Band theory of phase stratification

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A theory proposed here explains the stratification into phases in the high T_c superconductors as resulting from the existence of different insulating correlations, characterized by a long-range or short-range order. The onset of insulating properties is described in the band approach by a model with congruent sections of the Fermi surface. A self-consistent solution is found for a soliton in a system with a definitely multidimensional spectrum. The condition for a transition from a regime of periodic structures (soliton lattices) to a stratified state of insulating and metal droplets is determined. The size of the droplets and the structure of the stratified state are determined by a competition between the Coulomb energy of the charged droplets and the surface energy. A stratification can be induced by a superconducting transition. In a sample which is a superconductor in the sense that it exhibits a Meissner effect, application of a weak magnetic field gives rise to a resistance which is orders of magnitude greater than the resistance in the normal phase.

1. INTRODUCTION

The electronic properties, primarily the superconducting properties, of spatially inhomogeneous systems have attracted particular interest because of numerous high-T_c superconductor experiments which indicate the existence of various types of nonuniform structures in these compounds. Among these structures, one can distinguish two basic types: first, the superstructures (or superlattices) which are observed in bismuth ceramics,[1] thallium ceramics,[2] and barium-potassium ceramics[3] and also in the yttrium ceramics, near the crossover of the 60° and 90° phases;[4] second, the stratifications into different phases which can be detected directly by neutron diffraction in $La_2CuO_{4+\delta}$ (Ref. 5). There are also indications of a stratification in other high-T_c superconductors: the smearing of the superconducting transition temperature T_c and the hysteresis effects in a magnetic field, which were seen in the very first studies of the high-T_c superconductors[6] and which have since been observed in essentially all these superconductors; the plateau on the plot of T_c versus the composition of yttrium ceramics;[4] and the conductivity anomalies in $Ba_{1-x}K_xBiO_3$ in a magnetic field, in which case the resistance of the sample has been observed to increase significantly in a weak magnetic field after the transition to the superconducting phase (detected on the basis of the Meissner effect).[7]

Recent calculations show that both the formation of superstructures[8] and the stratification into phases in yttrium ceramics[9] can be explained on the basis of lattice atomic models which describe an ordering of oxygen vacancies in Cu–O chains. The interrelation between the structure of the inhomogeneous state and the superconducting properties remains an open question. A more comprehensive approach would start from a study of the electron subsystem. In the strong-coupling approximation, studied in Refs. 10 and 11, the stratification into phases (as well as the superconductivity) results from a mutual attraction of carriers. There is accordingly a competition between these two phenomena. Gor'kov and Sokol[12] link the stratification with a localization of carriers at the Jahn-Teller Cu^{2+} ions. Droplets of an insulating phase arise because of an attraction between localized holes through an elastic deformation. The same interaction might be responsible for the formation of local pairs which serve as sources of the superconducting pairing interaction of itinerant carriers.[13] In this paper we propose a band model in which the stratification does not compete with the superconductivity and may in fact be induced by the superconducting transition.

We start with a picture of the high T_c superconductors as doped semiconductors. To describe the conversion of the carrier spectrum into that of an insulator we use a model with a Fermi surface which approximately satisfies the "nesting" (or "congruence") condition.

An exact nesting of the Fermi surface is known to give rise to an instability with respect to a transition to a state with a charge density wave or a spin density wave. Such a state is described by introducing a uniform insulating order parameter $\Delta \sim \langle a^+_{\mathbf{k}+\mathbf{Q}} a_{\mathbf{k}} \rangle$, which determines the gap in the spectrum of elementary excitations. For the discussion below, it is sufficient that there be a pseudogap due to the establishment of a corresponding short-range order. The appearance of a gap gives rise to peaks in the density of states at the edges of the allowed bands. This fact, combined with the "softness" of the insulating order parameter with respect to doping, sets the stage for a stratification into different phases in these systems. Specifically, the elevated density of states at the edges of the allowed spectrum slows the increase in the kinetic energy of particles added to the insulating phase. At the same time, the gap size falls off rapidly:[14]

$$\Delta(n) = [\Delta_{D0}(\Delta_{D0} - 2\tilde{n})]^{1/2}$$

where Δ_{Do} is the order parameter in the undoped phase, $n = 2N(0)\tilde{n}$ is the concentration of the added particles, and $N(0)$ is the density of states at the Fermi surface.

As a result, the chemical potential μ decreases with doping: $\mu = \Delta_{Do} - \tilde{n}$. The condition $\partial\mu/\partial n < 0$ thus holds until the insulating gap closes ($\tilde{n} < \Delta_{Do}/2$).

Under the condition

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$$\frac{\partial\mu}{\partial n}=\frac{\partial^2 F}{\partial n^2}<0 \tag{1}$$

the uniform state of the system is absolutely unstable to the formation of macroscopic regions with an elevated particle density. It might seem that this situation should definitely result in a stratification of the system into homogeneous droplets of metallic and insulating phases.

However, we know from the exact solution of the one-dimensional model with nested regions of the Fermi surface (a Peierls insulator)[15] that a stratification into different phases does not occur in this case, and the ground state corresponds to a periodic soliton lattice.

The reason for this result is that at $D=1$ the nesting condition is always satisfied with a vector $q=2p_F$, regardless of the filling of the Fermi surface (two points). This condition results in a (logarithmic) instability with respect to the formation of a superstructure with a period of $(2p_F)^{-1}$. For this reason, the instability with $q=0$, responsible for the stratification, cannot occur.

In macroscopic terms, this behavior corresponds to a negative surface energy of droplets, which leads to a maximum possible disintegration of the droplets. From the soliton standpoint, the meaning is that the interaction between different self-localized states is repulsive. As a result, a periodic solution arises.

We thus see that the sole reason for the absence of a stratification into different phases with a macroscopic volume (despite the condition $\partial\mu/\partial n<0$) in the models for which an exact solution is known is the one-dimensional nature of the spectrum.

In any multidimensional system with a spectrum which satisfies the condition $\varepsilon(\mathbf{k}+Q)=-\varepsilon(\mathbf{k})$ a nesting of the Fermi surface, doping disrupts the nesting at a half filling. As we show below, this disruption of the nesting gives rise to a region corresponding to a stratified state on the phase diagram. The general appearance of the phase diagram of multidimensional models with nesting is discussed in Sec. 2; the corresponding diagram is shown in Fig. 3a. When a reservoir of carriers is introduced in the system, the stratification region in Fig. 3a shrinks; it eventually disappears entirely as the reservoir strength becomes infinite ($R\to\infty$). This situation apparently occurs in chromium, where the regions of the Fermi surface which have not become insulating constitute a large fraction of the Fermi surface. They serve as a reservoir. Consequently, there are only nonuniform solutions of the periodic-superstructure type.[16] The possible appearance of periodic solutions was ignored by Brankov *et al.*[17] in a discussion of the absolute instability of the model of Ref. 14.

We thus see that both types of nonuniformities which are found in the real high T_c superconductors are possible, depending on the parameter values of the model: periodic superlattices and a stratification into different phases, in the course of which a uniform insulating phase generally coexists with a metallic phase with a periodic superstructure. In addition to the model in which the insulating gap is formed exclusively by valence electrons, we discuss in Sec. 2 a model which incorporates a commensurate lattice potential, which results in the appearance of a seed gap. [In the high T_c superconductors, this role may be played by the "tilting" potential of the orthorhombic distortions (in a lanthanum ceramic) or by the potential of the chains (in an yttrium system).] We will see that this model, which is mathematically simpler, has a behavior qualitatively the same as that of the nesting model in the temperature range of interest here. To carry out a physically more transparent study of the stratified state and of the interrelationship between superconductivity and stratification, we formulate an isotropic version of this model in Sec. 3 and construct a corresponding phase diagram.

A stratification into metallic and insulating phases is accompanied by the formation of space charge. The disadvantage in terms of the Coulomb energy which arises as a result can be reduced by a breakup of the system into smaller droplets, which lead to electrical neutrality on the average at a smaller scale. In Sec. 4 we analyze the structure of the stratified state. We find the concentration and size of the droplets of the metallic and insulating phases.

In Sec. 5 we examine the interrelationships between superconductivity and the phase stratification. We will see that superconductivity may induce such a stratification. As a result, discrete superconducting droplets form in the system; they are separated from each other by insulating "interlayers" and coupled to each other by weak links.

2. STRATIFICATION INTO DIFFERENT PHASES IN MULTIDIMENSIONAL SYSTEMS WITH NESTED REGIONS OF THE FERMI SURFACE

1. We write the Hamiltonian of a system with a nesting of the Fermi surface as follows:

$$\hat{H}=\int d\mathbf{r}\left\{\sum_{\sigma,i}[\Psi_{i\sigma}^{+}(\mathbf{r})\varepsilon_i(\nabla)\Psi_{i\sigma}(\mathbf{r})+\Delta(\mathbf{r})\Psi_{1\sigma}^{+}(\mathbf{r})\Psi_{2\sigma}(\mathbf{r})\right.$$
$$\left.+\text{h.c.}+\frac{\Delta^2(\mathbf{r})}{g}\right\}. \tag{2}$$

Here $i=1,2$ corresponds to regions of the Fermi surface which can be brought into coincidence by translation through a vector $\mathbf{Q}$; $\Delta(\mathbf{r})$ is the insulating order parameter, which we assume to be real; $\psi_{i\sigma}(\mathbf{r})$ are field operators which annihilate particles; g is the coupling constant in the electron-hole channel;

$$\varepsilon_1(\mathbf{k})=\xi(\mathbf{k})-\mu,\quad \varepsilon_2(\mathbf{k})=-\xi(\mathbf{k})-\mu \tag{3}$$

are the seed dispersion relations; and μ is the chemical potential.

