Spatial correlation of conduction electrons near the electron–topological transition in a metal

D. I. Golosov[1)] and M. I. Kaganov

P. L. Kapitza Institute of Physics Problems, USSR Academy of Sciences
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The structure of the "density-density" correlation function of conduction electrons of a normal metal is explained. The connection between the asymptotic behavior of the correlation function and the local geometry of the Fermi surface is established. The reconstruction of the correlation function during an electronic topological transition is considered. It is shown that the asymptotic Ruderman-Kittel exchange integral can be expressed in terms of an asymptote of a correlation function.

1. INTRODUCTION

The effect of a complex geometry of the Fermi surface (FS) and of its variation as a result of the electron-topological transition (ETT)[1] on the "density-density" spatial correlation function of conduction electrons of a normal metal is analyzed in the present article. The results are valid at low temperatures and for sufficiently perfect crystals: thermal effects and finite mean free paths have not been taken into account. The validity range of the results is estimated below.

Let $\Delta n(\mathbf{r}) = n(\mathbf{r}) - \bar{n}$ be the deviation of the electron density $n(\mathbf{r})$ from its mean value $\bar{n}$. Then[2]

$$\nu(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\bar{n}} \langle \Delta n(\mathbf{r}_1) \Delta n(\mathbf{r}_2) \rangle - \delta(\mathbf{r}_1 - \mathbf{r}_2). \qquad (1)$$

Describing the stationary states of electrons in a metal by using Bloch wave functions

$$\psi_{\mathbf{q}s}(\mathbf{r}) = \exp\left(\frac{i}{\hbar}\mathbf{q}\mathbf{r}\right) u_{\mathbf{q}s}(\mathbf{r}), \qquad (2)$$

where $\mathbf{q}$ is the quasimomentum, s is the band number, and $u_{\mathbf{q}s}(\mathbf{r})$ is invariant to translational symmetry transformations of the crystal lattice, expression (1) can be written in the form (Fermi-liquid effects are neglected):

$$\nu(\mathbf{r}_1, \mathbf{r}_2) = -\frac{2}{\bar{n}} \left| \sum_s \int n_{\mathbf{q}s} \exp\left[\frac{i}{\hbar}\mathbf{q}(\mathbf{r}_2 - \mathbf{r}_1)\right] \times u_{\mathbf{q}s}^*(\mathbf{r}_1) u_{\mathbf{q}s}(\mathbf{r}_2) \frac{d^3q}{(2\pi\hbar)^3} \right|^2. \qquad (3)$$

The integral is carried out over the first Brillouin zone, while

$$n_{\mathbf{q}s} = \begin{cases} 1, & \varepsilon_s(\mathbf{q}) < \varepsilon_F, \\ 0, & \varepsilon_s(\mathbf{q}) > \varepsilon_F \end{cases} \qquad (4)$$

is the electron distribution function in quasimomentum at $T = 0$, ε_F is the Fermi energy, and $\varepsilon_s(\mathbf{q})$ is the electron energy in state (2). It is convenient to expand the function $u_{\mathbf{q}s}(\mathbf{r})$ in a Fourier series

$$u_{\mathbf{q}s}(\mathbf{r}) = \sum_{\mathbf{b}} e^{i\mathbf{b}\mathbf{r}} A_{\mathbf{q}s}(\mathbf{b}); \qquad (5)$$

where the summation is carried out over reciprocal lattice vectors $\mathbf{b}$ (if $\mathbf{a}$ is any lattice period, then $\mathbf{ab}/2\pi$ is an integer). Then

$$\nu(\mathbf{r}_1, \mathbf{r}_2) = -\frac{2}{\bar{n}} \left| \sum_{s\mathbf{b}\mathbf{b}'} \exp(-i\mathbf{b}\mathbf{r}_1 + i\mathbf{b}'\mathbf{r}_2) \times \int n_{\mathbf{q}s} \exp\left[\frac{i}{\hbar}(\mathbf{r}_2 - \mathbf{r}_1)\mathbf{q}\right] \times A_{\mathbf{q}s}^*(\mathbf{b}) A_{\mathbf{q}s}(\mathbf{b}') \frac{d^3q}{(2\pi\hbar)^3} \right|^2. \qquad (6)$$

It is seen that $\nu(\mathbf{r}_1, \mathbf{r}_2)$ is not a function of the difference of its arguments $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. Thus, for constant $\mathbf{r}$ the function $\nu(\mathbf{r}_1, \mathbf{r}_2)$ is periodic in $\mathbf{r}_1$, with periods equal to those of the crystal lattice.

Equation (6) generalizes the "density-density" correlation function of an electron gas in free space at $T = 0$. It is derived in the same way as the expression for the correlation function of a degenerate Fermi gas (cf. Ref. 2).

A characteristic feature of the correlation function of a degenerate electron gas at $T = 0$ is the nonexponential damping of oscillations with period $\hbar/2p_F$, where p_F is the radius of the Fermi-sphere (Friedel oscillations).[3] It can be said that Eq. (6) describes Friedel oscillations for the case of an electron gas in a metal.

The occurrence of nonexponentially damped correlations when r increases (where $r = |\mathbf{r}|$) is a consequence of the gradual filling of reciprocal space by electrons at $T = 0$. It is shown below that the complex shape of the FS leads not only to a change in the oscillation periods (in comparison with a free electron gas),[2,3] but also to their damping as $r \to \infty$.

The asymptotic behavior of the function $\nu(\mathbf{r}_1, \mathbf{r}_2)$ for large r is determined by the singularities of its Fourier-components $\nu(\mathbf{K}, \mathbf{k})$ as a function of $k = \mathbf{k} \cdot \mathbf{r}/r$ (V is the sample volume):

$$\nu(\mathbf{K}, \mathbf{k}) = \frac{1}{V^2} \int \nu(\mathbf{r}_1, \mathbf{r}_2) \exp(-i\mathbf{K}\mathbf{r}_1 - i\mathbf{k}\mathbf{r}) \, d^3r \, d^3r_1$$
$$= -\frac{2}{\bar{n}V} \sum \sum_{ss'} \iint A_{\mathbf{q}s}^*(\mathbf{b}_1) A_{\mathbf{q}s}(\mathbf{b}_2) A_{\mathbf{q}'s'}(\mathbf{b}_3) \times A_{\mathbf{q}'s'}^*(\mathbf{b}_4) n_{\mathbf{q}s} n_{\mathbf{q}'s'} \delta(\mathbf{q}' - \mathbf{q} + \hbar(\mathbf{k} - \mathbf{b})) \frac{d^3q' \, d^3q}{(2\pi\hbar)^3}. \qquad (7)$$

The second summation sign denotes summation over the reciprocal lattice vectors $\mathbf{b}$, $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, and $\mathbf{b}_4$ satisfying the condition $\mathbf{b} + \mathbf{b}_1 - \mathbf{b}_2 + \mathbf{b}_3 - \mathbf{b}_4 = 0$. Since $A_{\mathbf{q}s}(\mathbf{b}_i)$ is a smooth function of $\mathbf{q}$, we are dealing in fact with the singularities of the integrals, of the type

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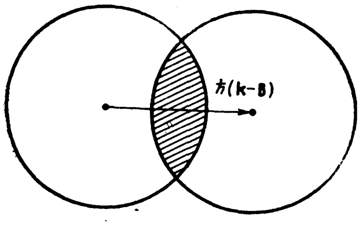


FIG. 1. Spherical Fermi surface and its shifted analog; volume of shaded region is the value of integral (8).

$$\Omega(\mathbf{k})=\int n_{\mathbf{q},s}n_{\mathbf{q}+\hbar(\mathbf{k}-\mathbf{b}),s'}\,d^3q, \tag{8}$$

where $\mathbf{b}$ is a reciprocal lattice vector. The value of the integral (8) is the volume of the intersection of the FS band s with the FS band s' shifted by $\hbar(\mathbf{k}-\mathbf{K})$ (this region is shaded in Fig. 1).

