Superconducting transitions due to Van Hove singularities in the electron spectrum

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Van Hove singularities in the electron spectrum can substantially raise the superconducting transition temperature. In cases in which the singularities lie near high-symmetry points at the boundary of the zone, transitions can occur to states which are coherent combinations of superconductivity, antiferromagnetism, and a charge density wave.

1. EXACT EQUATIONS

The high superconducting transition temperatures of multicomponent compounds based on La_2CuO_4 (or versions with other rare earths) have provoked a stream of papers regarding the mechanism for this increase in the temperature. In addition to the natural suggestions regarding strong coupling, studies by Jorgensen *et al.*[1] and Mattheiss[2] have attracted interest. Their papers link the increase in the transition temperature with the nature of the electron spectrum of La_2CuO_4, in particular, with Van Hove singularities. The results of my theoretical analysis of this possibility were reported in two letters.[4,5] The present paper furnishes the details which were omitted from Refs. 4 and 5.

Hirsch and Scalapino[3] pointed out that Van Hove singularities near the Fermi surface would alter the dependence of the superconducting transition temperature on a bare (in principle, weak) interaction. A Van Hove singularity, i.e., a point on a constant-energy surface where the electron velocity vanishes,

$$\frac{\partial \varepsilon}{\partial p_1}=\frac{\partial \varepsilon}{\partial p_2}=\frac{\partial \varepsilon}{\partial p_3}=0, \tag{1}$$

is generally a weak singularity, and in an essentially three-dimensional crystal it would not alter the superconducting transition temperature. The Cooper loop is proportional to

$$\left(g^2 \ln\frac{\bar\varepsilon}{T}\right)\int \frac{dS}{|\mathbf{v}|}, \tag{2}$$

where the integral — the state density $N(\varepsilon)$ — is over the entire Fermi surface ($\bar\varepsilon$ is the cutoff energy), and points corresponding to (1) could contribute only singlularities in the derivative of T_c with respect to the pressure. In layered crystals — a class which apparently includes[1,2] La_2CuO_4 — however, Van Hove singularities in the spectrum also generate singularities in the state density. Near a two-dimensional hyperbolic Van Hove point, the state density itself becomes logarithmic, $N(\varepsilon) \sim \ln(\bar\varepsilon/\varepsilon)$, and the magintude of the Cooper loop increases correspondingly:

$$g^2 \ln^2(\bar\varepsilon/T). \tag{2a}$$

The result is the desired increase in the transition temperature:

$$T_c \sim \bar\varepsilon \exp(-\mathrm{const}\cdot|g|^{-1/2}). \tag{3}$$

In other words, we get the BCS formula with $|g|^{1/2}$ in place of $|g|$. In the case of a repulsion, $g>0$, the superconducting transition does not occur, but the Van Hove singularity comes into play in the zero-sound channel, where the loop is given by

$$g^2\int\frac{d^2p}{|\varepsilon(\mathbf{p})|}\sim g^2\ln\frac{\bar\varepsilon}{T}. \tag{4}$$

This situation involves a transition to a state with a spin density wave or a charge density wave, at the temperature given by the standard BCS formula.

An alternative mechanism for the superconducting transition in La_2CuO_4— the so-called biexciton mechanism— also involves a two-dimensional Van Hove singularity. If we start from an insulating state, as in Ref. 6, we have an energy minimum lying near the bottom of the conduction band: an elliptical Van Hove point. For the Cooper loop we now have, instead of (2).

$$g^2\int\frac{d^2p}{\mathbf{p}^2}\sim g^2\ln\frac{\bar\varepsilon}{T}. \tag{2b}$$

The BCS formula for T_c which follows from (2b) is of course the same as the well-known formula for the energy of a bound state of two weakly interacting particles in the two-dimensional case.[7]

Hirch and Scalapino[3] also discussed how the transition temperature (3) depends on the proximity of the Van Hove singularity to the Fermi surface or, equivalently, on the chemical potential (or concentration). If we put the origin of the chemical-potential scale at the point at which the singularity lies on the Fermi surface, we find that the logarithm of the temperature in (2) would have to be replaced by the quantity

$$\xi=\frac{1}{2}\ln(\bar\varepsilon/\max(T,\mu)). \tag{5}$$

In the doubly logarithmic approximation, (2a), (3), we have $g\xi^2\sim 1$, which gives us a trivial quadratic state diagram (Fig. 1) with $T_c = |\mu_c|$. Finally, the three-dimensional effects associated with hops between layers will not be important as long as the corresponding energy satisfies

$$\varepsilon_{hop}\leqslant T_c,\ |\mu_c|.$$

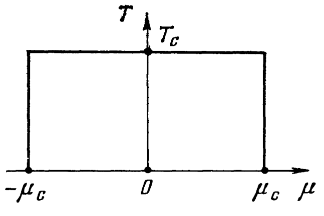

FIG. 1.

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A crucial point is that a Van Hove point is not a hyperbolic singularity of general position, according to Ref. 1. The asymptotes of the hyperbolas intersect at a right angle in it, and the point itself lies at the center of a face of a zone. This circumstance means that the electron spectrum of pure La_2CuO_4 can apparently be described very accurately in the nearest-neighbor approximation.

In the case of such an exclusively Van Hove singularity, both loops — the Cooper loop $C(2)$ and the zero-sound loop $Z(4)$ — became doubly logarithmic[3]:

$$C,\ Z \sim g^2\xi^2.$$

A measure of the accuracy of this assertion is the deviation of the angle between the asymptotes, α, from a right angle:

$$\varepsilon|\alpha-\pi/2| < T_c,\ |\mu_c|.$$

At this point the problem becomes rather complicated. We need to sum all the diagrams of the same order of magnitude in the doubly logarithmic approximation, $g\xi^2 \sim 1$. As was pointed out in Refs. 4 and 5, all such diagrams form a so-called parquet, which consists of all possible insertions of Cooper and zero-sound loops into each other (Fig. 2). The parquet summation problem, fortunately, is well-understood. In solid state physics, this problem was studied intensely in the theory of quasi-one-dimensional metals.[8,9] Since our case has the complication of the doubly logarithmic nature of the diagrams, however, we are forced to go through the calculations in some detail.