As we mentioned back in the Introduction, the governing difference between multidimensional models with congruent regions of the Fermi surface is the disruption of the exact nesting upon a deviation from a "half-filling" [in the model of Eqs. (2) and (3), a half-filling corresponds to a value $\mu=0$]. In the present section of the paper we show that this disruption can lead to a phase stratification. To do this, we consider a system with a transverse dispersion of the following (fairly general) type. We assume that $\xi(\mathbf{k})$ in (2) is given by

$$\xi(\mathbf{k})=v_{\mathbf{k}_\perp}k_x, \tag{4}$$

where k_x and $\mathbf{k}_\perp$ are the momenta which are respectively longitudinal and transverse with respect to the nesting vector $\mathbf{Q}=\mathbf{e}_xQ_x$, and $v_{\mathbf{k}_\perp}$ is a positive definite and otherwise arbitrary function.

It can be seen from (3) and (4) that the transverse-momentum dependence of the Fermi velocity has the result that the nesting condition $\varepsilon_1(\mathbf{k}+\mathbf{q}) = -\varepsilon_2(\mathbf{k})$ can be satisfied on the Fermi surface only at half filling, i.e., only at $\mu = 0$ (in contrast with the one-dimensional case, in which we have $v = \text{const}$, and there is a nesting with a vector $q = 2\mu/v$ for any value of μ).

The energy (W) of the system with Hamiltonian (2) is a functional of the parameter Δ:

$$W\{\Delta(\mathbf{r})\} = \sum_{E<\mu} E + \frac{L^{D-1}}{g}\int_{-L/2}^{L/2} \Delta^2(x)\,dx, \tag{5}$$

where D is the dimensionality, L is a linear dimension of the system, and the eigenvalues E are the eigenvalues of the system of equations

$$\begin{aligned} -iv_{\mathbf{k}_\perp}\frac{\partial}{\partial x}\varphi_{\mathbf{k}_\perp}(x) - i\Delta(x)\varphi_{\mathbf{k}}(x) &= E\psi_{\mathbf{k}_\perp}(x), \\ -iv_{\mathbf{k}_\perp}\frac{\partial}{\partial x}\psi_{\mathbf{k}_\perp}(x) + i\Delta(x)\psi_{\mathbf{k}_\perp}(x) &= E\varphi_{\mathbf{k}_\perp}(x). \end{aligned} \tag{6}$$

The dependence of the wave functions on the transverse coordinates has been singled out in the form $\varphi(r)$, $\psi(r) \sim \exp(i\mathbf{k}_\perp \mathbf{r}_\perp)\varphi_{\mathbf{k}_\perp}(x)$, $\psi_{\mathbf{k}_\perp}(x)$ in (6). The self-consistent potential $\Delta(x)$ must minimize the functional in (5).

We first consider the homogeneous state $[\Delta(x) = \text{const}]$. We then have the following expression for the energy density of the insulating phase, w_D:

$$w_D = \frac{W}{L^D} = \frac{2}{(2\pi)^D}\int E(\mathbf{k})\theta(\mu - E(\mathbf{k}))\,d\mathbf{k} + \frac{\Delta^2}{g}. \tag{7}$$

The chemical potential μ is found from the equation for the density (n) of particles in excess of a half-filled band ($\mu = 0$):

$$n = \frac{2}{(2\pi)^D}\int [\theta(\mu - E(\mathbf{k})) - \theta(-E(\mathbf{k}))]\,d\mathbf{k}. \tag{8}$$

Here

$$\begin{gathered} E(k) = \pm(v_{\mathbf{k}_\perp}{}^2 k_x{}^2 + \Delta^2)^{1/2}, \qquad \Delta^2 = \Delta_{D0}(\Delta_{D0} - 2\tilde{n}), \\ \Delta_{D0} = 2\tilde{\omega}\exp\left[-\frac{1}{N(0)g}\right], \qquad \tilde{n} = \frac{n}{2N(0)}, \qquad \mu = (\Delta^2 + \tilde{n}^2)^{1/2}. \end{gathered} \tag{9}$$

The density of states at the Fermi surface in the normal phase, $N(0)$, for dispersion relation (3), (4) is

$$N(0) = \frac{2}{(2\pi)^D}\int \frac{d\mathbf{k}_\perp}{v_{\mathbf{k}_\perp}} = \frac{\nu}{\pi L^{D-1}}\langle v^{-1}\rangle, \tag{10}$$

where $\nu = (L/2\pi)^{D-1}\int d k_\perp$ is the number of states in the transverse band, and where

$$\langle(\ldots)\rangle = \frac{1}{\nu}\left(\frac{L}{2\pi}\right)^{D-1}\int(\ldots)\,dk_\perp.$$

means an average over the transverse momentum.

For the energy of the uniform insulating state we find the following result from (7), also using (8) and (9):

$$w_D(n) = N(0)\{-\Delta_{D0}{}^2/2 + 2\tilde{n}\Delta_{D0} - \tilde{n}^2\}, \quad \tilde{n} \leqslant \Delta_{D0}/2. \tag{11}$$

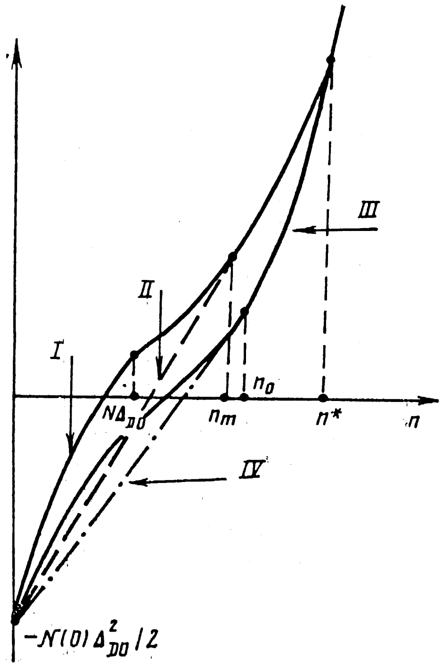

FIG. 1. Concentration dependence of the energy for a model with "nesting." I—Energy of uniform state; II—energy of system which has stratified into a uniform insulator and a uniform metal; III—energy of periodic solution under condition (17); IV—energy of a system which has stratified into an insulator and a phase with a periodic superstructure.

In (11), as well as everywhere below, the origin for the energy scale is taken to be the energy of the undoped ($n = 0$) metallic state.

The energy of the uniform insulating phase described by (11) is shown in Fig. 1 [line I corresponds to $n < N(0)\Delta_{D0}$]. At $n \geqslant N(0)\Delta_{D0}$, the system goes into a uniform metallic phase with an energy $w_M = \tilde{n}^2$ [line I, in the region $n > N(0)\Delta_{D0}$]. It follows from (11) that the uniform insulator is absolutely unstable, since the energy $w_D(n)$ is a convex function of the density:

$$\frac{\partial^2 w_D}{\partial n^2} = \frac{\partial\mu}{\partial n} = -\frac{1}{2N(0)} < 0.$$

It is thus natural to assume that the system stratifies into two stable phases:

1) a uniform metal ($\Delta = 0$) with an energy density $w_M = n^2/4N(0)$ and a relative volume $\eta = V_M/V$;

2) a uniform undoped insulator ($\Delta = \Delta_{D0}, n = 0$) with an energy $w_D(0) = -N(0)(\Delta_{D0}^2/2)$ and a relative volume of $1 - \eta$.

If we ignore the surface component, we can write the energy of this state as

$$w_{PS}(\eta) = -(1-\eta)N(0)\frac{\Delta_{D0}{}^2}{2} + \eta\frac{1}{4N(0)}\left(\frac{n}{\eta}\right)^2. \tag{12}$$

From the condition $\partial w_{PS}(\eta)/\partial\eta = 0$ we find the equilibrium volume of the metallic phase, η_m:

$$\eta_m = \frac{n}{2^{1/2}N(0)\Delta_{D0}} \equiv \frac{n}{n_m}. \tag{13}$$

Since $\eta_m \leqslant 1$, this stratification occurs under the condition $n \leqslant n_m = \sqrt{2}N(0)\Delta_{D0}$. The energy of the stratified state is

$$w_{PS}(\eta_m)=-N(0)\Delta_{D0}^2/2+\mu_0 n,\qquad \mu_0=2^{-1/2}\Delta_{D0}, \tag{14}$$

where μ_0 is the chemical potential of the stratified state.

The linear concentration dependence of the energy of the stratified state, w_{PS}, is general in nature and corresponds to a change in the volume of the droplets with the doping, at a constant concentration of the particles in a droplet. When the number of particles in the system reaches $n = n_m$, the metallic phase fills the entire volume ($\eta_m = 1$). As n is increased further, the concentration dependence of the energy corresponds to the energy of a uniform metal, $w_M(n)$ (line I in Fig. 1 at $n > n_m$). It can be seen from Fig. 1 that the energy of a system stratified as described above [see (14)] corresponds to the tangent to the function $w_M(n) = n^2/[4N(0)]$, which emerges from the point $-N(0)(\Delta_{Do}^2/2)$ at $n = 0$ (line II in Fig. 1).

We know that a stratification does not occur in the case $D = 1$. The ground state of the system corresponds to a periodic soliton lattice.[15] The formal reason for this result is that the polarization operator in the zero-sound channel, $\Pi(q)$, has a logarithmic singularity at $q = 2p_F$. This singularity is responsible for an instability with respect to the formation of a superstructure with this period. The concentration dependence of the energy of the soliton lattice which arises at small values of n starts from the point $N(0)(\Delta_{Do}^2/2)$ and is linear in the number of particles (the slope of this line as $n \to 0$ corresponds to the energy of an isolated soliton, $E_s^{D=1} = (2/\Pi)\Delta_{Do}$).[15] As n increases, this function remains at all times below lines II and I in Fig. 1, which correspond to stratified state (14) and to a uniform metal, respectively. This function has a positive second derivative, which indicates a repulsion of the solitons and a stability of the periodic superstructure at any concentration.