For simplicity it is assumed in the following that there exists only one conduction band in the metal, and the subscript s is omitted in all equations. The resultant equations can be easily extended to include a more general case.

For a given direction of the vector $\mathbf{r}$ the asymptote of the correlation function (6) is determined by the singularities of integral (8) taken over the two-component vector $\mathbf{k}_\perp=\mathbf{k}-k\mathbf{r}/r$, where $k=\mathbf{k}\cdot\mathbf{r}/r$, as a function of k. The k values at which the function

$$\Phi(k)=\int\Omega(\mathbf{k})\,d^2k_\perp$$

has singularities are those values of the wave vector components along the direction $\mathbf{r}/r$ for which the possibility appears (or disappears) of tangency (for some $\mathbf{k}_\perp$) of the FS to its shifted analog. We denote them by k_j. In the case of a free electron gas there exists only one k_j value, equal to $2p_F/\hbar$, determining the period of Friedel oscillations. In the general case the wave vectors of Friedel oscillations are the distances between the planes perpendicular to $\mathbf{r}$ and tangent to the FS.

The vectors in $\mathbf{q}$-space that join all possible pairs of points of planes tangent to the FS and parallel to each other determine not only the periods of the Friedel oscillations but also the values of wave vectors for which singularities are observed in the phonon spectrum. If the electron velocities are antiparallel at the tangency points, these are the well-known Migdal-Kohn singularities,[4,5] while if the velocities are parallel these are the commonly called Taylor singularities (see Refs. 6 and 7).

The use of expressions periodic in $\mathbf{q}$-space requires transition from the first Brillouin zone to an extended $\mathbf{q}$-space, and consequently the FS must be understood to mean a periodic surface[8] and not its portion within the first Brillouin zone.[2)] This fact alone complicates substantially the form of the correlation function and of the Friedel oscillations. We illustrate this with a simple example. Let the FS be a sphere (such as for Na, for example). At first glance this implies that, independently of the direction of $\mathbf{r}$, the wave period of Friedel oscillations is $\hbar/2p_F$ (as would have been the case for a Fermi-gas with an isotropic dispersion equation). From Fig. 2, however, it is seen that this is not the case: additional terms appear in the asymptote of the correlation function, while the wave-number oscillations corresponding to them depend substantially on the direction of the vector $\mathbf{r}$, and for

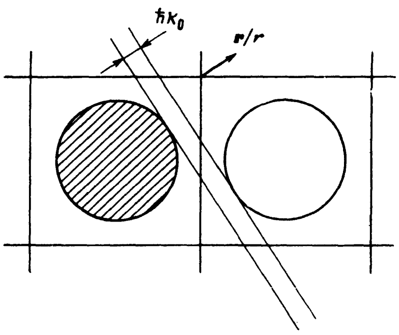


FIG. 2. Spherical Fermi surface periodically repeating in extended $\mathbf{q}$-space. Shaded part is the FS located in the first Brillouin zone. The asymptotic correlation function has a term oscillating with period $2\pi/k_0$, where $\hbar k_0$ is the distance between planes perpendicular to the direction of $\mathbf{r}/r$ and tangent to the FS at different cells of reciprocal space. The k_0 value depends on the direction of $\mathbf{r}/r$.

some of its directions they vanish linearly with the angle. These terms contain the coefficients $A_{\mathbf{q}}(\mathbf{b})$ in various combinations ($\mathbf{q}$ is located on the FS).

The law according to which Friedel oscillations decay as $r\to\infty$ (for a fixed direction of $\mathbf{r}$) is determined by the local FS geometry at the tangency points. Thus, if the FS is a sphere, the second derivative of the function $\nu(\mathbf{K},\mathbf{k})$ with respect to k has a jump at the singular points $\mathbf{k}_i$ (for example, at the point $\mathbf{K}_1=(\mathbf{r}/r)(2p_F/\hbar)$). In that case the damping of Friedel oscillations is determined by the factor r^{-4} (see Ref. 2). If the FS is cylindrical, and the vector $\mathbf{r}$ is perpendicular to its symmetry axis, the singularity of the function $\nu(\mathbf{K},\mathbf{k})$ is stronger (compare with Ref. 9): for $\mathbf{k}\to\mathbf{k}_i$

$$\partial\nu(\mathbf{K},\mathbf{k})/\partial k\propto|\mathbf{k}-\mathbf{k}_i|^{1/2},\quad \partial^2\nu(\mathbf{K},\mathbf{k})/\partial k^2\propto|\mathbf{k}-\mathbf{k}_i|^{-1/2}\to\infty. \tag{9}$$

In these cases the singularities of the quantities $\nu(\mathbf{K},\mathbf{k})$ as functions of k are alike at $\mathbf{k}=0$, namely, discontinuities of the first derivative.

It seems to us that in the considered problem of the effect of FS geometry on the correlation function of conduction electrons we must distinguish between two questions.

The first is the effect of the local FS geometry (the existence of parabolic points, flattening points, and so on),[10,11] manifested by the strong dependence of $\nu(\mathbf{r}_1,\mathbf{r}_2)$ on the direction of $\mathbf{r}/r$.

Section 2 is devoted to this question. The second is that of ETT effect on the correlation function (Sec. 4). The structure of the correlation function of conduction electrons is investigated primarily in Sec. 3.

In a comparatively crude description of an ETT due to formation of a new cavity, it can be sometimes assumed that a toroid, and not an ellipsoid, is formed.[12,13] How this affects the correlation function is considered in Sec. 5.

It is shown in Sec. 6 how the results of Sec. 2–5 can be used to investigate RKKY interactions.[14] Finally, in the concluding Sec. 7 we discuss the validity of the approach used and of the results.

The influence of local FS geometry and of topological and generalized topological transitions on the properties of metals has been discussed numerous times. Without being able to mention all the studies of this topic, we only point out several review articles, where the reader can find a relatively complete literature (see Refs. 10, 11, 15, 16), and we also point out one of the most recent publications known to us on the properties of metals during ETT.[17] The present paper is close in spirit to the articles quoted.

2. EFFECT OF LOCAL FS GEOMETRY ON THE FORM OF CORRELATION FUNCTIONS

According to (6), the correlation function is

$$\nu(\mathbf{r}_1,\mathbf{r}_2)=-\frac{1}{32\bar{n}\pi^6}\left|\sum_{\mathbf{b}\mathbf{b}'}\exp(-i\mathbf{b}\mathbf{r}_1+i\mathbf{b}'\mathbf{r}_2)I(\mathbf{b},\mathbf{b}',\mathbf{r})\right|^2, \tag{10}$$

where $\mathbf{r}=\mathbf{r}_2-\mathbf{r}_1$, while in the integral

$$I(\mathbf{b},\mathbf{b}',\mathbf{r})=\int e^{ikr}\left[\int A_{\hbar\mathbf{k}}^*(\mathbf{b})A_{\hbar\mathbf{k}}(\mathbf{b}')d^2k_\perp\right]dk \tag{11}$$

the integration is over the volume of the FS within the first Brillouin zone ($\mathbf{k}=\mathbf{q}/\hbar$, $k=\mathbf{k}\cdot\mathbf{r}/r$).