As always,[8,9] we take the transition temperature T_c to be the region where a two-particle function — a vertex — has a pole in T or, equivalently in ξ from (5). To find the vertices γ we need to sum the parquets (Fig. 2). As was pointed out previously,[4] doubly logarithmic contributions to Cooper and zero-sound diagrams come exclusively from the vicinity of the centers of the faces of the zone: points $ABCD$ in Fig. 1a in Ref. 4. On the other hand, we cannot ignore the fact that AC and BD are periods of the reciprocal lattice, so we require the corresponding periodicity of the vertices: $\gamma(ACCA) = \gamma(AAAA)$, $\gamma(BDDB) = \gamma(BBBB)$, $\gamma(ABCD) = \gamma(ABAB)$, $\gamma(ACBD) = \gamma(AABB)$, etc. It is also clear that the only a symmetric solution, $\gamma(BBBB)$, would be of interest. The periodicity of the vertices γ makes it possible to glue point A to C and B to D in Fig. 1a in Ref. 4 and to use Fig. 1b of Ref. 4.

We write the spectrum near points A and B in terms of dimensionless momentum projections, x_1, x_2:

$$\varepsilon_A = -vp_0x_1x_2, \qquad \varepsilon_B = vp_0x_1x_2.$$

The Cooper loop C_{AA} and the zero-sound loop Z_{AB} are given by

$$C_{AA} = \frac{p_0}{4\pi^2 v}\int\frac{dx_1\,dx_2}{|x_1x_2|} = \frac{p_0}{4\pi^2 v}\xi_1\xi_2, \tag{6}$$

$$Z_{AB} = \frac{p_0}{2\pi^2 v}\int\frac{dx_1\,dx_2}{|x_1x_2|} = \frac{p_0}{2\pi^2 v}\xi_1\xi_2,$$

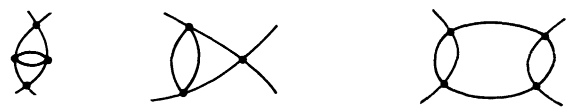

FIG. 2.

$$\xi_{1,2} = \ln(\Lambda/|x_{1,2}|),$$

where $x_{1,2}$ are the projections of the external momentum in the diagram, and Λ is a dimensionless cutoff. If the external momentum $x_{1,2}$ is zero, we would replace $\xi_{1,2}$ in (6) by ξ from (5) with $\bar{\varepsilon} = vp_0\Lambda^2$. The most effective method for solving the equations of an ordinary single-logarithm parquet is the Sudakov method. In this method (Refs. 8 and 9, for example) one begins with a calculation of the simplest vertex, all of whose momenta are of the same order. For this case there is a simple differential equation. The other vertices — vertices with unequal external momenta — and the responses can be calculated quite easily on the basis of the simplest vertex (cf. Ref. 9). In our doubly logarithmic case, as can be seen even from (6), we can take the Sudakov approach only for one of the momentum projections, say x_1. The equations which result are integrodifferential equations: differential in ξ_1 and integral in x_2. There is no particular difficulty in writing the equations; it is sufficient to repeat the derivation of the equations for a so-called fast parquet, as carried out previously in the theory of the magnetism of metals[10] and of quasi-one-dimensional metals.[11]

We begin with an accurate determination of the spin structure of the quantities which appear in the equations. The parquet is specified by the diagrams in Fig. 2 or Ref. 4. There are three vertices here: $\gamma(AAAA)$, $\gamma(AABB)$, and $\gamma(ABBA)$. If all the momenta are comparable in magnitude, as in Ref. 4, there are four independent functions. In the case of vertices with different momenta, which appear in the parquet equations, however, the number of independent functions is a maximum, equal to six:

$$\begin{aligned}\gamma(AAAA) &= \gamma_1\delta_{\alpha\gamma}\delta_{\beta\delta} - \gamma_{-1}\delta_{\alpha\delta}\delta_{\beta\gamma},\\ \gamma(AABB) &= \gamma_2\delta_{\alpha\gamma}\delta_{\beta\delta} - \gamma_{-2}\delta_{\alpha\delta}\delta_{\beta\gamma},\\ \gamma(ABBA) &= \gamma_3\delta_{\alpha\gamma}\delta_{\beta\delta} - \gamma_4\delta_{\alpha\delta}\delta_{\beta\gamma}.\end{aligned} \tag{7}$$

Here we have retained the notation of Ref. 4 to the extent possible. For the case of equal momenta we have $\gamma_{1,2} = \gamma_{-1,-2}$. However, we are left with four bare charges: $g_{-1,-2} = g_{1,2}$. The vertices and the charges will be expressed below in units of $2\pi^2 v/p_0$.

By assumption, the vertices γ_k depend on the momentum projections x_1 only through ξ_1. The dependence on the projections x_2 must be specified by three equivalent sets of variables (Fig. 3), depending on the particular channel along which the parquet diagram is sliced: 1) a Cooper sum $c = l_1 + l_2$ and $l_1 l_3$; 2) a zero-sound difference $z = l_3 - l_1$ and l_1, l_2; 3) another zero-sound difference $\bar{z} = l_4 - l_1$ and l_1, l_2. Correspondingly, logarithmic variables are introduced:

$$\begin{aligned}\xi_2(c) &= \ln(\Lambda/|c|),\quad \xi_2(z) = \ln(\Lambda/|z|),\quad \xi_2(\bar{z}) = \ln(\Lambda/|\bar{z}|),\\ \eta_1 &= \ln(\Lambda/|l_1|),\quad \eta_2 = \ln(\Lambda/|l_2|),\quad \eta_3 = \ln(\Lambda/|l_3|).\end{aligned} \tag{8}$$

The equations of a fast parquet are conveniently written separately for the parts which are sliced along Cooper (Z_k)

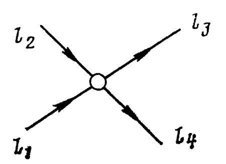

FIG. 3.