The appearance of even a slight deviation from a one-dimensional nature smears out the singularity in the polarization operator at all filling levels which do not correspond to exact nesting. As a result, the ground state at large values of n corresponds to a uniform metal. However, the maximum on the $\Pi(q)$ curve at $q \neq Q$ (instead of the "integrated" singularity) causes a phase transition (at the point $n = n^*$) as the concentration is reduced. This transition goes to a state with a periodic superstructure. A transition of this sort was first discussed in Refs. 18 and 19 in connection with the appearance of a nonuniform state of a superconductor with an internal magnetic field. That case is formally equivalent to an isotropic model with nesting and a given value of μ.

The energy of this periodic phase, $W_{SL}(n)$, can be calculated by expansion in $(n^* - n)/n^*$ near the transition point n^* (Ref. 19). It has a positive curvature (line III near the point III in Fig. 1). In general, the point n^* may lie above the point of a stratification into a uniform metal and a uniform insulator, i.e., n_m (this is what happens in the isotropic case). In such a case, the stratification described above does not occur, but if the curvature of the energy of the periodic superstructure which forms at $n < n^*$, i.e., $W_{SL}(n)$, changes sign with decreasing n, the system stratifies into an insulator and a phase with a superlattice. Since the solution is formed in the limit $n \to 0$ because of the appearance of distinct, self-localized states and an interaction among them, the negative value of $\partial^2 W_{SL}/\partial n^2$ corresponds to an attraction. This attraction leads to a stratification.

As $n \to 0$, the energy of the periodic structure is the sum of the energies of the individual solitons:

$$W_{SL}\approx -N(0)\Delta_{D0}^2/2+E_S n,\quad n\to 0. \tag{15}$$

It can be seen from Fig. 1 that there exists a critical slope E_S^c of the $W_{SL}(n \to 0)$ curve: If $E_S > E_S^c$, then a necessary condition for a smooth joining of the known asymptotic expressions for the function $W_{SL}(n)$ as $n \to n^*$ and $n \to 0$ [see (12)] is that there be a point $n_c < n^*$ such that at $n < n_c$ the condition $\partial^2 W_{SL}(n)/\partial n^2 < 0$ holds. If the condition $n^* \geqslant n_m$ holds, then

$$E_S^c<\mu_0=2^{-1/2}\Delta_{D0}. \tag{16}$$

The following is then clearly a sufficient condition for stratification of the system:

$$E_S\geqslant\mu_0=2^{-1/2}\Delta_{D0}. \tag{17}$$

Line III in Fig. 1 shows a qualitative plot of the n dependence of the energy of the periodic structure under condition (17). The energy of the system after it has stratified into an insulator and a metal with a superlattice corresponds to the tangent to line III (line IV in Fig. 1).

These arguments thus make it possible to analyze the stability of the periodic solution with respect to phase stratification simply by calculating the energy of one self-localized state, E_S, and by testing condition (17); it is not at all necessary to go into the difficult multisoliton problem.

To calculate the energy of the self-localized state in a multidimensional system with energy (5), we use a method like that proposed in Ref. 20 for finding the energy of a soliton in the case $D = 1$.

The energy of one soliton [which determines the coefficient of the term in (15) which is linear in n] is found as half the formation energy of two domain walls separated by a large distance, divided by the number of states in the transverse band:

$$E_S=\frac{1}{\nu}\left\{\Sigma(E-E^{(0)})+\frac{L^{D-1}}{g}\int_{-\infty}^{\infty}(\Delta^2(x)-\Delta_{D0}^2)\,dx\right\}, \tag{18}$$

where

$$E^{(0)}=(v_{\mathbf{k}_\perp}^2k_x^2+\Delta_{D0}^2)^{1/2}.$$

The discrete spectrum and the phase shifts in the continuous spectrum, which determine the change in the density of states, are found from the second-order equation for one of the functions in (6), with periodic boundary conditions:

$$\begin{gathered}-\frac{d^2}{d\xi^2}\varphi_{\mathbf{k}_\perp}(\xi)+\left\{W^2(v_{\mathbf{k}_\perp}\xi)-\frac{d}{d\xi}W(v_{\mathbf{k}_\perp}\xi)\right\}\varphi_{\mathbf{k}_\perp}(\xi)\\ =(p_{\mathbf{k}_\perp}^2+1)\varphi_{\mathbf{k}_\perp}(\xi),\\ W(\pm\infty)=\pm1,\end{gathered} \tag{19}$$

where

$$E^2=\Delta_{D0}^2(p_{\mathbf{k}_\perp}^2+1),\qquad \xi=\frac{\Delta_{D0}x}{v_{\mathbf{k}_\perp}},\qquad W(v_{\mathbf{k}_\perp}\xi)=\frac{\Delta(x)}{\Delta_{D0}}. \tag{20}$$

We make use of the circumstance that the potential in the Schrödinger equation can be reconstructed from scattering data,[21] and we use the set of scattering data for problem (19) to express both terms in (18).

By virtue of the supersymmetry of the potential in (19), there is a zero mode

$$E_0^2=\Delta_{D0}^2(1-p_0^2)=0. \tag{21a}$$

in the discrete spectrum of all the equations (for any value of $v_{\mathbf{k}_\perp}$). We further assume that for each point $\mathbf{k}_\perp$ there are $M_{\mathbf{k}_\perp}$ discrete levels

$$E_{\mathbf{k}_\perp l}=\Delta_{D0}^2(1-p_{\mathbf{k}_\perp l}^2),\quad l=1\ldots M_{\mathbf{k}_\perp}. \tag{21b}$$

Denoting the phase shift in the states of the continuous spectrum by $\delta_{\mathbf{k}_\perp}(p)$ and using (21a) and (21b), we find the following result from (18) (by analogy with Ref. 19):

$$\begin{aligned}E_S=\Delta_{D0}\frac{1}{\nu}\left(\frac{L}{2\pi}\right)^{D-1}\int d\mathbf{k}_\perp\\ \times\Bigg\{-2\sum_{l=1}^{M_{\mathbf{k}_\perp}}(1-p_{\mathbf{k}_\perp l})^{1/2}+2M_{\mathbf{k}_\perp}+1\\ -\frac{2}{\pi}\int_0^{\tilde{\omega}/\Delta_{D0}}\delta_{\mathbf{k}_\perp}(p)\frac{d}{dp}(p^2+1)^{1/2}dp\Bigg\}\\ +\frac{L^{D-1}}{\nu g}\int_{-\infty}^{\infty}(\Delta^2(x)-\Delta_{D0}^2)\,dx.\end{aligned} \tag{22}$$

The phase shift can be written as

$$\delta_{\mathbf{k}_\perp}(p)=\arg a_{\mathbf{k}_\perp}(p)+\operatorname{arctg}\frac{1}{p},$$

where $a_{\mathbf{k}_\perp}(p)$ is the coefficient in the asymptotic expression for the Jost solutions in the presence of one soliton:

$$\varphi_{\xi\to\infty}\approx e^{ip\xi},\quad \varphi_{\xi\to-\infty}\approx a(p)e^{ip\xi}+b(p)e^{-ip\xi},$$
$$|a(p)|^2-|b(p)|^2=1,\quad |a(p)|^2=(1-|r(p)|^2)^{-1}.$$

Here $r(p)$ is a reflection coefficient.

We then find[21]

$$\begin{aligned}\delta_{\mathbf{k}_\perp}(p)=-\operatorname{arctg}\frac{1}{p}-2\sum_{l=1}^{M_{\mathbf{k}_\perp}}\operatorname{arctg}\frac{p_{\mathbf{k}_\perp l}}{p}\\ -\int_{-\infty}^{\infty}\frac{\ln|a_{\mathbf{k}_\perp}(q)|}{q-p}\frac{dq}{\pi}.\end{aligned} \tag{23}$$

Following Ref. 20, we express the last term in (22) in terms of the scattering data:

$$J\equiv\int_{-\infty}^{\infty}(\Delta^2(x)-\Delta_{D0}^2)\,dx=\Delta_{D0}v_{\mathbf{k}'_\perp}\{-2I_{\mathbf{k}'_\perp 1}+2\},$$

where

$$I_{\mathbf{k}'_\perp 1}=-\frac{1}{2}\int_{-\infty}^{\infty}u_{\mathbf{k}'_\perp}(\xi)\,d\xi$$

is one of the integrals of motion of the Korteweg-de Vries equation, and

$$u_{\mathbf{k}_\perp}(\xi)=W^2(v_{\mathbf{k}_\perp}\xi)-\frac{d}{d\xi}W(v_{\mathbf{k}_\perp}\xi)-1 \tag{24}$$

is the potential in Schrödinger equation (19). Using the explicit expressions for the integrals of motion in terms of the scattering data,[21] we find

$$\begin{aligned}J\equiv\int_{-\infty}^{\infty}(\Delta^2(x)-\Delta_{D0}^2)\,dx=2\Delta_{D0}v_{\mathbf{k}'_\perp}\\ \times\left\{-1-2\sum_{l=1}^{M_{\mathbf{k}_\perp}}p_{\mathbf{k}'_\perp l}+\int_{-\infty}^{\infty}\ln|a_{\mathbf{k}'_\perp}(q)|\frac{dq}{\pi}\right\}.\end{aligned} \tag{25}$$