The asymptotic behavior of the function $\nu(\mathbf{r}_1,\mathbf{r}_2)$ at large r is determined by the singularities of the internal integral[3)] (over $\mathbf{k}_\perp$) as a function of k. Owing to the smoothness of the function $A_{hk}(\mathbf{b})$, these singularities coincide with those of the area $S(k,\varepsilon_F)$ of the intersection of the FS with the plane $k=$ const as k tends to k_j, where $k_j=\mathbf{k}_j\cdot\mathbf{r}/r$ and $\mathbf{k}_j=\mathbf{k}_j(\mathbf{r}/r)$ are tangency points of the FS with the secant plane. At large r the asymptote of integral (11) is

$$I(\mathbf{b},\mathbf{b}',\mathbf{r})\approx\sum_j A_{\hbar\mathbf{k}_j}^*(\mathbf{b})A_{\hbar\mathbf{k}_j}(\mathbf{b}')I_j(r)\exp(ik_jr). \tag{12}$$

Our task is to explain how the local FS geometry at the tangency point $\mathbf{k}=\mathbf{k}_j$ affects the shape of the function $I_j(r)$ corresponding to this point.

If the FS can be approximated near the tangency point by a second-order surface, this point is hyperbolic or elliptic.[18] We consider these and other cases in succession.

a) Hyperbolic point

We select the ξ_3 axis in $\mathbf{k}$-space along $\mathbf{r}/r$, so that $\xi_3=0$ at the tangency point ($k=k_h$). In the plane $\xi_3=0$ the ξ_1 and ξ_2 axes are selected along the FS lines of curvature.[18] The FS deflection from the plane $k=k_h$ near the tangency point is then

$$\xi_3(\xi_1,\xi_2)=-A\xi_1^2+B\xi_2^2,\quad AB>0. \tag{13}$$

We assume that $A>0$ and $B>0$.[4)] Besides, it is assumed [here and in Eqs. (26), (28), (32), (35) below] that $\varepsilon[\hbar(\mathbf{k}_h+\xi)]<\varepsilon_F$ with $\xi_3>\xi_3(\xi_1,\xi_2)$; in the opposite case the sign of the response must be reversed [see Eq. (24) below, and, correspondingly, Eqs. (27), (34), (38), (41)]. Following variable replacement we have

$$\xi_3=\rho^2-\eta^2. \tag{14}$$

Our purpose is to calculate the integral

$$\tilde{I}_h(r)=\int_{-\delta}^{\delta}e^{i\xi_3r}\left[\int d^2k_\perp\right]d\xi_3 \tag{15}$$

in a small neighborhood ($\delta\ll k_F$) of the point $\xi_3=0$. The integration over $d^2k_\perp$ is carried out over the area of the FS intersection with the plane $\xi_3=$ const. To distinguish the singularity of interest, one may take the integral not over the entire area of this cross section, but over a small portion of it, for which

$$\rho^2<\gamma,\quad \eta^2<\gamma\quad(\gamma>0,\quad \gamma\ll k_F). \tag{16}$$

Denoting the area of this part of the cross section by $S_\gamma(k_h+\xi_3,\varepsilon_F)$, one has

$$\tilde{I}_h(r)\approx\int_{-\delta}^{\delta}e^{i\xi_3r}S_\gamma(k_h+\xi_3,\varepsilon_F)d\xi_3. \tag{17}$$

In the neighborhood of the tangency point, where $|\xi_3|<\delta$ and condition (16) is satisfied, one may use Eq. (14):

$$(AB)^{1/2}S_\gamma=\begin{cases}2\gamma^{1/2}(\xi_3+\gamma)^{1/2}+\xi_3\ln\left|\dfrac{\gamma^{1/2}+(\xi_3+\gamma)^{1/2}}{-\gamma^{1/2}+(\xi_3+\gamma)^{1/2}}\right|, & \xi_3<0,\\[2ex] 4\gamma-2\gamma^{1/2}(\gamma-\xi_3)^{1/2}+\xi_3\ln\left|\dfrac{\gamma^{1/2}+(\gamma-\xi_3)^{1/2}}{-\gamma^{1/2}+(\gamma-\xi_3)^{1/2}}\right|, & \xi_3>0.\end{cases} \tag{18}$$

With the intention of calculating the leading term in the asymptote of the integral $\tilde{I}_h(r)$, we can retain in (17) only those terms of expression (18) for S_γ, whose singularity at $\xi_3=0$ is the most pronounced. Rewriting (17) in the form

$$\tilde{I}_h(r)\approx\int_0^\delta[e^{i\xi_3r}S_\gamma(k_h+\xi_3,\varepsilon_F)+e^{-i\xi_3r}S_\gamma(k_h-\xi_3,\varepsilon_F)]d\xi_3, \tag{19}$$

we have

$$\tilde{I}_h(r)\approx\frac{2i}{(AB)^{1/2}}\int_0^\delta\sin(\xi_3r)\cdot\xi_3\ln\left|\frac{(\gamma-\xi_3)^{1/2}+\gamma^{1/2}}{(\gamma-\xi_3)^{1/2}-\gamma^{1/2}}\right|d\xi_3. \tag{20}$$

Finally, putting $\delta\ll\gamma$, expanding the logarithmic argument in ξ_3/γ, and carrying out the integration,[5)] we obtain

$$I_h(r)\approx\frac{i\pi}{(AB)^{1/2}r^2}, \tag{21}$$

and the corresponding contribution to the asymptotic integral (11) is [see Eq. (12)]

$$A_{\hbar\mathbf{k}_h}^*(\mathbf{b})A_{\hbar\mathbf{k}_h}(\mathbf{b}')\exp(ik_hr+i\pi/2)\frac{\pi}{r^2(AB)^{1/2}}. \tag{22}$$

It is noted that the quantities A and B can be expressed in terms of the coefficients of the second quadratic FS form at the tangency point.[18]

We estimate the range of validity of the results (21), (22). For this it is necessary to determine when the terms discarded from (13) and (14) are, indeed, insignificant.

Let, for example,

$$\xi_3(\xi_1,\xi_2)=-A\xi_1^2+B\xi_2^2+C\xi_1^3, \tag{23}$$

i.e., following variable replacement we have

$$\xi_3=\rho^2-\eta^2+CA^{-3/2}\eta^3. \tag{24}$$

Estimating the correction appearing in the expression for S_γ, isolating in it the singular term, and requiring smallness of the contribution of this term to the integral $I_h(r)$, we obtain the condition

$$r \gg C^2/A^3. \qquad (25)$$

If the FS is such that there exists a single scale $\sim \hbar k_F$, we then obtain from (25) the condition $r \gg 1/k_F$ (see footnote[4]); in this case the validity conditions of Eqs. (27), (31), (33), (36) that will be derived below are similar.

We have treated in particular detail the case of a parabolic tangency point, so as to demonstrate the method of singularity extraction. Results similarly obtained for other cases are provided below.

b) Elliptic point

At an elliptic tangency point we have, instead of (13),

$$\xi_3(\xi_1, \xi_2) = A\xi_1^2 + B\xi_2^2. \qquad (26)$$

This case is much simpler than the preceding one. Instead of (21) one easily obtains:

$$I_e(r) = -\frac{\pi}{r^2 (AB)^{1/2}}. \qquad (27)$$

The validity condition (25) refers to this case as well.

c) Parabolic point

The regions of elliptic and hyperbolic points on the FS are separated by lines of parabolic points.