and zero-sound lines (Z_k along z and $\bar{Z}_k$ along $\bar{z}$; here $k = \pm 1, \pm 2, 3, 4$). The complete vertices in this case are

$$\gamma_k = g_k + C_k + Z_k + \bar{Z}_k.$$

The equations corresponding to the diagrams in Fig. 2 of Ref. 4 are

$$\frac{\partial \gamma_1}{\partial \xi_1} = -\frac{1}{2}\int_0^{\xi_2(c)} d\zeta \{\gamma_1(\eta_1,\zeta)\gamma_{-1}(\zeta,\eta_3) + \gamma_2(\eta_1,\zeta)\gamma_{-2}(\zeta,\eta_3) + \eta_1 \rightleftarrows \eta_3\},$$

$$\frac{\partial \gamma_{-1}}{\partial \xi_1} = -\frac{1}{2}\int_0^{\xi_2(c)} d\zeta \{\gamma_1(\eta_1,\zeta)\gamma_1(\zeta,\eta_3) + \gamma_{-1}(\eta_1,\zeta)\gamma_{-1}(\zeta,\eta_3) + \gamma_2(\eta_1,\zeta)\gamma_2(\zeta,\eta_3) + \gamma_{-2}(\eta_1,\zeta)\gamma_{-2}(\zeta,\eta_3)\},$$

$$\frac{\partial C_2}{\partial \xi_1} = -\frac{1}{2}\int_0^{\xi_2(c)} d\zeta \{\gamma_1(\eta_1,\zeta)\gamma_{-2}(\zeta,\eta_3) + \gamma_{-1}(\eta_1,\zeta)\gamma_2(\zeta,\eta_3) + \eta_1 \rightleftarrows \eta_3\},$$

$$\frac{\partial C_{-2}}{\partial \xi_1} = -\frac{1}{2}\int_0^{\xi_2(c)} d\zeta \{\gamma_1(\eta_1,\zeta)\gamma_2(\zeta,\eta_3) + \gamma_{-1}(\eta,\zeta)\gamma_{-2}(\zeta,\eta_3) + \eta_1 \rightleftarrows \eta_3\},$$

$$\frac{\partial Z_2}{\partial \xi_1} = \int_0^{\xi_2(z)} d\zeta \{-(2\gamma_2(\eta_1,\zeta) - \gamma_{-2}(\eta_1,\zeta))\gamma_3(\zeta,\eta_2) + \gamma_2(\eta_1,\zeta)\gamma_4(\zeta,\eta_2) + \eta_1 \rightleftarrows \eta_2\},$$

$$\frac{\partial Z_{-2}}{\partial \xi_1} = \int_0^{\xi_2(z)} d\zeta \{\gamma_{-2}(\eta_1,\zeta)\gamma_4(\zeta,\eta_2) + \eta_1 \rightleftarrows \eta_2\}, \qquad (9)$$

$$\frac{\partial \bar{Z}_2}{\partial \xi_1} = \int_0^{\xi_2(\bar{z})} d\zeta \{\gamma_2(\eta_1,\zeta)\gamma_4(\zeta,\eta_2) + \eta_1 \rightleftarrows \eta_2\},$$

$$\frac{\partial \bar{Z}_{-2}}{\partial \xi_1} = \int_0^{\xi_2(\bar{z})} d\zeta \{-(2\gamma_{-2}(\eta_1,\zeta) - \gamma_2(\eta_1,\zeta))\gamma_3(\zeta,\eta_2) + \gamma_{-2}(\eta_1,\zeta)\gamma_4(\zeta,\eta_2) + \eta_1 \rightleftarrows \eta_2\},$$

$$\frac{\partial \gamma_3}{\partial \xi_1} = -\int_0^{\xi_2(z)} d\zeta \{\gamma_3(\eta_1,\zeta)(\gamma_3(\zeta,\eta_2) - \gamma_4(\zeta,\eta_2)) + \gamma_2(\eta_1,\zeta)(\gamma_2(\eta_2,\zeta) - \gamma_{-2}(\eta_2,\zeta)) + \eta_1 \rightleftarrows \eta_2\},$$

$$\frac{\partial \gamma_4}{\partial \xi_1} = \int_0^{\xi_2(z)} d\zeta \{\gamma_4(\eta_1,\zeta)\gamma_4(\zeta,\eta_2) + \gamma_{-2}(\eta_1,\zeta)\gamma_{-2}(\zeta,\eta_2)\};$$

$$\gamma_{\pm 2} = g_2 + C_{\pm 2} + Z_{\pm 2} + \bar{Z}_{\pm 2}.$$

2. MOVING AND NONMOVING POLES

Equations (9) can be used to derive the results regarding the poles which were reported in Ref. 4. For this purpose it is sufficient to find the solutions with a pole in ξ_1 with (in principle) different projections x_2 and then transform from ξ_1 to ξ using (5), setting x_1 and some (or all) of the momenta x_2 equal to zero. There are two types of pole solutions of Eqs. (9): moving poles and nonmoving poles in ξ_1 (cf. Refs. 10 and 11). In the latter, the pole position ξ_0 does not depend on the momenta x_2, while in the former it does.

We begin with the moving poles. There are three types, in accordance with the number of sections of the parquet diagrams: along c, along z, and along $\bar{z}$. The first type is formed primarily as a result of the particle-particle interaction, and its position (trajectory depends only on $c - \xi_0(c)$. In the two other types, the poles are due to a particle-hole interaction, and their trajectories depend on $z - \xi_0(z)$ or $\bar{z} - \xi_0(\bar{z})$, respectively. In terms of their physical meaning, the poles in $\xi_0(c)$ are present only in the equations for γ_{w1} and C_{w2} in (9); the poles in $\xi_0(z)$ only in the equations for Z_{w2}, γ_3, and γ_4; and the poles in $\xi_0(\bar{z})$ only in the equations for $\bar{Z}_{\pm 2}$, γ_3, and γ_4.