By definition, J in (25) is independent of $\mathbf{k}_\perp$. Using the representation for $1/g$ in terms of the self-consistency equation in the uniform case, we then find

$$\begin{aligned}\frac{L^{D-1}}{g}J=2\Delta_{D0}v_{\mathbf{k}'_\perp}\left\{-1-2\sum_{l=1}^{M_{\mathbf{k}'_\perp}}p_{\mathbf{k}'_\perp l}+\int_{-\infty}^{\infty}\ln|a_{\mathbf{k}'_\perp}(q)|\frac{dq}{\pi}\right\}\\ \times\frac{1}{\pi}\left(\frac{L}{2\pi}\right)^{D-1}\int\frac{dk_\perp}{v_{\mathbf{k}_\perp}}\int_0^{\tilde{\omega}/\Delta_{D0}}\frac{dp}{(p^2+1)^{1/2}}\\ =\nu\Delta_{D0}\Big\langle\frac{2}{\pi}\Big(-1-2\sum_{i=1}^{M_{\mathbf{k}_\perp}}p_{\mathbf{k}_\perp l}\\ +\int_{-\infty}^{\infty}\ln|a_{\mathbf{k}_\perp}(q)|\frac{dq}{\pi}\Big)\int_0^{\tilde{\omega}/\Delta_{D0}}\frac{dp}{(p^2+1)^{1/2}}\Big\rangle.\end{aligned} \tag{26}$$

Using (23) and (26), we can put (22) in the form

$$E_S=\frac{2}{\pi}\Delta_{D0}(1+\langle\Phi(v_{\mathbf{k}_\perp})\rangle), \tag{27}$$

$$\begin{aligned}\Phi(v_{\mathbf{k}_\perp})=\int_0^{\infty}\frac{q}{(q^2+1)^{1/2}}\ln\frac{(q^2+1)^{1/2}+q}{(q^2+1)^{1/2}-q}\ln|a_{\mathbf{k}_\perp}(q)|\frac{dq}{\pi}\\ +2\sum_{l=1}^{M_{\mathbf{k}_\perp}}\left\{p_{\mathbf{k}_\perp l}-[1-p_{\mathbf{k}_\perp l}^2]^{1/2}\left[\frac{\pi}{2}-\operatorname{arctg}\frac{(1-p_{\mathbf{k}_\perp l}^2)^{1/2}}{p_{\mathbf{k}_\perp l}}\right]\right\}.\end{aligned} \tag{28}$$

The first term in (27) is the energy of a soliton for $D=1$:

$$E_S^{D=1}=2\Delta_{D0}/\pi.$$

The expression for E_S in (27) is a functional with respect to the scattering data at some single point $\mathbf{k}_\perp$, since the quantities $|a_{\mathbf{k}_\perp}(q)|$, $M_{\mathbf{k}_\perp}$, and $p_{\mathbf{k}_\perp l}$, for the various values of $\mathbf{k}_\perp$ are unambiguously related by virtue of the coupling of the potentials in (24). This relationship cannot be determined for the general case, but it is possible to advance the following arguments, which indicate the form of the exact solution.

Both terms in $\Phi(v)$ in (28) are positive or zero, so we have $\Phi(v)\geqslant 0$. The asymptotic expressions for $\Phi(v)$ do not depend on the particular trial function $W(\xi)$. To demonstrate the point, we assume that the potential $W(\xi)$ has a characteristic width v_0. As $v\to\infty$, we have $W(v\xi)\to\operatorname{sign}(\xi)$ $[u_v(\xi)\to 2\delta(\xi)]$. For $\Phi(v)$ we thus have

$$\lim_{v\to\infty} \Phi(v) = \pi/2 - 1.$$

As $v\to 0$, we find a potential $u_v(\xi)$ from (24) with a depth ~ 1 and a width which goes off to ∞. In this case we have

$$|a_v(q)|\to 1, \quad M_v\to\infty.$$

It then follows from (28) that as $v\to 0$ the function $\Phi(v)$ goes off to infinity by a power law. In addition, $\Phi(v)$ vanishes in only a single case: $M_v = 0$, $|a_v(q)| = 1$. This case corresponds to a reflectionless potential with one level (a zero mode):

$$W(v\xi) = \operatorname{th}\xi.$$

Figure 2 shows the function $\Phi_0(v)$ for the potential $W_0(\xi) = \operatorname{th}\xi/v_0$. According to the discussion above, $\Phi_0(v)$ touches the abscissa at the point $v = v_0$. In contrast, the functions $\Phi(v)$ for any other potential which has the same asymptotic behavior never vanish $[\Phi(v) > 0]$.

These arguments indicate that the minimum of E_S is apparently realized in the case of the potential

$$W_0(v_{\mathbf{k}_\perp}\xi) = \operatorname{th}\left(\frac{v_{\mathbf{k}_\perp}}{v_0}\xi\right). \tag{29}$$

The minimization in (27) then reduces to solving the algebraic equation

$$\frac{d}{dv_0}\langle\Phi_0(v_{\mathbf{k}_\perp})\rangle = 0 \tag{30}$$

where $\Phi_0(v_{\mathbf{k}_\perp})$ in (28) is now known explicitly. The reason is that for $W_0(v_{\mathbf{k}_\perp}\xi)$ as in (29) we have

$$|a_{\mathbf{k}_\perp}(q)|^2 = 1 - \frac{\sin^2 \pi v_0/v_{\mathbf{k}_\perp}}{\operatorname{sh}\pi q},$$

$$p^2_{\mathbf{k}_\perp l} = \frac{v_{\mathbf{k}_\perp}}{v_0}\left(1 - \frac{v_{\mathbf{k}_\perp}}{v_0} l\right), \quad l < \frac{v_0}{v_{\mathbf{k}_\perp}}.$$

We now write stratification condition (17) as follows, where we are using (27):

$$\langle\Phi_0(v_{\mathbf{k}_\perp})\rangle \geqslant 2^{-1/2}\pi - 1 \approx 0{,}11. \tag{31}$$

That (31) can hold in principle is clear simply from the asymptotic behavior of the function $\Phi(v)$:$\Phi(v\to 0)\to\infty$, $\Phi(\infty)\to\pi/2 - 1$. This behavior is independent of the particular odd function $\Delta(x)$ which satisfies the condition $|\Delta(\pm\infty)| = \Delta_{D_0}$. Furthermore, the small value of the quantity on the right side of (31) and the fact that condition (17) overestimates the value of the critical slope E_S^c raise the hope that a stratification would occur in the case of a fairly weak transverse dispersion.

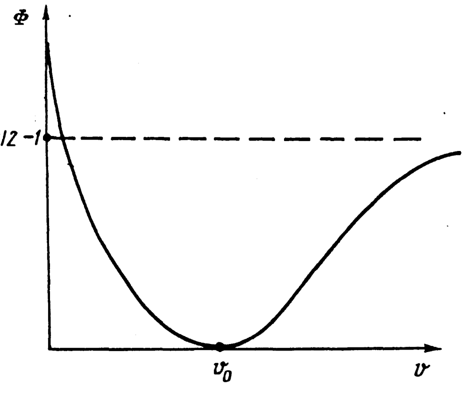

FIG. 2. The $\Phi_0(v)$ dependence in (28) for the potential $W_0(\xi)$ is $\tanh(\xi/v_0)$.

Consequently, if the deviation of a system with nesting from a one-dimensional nature is such that condition (31) holds, there will be a stratification region on the phase diagram. Figure 3a is a qualitative sketch of the phase diagram of a system of this sort.

2. We turn now to a mathematically simpler model whose behavior is similar to that of the system with nesting discussed above. This model can be found from the model with congruent sections of the Fermi surface by taking account of a commensurate potential Δ_{DS}, which gives rise to a seed gap in the spectrum. The appearance of a commensurate lattice potential is described by adding a term

$$\hat{H}_S = -\int \frac{2\Delta(\mathbf{r})\Delta_{DS}}{g}\,d\mathbf{r}, \tag{32}$$

to Hamiltonian (2). This term gives rise to a source in the self-consistency equation for the parameter $\Delta(\mathbf{r})$. The latter is found from the condition

$$\frac{\delta\langle\hat{H}+\hat{H}_S\rangle}{\delta\Delta(\mathbf{r})} = 0.$$

An integration of the self-consistency equation in the uniform case leads to

$$\frac{\Delta_{DS}}{N(0)g} = \Delta\ln\frac{\tilde{n} + (\Delta^2+\tilde{n}^2)^{1/2}}{\Delta_{D0}}. \tag{33}$$

Differentiating the expression for the chemical potential $\mu = \sqrt{\Delta^2 + \tilde{n}^2}$, and using (33), we find

$$\frac{\partial\mu}{\partial\tilde{n}} = -\frac{\Delta^3 - (1/N(0)g)\Delta_{DS}\tilde{n}(\tilde{n}+\mu)}{\Delta^3 + (1/N(0)g)\Delta_{DS}\mu(\tilde{n}+\mu)}. \tag{34}$$

It follows that for any Δ_{DS} we can find an $\tilde{n}$ for which the condition $\partial\mu/\partial n > 0$ holds and for which a uniform phase is stable. In the limit

$$\frac{1}{N(0)g}\frac{\Delta_{DS}}{\Delta_0} \gg 1$$

[here $\Delta_0 = \Delta(n=0)$], the sign of $\partial\mu/\partial n$ changes at

$$\frac{\tilde{n}}{\Delta_0} \approx N(0)g\frac{\Delta_0}{\Delta_{DS}} \approx \ln^{-1}\frac{\Delta_0}{\Delta_{DS}} \ll 1. \tag{35}$$

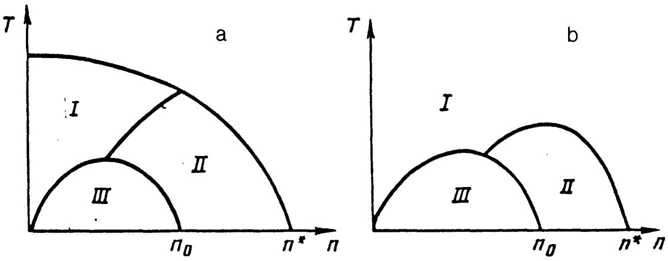

FIG. 3. (T, n) phase diagrams. a—For a system with nesting. b—For a model with a source of an insulating gap. Region I—Uniform insulator; II—phase with a periodic structure; III—stratified state.

