is the dimension of the system in the x direction, we obtain

$$1=-\overline{U}A(\varepsilon_0), \tag{62}$$

$$A(\varepsilon_0)=\frac{2M(\varepsilon_0)}{\pi\gamma\varepsilon_+\varepsilon_0}\left[\varepsilon_0\operatorname{sn}(x_0,\gamma)+\varepsilon_0^2-\frac{1}{4}\left(1+\frac{1}{\gamma^2}\right)+\frac{1}{2}\operatorname{sn}^2(x_0,\gamma)\right], \tag{63}$$

$$M(\varepsilon_0)=\Pi(\varepsilon_0^2/\varepsilon_+^2;\ \varepsilon_-/\varepsilon_+)+\Pi(\varepsilon_-^2/\varepsilon_0^2;\ \varepsilon_-/\varepsilon_+)-K(\varepsilon_-/\varepsilon_+), \tag{64}$$

$$\overline{U}=\pi U/v_F a_y a_z, \tag{65}$$

$\Pi(\varphi,\varepsilon_-/\varepsilon_+)$ is a complete elliptic integral of the third kind. The function $M(\varepsilon_0)$ is such that $M(\varepsilon_0)=0$ at $\varepsilon_0^2>\varepsilon_+^2$ and $\varepsilon_0^2<\varepsilon_-^2$ (we recall that ε_+ and ε_- are the end points of the single-electron spectrum in systems with soliton solutions). Solutions of (63) exist thus only at energies $\varepsilon_-^2\leqslant\varepsilon_0^2\leqslant\varepsilon_+^2$, i.e., in the forbidden band.

Let us investigate some limiting cases. As $\gamma\to 1$ (the limit of a loose-mesh soliton lattice) Eq. (63) takes the form

$$1=-\frac{\overline{U}}{\varepsilon_0(1-\varepsilon_0^2)^{1/2}}\left[\varepsilon_0\operatorname{th}x_0+\varepsilon_0^2-\frac{1}{2}(1-\operatorname{th}^2 x_0)\right], \tag{66}$$

while $\Delta(x)=\Delta_1\tanh x$. Assume that the impurity site is in the region of the positive half of the CDW, i.e., $x_0>0$ (the chosen amplitude is assumed to be $\Delta_1>0$). Far from the soliton wall, the bound state occurs at $\overline{U}<0$, and its energy is

$$\varepsilon_0=(1-\overline{U}^2)/(1+\overline{U}^2), \quad x_0\to+\infty. \tag{67}$$

Similarly, in the negative half-wave region the bound state sets in at $\overline{U}>0$:

$$\varepsilon_0=-(1-\overline{U}^2)/(1+\overline{U}^2), \quad x_0\to-\infty. \tag{68}$$

The results (67) and (68) agree with those known for homogeneous structures.[19] If, however, the defect is near a soliton wall, the situation is in principle different. Let the impurity site be at the center of the wall ($x_0=0$). In this case we have two roots:

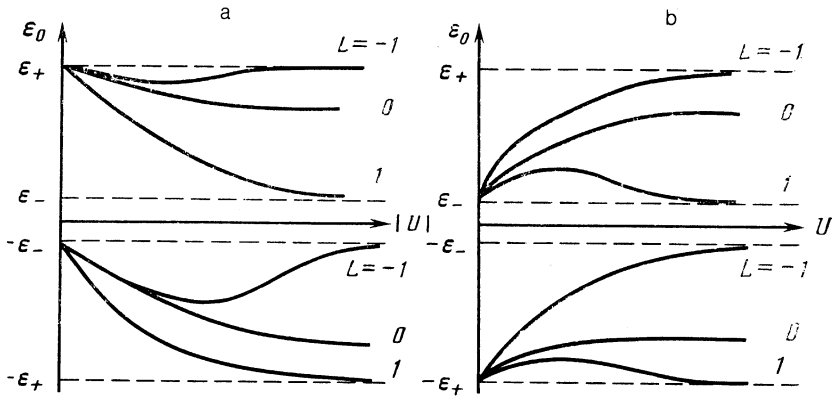

FIG. 3. Plots of $\varepsilon_0(U)$ for different x_0: $a - U\leqslant 0$, $\delta - U>0$; $L=\mathrm{sn}(x_0,\gamma)$

$$\varepsilon_0^{(1,2)}=\pm\frac{1}{2^{1/2}}\left[1\mp\frac{\operatorname{sign}\overline{U}}{(1+\overline{U}^2)^{1/2}}\right]^{1/2}. \tag{69}$$