The doubly logarithmic nature of our problem makes it possible to find trajectories for the moving poles. For this purpose it is sufficient to consider the vertices in the asymmetric regions of the projections x_2. For the pole $\xi_0(x)$ this is a region in which we have (for example) $l_1 \sim l_2 \sim c \ll \Lambda$, and the momenta $l_3 \sim l_4 \sim \Lambda$ are large. In it we have $\eta_1 = \eta_2 = \xi_2(c)$ and $n_3 = \eta_4 = 0$. On the other hand, it is clear from the structure of the perturbation-theory series that the vertex depends only on $\xi_1\xi_2(c)$ in this region. The trajectory thus has the behavior $\xi_0(c) \sim \text{const}/\xi_2(c)$, and the pole part of γ is written in the form

$$\gamma_k \approx C_k \approx \frac{\Gamma_k(\eta_1,\eta_3)}{\xi_1\xi_2(c) - \xi_0^2}, \quad k = \pm 1, \pm 2, \qquad (10)$$

where ξ_0^2 is a constant which depends on the bare charges and which will be determined shortly.

Similarly, setting $l_1 \sim l_3 \sim z$, $l_2 \sim l_4 \sim \Lambda$ or $l_1 \sim l_4 \sim \bar{z}$, $l_2 \sim l_3 \sim \Lambda$, we find the following results for the poles in the Z channels:

$$\gamma_k \approx Z_k, \bar{Z}_k \approx \frac{\Gamma_k(\eta_1,\eta_2)}{\xi_1\xi_2(z,\bar{z}) - \xi_0^2}, \quad k = \pm 2, 3, 4. \qquad (11)$$

To calculate the constants we need to solve Eqs. (9) numerically. We will restrict the discussion here to an evaluation in the ladder approximation.

The Cooper ladder with $\eta_3 = \eta_4 = 0$ is

$$\omega\gamma_1 = \omega g_1 - {}^1/_2 g_1(\gamma_1 + \gamma_{-1}) - {}^1/_2 g_2(\gamma_2 + \gamma_{-2}),$$
$$\omega\gamma_2 = \omega g_2 - {}^1/_2 g_1(\gamma_2 + \gamma_{-2}) - {}^1/_2 g_2(\gamma_{-1} + \gamma_1). \qquad (12)$$

With $g_{-1} = g_1$, the equations for γ_{-1} and γ_{-2} are the same as (12), so we have $\gamma_{-1} = \gamma_1, \gamma_{-2} = \gamma_2$. Here we have used $\omega = 1/\xi_1\xi_2(c)$. The solution is trivial:

$$\gamma_1 \pm \gamma_2 = (g_1 \pm g_2)/[1 + (g_1 \pm g_2)\xi_1\xi_2(c)], \quad \xi_0^{-2} = -g_1 \mp g_2. \qquad (13)$$

The pole (13) clearly describes singlet superconductivity. In the Z channel with $\eta_2 = \eta_4 = 0$ we have $\omega = 1/\xi_1\xi_2(z)$

$$\omega\gamma_2 = \omega g_2 - (2g_3 - g_4)\gamma_2 + g_3\gamma_{-2} - g_2\gamma_3 + g_2\gamma_4,$$
$$\omega\gamma_{-2} = \omega g_2 + g_2\gamma_4 + g_4\gamma_{-2},$$
$$\omega\gamma_4 = \omega g_4 + g_4\gamma_4 + g_2\gamma_{-2},$$
$$\omega\gamma_3 = \omega g_3 - (2g_3 - g_4)\gamma_3 + g_3\gamma_4 - g_2\gamma_2 + g_2\gamma_{-2}.$$

They have solutions of two types: spin density waves,

$$\gamma_4 \pm \gamma_{-2} = (g_4 \pm g_2)/[1 - (g_4 \pm g_2)\xi_1\xi_2(z)], \quad \xi_0^{-2} = g_4 \pm g_2, \qquad (14)$$

and charge density waves,

$$2\gamma_3-\gamma_4\pm2\gamma_2\mp\gamma_{-2}=(2g_3-g_4\pm g_2)/[1+(2g_3-g_4\pm g_2)\xi_1\xi_2(z)],$$
$$\xi_0^{-2}=-2g_3+g_4\mp g_2. \qquad (15)$$

The division of the moving poles into pure singlet superconductivity, spin density waves, and charge density waves is in a sense retained beyond the ladder approximation. The exact Eqs. (9) can be rewritten in diagonalized form:

$$\frac{\partial}{\partial\xi_1}(\gamma_1+\gamma_{-1}\pm C_2\pm C_{-2})=-\frac{1}{2}\int d\zeta(\gamma_1+\gamma_{-1}\pm\gamma_2\pm\gamma_{-2})^2, \quad (16)$$

$$\frac{\partial}{\partial\xi_1}(\gamma_1-\gamma_{-1}\pm C_2\mp C_{-2})=\frac{1}{2}\int d\zeta(\gamma_1-\gamma_{-1}\pm\gamma_2\mp\gamma_{-2})^2, \quad (16')$$

$$\frac{\partial}{\partial\xi_1}(\gamma_4\pm Z_{-2})=\int d\zeta(\gamma_4\pm\gamma_{-2})^2, \quad (17)$$

$$\frac{\partial}{\partial\xi_1}(2\gamma_3-\gamma_4\pm2Z_2\mp Z_{-2})=-\int d\zeta(2\gamma_3-\gamma_4\pm2\gamma_2\mp\gamma_{-2})^2. \quad (18)$$

There is a shorthand notation for the integrals on the right sides:

$$\int\gamma^2 d\zeta\equiv\int_0^{\xi_2(c),\xi_2(z)}\gamma(\eta_1,\zeta)\gamma(\zeta,\eta_{3,2})d\zeta \text{, etc.}$$

recalling the old results,[10,11] we immediately see that a pole solution in (16) corresponds to a pole in the temperature in the response χ_{SS}, the solution in (17) corresponds to a pole in the response χ_{SDW}, and solution (18) corresponds to a pole in the response χ_{CDW}.