Because of the small parameter in (35), we can restrict the discussion to a single band in the phase which has become an insulating phase. We seek a solution for the insulating gap in the form

$$\Delta(\mathbf{r})=\Delta_0+d(\mathbf{r}),\qquad d(\mathbf{r})/\Delta_0\ll 1. \tag{36}$$

We diagonalize the uniform part of the Hamiltonian $\hat{H}+\hat{H}_S$ by means of a standard canonical transformation. Assuming that the length scales for the spatial variations in the system are on the order of v_F/d, we carry out an expansion in the parameter $d/\Delta_0\ll 1$, retaining the first nonvanishing terms, as is done in the effective-mass method. As a result we find the following effective Hamiltonian for quasiparticles in the conduction band (or, in the case $\mu<0$, in the valence band):

$$\hat{H}_{eff}=\int d\mathbf{r}\left\{\sum_\sigma \varphi_\sigma^+(\mathbf{r})\left[\frac{\xi^2(\nabla)}{2\Delta_0}-\tilde{\mu}+d(\mathbf{r})\right]\varphi_\sigma(\mathbf{r})+\frac{d^2(\mathbf{r})}{\tilde{n}_c}\right\}, \tag{37}$$

The operator $\varphi_\sigma^+(\mathbf{r})$ creates a quasiparticle; $\tilde{\mu}=\mu-\Delta_0$ is the chemical potential reckoned from the edge of the band at $n=0$; and we have introduced

$$\tilde{n}_c=g\frac{\Delta_0}{\Delta_{DS}},\qquad N(0)\tilde{n}_c\ll 1.$$

Varying average Hamiltonian (37), we find the self-consistency equation

$$d(\mathbf{r})=-{}^1/_2\tilde{n}_c\sum_\sigma\langle\varphi_\sigma^+(\mathbf{r})\varphi_\sigma(\mathbf{r})\rangle. \tag{38}$$

The equation which determines the number of particles is

$$n(\mathbf{r})=\sum_\sigma\langle\varphi_\sigma^+(\mathbf{r})\varphi_\sigma(\mathbf{r})\rangle. \tag{39}$$

A comparison of (38) and (39) shows that the self-consistent potential which determines the position of the edge of the allowed band is

$$d(\mathbf{r})=-{}^1/_2\tilde{n}_c n(\mathbf{r}). \tag{40}$$

Before we go into a detailed study of the model which we have constructed, (37), we note that this model could be analyzed without any direct linkage with systems which have a Fermi-surface nesting. The model phenomenologically describes the following physical situation. There is a peak in the density of states (for simplicity, we assume a one-dimensional peak) at the edge of the conduction band. If the position of the edge depends on the doping [as $n\to 0$, a linear dependence as in (40) is natural], a stratification can occur in a system of this sort, for the same physical reasons as in the nesting model (see the Introduction).

Taking an average of (37), we find the energy functional

$$W=\sum_{E<\mu}E+\frac{1}{\tilde{n}_c}\int d^2(\mathbf{r})d\mathbf{r}, \tag{41}$$

where the eigenvalues E are the eigenvalues of the Schrödinger equation

$$-\frac{v_{\mathbf{k}_\perp}}{2\Delta_0}\frac{d^2}{dx^2}\varphi_{\mathbf{k}_\perp}(x)+d(x)\varphi_{\mathbf{k}_\perp}(x)=E\varphi_{\mathbf{k}_\perp}(x). \tag{42}$$

The seed dispersion relation $\xi(\mathbf{k})$ in (41) and (42) is of the form in (4), as before.

A calculation of the energy density in the uniform system ($d=\text{const}$) yields

$$w=\frac{1}{4}\left(\frac{n^3}{6\Delta_0N^2(0)}-\tilde{n}_cn^2\right). \tag{43}$$

From (43) we find an expression for $\partial\mu/\partial n$:

$$\frac{\partial\mu}{\partial n}=\frac{\partial^2w}{\partial n^2}=\frac{1}{2}\left(\frac{n}{2\Delta_0N^2(0)}-\tilde{n}_c\right). \tag{44}$$

In the case $n<2\Delta_0N^2(0)\tilde{n}_c$, the uniform state is unstable, and the system may stratify into a metallic phase with a relative volume η and an insulating phase with a relative volume $1-\eta$. As in (12) we write the energy of the state as

$$w_{PS}=\eta w\left(\frac{n}{\eta}\right) \tag{45}$$

Minimizing with respect to η, we find the condition

$$w\left(\frac{n}{\eta}\right)-\frac{n}{\eta}w'\left(\frac{n}{\eta}\right)=0. \tag{46}$$

Solving (46), using (43), we find the equilibrium volume of the metallic phase, η_m, and the concentration (n_m) below which stratification occurs:

$$\eta_m=\frac{1}{3}\frac{n}{\Delta_0N^2(0)\tilde{n}_c}=\frac{n}{n_m},\qquad n_m=3\Delta_0N^2(0)\tilde{n}_c. \tag{47}$$

As in (14), the energy of the stratified phase is linear in the concentration:

$$w_{PS}=\mu_0n,$$

$$\mu_0=-\frac{3}{2}\Delta_0\left(\frac{N(0)\tilde{n}_c}{2}\right)^2\equiv-\frac{3}{2\pi^2}\Delta_0\left(\frac{\nu\tilde{n}_c}{2L^{D-1}}\right)^2\langle v^{-1}\rangle^2. \tag{48}$$

In the expression in (48) for the chemical potential of the stratified state, μ_0, we have made use of the explicit expression for the density of states $N(0)$ from (10).

With $D=1$, Hamiltonian (37) corresponds to the Fröhlich model for a one-dimensional metal with an electron-phonon interaction. The ground state for this model is a periodic superstructure.[22] As in Sec. 1, the circumstance is associated with the congruence of the Fermi surface during doping. Because of the deviation from a one-dimensional situation [which stems from the $\mathbf{k}_\perp$ dependence of the mass in (42)], the uniform phase is stable at large values of n. It goes into a state with a superlattice at $n\leqslant n^*$.

As $n\to 0$, the energy of the periodic phase [as in (15)] is

$$W_{SL}=E_Sn.$$

For the general case $n^*>n_m$ [see (47)], we find the following condition for stratification into a phase with $n=0$ and a metallic phase with a periodic superstructure:

$$E_S\geqslant\mu_0. \tag{49}$$

We can show that even a slight transverse dispersion is sufficient to satisfy this condition.

Let us assume that the zeroth approximation corresponds to a dispersion-free transverse band: $v_{\mathbf{k}_\perp}^{(0)} = 1$.

Expressing the energy in (41) in terms of the scattering data of problem (42), and minimizing with respect to these data, we find that a one-soliton solution corresponds to

$$E^{(0)}=-\frac{\varkappa^{(0)2}}{2\Delta_0}=-\frac{1}{2}\Delta_0\left(\frac{\nu\tilde{n}_c}{2L^{D-1}}\right)^2, \qquad |a^{(0)}(q)|=1,$$
$$d^{(0)}(x)=-\frac{\varkappa^{(0)}/\Delta_0}{\mathrm{ch}^2\,\varkappa^{(0)}x}, \qquad E_S^{(0)}=-\frac{1}{6}\Delta_0\left(\frac{\nu\tilde{n}_c}{2L^{D-1}}\right). \tag{50}$$

We introduce a transverse dispersion:

$$v_{\mathbf{k}_\perp=0}=1, \quad v_{\mathbf{k}_\perp}\geqslant 1.$$

We seek the first perturbation-theory correction to the energy $E_S^{(0)}$ in (50). For the eigenvalues we find

$$E_{\mathbf{k}_\perp}=-\frac{\varkappa^{(0)2}}{2\Delta_0}\left[\frac{4}{(v_{\mathbf{k}_\perp}^2+8)^{1/2}+v_{\mathbf{k}_\perp}}\right]^2.$$

For the energy of the soliton we then have

$$E_S=E_S^{(0)}\left\langle 3\left[\frac{(v_{\mathbf{k}_\perp}^2+8)^{1/2}-v_{\mathbf{k}_\perp}}{2}\right]^2-2\right\rangle. \tag{51}$$

Under the condition for the applicability of a perturbation theory we have

$$1-\left\langle 3\left[\frac{(v_{\mathbf{k}_\perp}^2+8)^{1/2}-v_{\mathbf{k}_\perp}}{2}\right]^2-2\right\rangle\ll 1. \tag{52}$$

Comparing E_S from (51) with μ_0 from (48), we find from (49) a condition (on the transverse dispersion) under which stratification occurs:

$$\langle v_{\mathbf{k}_\perp}^{-1}\rangle\geqslant\left(\frac{\pi}{3}\right)^2\left\langle 3\left[\frac{(v_{\mathbf{k}_\perp}^2+8)^{1/2}-v_{\mathbf{k}_\perp}}{2}\right]^2-2\right\rangle. \tag{53}$$

Let us demonstrate that (53) and (52) can hold simultaneously in the particular case of a transverse dispersion. We assume that the relative phase volume in which we have $v_{\mathbf{k}_\perp}\neq 1$ (it has values $v>1$) is small: $\beta\ll 1$. Then (52) and (53) become, respectively,

$$3\beta\left\{1-\left[\frac{(v^2+8)^{1/2}-v}{2}\right]^2\right\}\ll 1$$

which is the condition for the applicability of a perturbation theory, and

$$3\beta\left\{1-\frac{6}{\pi}\frac{v-1}{v}-\left[\frac{(v^2+8)^{1/2}-v}{2}\right]^2\right\}\geqslant 1-\left(\frac{3}{\pi}\right)^2\approx 0{,}09$$

which is the stratification condition.