It is quite understandable that for any sign of the potential $\overline{U}$ there exist within the forbidden bands two local levels separated from the conduction (valence) band and from the central soliton band. In the limits $\gamma\to 1$, $x_0\to\pm\infty$ one of the levels merges with the soliton band and is lost. Figure 3 shows plots of $\varepsilon_0(\overline{U})$ for different x_0 (a limit $|x_0|=2K(\gamma)$ is imposed by the fact that $sn\,x$ is periodic function). The general properties of the impurity states in the soliton lattice allows them to be grouped into several blocks. At $\overline{U}<0$ a level in the energy interval $\varepsilon_0^{(+)}\leqslant\varepsilon_0\leqslant\varepsilon_+$ is separated from the conduction band, and a level in the interval $\varepsilon_0^{(-)}\leqslant\varepsilon_0\lesssim-\varepsilon$ is separated from the central soliton band. At $U>0$ the levels separated from the valence and soliton bands have respective energies $\varepsilon_+\leqslant\varepsilon_0\leqslant\varepsilon_0^{(-)}$ and $\varepsilon_-\leqslant\varepsilon_0\leqslant\varepsilon_0^{(+)}$. Energies $\varepsilon_0^{(+)}$ are obtained as asymptotic values as $\overline{U}\to\pm\infty$:

$$\varepsilon_0^{(\pm)}={}^1/_2\{-\mathrm{sn}(x_0,\gamma)\pm[1+\gamma^{-2}-\mathrm{sn}^2(x_0,\gamma)]^{1/2}\}. \tag{70}$$

If the defect locations in the lattice are not correlated, the coordinate x_0 runs randomly through all the values in the interval from 0 to $2K(\gamma)$. The impurity levels $\varepsilon_0(x_0)$ are therefore spread over the entire forbidden band. The form of the impurity-state density depends on the ratio of the sizes of the soliton wall and of the region of almost constant amplitude value of $\tilde{\Delta}(x)$. In the limit of a loose-mesh lattice, the density of the impurity states takes the form of an abrupt maximum at energies ε_0 with a spread region $\delta\varepsilon_0\sim\mathrm{K}^{-1}$.

Let us estimate the range of validity of the results. We calculate the correction to the CDW amplitude at the defect location. In the limit of a loose-mesh lattice we have $\delta\Delta(x_0)=f(\overline{U})\Delta_\gamma$, where $f(\overline{U})\approx-2\overline{U}^2$ for $|\overline{U}|\ll 1$ and $f(\overline{U})\approx-\frac{1}{2}$ for $|\overline{U}|\gg 1$. We actually have $|\delta\tilde{\Delta}(x_0)|\sim\Delta_\gamma$ already at $|\overline{U}|\gtrsim 1$, and all the results of §6 are approximate, so that for a more rigorous analysis the impurity potential must be made self-consistent.

In systems with SDW, the entire analysis is almost entirely similar to the case of CDW. The only difference lies in the spin polarization of the impurity states, which results in a magnetic moment for the defect.[20]

Allowance for the corrugation of $\eta_+(\mathbf{q}_\perp)$ does not lead to qualitative differences in the results if $|\eta_+|\lesssim|\varepsilon_0|$. In the opposite case $|\eta|\gtrsim\varepsilon_0|$, it can be readily seen that the impurity states become damped because of the intersection of the energy ε_0 of the local state located inside the gap with the itinerant-electron spectrum which is corrugated in the transverse direction. A more detailed analysis calls for knowledge of $\eta_+(\mathbf{q}_\perp)$ in explicit analytic form and is not presented here.