However, we must not forget another possibility: In writing Eqs. (10) and (11) we tacitly assumed that the residues γ at poles of the type $\xi_1\sim\text{const}/\xi_2$ are nonzero in the corresponding asymmetric regions, e.g., $\eta_3=\eta_4=0$. If the residues are instead zero here, it becomes impossible to make assertions of any sort regarding the trajectories of the poles. Both the trajectories and the residues must be found by integrating (9) numerically. The responses of course remain simple poles in the temperature, by virtue of (16)–(18).

It is not such a simple matter to resolve the question regarding the nonmoving poles. It is necessary to carry out a complete numerical study of Eqs. (9). In the present paper we will simply show that Eqs. (9) actually have a singular solution which has all the properties of the nonlinear solution found by an approximate method in Ref. 4.

We now assume that not only the momenta x_1 but also x_2 have comparable magnitude (ξ_2). We then obviously have $\gamma_{-1,2}=\gamma_{1,2}$, $C_{-1,2}=C_{1,2}$, $Z_{-1,2}=\overline{Z}_{-1,2}=Z_{1,2}=\overline{Z}_{1,2}$. Furthermore, it can be seen by direct substitution into (9) that in the case of equal momenta there is a solution of the form

$$\gamma_k=\Gamma_k\delta(\eta_1-\eta_3)\equiv\Gamma_k\delta(\eta_1-\eta_2), \qquad k=1,\,2,\,3,\,4,$$

with constants Γ_k which satisfy the relations

$$\Gamma_1=\Gamma_1^2+\Gamma_2^2, \quad \Gamma_2=2\Gamma_2(\Gamma_1+\Gamma_3-2\Gamma_4),$$
$$\Gamma_3=2\Gamma_3(\Gamma_3-\Gamma_4), \quad \Gamma_4=-\Gamma_4^2-\Gamma_2^2.$$

These equations have the solutions $(\Gamma_1\Gamma_2\Gamma_3\Gamma_4)$

$$(1000),\left(00\frac{1}{2}0\right),\left(00-\frac{1}{2}-1\right),(100-1),$$
$$\left(\frac{1}{6}\pm\frac{\sqrt{5}}{6}0-\frac{1}{6}\right), \qquad (19)$$

which are the same as the corresponding set in Ref. 4. An approximate estimate of ξ_0 in the Hubbard model ($g_1=g_2=g_3=g$) yields $\xi_0=2.5g,\ -2.13g$.

It remains to calculate the responses. As in writing the parquet equations (9), we use the Sudakov method. We again assume that all the projections x_1 are of the same order of magnitude, ξ_1. The singlet-superconductivity response then depends on ξ_1 and $\xi_2(c)$, while the responses of the charge and spin density waves depend on ξ_1 and $\xi_2(z)$. Repeating the arguments from an old paper of Larkin and the present author[9] word by word, we find the following results for the responses, by analogy with (9):

$$\frac{\partial}{\partial\xi_1}\chi_{SS}\sim\int_0^{\xi_2(c)}\Delta^2(\eta)d\eta,$$
$$\frac{\partial}{\partial\xi_1}\chi_{SDW}\sim\int_0^{\xi_2(z)}\sigma^2(\eta)d\eta, \qquad (20)$$
$$\frac{\partial}{\partial\xi_1}\chi_{CDW}\sim\int_0^{\xi_2(z)}n^2(\eta)d\eta.$$

The functions Δ, σ, and n, which are analogous to the vertices in (9), satisfy integrodifferential equations (we recall that we now have $\gamma_{-1,2}=\gamma_{1,2}$):

$$\frac{\partial\Delta(\eta)}{\partial\xi_1}=-\int_0^{\xi_2(c)}d\zeta\,\Delta(\zeta)[\gamma_1(\zeta,\eta;c)\pm\gamma_2(\zeta,\eta;c)],$$

$$\frac{\partial\sigma(\eta)}{\partial\xi_1}=\int_0^{\xi_2(z)}d\zeta\,\sigma(\zeta)[\gamma_4(\zeta,\eta;z)\pm\gamma_2(\zeta,\eta;z)], \quad (21)$$

$$\frac{\partial n(\eta)}{\partial\xi_1}=-\int_0^{\xi_2(z)}d\zeta\,n(\zeta)[2\gamma_3(\zeta,\eta;z)-\gamma_4(\zeta,\eta;z)\pm\gamma_2(\zeta,\eta;z)].$$

Now substituting the quantities γ_k in the form of δ-functions into (21), we see that the dependence of Δ, σ, and n on the momentum η is arbitrary and that we have

$$\Delta\sim(\xi_0^2-\xi_1\xi_2)^{-\Gamma_1-|\Gamma_2|},$$
$$\sigma\sim(\xi_0^2-\xi_1\xi_2)^{\Gamma_4-|\Gamma_2|}, \qquad (22)$$
$$n\sim(\xi_0^2-\xi_1\xi_2)^{-2\Gamma_3+\Gamma_4-|\Gamma_2|}.$$

We then find from (20)

$$\chi_{SS}\sim(\xi_0-\xi)^{-2\Gamma_1-2|\Gamma_2|+1},$$
$$\chi_{SDW}\sim(\xi_0-\xi)^{2\Gamma_4-2|\Gamma_2|+1}, \qquad (23)$$
$$\chi_{CDW}\sim(\xi_0-\xi)^{-4\Gamma_3+2\Gamma_4-2|\Gamma_2|+1}$$

with ξ from (5). The first points in (19) give, respectively, the independent singlet superconductivity, charge density waves, and spin density waves. It can be seen that the (100–1) solution corresponds to retention of a metallic state. Finally, the last nontrivial point gives us the expression presented in Ref. 4:

$$\chi_{SS}\sim\chi_{SDW}\sim\chi_{CDW}\sim(\xi_0-\xi)^{-(\sqrt{5}-2)/3}. \qquad (24)$$

3. MAXIMUM INCREASE IN THE TRANSITION TEMPERATURE

I recently examined the still hypothetical case of a body-centered cubic crystal in which the increase in T_c reaches the maximum possible value in the weak-coupling region.[5] Below, as in Secs. 1 and 2, we present the details omitted from Ref. 5. The arguments are nearly a literal repetition of those in Secs. 1 and 2, so we will write only the key equations, keeping the words to a minimum.