These conditions can hold simultaneously by virtue of the small quantity on the right side of the stratification condition [cf. (31)].

It has thus been shown that the introduction of a slight deviation from a one-dimensional situation gives rise to a stratification region in the phase diagram, as shown approximately in Fig. 3b.

We thus see that the common physical mechanism for the stratification in the nesting model and in the model in (37) results in similar phase diagrams in the two cases (Figs. 3a and 3b), except near the transition to a uniform insulating phase in Fig. 3a. Since we will be interested below in the region of T and n values far from the line of the insulating transition, the entire discussion below will be based on simple model (37). Specifically, the isotropic version of this model (Sec. 3) will be discussed, since it demonstrates most clearly the physical features associated with phase stratification.

3. PHASE DIAGRAM OF AN ISOTROPIC MODEL WITH A SOURCE

Let us consider the isotropic version of uniform Hamiltonian (37). We assume that the spectrum $\xi(\mathbf{k})$ in (37) is

$$\xi(\mathbf{k})=v_F(|\mathbf{k}|-k_F). \tag{54}$$

The density of states $N(0)$ in the seed phase is then

$$N(0)=\frac{k_F^2}{\pi v_F}.$$

instead of that in (10). At this point it is convenient to introduce some dimensionless variables: We express all energies in units of Δ_0, and we take n to be the concentration normalized by $n=\tilde{n}/\Delta_0$. Using (40), we then find from (37)

$$\tilde{H}_{eff}=\frac{H_{eff}}{2N(0)\Delta_0^2}=\int d\mathbf{r}$$
$$\times\left\{\frac{1}{2N(0)\Delta_0}\sum_\sigma\varphi_\sigma^+(r)\left[\frac{\xi^2(\nabla)}{2}-\mu+n_cn\right]\right.$$
$$\left.\times\,\varphi_\sigma(\mathbf{r})+\frac{1}{2}n_cn^2(\mathbf{r})\right\}, \tag{55}$$

where $n_c=N(0)\tilde{n}_c$.

To construct a (T, n) phase diagram and to find the region corresponding to stratification, we calculate the free energy of the uniform phase, $f_T(n)$. By definition we have

$$f_T(n)=\Omega_T(\mu)+\mu n,$$

where

$$\Omega_T(\mu)=\langle\tilde{H}_{eff}\rangle=-\frac{T}{N(0)\Delta_0}\int\frac{d\mathbf{k}}{(2\pi)^3}\ln\left[1+\exp\left(\frac{\mu'-\varepsilon_\mathbf{k}}{T}\right)\right]$$
$$+\frac{1}{2}n_cn^2, \tag{56}$$
$$\varepsilon_\mathbf{k}=\xi^2(\mathbf{k})/2, \quad \mu'=\mu+n_cn.$$

This system was studied above for the case $T=0$; stratification conditions (47) and the energy of the stratified state (48), were found. In terms of the new variables we find the following results from (47) and (48): For the energy of the stratified phase, F_0, we find

$$F_0(n)=\frac{w_{PS}}{2N(0)\Delta_0}=-\frac{3}{8}n_c^2n\equiv\mu_0n \tag{57}$$

and for the concentration (n_0) below which a stratification occurs we find

$$n_0=\frac{n_m}{2N(0)\Delta_0}=\frac{3}{2}n_c. \tag{58}$$

The boundary found here for the region in which a stratified state exists, (58) should be compared with the point n^* of the transition to the nonuniform periodic phase. For this purpose, we examine the coefficient $\alpha(q)$ of the term d_q^2 in the power-series expansion of the thermodynamic potential in d_q. The change in the sign of $\alpha(q)$ at $q\neq 0$ means an instability with respect to the formation of a periodic structure with this wave vector. The expansion of the thermodynamic potential is

$$\Omega(q)=\alpha(q)d_q^2+O(d^4), \tag{59}$$

$$\alpha(q)=\frac{1}{g}\frac{\Delta_{DS}}{\Delta_0}-\Pi(q),$$

where $\Pi(q)$ is a polarization operator. In model (55) with (54), we find the following expression for $\alpha(q)$:

$$\alpha(p)=\frac{N(0)}{n_c}\left\{1-\frac{3n_c}{2n}\gamma(p)\right\},$$

$$\gamma(p)=\frac{1}{3p}\int_0^p \ln\left|\frac{x+1}{x-1}\right|\frac{dx}{x},\qquad p=\frac{q}{2n}. \tag{60}$$

The function $\gamma(p)$ is less than one for all $p>0$ and has a maximum at the point $p^*\approx 1.14$, at which its value is $\gamma^*=\gamma(p^*)\approx 0.87$. It can be seen from (60) that α first vanishes at $n=n^*=\frac{3}{2}n_c\gamma^*\approx 1.3n_c$. This point corresponds to an instability with respect to the formation of a periodic structure with $q=q^*=2n^*p^*$.

Since $\gamma^*<1$, the critical concentration n^* associated with this instability is smaller than the value $n=n_0=(3/2)n_c$, at which a stratification of the system becomes favorable. In addition, it can be shown that at $T\neq 0$ the line of the transition to the phase with a periodic structure on the (T, n) phase diagram lies below the line of the first-order phase transition to a stratified state. In this case the system thus stratifies into a uniform insulator and a uniform metal with a concentration $n=n_0$. A positive value of the coefficient α_q at this concentration means that the surface energy is positive.

We now consider a nonzero temperature $T\neq 0$, and we construct a (T, n) phase diagram. From (56) we find the following asymptotic expressions in different limits in the parameter T/n^2. At $T/n^2\ll 1$ we find

$$f_T(n)\approx\frac{1}{6}n^3-\frac{1}{2}n_cn^2-\frac{\pi^2}{6}\frac{T^2}{n},$$

$$\mu(n)\approx\frac{1}{2}n^2-n_cn+\frac{\pi^2}{6}\frac{T^2}{n^2}, \tag{61}$$

and at $T/n^2\gg 1$ we find

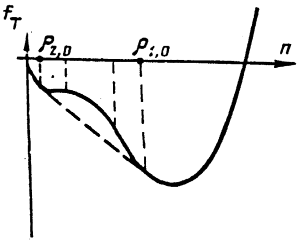

FIG. 4. Concentration dependence of the free energy for a model with a source. Solid line—Uniform state; dashed line—stratified state.

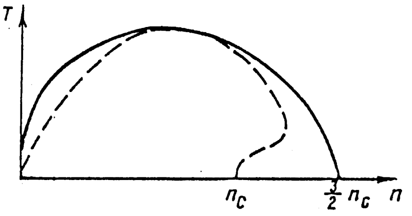

FIG. 5. Phase diagram of an isotropic model with a source. Solid line—Line of transition to a stratified state; dashed line—line of an absolute instability of the uniform phase $(\partial\mu/\partial n=0)$.

$$f_T(n)\approx-\frac{1}{2}n_cn^2-nT-nT\ln\frac{1}{n}\left(\frac{\pi T}{2}\right)^{1/2}+\frac{1}{2}n^2\left(\frac{T}{\pi}\right)^{1/2},$$

$$\mu(n)\approx-n_cn-T\ln\frac{1}{n}\left(\frac{\pi T}{2}\right)^{1/2}+n\left(\frac{T}{\pi}\right)^{1/2}. \tag{62}$$

Figure 4 shows the function $f_T(n)$ at a nonzero temperature. It can be seen from expression (62) for $\mu(n)$ that the condition $\partial\mu/\partial n>0$ holds at concentrations small in comparison with the thermal concentration, so the uniform state is stable. The meaning here is that the stratification should give rise to two equilibrium phases with a nonzero carrier density: an insulating phase (in which n is exponentially small) and a metallic phase (with $n>n_c$). The energy of the stratified state is thus

$$F_T(\eta)=\eta f_T\left(\frac{n_1}{\eta}\right)+(1-\eta)f_T\left(\frac{n-n_1}{1-\eta}\right). \tag{63}$$

Here η and n_1 are the relative volume and the number of particles in the metallic phase. From the condition for a minimum of the function F_T with respect to the variables η and n_1, at a given total number of particles, n, we find the equations

$$f_T'(\rho_1)=f_T'(\rho_2), \tag{64}$$

$$f_T(\rho_1)-\rho_1f_T'(\rho_1)=f_T(\rho_2)-\rho_2f_T'(\rho_2),$$

where $\rho_1=n_1/\eta$ and $\rho_2=(n-n_1)/(1-\eta)$ are the particle densities in the separate phases. The first equation in (64) corresponds to the equality of the chemical potentials in the two phases. Together, these equations determine those points ($\rho_{1,0}$ and $\rho_{2,0}$) at which the function $f_T(\rho)$ has a common tangent. In the concentration interval

$$\rho_{2,0}(T)<n<\rho_{1,0}(T) \tag{65}$$

the energy of the stratified state is lower than that of a uniform phase. Figure 4 shows the energy of the nonuniform state as a function of n. With increasing T, the points $\rho_{1,0}$ and $\rho_{2,0}$ move closer together, and at a certain temperature they merge. As the temperature is raised further we have $\partial\mu/\partial n>0$. At sufficiently low temperatures $(T/n^2\ll 1)$ we have

$$\frac{\rho_{1,0}^2}{T}\gg 1,\qquad\frac{\rho_{2,0}^2}{T}\ll 1.$$

We can thus use asymptotic expressions (61) and (62) in solving equations (64). As a result we find

$$\begin{aligned} \rho_{1,0} &\approx \frac{3}{2} n_c - \frac{8\pi^2}{27} \frac{T^2}{n_c^3}, \\ \rho_{2,0} &\approx \left(\frac{\pi T}{2}\right)^{1/2} \exp\left(\frac{\mu_0}{T}\right), \\ \mu_0(T) &\approx -\frac{3}{8} n_c^2 - \frac{2\pi^2}{27} \frac{T^2}{n_c^2}. \end{aligned} \tag{66}$$

We can use these results to construct a phase diagram of the system in the coordinates (T, n) (Fig. 5).