At a parabolic point one of the principal curvatures of the surface vanishes, and for the deviation of the FS from the tangent plane near the point of tangency one has

$$\xi_3(\xi_1, \xi_2) = C\xi_1^3 + B\xi_2^2; \qquad (28)$$

for definiteness it is assumed that $B > 0$.[6] We note that Eq. (28) has been written down for the case in which the tangency point is a parabolic point of general position [see Eq. (61) below]. Changing variables, we obtain

$$\xi_3 = \rho^3 + \eta^2. \qquad (29)$$

Further calculations are carried out as in the case of a hyperbolic point. We only note that in determining the quantity S_γ one must replace here (16) by

$$|\rho^3| < \gamma, \quad \eta^2 < \gamma. \qquad (30)$$

As a result, the function $I(r)$ in (12) corresponding to the parabolic tangency point is given by

$$I_p(r) \approx \frac{2\mathscr{K}[\sin(\pi/12)]\Gamma(5/6)}{3^{1/4}|C|^{1/3}B^{1/2}} r^{-11/6} e^{3\pi i/4}. \qquad (31)$$

Here Γ is an Euler integral of the second kind, and $\mathscr{K}$ is a complete elliptic integral ($\Gamma(5/6) \approx 0.94$, $\mathscr{K}[\sin(\pi/12)] \approx 1.60$).[19]

d) Flattening point upon "Crater" formation on the FS[10]

The Fermi surface possessing a flattening point can be separated into convex equal-energy surfaces and equal-energy surfaces with "craters." The flattening point is then a point to which small loops have contracted, meaning lines of parabolic points (Fig. 3). As a rule, a symmetry axis of the reciprocal lattice passes through such an FS point. If it is a two-, four-, or sixfold axis, the FS deviation from the tangent plane (being always a fourth order function of ξ_1, ξ_2) can be expressed near the flattening point in the form

$$\xi_3(\xi_1, \xi_2) = A\xi_1^4 + B\xi_2^4 + 2\Phi(|AB|)^{1/2}\xi_1^2\xi_2^2. \qquad (32)$$

If the symmetry axis is twofold, no conditions are imposed on the coefficients A, B, and Φ in (32); if it is fourfold, one must have $A = B$; and if it is sixfold we must also have $\Phi = 1$. We assume that the form (32) is sign-definite: $AB > 0$, $\Phi > -1$. The corresponding flattening point of the function $I(r)$ in Eq. (12) is then

$$I_{pl} \approx \left(\frac{\pi^2}{AB}\right)^{1/4} J r^{-3/2} e^{3\pi i/4}, \qquad (33)$$

where

$$J = \begin{cases} \mathscr{K}\left[\left(\frac{1-\Phi}{2}\right)^{1/2}\right], & \Phi \leq 1, \\ \left(\frac{2}{\Phi+1}\right)^{1/2} \mathscr{K}\left[\left(\frac{\Phi-1}{\Phi+1}\right)^{1/2}\right], & \Phi > 1. \end{cases} \qquad (34)$$

It is understood that not any fourth order form can be reduced to (32), but, obviously, the power of r is independent of the specific form of (32).

e) Intersection point of lines of parabolic points

Even though lines of parabolic points do not intersect in the ETT model considered in Sec. 3, such intersections may indeed occur due to FS "corrugation," as well as in a generalized topological transition.[20] Let the FS deflection from the tangent plane, described by a third order form, be

$$\xi_3(\xi_1, \xi_2) = C\xi_1^3 + D\xi_2^3. \qquad (35)$$

As in the preceding subsection, we consider a particular case convenient for our purposes.

The corresponding function $I(r)$ in the asymptotic expansion (12) is

$$I_{0r}(r) \approx \frac{2\alpha\Gamma(2/3)}{3(CD)^{1/3}} r^{-5/3} e^{5\pi i/6}, \qquad (36)$$

where

$$\alpha = \int_{-\infty}^{\infty} [(1-\xi^3)^{1/3} + \xi] d\xi \approx 2{,}65. \qquad (37)$$

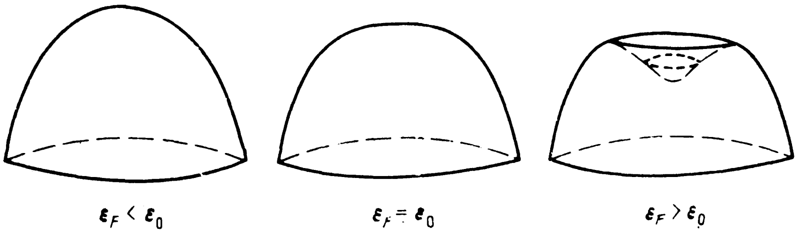


FIG. 3. "Crater" formation on the FS. A flattening point exists for $\varepsilon_F = \varepsilon_0$ at the FS, and a crater for $\varepsilon_F > \varepsilon_0$. The thick dashed line is the line of parabolic points, existing for $\varepsilon_F > \varepsilon_0$.

Concluding this list of different types of tangency points, we note that in Sec. 5 we will encounter a situation in which the FS is tangent to a plane not at an isolated point, but along lines of parabolic points.

3. STRUCTURE OF ELECTRON CORRELATION FUNCTIONS IN A METAL

Using the results derived above one can, in principle, write down the asymptote of the function $\nu(\mathbf{r}_1,\mathbf{r}_2)$ at large $r=|\mathbf{r}_2-\mathbf{r}_1|$, given the crystal structure and the FS shape. This quantity, however, depends on its arguments in a very complex manner. We first average it over $\mathbf{r}_1$:

$$\nu(\mathbf{r})=\frac{1}{v}\int \nu(\mathbf{r}_1,\mathbf{r}_1+\mathbf{r})d\mathbf{r}_1, \qquad (38)$$

where the integration is carried out over the volume v of a unit cell. We have

$$\nu(\mathbf{r})\doteq-\frac{1}{32\bar{n}\pi^6}\sum \exp[i(\mathbf{b}_2-\mathbf{b}_4)\mathbf{r}]I(\mathbf{b}_1,\mathbf{b}_2,\mathbf{r})I^*(\mathbf{b}_3,\mathbf{b}_4,\mathbf{r}), \qquad (39)$$

with the summation performed over the reciprocal-lattice vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, and $\mathbf{b}_4$ satisfying the condition $-\mathbf{b}_1+\mathbf{b}_2+\mathbf{b}_3-\mathbf{b}_4=0$.

For a given direction of the vector $\mathbf{r}$, let some points $\varkappa_j$ from among all the tangency points $\mathbf{k}_i$ of the FS with planes perpendicular to the radius-vector be close to each other: $|\varkappa_j-\varkappa_l|\ll k_F$. It is precisely this case which is of interest to us in Secs. 4–6 below: near the ETT points the FS has either small cavities (if the ETT is due to formation of a new cavity), or, in any case, small extremal diameters.

Let, furthermore, the point $\varkappa_j$ be located far away from all other tangency points $\mathbf{K}_l$:

$$|\varkappa_j-\mathbf{K}_l+\mathbf{b}|\gtrsim k_F,$$

where $\mathbf{b}$ is some reciprocal lattice vector,[7] and point $\mathbf{K}_l$ are far from each other:

$$|\mathbf{K}_l-\mathbf{K}_m+\mathbf{b}|\gtrsim k_F \text{ when } l\neq m.$$

At large r the asymptote of the correlation function $\nu(\mathbf{r})$ is a sum of oscillating contributions from all possible pairs of tangency points in the extended $\mathbf{k}$-space and of monotonically decreasing terms resulting from the singularities of the Fourier-component of the correlation function (7) at $\mathbf{k}=0$. The pairs of tangency points can be separated into three groups.

1) Those pairs of tangency points for which the distance between the corresponding planes tangent to the FS is large:

$$|k_j-k_l+\mathbf{b}'\mathbf{r}/r|\gtrsim k_F,\quad k_j=\mathbf{k}_j\mathbf{r}/r,$$

where $\mathbf{b}'$ is some reciprocal-lattice vector. We recall that $\mathbf{k}_j$ can be one of the points K_l, or one of the points $\varkappa_m$.