Reference 5 deals with the theoretical electron spectrum of a BCC metal which incorporates only the abbreviated jump from a vertex of the cube to its center:

$$\varepsilon(\mathbf{p})=\varepsilon_0 \cos\frac{\pi p_1}{2}\cos\frac{\pi p_2}{2}\cos\frac{\pi p_3}{2}.$$

If there is precisely one electron per cell, the Fermi surface is a cube with corners A—111, B—$\bar{1}\bar{1}\bar{1}$, $C-\bar{1}11$,.... The periods of the reciprocal FCC lattice are the vectors [220,..., and [400],.... The Cooper loop C and zero-charge loops Z are now proportional to the cubes of logarithms, which receive contributions only from the neighborhoods of corners A, B, C,.... Considering the periodicity of the vertices explicitly, as in Sec. 1, we can glue the points 111, $\bar{1}\bar{1}1$, $1\bar{1}\bar{1}$, and $\bar{1}1\bar{1}$ into a single point A, and we can glue the four other points, $\bar{1}\bar{1}\bar{1}$, $\bar{1}11$, $1\bar{1}1$, and $11\bar{1}$, into another point, B. We are accordingly again dealing with a Fermi surface which consists of two points, A and B, this time in three-dimensional space. Near the Fermi surface we have, in constrast with Sec. 1,

$$\varepsilon_A=-vp_0x_1x_2x_3, \quad \varepsilon_B=vp_0x_1x_2x_3.$$

The parquet equations of the problem are shown in Fig. 1 in Ref. 5. There are only a single Cooper loop and a single zero-sound loop:

$$C_{AB}=Z_{AB}=\frac{p_0^2}{2\pi^3 v}\xi_1\xi_2\xi_3,$$
$$\xi_l=\ln\frac{\Lambda}{|x_l|}, \quad l=1,2,3.$$

The parquet equations include two vertices: $\gamma(ABBA)$ and the interchange $\gamma(AABB)$. Their spin structure in the case of different momenta is more complicated than in Ref. 5 [cf. (7)]:

$$\gamma(ABBA)=\gamma_1\delta_{\alpha\gamma}\delta_{\beta\delta}-\gamma_2\delta_{\alpha\delta}\delta_{\beta\gamma},$$
$$\gamma(AABB)=\gamma_3\delta_{\alpha\gamma}\delta_{\beta\delta}-\gamma_{-3}\delta_{\alpha\delta}\delta_{\beta\gamma}.$$

In the case of equal momenta we would naturally have $\gamma_{-3}=\gamma_3$, while the bare charges would always be $g_{-3}=g_3$. Both the vertices and the charges are expressed below in units of $\pi^3 v/p_0^2$.

We again take the Sudakov approach, assuming that all the projections x_1 are equal (ξ_1), while the projections x_2 and x_3 are different. The entire text preceding Eq. (9) can be repeated here intact. The only difference is that the quantities l, and, correspondingly, η and ζ become two-dimensional vectors in the space x_2, x_3. Instead of Eqs. (9) we now find

$$\frac{\partial C_1}{\partial\xi_1}=-\frac{1}{2}\int_0^{\xi_{2,3}(c)} d^2\zeta\{\gamma_1(\eta_1,\zeta)\gamma_2(\zeta,\eta_3)+\eta_1\rightleftarrows\eta_3\},$$

$$\frac{\partial C_2}{\partial\xi_1}=-\frac{1}{2}\int_0^{\xi_{2,3}(c)} d^2\zeta\{\gamma_1(\eta_1,\zeta)\gamma_1(\zeta,\eta_3)+\gamma_2(\eta_1,\zeta)\gamma_2(\zeta,\eta_3)\},$$

$$\frac{\partial Z_1}{\partial\xi_1}=-\frac{1}{2}\int_0^{\xi_{2,3}(z)} d^2\zeta\{\gamma_1(\eta_1,\zeta)(\gamma_1(\zeta,\eta_2)-\gamma_2(\zeta,\eta_2)) +\gamma_3(\eta_1,\zeta)(\gamma_3(\zeta,\eta_2)-\gamma_{-3}(\zeta,\eta_2))+\eta_1\rightleftarrows\eta_2\},$$

$$\frac{\partial Z_2}{\partial\xi_1}=\frac{1}{2}\int_0^{\xi_{2,3}(z)} d^2\zeta\{\gamma_2(\eta_1,\zeta)\gamma_2(\zeta,\eta_2)+\gamma_{-3}(\eta_1,\zeta)\gamma_{-3}(\zeta,\eta_2)\},$$

$$\frac{\partial Z_3}{\partial\xi_1}=\frac{1}{2}\int_0^{\xi_{2,3}(z)} d^2\zeta\{-(2\gamma_3(\eta_1,\zeta)-\gamma_{-3}(\eta_1,\zeta))\gamma_1(\zeta,\eta_2) +\gamma_3(\eta_1,\zeta)\gamma_2(\zeta,\eta_2)+\eta_1\rightleftarrows\eta_2\}, \quad (25)$$

$$\frac{\partial Z_{-3}}{\partial\xi_1}=\frac{1}{2}\int_0^{\xi_{2,3}(z)} d^2\zeta\{\gamma_{-3}(\eta_1,\zeta)\gamma_2(\zeta,\eta_2)+\eta_1\rightleftarrows\eta_2\},$$

$$\frac{\partial \bar{Z}_3}{\partial\xi_1}=\frac{1}{2}\int_0^{\xi_{2,3}(\bar{z})} d^2\zeta\{\gamma_3(\eta_1,\zeta)\gamma_2(\zeta,\eta_2)+\eta_1\rightleftarrows\eta_2\},$$

$$\frac{\partial \bar{Z}_3}{\partial\xi_1}=\frac{1}{2}\int_0^{\xi_{2,3}(\bar{z})} d^2\zeta\{-(2\gamma_{-3}(\eta_1,\zeta)-\gamma_3(\eta_1,\zeta))\gamma_1(\zeta,\eta_2) +\gamma_{-3}(\eta_1,\zeta)\gamma_2(\zeta,\eta_2)+\eta_1\rightleftarrows\eta_2\};$$
$$\gamma_{1,2}=g_{1,2}+C_{1,2}+Z_{1,2}, \quad \gamma_{\pm3}=g_3+Z_{\pm3}+\bar{Z}_{\pm3}.$$