We have been discussing the simplest version of phase stratification. In principle, we should allow for the possibility that the nature of the insulating order changes upon doping. In different concentration regions, different types of stratified states may thus arise, with metallic and insulating regions with different properties. In this case a plot of several parameters of the system (in particular, the transition temperature T_c) versus the doping level should have a series of plateaus corresponding to different types of insulating order. The presence of these plateaus is in this case a consequence of a pinning of the chemical potential in the stratified state. This is apparently the situation which prevails in $YBa_2Cu_3O_{7-x}$. Furthermore, in this model there is the possibility of a stratification into two (or more) metallic phases. The stability of the phase with the lower concentration in this case may result from a smearing of the peak in the density of states at the edge of the filling band. We then have $\partial\mu/\partial n > 0$ at small values of n, but this derivative changes sign as the concentration is raised. The change in the amplitude of the source in (32) upon doping may also lead to stability of a metallic phase with a lower density.

4. SPACE CHARGE AND STRUCTURE OF THE STRATIFIED STATE

Let us examine the structure of the stratified state. In the region in which the uniform phase is stable ($\Pi(q) < 1/g$, $\alpha_q > 0$) the surface energy is positive, and mobile carriers in the metallic phase would tend to merge into a common droplet. This merging would be opposed by the Coulomb interaction between the space-charge regions which would form in the process. Let us first calculate the Coulomb energy E_C of negatively charged spherical droplets against the background of a positive charge. We write

$$E_C = W_b + W_d + W_{bd}. \tag{67}$$

The first and second terms here are the Coulomb energies of the background and of the droplets, respectively, and the last term is the energy of the background-droplet interaction. We denote by V the volume of the system, by V_d the volume of the droplets ($V_d/V < 1$), by $\rho = en$ the charge density of the background, and by $\rho_0 = \rho v/v_d = en_0$ the density of the negative charge in the droplets. We then have

$$W_b = \frac{1}{2} \int \rho \varphi_b(\mathbf{r}) d\mathbf{r}, \tag{68}$$

where $\varphi_b = \int_V \rho d\mathbf{r}'/(\varepsilon|\mathbf{r} - \mathbf{r}'|)$ is the potential of the background, and ε is the dielectric constant of the background. We also have

$$\begin{aligned} W_{bd} &= -\frac{1}{2} \int \rho_d(\mathbf{r}) \varphi_b(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \rho \varphi_d(\mathbf{r}) d\mathbf{r} \\ &= -\int \sum_{i=1}^{p} \rho_i(\mathbf{r} - \mathbf{r}_i) \varphi_{bd}(\mathbf{r}) d\mathbf{r}, \end{aligned} \tag{69}$$

where $\rho_i = \rho_0 \theta(r - R_i)$ is the charge density inside a droplet, $R_i = ((3/4\pi)(V_d/p))^{1/3}$ is the radius of a droplet, and $\varphi_k(\mathbf{r}) = \int \rho_k(\mathbf{r}') d\mathbf{r}'/(\varepsilon|\mathbf{r} - \mathbf{r}'|) = \int \Sigma_{i=1}^{p} \times [\rho_i(\mathbf{r}_i - \mathbf{r}')/\varepsilon|\mathbf{r} - \mathbf{r}'|] d\mathbf{r}'$ is the potential of the droplets. Finally, we have

$$W_d = \frac{1}{2} \int \rho_d(\mathbf{r}) \varphi_k(\mathbf{r}) d\mathbf{r} = \frac{1}{2} \int \sum_{i=1}^{p} \rho_i(\mathbf{r} - \mathbf{r}_i) \varphi_d(\mathbf{r}) d\mathbf{r}. \tag{70}$$

In the limit $p \to \infty$, the sums in (69) and (70) become integrals, and E_C vanishes by virtue of the electrical neutrality of the system. However, the increase in the number of droplets, p, is limited by the surface energy. Let us calculate E_C in the first nonvanishing order in $1/p$. Assuming that the lattice of droplets has a cubic symmetry, we find from (70) and (69)

$$\begin{aligned} W_d &= W_b + \frac{\pi}{3} \frac{1}{\varepsilon} \rho(\rho + \rho_0) V^{5/3} \left\{1 - \frac{4\pi}{5} \frac{\rho_0}{\rho} \left(\frac{3}{4\pi} \frac{V_d}{V}\right)^{5/3}\right\} \frac{1}{p^{2/3}}, \\ W_d &= -2W_b - \frac{2\pi}{3} \frac{1}{\varepsilon} \rho^2 V^{5/3} \left\{1 - \frac{4\pi}{5} \frac{\rho_0}{\rho} \left(\frac{3}{4\pi} \frac{V_d}{V}\right)^{5/3}\right\} \frac{1}{p^{2/3}}. \end{aligned}$$

Finally, for the Coulomb energy of p negatively charged droplets, each having a charge density $\rho_0 = en_0$, against a positive background $\rho = en$, we find

$$\begin{aligned} E_C^{(-)} &= \frac{\pi}{3} \frac{e^2}{\varepsilon} n(n_0 - n) \\ &\times \left\{1 - \frac{3}{5} \left(\frac{3}{4\pi} \frac{n}{n_0}\right)^{2/3}\right\} \frac{V^{5/3}}{p^{2/3}} = \tau(n, n_0) \frac{V^{5/3}}{p^{2/3}}. \end{aligned} \tag{71}$$

If, on the other hand, the background breaks up into droplets (i.e., if uniformly distributed insulating droplets with a total volume $V - V_d$ appear), the expression for the Coulomb energy of the system, $E_C^{(+)}$, is found from (71) by making the substitution $n \to n_0 - n$. A comparison of the expressions for $E^{(-)}$ and $E^{(+)}$ shows that, as n decreases from n_0, a lattice of voids with a positive charge first appears. At $n \leqslant n_0/2$, the formation of a structure of isolated droplets against a positive background becomes more favorable.

Let us calculate the equilibrium number of droplets, p, taking the surface energy E_{surf} into account. The expression for E_{surf} is

$$E_s = \sum_{i=1}^{p} \sigma v_i^{2/3} = \sigma \left(\frac{n}{n_0}\right)^{2/3} V^{2/3} p^{1/3}. \tag{72}$$

Here $v_i = V_d/p = (V/p)(n/n_0)$ is the volume of a droplet, and the surface tension σ satisfies $\sigma \sim u_{\text{surf}} l$, where u_{surf} is the energy density inside the transition layer, and l is the thickness of this layer (the boundary of the droplet). From the condition for a minimum of the total energy $E = E_C + E_{\text{surf}}$ we find

$$p = 2 \frac{\tau(n, n_0)}{(n/n_0)^{2/3} \sigma} V \sim \frac{e^2 n_0^2}{\varepsilon \sigma} V. \tag{73}$$

The function $\tau(n,n_0)$ is given in (71). To estimate the droplet radius $R_i \sim (V/p)^{1/3}$, we assume that the energy density inside the transition layer, u_{surf}, is on the order of the bulk energy: $u_{\text{surf}} \sim \mu_0 n_0$. We then have $\sigma \sim \mu_0 n_0 l$ and

$$R_i \sim \left(\frac{\mu_0 l \varepsilon}{e^2 n_0}\right)^{1/3}. \tag{74}$$

The quantity l is on the order of the insulating correlation length of the model of (55), $l \sim (v_F/\Delta_0)(1/n_c)$, where v_F is the Fermi velocity in the two-band model, (2), which is the starting point for (55). If we are to treat the droplet as a macroscopically uniform volume, we must satisfy the condition

$$\frac{l}{R_i} \sim \left[\frac{e^2}{\varepsilon v_F}\left(\frac{E_F}{\Delta_0}\right)^2 n_c^{-3}\right]^{1/3} \ll 1. \tag{75}$$

In deriving (75) we used the estimates $n_0 \sim N(0)\Delta_0 n_c$ and $\mu_0 \sim \Delta_0 n_c^2$. The static dielectric constant which appears in the expression for the droplet radius, (74), and also in condition (75) is large in the layered perovskite ceramics, even in the insulating phase. Doping will cause a further increase in the screening, not only because of the mobile carriers in the band but also because of a redistribution of the charge in the localized states which serve as sources of mobile charge carriers.