2) Pairs of tangency points far from each other, for which the corresponding tangent planes are close:

$$|\mathbf{k}_j-\mathbf{k}_l+\mathbf{b}'|\gtrsim k_F,\quad |k_j-k_l+\mathbf{b}'\mathbf{r}/r|\ll k_F. \qquad (40)$$

3) Pairs of points $\varkappa_j$ close to each other.

Correspondingly, the asymptote of the function $\nu(\mathbf{r})$ is conveniently represented as a sum of three terms:

$$\nu(\mathbf{r})=\nu_0(\mathbf{r})+\nu_1(\mathbf{r})+\nu_{an}(\mathbf{r}), \qquad (41)$$

the first of which containing contributions from the first group of pairs of tangency points, the second—from the second group, and the third—from pairs of points $\varkappa_j$.

The monotonically decreasing terms in $\nu(\mathbf{r})$ are sums of contributions of those pairs of points $\mathbf{k}_i$, $\mathbf{k}_j$, for which

$$k_i=k_j+\mathbf{b}'\mathbf{r}/r. \qquad (42)$$

If in that case $\mathbf{k}_i=\mathbf{k}_j$ and it is one of the points $\mathbf{K}_l$, while $\mathbf{b}'=0$, we shall assume that the corresponding term enters in the function $\nu_0(\mathbf{r})$. If $\mathbf{b}'=0$, and the points $\mathbf{k}_i$ and $\mathbf{k}_j$ enter in a group of points $\mathbf{k}_l$ that are close to each other, then we include the corresponding contribution in $\nu_{\text{an}}(\mathbf{r})$. In the other cases, we will assume that this pair of points gives a contribution to $\nu_1(\mathbf{r})$.

The function $\nu_0(\mathbf{r})$ contains the Friedel oscillations with small periods (the wave vector is $\gtrsim k_F$). Taking an average over $\Delta r\sim k_F^{-1}$, we obtain the expression for its mean value

$$\langle\nu_0(\mathbf{r})\rangle=-\frac{1}{32\bar{n}\pi^6}\sum_l |I_l(r)|^2, \qquad (43)$$

where l specifies the points $\mathbf{K}_l$. We recall that the monotonically decreasing functions $I_i(r)$ and $I_l(r)$ depend on the direction of $\mathbf{r}$.

If there are no parabolic or other singular points among the points $\mathbf{K}_l$, then $\langle\nu_0(\mathbf{r})\rangle$ will decrease as r^{-4} as $r\to\infty$.

Let us consider the function $\nu_1(\mathbf{r})$, which contains long-period contributions from the pairs of widely separated tangency points [see Eq. (40)]. In particular, these may be the tangency points which lie in different cells of the reciprocal space. It is easy to see that the corresponding terms in the function $\nu_1(\mathbf{r})$ contain factors of the type

$$A_{\mathbf{q}_1}(\mathbf{b})A_{\mathbf{q}_2}(\mathbf{b}+\mathbf{b}'), \qquad (44)$$

where $\mathbf{b}'$ is the reciprocal-lattice vector which links the cell centers. The coefficients $A_q(\mathbf{b})$ obey the normalization condition

$$\sum_{\mathbf{b}} |A_{\mathbf{q}}(\mathbf{b})|^2=1, \qquad (45)$$

therefore the quantity (41) decreases quickly with increasing $(\mathbf{b}')$. Thus, only the terms corresponding to the first $b'\neq 0$ are important.

For a given direction of the vector $\mathbf{r}$ let some pair of tangency points satisfy condition (40). If the change of the angle specifying the direction of the vector $\mathbf{r}$, is of the order of unity, we obtain instead of (40)

$$|k_j-k_l+\mathbf{b}'\mathbf{r}/r|\gtrsim k_F,$$

i.e., the contribution of this pair of tangency points becomes a short-period one and appears not in $\nu_1(\mathbf{r})$ but in $\nu_0(\mathbf{r})$.

Thus, we reach the following conclusion: the function $\nu_1(\mathbf{r})$, containing long-period oscillations, differs substantially from zero only if the angles specifying the direction of the vector $\mathbf{r}$ are contained in quite narrow intervals. A characteristic feature of the oscillations contained in $\nu_1(r)$ is that upon approaching some specific direction of the radius-vector their wave number vanishes linearly with the angle. In that case additional monotonically decreasing terms appear in $\nu_1(r)$.

The third term in the right-hand side of Eq. (41), which we call the anomalous part of the correlation function, contains long-period oscillations resulting from pairs of tangency points $\varkappa_j$ adjacent to each other. Using Eqs. (12) and

(45), we obtain the following expression for the asymptote of the anomalous part:

$$\nu_{an}(\mathbf{r}) = -\frac{1}{32\bar{n}\pi^6}\sum_{jj'} I_j(r)I_{j'}^*(r)\exp[i(\varkappa_j-\varkappa_{j'})r]. \quad (46)$$

We note that if for a given direction of $\mathbf{r}/r$ there exist not one but several groups of adjacent tangency points, the results of the present section remain valid, except that the anomalous part of the correlation function must be understood to be the quantity

$$\nu_{an}(\mathbf{r}) = \sum_l \nu_{an}^{(l)}(\mathbf{r}),$$

$$\nu_{an}^{(l)}(\mathbf{r}) = -\frac{1}{32\bar{n}\pi^6}\sum_{jj'} I_j(r)I_{j'}^*(r)\exp[i(\varkappa_j^{(l)}-\varkappa_{j'}^{(l)})r].$$

Here the superscript l numbers groups of adjacent tangency points, and the subscripts j and j' number tangency points belonging to the lth group. It is assumed here that tangency points belonging to different groups are sufficiently far from each other: for $l \neq l'$ we have the inequality $|\varkappa_j^{(l)} - \varkappa_{j'}^{(l')} + \mathbf{b}| \gtrsim k_F$, where $\mathbf{b}$ is a reciprocal-lattice vector. The following two sections are devoted to an investigation of the anomalous part of the correlation function when its generation results from proximity to an ETT.

4. FORM OF ANOMALOUS PART OF THE CORRELATION FUNCTION NEAR ETT POINTS

Owing to the presence of extremal FS cross sections of a small diameter, the function $\nu(\mathbf{r})$ contains near an ETT point[1] long-wave terms. This means that averaging over distances of the order of k_F^{-1} does not remove the oscillations of $\nu(\mathbf{r})$.

If the variation in the FS topology consists of the appearance (or disappearance) of FS cavities, the anomalous part (46) of the correlation function (41) containing these oscillations decreases as r^{-4} regardless of the direction of $\mathbf{r}$. In that case the anomalous terms can be obtained, by changing variables, from the standard expression for the correlation function of an isotropic Fermi-gas (Ref. 21)[8)]

Less trivial is the case in which the ETT results from a break (generation) of an FS bridge. It is assumed that near a saddle point $\mathbf{q}_{cr}$ of the dispersion relation $\varepsilon(\mathbf{q})$ the FS can be approximated by a surface of revolution symmetric with respect to a plane perpendicular to the axis of rotation and passing through the point $\mathbf{q}_{cr}$. It is, thus, described by the equation

$$z \approx \frac{p_\perp^2}{2m_\perp} - \frac{p_3^2}{2m_\parallel} + \frac{\beta}{4m_\parallel^2}p_3^4, \quad [\beta] = \mathrm{erg}^{-1}, \qquad (47)$$

where

$$z = \varepsilon_F - \varepsilon_{cr}, \quad \varepsilon_{cr} = \varepsilon(\mathbf{q}_{cr}), \qquad (48)$$

$m_\perp$ and $m_\parallel$ are the electron effective masses at the origin $\mathbf{q}_{cr}$ of the vector $\mathbf{p}$. For simplicity it is assumed below that $m_\perp > 0$, $m_\parallel > 0$, and $\mathbf{q}_{cr} = 0$. It follows from Eq. (47) that the electron bridge of the FS existing at $z > 0$ is absent at $z < 0$.