What are the moving poles now? Instead of (10) we have

$$\gamma_k\approx C_k\approx\frac{\Gamma_k(\eta_1,\eta_3)}{\xi_1\xi_2(c)\xi_3(c)-\xi_0^3}, \quad k=1,2, \quad (26)$$

in the Cooper channel, and instead of (11) we have

$$\gamma_k\approx Z_k\approx\frac{\Gamma_k(\eta_1,\eta_2)}{\xi_1\xi_2(z)\xi_3(z)-\xi_0^3}, \quad k=1,2,\pm3, \quad (27)$$

in the zero-charge channels (there are corresponding expressions for $\bar{Z}$).

The constants ξ_0^3 are again estimated from ladders. The Cooper ladder ($\omega=1/\xi_1\xi_2\xi_3$)

$$\omega\gamma_1=\omega g_1-(g_1\gamma_2+g_2\gamma_1)/2,$$
$$\omega\gamma_2=\omega g_2-(g_1\gamma_1+g_2\gamma_2)/2$$

has two solutions. The solution

$$\gamma_2+\gamma_1=(g_2+g_1)/[1+(g_2+g_1)\xi_1\xi_2\xi_3/2], \quad \xi_0^{-3}=-(g_1+g_2)/2 \quad (28)$$

corresponds to singlet pairing, while

$$\gamma_2-\gamma_1=(g_2-g_1)/[1+(g_2-g_1)\xi_1\xi_2\xi_3/2], \quad \xi_0^{-3}=(g_1-g_2)/2 \quad (29)$$

corresponds to triplet pairing.

The zero-sound ladder

$$\omega\gamma_1=g_1\omega+(-g_1+{}^1/_2g_2)\gamma_1+{}^1/_2g_1\gamma_2-{}^1/_2g_3(\gamma_3-\gamma_{-3}),$$
$$\omega\gamma_2=\omega g_2+{}^1/_2g_2\gamma_2+{}^1/_2g_3\gamma_{-3},$$
$$\omega\gamma_3=\omega g_3-{}^1/_2g_3\gamma_1+{}^1/_2g_3\gamma_2+(-g_1+{}^1/_2g_2)\gamma_3+{}^1/_2g_1\gamma_{-3},$$
$$\omega\gamma_{-3}=\omega g_3+{}^1/_2g_3\gamma_2+{}^1/_2g_2\gamma_{-3}$$

also has two solutions. The solution

$$\gamma_2\pm\gamma_{-3}=(g_2\pm g_3)/[1-{}^1/_2(g_2\pm g_3)\xi_1\xi_2\xi_3], \quad \xi_0^{-3}={}^1/_2(g_2\pm g_3) \quad (30)$$

corresponds to a spin density wave, while

$$\gamma_1-{}^1/_2\gamma_2\pm\gamma_3\mp{}^1/_2\gamma_{-3} =(g_1-{}^1/_2g_2\pm{}^1/_2g_3)/[1+{}^1/_2(2g_1-g_2\pm g_3)\xi_1\xi_2\xi_3], \quad (31)$$
$$\xi_0^{-3}=-g_1+{}^1/_2g_2\mp{}^1/_2g_3$$

corresponds to a charge density wave.

The responses for the moving poles are calculated by the same procedure as in the corresponding place in Sec. 2. In particular, (16)–(18) are replaced by

$$\frac{\partial}{\partial \xi_1}(C_2 \pm C_1) = -\frac{1}{2}\int d^2\zeta(\gamma_2 \pm \gamma_1)^2 \tag{32}$$

for singlet and triplet superconductivity,

$$\frac{\partial}{\partial \xi_1}(Z_2 \pm Z_{-3}) = \frac{1}{2}\int d^2\zeta(\gamma_2 \pm \gamma_{-3})^2 \tag{33}$$

for a spin density wave, and, finally

$$\frac{\partial}{\partial \xi_1}\left(Z_1 - \frac{1}{2}Z_2 \pm Z_3 \mp \frac{1}{2}Z_{-3}\right)$$
$$= -\int d^2\zeta\left(\gamma_1 - \frac{1}{2}\gamma_2 \pm \gamma_3 \mp \frac{1}{2}\gamma_{-3}\right)^2$$

for a charge density wave.

For nonmoving poles, we again consider the case of equal momenta and singular solutions of the type

$$\gamma_k = \Gamma_k \delta(\eta_1 - \eta_3) = \Gamma_k \delta(\eta_1 - \eta_2), \quad k = 1, 2, 3.$$

The equations for Γ_k now take the form

$$\Gamma_1 = \Gamma_1^2, \ \Gamma_2 = {}^1/_2\Gamma_1^2 - {}^1/_2\Gamma_3^2, \ \Gamma_3 = \Gamma_3(\Gamma_1 - 2\Gamma_2),$$

and their solutions $(\Gamma_1\Gamma_2\Gamma_3)$ are

$$(1\ {}^1/_2\ 0),\ (0\ -{}^1/_2\ \pm 1). \tag{34}$$

The calculation of the responses is similar to (23) (cf. also Ref. 9):

$$\chi_{SS} \sim (\xi_0 - \xi)^{-\Gamma_1 - \Gamma_2 + 1},$$
$$\chi_{SDW} \sim (\xi_0 - \xi)^{\Gamma_2 - |\Gamma_3| + 1},$$
$$\chi_{CDW} \sim (\xi_0 - \xi)^{-2\Gamma_1 + \Gamma_2 - |\Gamma_3| + 1}.$$

The set of points (34) and the corresponding responses

$$\chi_{SS} \sim \chi_{CDW} \sim (\xi_0 - \xi)^{-1/2}, \quad (1\ {}^1/_2\ 0),$$
$$\chi_{SDW} \sim \chi_{CDW} \sim (\xi_0 - \xi)^{-1/2}, \quad (0\ -{}^1/_2\ \pm 1) \tag{35}$$

are the same as those given in Ref. 5.