Let us estimate the ratios of the surface energy and the Coulomb energy, on the one hand, to the bulk energy, on the other

$$\frac{E_C+E_s}{\mu_0 n V} \sim \left(\frac{e^2 n_0^2 \sigma^2}{\varepsilon \mu_0^3 n_0}\right)^{1/3} \sim \left(\frac{e^2 n_0 l}{\mu_0}\right)^{1/3} \sim \frac{e^2 n_0 R_i}{\mu_0} \sim \frac{l}{R_i}. \tag{76}$$

Under condition (70), the bulk properties of a droplet are thus determined completely by the microscopic correlation energy (63). The Coulomb energy of the space charge and the surface energy, which determine the size and relative arrangement of the droplets, can be treated independently. We can show that the same parameter (l/R_i) determines the extent to which the charge distribution inside a droplet is nonuniform. From the condition that the total force acting on a charge at the given point vanish, we find the relation

$$\frac{\partial \mu}{\partial n}\frac{\partial}{\partial r}\delta n(r) = \frac{4}{3}\pi e^2\left[(n_0-n)r + \frac{3}{r^2}\int_0^r \delta n(x) x^2\,dx\right]. \tag{77}$$

Here $\delta n(r)$ is the deviation of the distribution of the negative charge in a droplet from a uniform distribution. The term on the left side of (77) is the force which arises because of the increase in bulk energy (55) upon the appearance of a nonuniformity of the order parameter. The terms on the right side describe the forces exerted on the charge by the background and by the moving negative charge in the droplet. We know that the net charge on a metal sphere concentrates at the surface. This classical solution follows directly from (77) when we set the left side equal to zero. If the bulk energy is instead large in comparison with the Coulomb energy from (77), we find the following expression for $\delta n(r)$:

$$\frac{\delta n(r)}{n_0} = \frac{4\pi}{3}\frac{e^2 R_i}{\partial\mu/\partial n}\left(1-\frac{n}{n_0}\right)\left[\left(\frac{r}{R_i}\right)^2 - \frac{3}{5}\right] \sim \frac{l}{R_i}. \tag{78}$$

Expression (78) means that under condition (75) a nonuniform charge distribution and the associated nonuniformity of the order parameter are unfavorable from the energy standpoint, and the charge in a droplet can be assumed uniform.

5. STRATIFICATION INTO PHASES AND SUPERCONDUCTING DROPLETS

Under what conditions does a stratified state arise in the presence of superconductivity? The effective Hamiltonian (55) of the one-band model, supplemented with terms to describe the superconducting pairing, is

$$\mathcal{H}_{eff} = \sum_\sigma \int d\mathbf{r}\left\{\frac{1}{2N(0)\Delta_0}\left[\varphi_\sigma^+(\mathbf{r})\left(\frac{\xi^2(\nabla)}{2} - \mu - n_c n(\mathbf{r})\right)\right.\right.$$
$$\left.\left.\cdot\varphi_\sigma(\mathbf{r}) + \delta(\mathbf{r})\varphi_\uparrow^+(\mathbf{r})\varphi_\downarrow^+(\mathbf{r}) + \text{h.c.}\right] + \frac{1}{2}n_c n^2(\mathbf{r}) - \frac{1}{2}\frac{\delta^2(\mathbf{r})}{\lambda}\right\}. \tag{79}$$

Here $\delta(\mathbf{r})$ is the superconducting order parameter, normalized to the size of the insulating gap, and λ is the magnitude of the coupling constant in the Cooper channel. The self-consistency equation for $\delta(r)$ is written in the usual way:

$$\delta(\mathbf{r}) = \frac{\lambda}{N(0)\Delta_0}\langle\varphi_\uparrow(\mathbf{r})\varphi_\downarrow(\mathbf{r})\rangle. \tag{80}$$

To calculate the free energy f_0, we use standard expression (56), in which we should use (79) as the Hamiltonian. Going over to the variable $\varepsilon = \xi^2(\mathbf{k})/2$ in the integrals, we find the following equations for determining f_0, μ, δ in the dependence on the concentration n:

$$f_0 = I_1 - {}^1\!/_2 n_c n^2 - {}^1\!/_2 \delta^2/\lambda, \tag{81}$$

$$n = I_2, \tag{82}$$

$$\frac{1}{\lambda} = I_3, \tag{83}$$

where

$$I_1 = \frac{1}{2}\int_0^\infty \left\{1 - \frac{\varepsilon-\mu'}{[(\varepsilon-\mu')^2+\delta^2]^{1/2}}\right\}\frac{\varepsilon\,d\varepsilon}{(2\varepsilon)^{1/2}}, \tag{84a}$$

$$I_2 = \frac{1}{2}\int_0^\infty \left\{1 - \frac{\varepsilon-\mu'}{[(\varepsilon-\mu')^2+\delta^2]^{1/2}}\right\}\frac{d\varepsilon}{(2\varepsilon)^{1/2}}, \tag{84b}$$

$$I_3 = \frac{1}{2}\int_0^\infty \frac{d\varepsilon}{\{2\varepsilon[(\varepsilon-\mu')^2+\delta^2]\}^{1/2}}. \tag{84c}$$

Here we have introduced an effective chemical potential

$$\mu' = \mu + n_c n.$$

We will first find solutions of the self-consistency equations for δ and μ, working from (82) and (83), in the asymptotic limits in terms of the parameter δ/n^2. The case of large values of this parameter corresponds to the situation in which the superconducting pairing, while smearing out the distribution function to a great extent, causes the chemical potential μ' to descend into the band gap (μ' becomes negative). If the condition $(\delta/\mu')^2 \ll 1$ $(\mu' < 0)$ also holds, then by using the corresponding asymptotic expressions for the integrals in (84b) and (84c) we can put Eqs. (82) and (83) in the form

$$n = \frac{\pi}{4}\frac{\delta^2}{(2|\mu'|)^{3/2}}, \tag{82a}$$

$$\frac{1}{\lambda}=\frac{\pi}{2}\frac{1}{(2|\mu'|)^{1/2}}. \tag{83a}$$

Solving these equations for δ and μ', we find

$$\delta(n)=\pi\lambda^{3/2}(n/2)^{1/2}, \tag{85}$$
$$\mu'=-\pi^2\lambda^2/8.$$

It follows from (56) that the relation $(\delta/\mu')^2\ll 1$ holds if $\delta/n^2\gg 1$ or $n/\lambda\ll 1$. In the opposite limit

$$\delta/n^2\ll 1$$

we have a solution which was first found in Ref. 23 and which has been studied in several places:

$$\delta(n)\approx 4n^2\exp(-n/\lambda), \tag{86}$$
$$\mu'\approx {}^1/_2 n^2+{}^1/_2\delta^2/\lambda n.$$

According to (85) and (86), the function $\delta(n)$ increases with increasing n at $n/\lambda\ll 1$, goes through a maximum at $n\sim 2\lambda$, and then falls off with further increase in the carrier density. In this model, near the maximum, the amplitude of the superconducting order parameter may be substantially greater than the corresponding value in the BCS theory (see Ref. 23 for details).

A calculation of the free energy and the chemical potential in the limit $n/\lambda\ll 1$ yields

$$f_0(n)=-{}^1/_8\pi^2\lambda^2 n-{}^1/_2 n_c n^2, \tag{87}$$
$$\frac{\partial\mu}{\partial n}=\frac{\partial^2 f_0}{\partial n^2}=-n_c.$$

The condition for an instability to phase stratification, $\partial\mu/\partial n<0$, thus holds over the entire concentration range $n/\lambda\ll 1$ in the presence of superconducting pairing. As we have already mentioned, a factor which determines the behavior of the chemical potential μ upon the appearance of a superconductivity is the smearing of the Fermi distribution as δ increases. At $n/\lambda\ll 1$, this effect causes the chemical potential to descend below the boundary of the allowed band. As n increases, δ increases in this region, the smearing increases, and μ decreases.

Under the condition $n/\lambda\gg 1$ we have

$$f_0(n)={}^1/_6 n^3-{}^1/_2 n_c n^2-\delta^2/4n, \tag{88}$$
$$\frac{\partial\mu}{\partial n}=n-n_c-16\frac{n^3}{\lambda}\exp\left(-\frac{2n}{\lambda}\right)\approx n-n_c^*, \quad n_c^*>n_c.$$

We see that again in this limit the stability boundary is shifted toward higher concentrations by the superconductivity. In contrast with the preceding case, the smearing of the Fermi step at $\delta/n^2\ll 1$ $(n/\lambda\gg 1)$ due to the decrease in the density of states with increasing energy leads to an increase in the chemical potential (at a fixed value of n). With increasing value of n, the order parameter δ decreases, the smearing becomes less extensive, and μ also decreases.

6. CONCLUSION

In this paper it has been demonstrated that the electron subsystem plays an important role in shaping various nonuniform states. It has been shown that correlations between carriers in systems with certain particular band features, such as the presence of congruent regions of the Fermi surface, can lead to a phase stratification. The most interesting manifestation of the fact that collectivized carriers are responsible for the formation of a nonuniform state is the interrelationship between the phase stratification and the superconductivity. Specifically, it follows from Eqs. (87) and (88) of Sec. 5 that the appearance of a superconducting order parameter expands the range of instability of the uniform state. As a result, the superconducting transition may cause a sample which is metallic in its normal phase to stratify into superconducting metallic droplets which are separated from each other by insulating "interlayers" and coupled with each other weakly. The disruption of this coupling by a weak magnetic field gives rise to a resistance of the sample while it is in the superconducting phase (according to the Meissner effect). This resistance is larger than that in the normal metallic state, since it is determined by the resistance of the insulating interlayers.[7,24]

The estimates of the droplet size in Sec. 4 were based on the assumption of immobile, uniformly distributed impurities. In real systems, in contrast, a space charge which arises from the stratification may be screened by a redistribution of impurity atoms. This situation is possible in $La_2CuO_{4+\delta}$, in which added oxygen atoms take positions between lanthanum layers and may have a high mobility.

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