In the following it is assumed that

$$|\beta z|^{1/2} \ll 1. \qquad (49)$$

In Fig. 4 (see Ref. 21) we show the shape of the FS near the point $\mathbf{p} = 0$ for different signs of z and β.

We calculate now the anomalous terms $\nu_{an}(\mathbf{r})$ (46) of the correlation function $\nu(\mathbf{r})$ by using Eqs. (11) and (12). As shown in Sec. 1, the wave numbers $\varkappa_i - \varkappa_j$ describing the oscillations of these terms about r are the distances between the tangents to the FS planes perpendicular to $\mathbf{r}$. These planes, the distances between them, and the tangency points themselves are easily found for any value of the angle θ between the vector $\mathbf{r}$ and the p_3 axis.[9)] Next, using the obvious fact that one of the principal directions on a surface of revolution always lies in a plane containing the revolution axis, one can describe with the required accuracy the FS deflec-

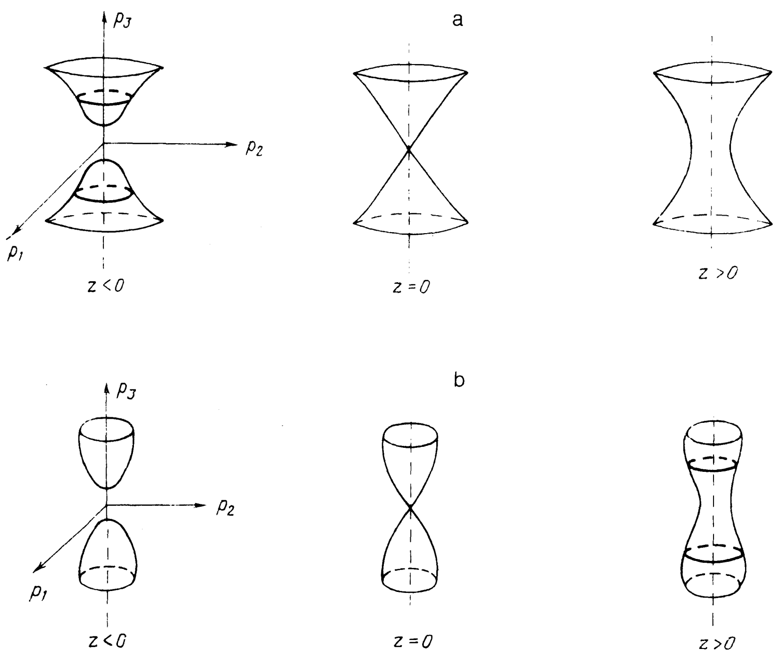
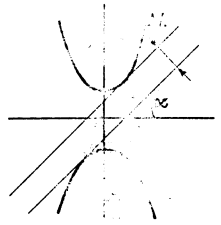
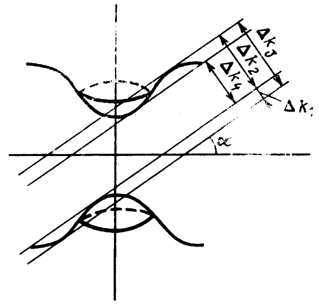


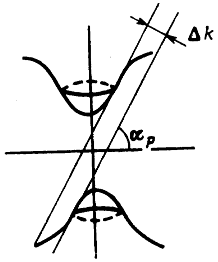
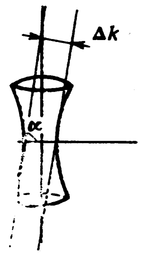
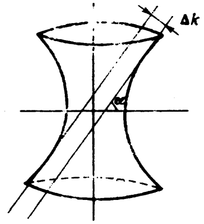
FIG. 4. Disappearance (a) and appearance (b) of line of parabolic points during bridge formation (marked by thick lines).[21]

TABLE I.

Sign of z and range of angle values	Estimate of periods Λ and $\nu_{an}(R,\alpha)$ oscillations	Estimate of amplitude of $\nu_{an}(R,\alpha)$ oscillations	Diagram
$z<0$, $1-\mathrm{tg}\,\alpha \gg \lvert\beta z\rvert^{1/2}$	$\Lambda \propto (\lvert z\rvert \cos 2\alpha)^{-1/2}$	$\dfrac{m_\perp^2 m_\parallel}{\bar{n}R^4}\,\dfrac{\lvert z\rvert}{\cos^2 2\alpha}$	
$z<0$, $2\Delta\alpha < -(3\beta z)^{1/2}$ $\left\lvert \dfrac{2\Delta\alpha}{(3\beta z)^{1/2}}+1\right\rvert \ll 1$	$\Lambda_1 \propto \lvert z\rvert^{-3/4}\lvert\beta\rvert^{-1/4}\cdot \left\lvert \dfrac{2\Delta\alpha}{(3\beta z)^{1/2}}+1\right\rvert^{-3/2}$, $\Lambda_2 \propto \lvert z\rvert^{-3/4}\lvert\beta\rvert^{-1/4}$, $\Lambda_{3,4} = (\Lambda_2^{-1} \pm \Lambda_1^{-1})^{-1}$	$\dfrac{m_\perp^2 m_\parallel}{\bar{n}\lvert\beta\rvert} R^{-4}\cdot \left\lvert \dfrac{2\Delta\alpha}{(3\beta z)^{1/2}}+1\right\rvert^{-1/2}$ (for all Λ_j)	

(*continued*)

TABLE I.—Continued

Sign of z and range of angle values	Estimate of periods Λ and $\nu_{an}(R,\alpha)$ oscillations	Estimate of amplitude of $\nu_{an}(R,\alpha)$ oscillations	Diagram
$z<0$, $2\Delta\alpha=-(3\beta z)^{1/2}$	$\Lambda\propto\lvert z\rvert^{-3/4}\lvert\beta\rvert^{-1/4}$	$\frac{m_\perp^2 m_\parallel}{\bar n}\lvert z\rvert^{1/4}\lvert\beta\rvert^{-11/12}R^{-11/3}$	
$z<0,\ 2\Delta\alpha>-(3\beta z)^{1/2}$	—	$\nu_{an}(R,\alpha)\approx 0$	—
$z>0$, $\mathrm{tg}\,\alpha-1\gg\lvert\beta z\rvert^{1/2}$	$\Lambda\propto(z\lvert\cos 2\alpha\rvert)^{-1/2}$	$\frac{m_\perp^2 m_\parallel}{\bar n R^4}\ \frac{z}{\cos^2 2\alpha}$	
$z>0$, $2\lvert\Delta\alpha\rvert\lessapprox\lvert\beta z\rvert^{1/2}$	$\Lambda\propto z^{-3/4}\lvert\beta\rvert^{-1/4}\times\left\lvert\frac{2\Delta\alpha}{\lvert\beta z\rvert^{1/2}}+1\right\rvert^{-1}$	$\frac{m_\perp^2 m_\parallel}{\bar n\beta}R^{-4}$	

Notation: $\Delta k_i=2\pi/\Lambda_i$ wave numbers of oscillations of $\nu_{an}(R,\alpha)$; the thick lines in the diagrams are lines of parabolic points. The tangency points are parabolic for $d=dp$, where $dp=\Delta dp+\pi/4$; see Eq. (53).

tion from the tangent plane near tangency points and, thus, find the coefficients in Eqs. (13), (23), (26), and (28). Calculating then by using Eqs. (21), (27), and (31) the corresponding tangency points $\varkappa_i$ of the function $I_i(r)$, which determine the asymptote (12) of integral (11), one obtains from Eq. (46) an expression for $\nu_{\rm an}(\mathbf{r})$.