CONCLUSION

The theory developed here is not yet capable of describing the vicinity of the phase transition or of supporting microscopic calculations on physical effects at low temperatures. Correcting these deficiencies will require abandoning the parquent approximation. We will accordingly restrict the discussion to a very simple phenomenological symmetry analysis of the situation.

Phenomenologically, a state can be described by three gaps: a superconducting gap Δ_{SS}, a spin-density-wave gap Δ_{SDW}, and a charge-density-wave gap Δ_{CDW}. The latter two gaps depend on the coordinates,

$$\Delta^{\pm}_{SDW}, \Delta^{\pm}_{CDW} \sim \begin{pmatrix} \cos \mathbf{Qr} \\ \sin \mathbf{Qr} \end{pmatrix}, \quad Q = \frac{\pi}{a},$$

and change sign as a result of a displacement equal to the period of the original crystal, a.

A mixture of singlet superconductivity and a charge density wave has no macroscopic manifestations. An insulating state of a spin density wave plus a charge density wave is the richest. If a transition conserves spatial inversion, i.e., if Δ_{SDW} and Δ_{CDW} have identical upper indices, $\Delta^{+}_{SDW}, \Delta^{+}_{CDW}$ ($\Delta^{-}_{SDW}, \Delta^{-}_{CDW}$), the substance unavoidably acquires a spontaneous magnetic moment:

$$\mathbf{M} \propto \Delta^{\pm}_{SDW}\Delta^{\pm}_{CDW}. \tag{36}$$

This ferromagnetism is evidently weak near the transition point. The physical picture is not disrupted as long as the Fermi surfaces do not shift by more than T_c. If the spatial inversion is disrupted (i.e., if the signs of Δ_{SDW} and Δ_{CDW} are opposite), we could in principle replace (36) by an expression for the electric current:

$$\mathbf{j} \propto \Delta^{\pm}_{SDW}\Delta^{\mp}_{CDW}. \tag{37}$$

Since the left and right sides of (2) have the same spatial and temporal parity, phenomena of this sort also fall in the category of so-called magnetokinetic phenomena; they were classified in detail from the symmetry standpoint some time ago.[12] In insulators, of course, an electric current could be only dissipative, so that a symmetry which allows relations like (37) in the case with dissipation[1)] would make the substance a ferroelectric in which the magnitude of the spontaneous polarization $\mathbf{P}$ is inversely proportional to the electron lifetime τ_e:

$$\mathbf{P} \propto \frac{1}{\tau_e}\Delta^{\pm}_{SDW}\Delta^{\mp}_{CDW}. \tag{38}$$

Depending on the scattering mechanism, $1/\tau_e$ would be proportional to either the number of phonons, $N_{ph} \sim T^3$, or the impurity concentration N_{imp} (i.e., it would be finite even at a vanishing temperature), but it would not depend on the number of conduction electrons. The following simple argument leads to (38): The current $\mathbf{j}$ is proportional to the number of conduction electrons,

$$\mathbf{j} \propto N_e \Delta_{SDW}\Delta_{CDW},$$

while on the other hand we have $\mathbf{j} \propto N_e \tau_e \mathbf{P}$.

Relation (37) also implies that there is an effect in the substance which is weaker than that in (38): a magnetoelectric effect. To see this, we note that (37) can always be put in the form

$$\mathbf{P} \propto [\mathbf{H}\Delta^{\pm}_{SDW}]\Delta^{\mp}_{CDW}, \quad \mathbf{M} \propto [\mathbf{E}\Delta^{\pm}_{SDW}]\Delta^{\mp}_{CDW}. \tag{39}$$

In contrast with the ferroelectricity (38), the magnetoelectric effect in (39) is not dissipative.

If consinusoidal and sinusoidal waves are mixed in both the spin and charge channels, the substance will of course become a ferromagnetic ferroelectric.

The coexistence of singlet superconductivity, spin density waves, and a charge density waves leads to two effects in the surface impedance. The first is anisotropy of the penetration depth.

$$\mathbf{j} \propto \Delta_{SDW}(\mathbf{A}\Delta_{SDW}). \tag{40}$$

Whether the anisotropy can be observed depends on the relation between the magnitude of the penetration depth, δ, and the magnetic-anisotropy energy α [expressed in terms of the effective domain-wall thickness $\delta_d \sim (T_c/\alpha)^{1/2}$]. If

$\delta \ll \delta_d$, the gap Δ_{SDW} at the surface will always adjust itself to the direction of the magnetic field in such a way that δ is maximized. The orientation of the spins in the interior of the sample, in constrast, will go to the easy-magnetization axis at distances on the order of δ_d. If the relation is reversed, $\delta \gg \delta_d$, the orientation of the spins Δ_{SDW} at the surface is set by the anisotropy of the crystal.

The second effect is more interesting: an anomalous Hall effect in the impedance,

$$\mathbf{j} \propto [\mathbf{E}\Delta^{\pm}_{SDW}]\Delta^{\pm}_{CDW}, \qquad (41)$$

which results in a rotation of the polarization plane upon reflection. Unfortunately, in our parquent approximation we are unable to calculate the frequency or momentum dependence of the coefficients in (40) and (41). These equations are therefore symbolic in nature, reflecting only the crude consequences of the symmetry.

There is nothing to prevent a superconductor in a state with singlet superconductivity plus a spin density wave plus a charge density wave from being a ferromagnet as in (36) [or a ferroelectric as in (38)].

[1)] A magnetoelectric effect of dissipative origin in metals was recently studied by Levitov *et al.*[13]

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