The problem of localized defects on planar defects (e.g., on the surface of the sample) in crystals with soliton lattices has much in common with the case of a pointlike impurity. It is not necesary here, however to sum over the transverse quasimomentum (the planar defect is assumed oriented perpendicular to the x axis). The corrugation leads now to formation of a two-dimensional electron band with a dispersion $\varepsilon(\mathbf{q}_\perp)=\varepsilon_0+\eta_+(\mathbf{q}_\perp)$ along the plane of the defect. Thus, particularly in band antiferromagnets, spin-polarized surface states can be formed on the sample boundary or on the domain walls, and surface magnetization results.

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APPENDIX 1

Equations for the coefficients in the Ginzburg-Landau functional $\mathcal{F}$ are obtained by the standard temperature Green's function method. The dimensionless variables are defined as $\psi\to\psi_0\varphi, x\to\psi_0 x/v_F$, where v_F is the velocity on the Fermi surface, and ψ_0 is the order parameter in the BCS model for $T=\mu=0$. In this notation,

$$\mathcal{F}(\varphi)=\int\{C_1\varphi^2+C_2(\varphi^4+\varphi'^2)+C_3(5\varphi^2\varphi'^2+\varphi^6+\varphi''^2/2) - \Gamma[\varphi(0)]\delta(x)\}dx, \tag{A.1}$$

$$C_1=\frac{\tau}{2}\left(1-\frac{4\mu}{\pi T}\tilde{\varphi}_1\right),\quad C_2=\frac{\psi_0^2\tilde{\varphi}_2}{4(\pi T)^2},\quad C_3=\frac{\psi_0^4\varphi_4}{8(\pi T)^4},\quad \tau=\frac{T-T_0}{T_0}, \tag{A.2}$$

$$\tilde{\varphi}_1=\sum_{n\geqslant 0}\frac{\mu}{\omega_n}(2n+1)^{-2}\left(1+\frac{\mu^2}{\omega_n^2}\right)^{-2};$$

$$\tilde{\varphi}_2=\sum_{n\geqslant 0}(1-3\mu^2/\omega_n^2)\,(2n+1)^{-3}(1+\mu^2/\omega_n^2)^{-3},$$

$$\tilde{\varphi}_4=\sum_{n\geqslant 0}(10\mu^2/\omega_n^2-5\mu^4/\omega_n^4-1)\,(2n+1)^{-5}(1+\mu^2/\omega_n^2)^{-5}, \tag{A.3}$$

$$\omega_n=\pi T(2n+1).$$

For the case of a point defect of the "local field" type, the source function $\Gamma(\varphi)$ takes in the SDW model the form

$$\Gamma_0(\varphi)=F_0\varphi,\quad F_0=-2\bar{U}/(1+\bar{U}^2)\bar{g}. \tag{A.4}$$

For the case of a defect of "local temperature" type we have in the SDW model

$$\Gamma_1(\varphi)={}^1/_2F_1\varphi^2,$$

$$F_1=\frac{\psi_0}{T}\frac{\bar{U}}{(1+\bar{U}^2)^2}\left[\frac{4\tilde{\varphi}_1}{\pi}(1-\bar{U}^2)-\frac{\pi\bar{U}}{2}\operatorname{sech}^2\frac{\mu}{2T}\right]. \tag{A.5}$$

In (A.4) and (A.5) $\bar{U}=\pi Uv_F^{-1}$, and U is the potential of the defect [in (A.4), $U=JM$ where M is the local frozen-in magnetization and J is the effective exchange intergral; in (A.5), U is the potential of the nonmagnetic defect].

APPENDIX 2.

The nonlinear-transformation equations used in §5 were taken from Ref. 15. The solutions $u_0(x)$ and $u_j(x)$ $(J=1,2)$ of the KdV equation are connected by the Bäcklund transformation if

$$W_0'(x)+W_j'(x)={}^1/_2[W_0(x)-W_j(x)]^2+{}^1/_2[4d_j-W_0(x)+W_j(x)], \tag{A.6}$$

where

$$W(x)=\int_x^\infty u(y)\,dy,$$

and d_j are the transformation parameters. By algebraic transformations we can obtain from (A.6) a new solution of the KdV equation:

$$W_{12}(x)=W_0(x)-\frac{(d_1+d_2)[W_1(x)-W_2(x)]}{d_1-d_2+{}^1/_2[W_1(x)-W_2(x)]}. \tag{A.7}$$

Equation (A.7) is known as the nonlinear superposition principle for solutions of the KdV equations.

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