The results of these calculations for different angles θ $(0<\theta<\pi/2)$ and $\beta<0$ are given in Table I.[10] The equations are given in the Appendix. The following notation is used ($\hbar=1$):

$$\operatorname{tg}\alpha=\left(\frac{m_\perp}{m_\parallel}\right)^{1/2}\operatorname{tg}\theta, \tag{50}$$

$$R=(2m_\parallel\cos^2\theta+2m_\perp\sin^2\theta)^{1/2}r, \tag{51}$$

$$\Delta\alpha=\alpha-\pi/4. \tag{52}$$

Table I lists order-of-magnitude estimates for the spatial oscillation periods of the anomalous term of the correlation function and for the amplitudes of these oscillations.[11] These results are valid for R values much larger than the largest period (for given θ, z, β) of the spatial oscillations of the function $\nu(R,\alpha)$. The last column of the table shows schematically the corresponding planes tangent to the FS. The complete equations for $\nu_{\rm an}(R,\alpha)$ are gathered in the Appendix.

It is seen from Table I that both the amplitude and the oscillation periods of the anomalous term $\nu_{\rm an}(\mathbf{r})$ depend substantially on the direction of the radius vector. This dependence is radically changed when the sign of z is reversed: the replacement $z\to -z$ is similar in some sense to the formal replacement $\alpha\to\pi/2-\alpha, \beta\to-\beta$ (the latter denotes a transition to another crystal). Upon approaching the ETT point (i.e., with decreasing $|z|$) the oscillation wave-length naturally increases.

Lines of parabolic points (see Fig. 4) appear on the FS near the point $\mathbf{q}_{\rm cr}$ when $\beta z>0$. The tangency points (Sec. 2) are parabolic for

$$\Delta\alpha=\Delta\alpha_p=\begin{cases}-\dfrac{1}{2}(3\beta z)^{1/2}, & z<0,\\[2mm] \dfrac{1}{2}(3\beta z)^{1/2}, & z>0.\end{cases} \tag{53}$$

For angles $\Delta\alpha$ near $\Delta\alpha_p$ the form of the function $\nu_{\rm an}(\mathbf{r})$ changes correspondingly. When α approaches $\Delta\alpha_p+\pi/4$ from the same side as $\Delta\alpha\cdot\Delta\alpha_p>\frac{3}{4}\beta z$, two tangency points appear near each line of parabolic points. Thus, in this case the number of planes perpendicular to the vector $\mathbf{r}$ and tangent to the FS near the point $\mathbf{q}_{\rm cr}$, is equal to four. When $\alpha\to\Delta\alpha_p+\pi/4$ the tangency points approach each other, while the period of the corresponding oscillations in $\nu_{\rm an}(\mathbf{r})$ increases like $|\Delta\alpha-\Delta\alpha_p|^{-3/2}$ (see Table I). If the angle α is located on the other side of $\Delta\alpha_p+\pi/4$, the plane tangent to the FS near the point $\mathbf{q}_{\rm cr}$ does not exist at all. Consequently, there exist no corresponding long-wave oscillations.

If the direction of the vector $\mathbf{r}$ corresponds to the parabolic tangency point (53), the anomalous terms decrease with increasing r like $r^{-11/3}$, i.e., more slowly than the basic term ν_0 [see Eqs. (43), (45); $\nu_0(\mathbf{r})$ decreases like r^{-4} as $r\to\infty$].

We note that for $\beta z<0$, when there are no parabolic points near $\mathbf{q}_{\rm cr}$, there exists an angle

$$\Delta\alpha_0=\begin{cases}\frac{1}{2}|\beta z|^{1/2}, & z<0,\\ -\frac{1}{2}|\beta z|^{1/2}, & z>0,\end{cases} \tag{54}$$

at which both tangential planes coincide,[12] and thus $\nu_{\rm an}(\mathbf{r})$ is a monotonically decreasing function of r if $\Delta\alpha=\Delta\alpha_0$.

The wave number corresponding to oscillations of $\nu_{\rm an}(\mathbf{r})$ as a function of r reaches, at $z<0$, its maximum (at $z=$ const) value $(2m_\parallel|z|)^{1/2}/\hbar\ll k_F$ when the vector $\mathbf{r}$ is directed along the $\mathbf{p}_3$ axis ($\theta=0$). If $z<0$, a maximum will be reached at $\theta\approx\pi/2$ (i.e., $\mathbf{r}\perp\mathbf{p}_3$).

As mentioned in Sec. 3, along with the fundamental term $\nu_0(\mathbf{r})$ [Eq. (41)] (containing short-period oscillations) and the anomalous term $\nu_{\rm an}(\mathbf{r})$ (both in the presence of ETT and in its absence), for some directions of $\mathbf{r}$ there appears in the function $\nu(\mathbf{r})$ one more term containing long-wave oscillations. The wave number of these oscillations can correspond to a distance between planes tangent to the FS at different unit cells of reciprocal space, or tangent to different FS cavities in one and the same cell, and at any rate vanishing linearly with angle. For variation of the angle θ by less than or by an order of unity the wave number reaches values of the order of k_F, and, thus, the corresponding term drops out of the correlation function averaged over $\Delta r\sim k_F^{-1}$. These are so to speak "random" long-period oscillations. The long-period oscillations contained in $\nu_{\rm an}(\mathbf{r})$ behave differently. Their main characteristic feature is rearrangement under ETT action (when the sign of the parameter z is reversed).

If several FS bridges are generated (broken) in a unit cell of the reciprocal lattice simultaneously at $\varepsilon_F=\varepsilon_{\rm cr}$ the anomalous term in the function $\nu(\mathbf{r})$ is (see Sec. 3)

$$\nu_{an}(\mathbf{r})=\sum_i\nu_{an}^{(i)}(\mathbf{r}), \tag{55}$$

where the superscript i labels the points $q_{\rm cr}^{(i)}$, and the function $\nu_{\rm an}^{(i)}(\mathbf{r})$ should be selected from the Appendix.

In the approximate dispersion relation (47) of an electron near a critical point we have assumed that near the point $\mathbf{q}_{\rm cr}$ the FS can be approximated by a mirror-symmetric surface. Generally speaking, this occurs only if $\mathbf{q}_{\rm cr}$ is an enhanced-symmetry point. In all remaining cases it is not justified to neglect the cubic term in the expansion of z in the quasimomentum $\mathbf{p}$, i.e., instead of (47) one must write (it is assumed, as previously, that the FS can be approximated by a surface of revolution)

$$z\approx\frac{p_\perp^2}{2m_\perp}-\frac{p_3^2}{2m_\parallel}+\frac{\gamma}{(2m_\parallel)^{3/2}}p_3^3,\qquad [\gamma]=\mathrm{erg}^{-1/2}. \tag{56}$$

Assuming that z is quite small, we have omitted the term containing p_3^4: for this case the FS near the point $\mathbf{q}_{\rm cr}$ is shown in Fig. 5.

We assume that the following inequality is valid

$$|z\gamma^2|^{1/3}\ll 1. \tag{57}$$

Expressions for $\nu_{\rm an}(\mathbf{r})$ are given in the Appendix for various directions of $\mathbf{r}$.

We note that from the geometrical point of view this case differs from the preceding one in that, besides the dependences on the signs of γ and z near the point $\mathbf{q}_{\rm cr}$, there always exists one line of parabolic points (see Fig. 5). There-

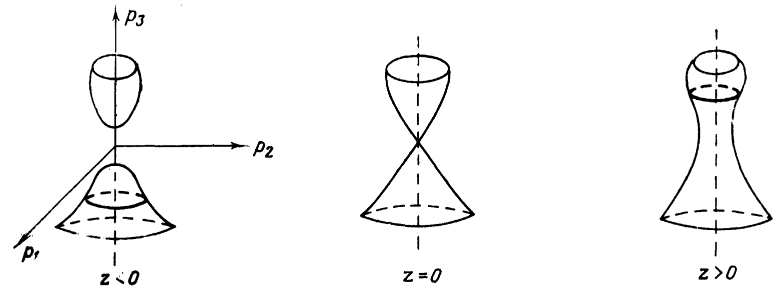


FIG. 5. Formation of nonsymmetric FS bridge [see Eq. (56) with $\gamma>0$ in text]. The heavy lines are lines of parabolic points.

fore, if the vector $\mathbf{r}$ is parallel to the normal to the FS at a parabolic point:

$$\Delta\alpha_{cr}={}^3/_4(z\gamma^2)^{1/3}, \qquad (58)$$

then only one of the two adjacent tangency points $\varkappa_{1,2}$ is parabolic; as a result, the long-period term in the function $\nu_{an}(\mathbf{r})$ decreases like $r^{-11/6}r^{-2}=r^{-23/6}=r^{-4+1/6}$ as $r\to\infty$.

In this section we have assumed that even if several cavities or several bridges are generated in a topological transition, they are quite far from each other. In wurtzite-type crystals two ETTs are located near each other. Several ellipsoids are generated as a result of the first and coalesce into a toroidal surface as a result of the second.[12,13] It can be assumed somewhat roughly that a toroidal FS cavity is formed directly (as a result of a single transition). In the following section we consider the effect of such a transition on the properties of the correlation function.

5. LOOP OF EXTREMA OF THE DISPERSION RELATION

Let an extremum of the dispersion relation be continuously degenerate, i.e., the extremum points form a line in reciprocal space. In that case the ETT is manifested more sharply than in the case of isolated extremum points, for instead of having a square-root singularity ($\propto(\varepsilon-\varepsilon_{cr})^{1/2}$) the electron density of states changes jumpwise at the point $\varepsilon=\varepsilon_{cr}$.[22]

If the line of extrema corresponds to a minimum (maximum) of the dispersion relation $\varepsilon(\mathbf{q})$, then for $\varepsilon>\varepsilon_{cr}$ ($\varepsilon<\varepsilon_{cr}$) a new FS cavity in the shape of a tube is generated. If the line of extrema is a closed curve, or if it is infinite in extended reciprocal space, it can be stated that lines of parabolic points exist on this tube. We recall that lines of parabolic points are generated near an isolated extremum point only if the extremum is a saddle point.

Consider the case in which the line of minima of the dispersion relation in reciprocal space is a circle, and the dispersion relation near it is

$$z\equiv\varepsilon-\varepsilon_{cr}=\frac{(p_\perp-p_0)^2}{2m_\perp}+\frac{p_3^2}{2m_\parallel}, \qquad (59)$$

where $m_\parallel>0$ and $m_\perp>0$ are the effective masses, and the third-coordinate axis of the dependent variable is perpendicular to the plane containing the line of extrema—a circle of radius p_0 (Fig. 6).

We shall assume that

$$(2m_\perp z)^{1/2}<p_0,\quad p_0-(2m_\perp z)^{1/2}\leqslant p_0, \qquad (60)$$

so that the FS tube has the shape of a torus; the lines of parabolic points are two circles with $p_\perp=p_0$ and $p_3=\pm(2m_\parallel z)^{1/2}$; from the mirror symmetry of the FS tube with respect to the plane containing the p_3 axis it follows that these points cannot be parabolic points of general form [see (28)]. Indeed, the FS deflection from the tangential plane near a parabolic tangency point is given here by the following equation:

$$\xi_3(\xi_1,\xi_2)=A\xi_1^2+B\xi_2^4+C\xi_1\xi_2^2, \qquad (61)$$

where the ξ_1 and ξ_2 axes are respectively parallel and tangent to the radius of the circle of extrema.

We present expressions for the anomalous term $\nu_{an}(\mathbf{r})$ in the correlation function $\nu(\mathbf{r})$ (41). If the vector $\mathbf{r}$ is directed along the p_3 axis ($\theta=0$), then we obtain by exact integration in a cylindrical coordinate system

$$\nu_{an}(\mathbf{r})=-\frac{m_\perp p_0^2 z}{\hbar\pi^2r^2}\{J_1[r(2m_\parallel z)^{1/2}]\}^2, \qquad (62)$$

where J_1 is a Bessel function and $\hbar=1$. For $r(2m_\parallel z)^{1/2}\gg1$ we obtain from (62)

$$\nu_{an}(R,\alpha)\approx-\frac{4}{\hbar}m_\parallel m_\perp\frac{p_0^2z^{1/2}}{\pi^3R^3}\cos^2\left(Rz^{1/2}-\frac{3\pi}{4}\right), \qquad (63)$$

where the notation (50), (51) is used. Proceeding as in Sec. 3, we have[13] for $\pi/2>\alpha>0$

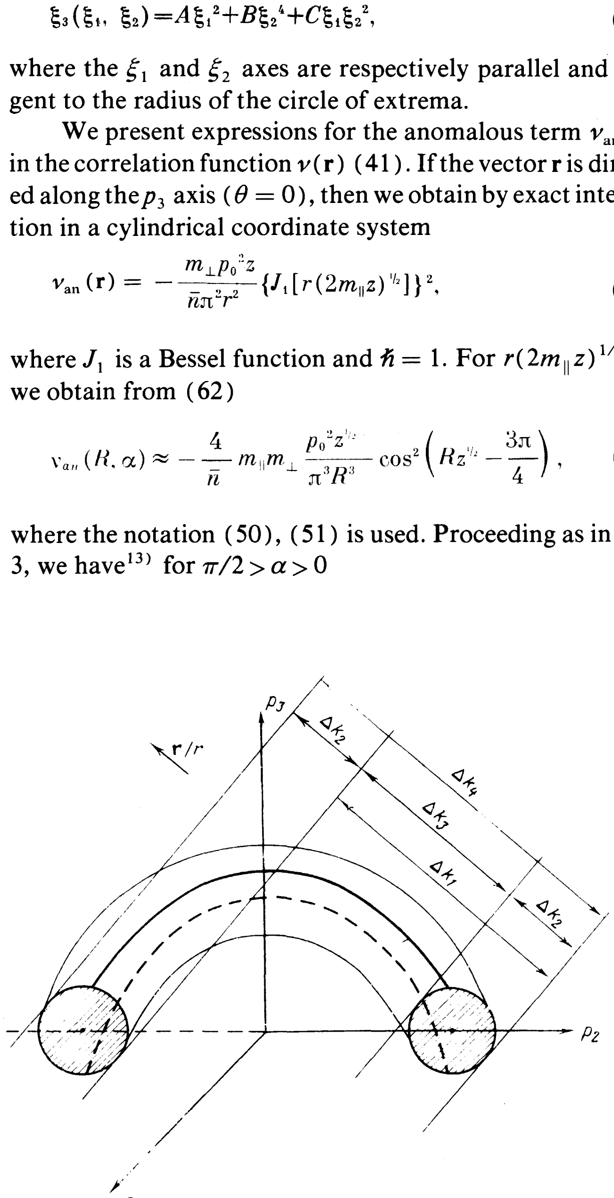


FIG. 6. Toroidal FS cavity in the case $m_\parallel=m_\perp$ [see Eq. (59)]. The thick lines are lines of parabolic points; Δk_i are wave numbers of oscillations of $\nu_{an}(\mathbf{r})$ for a given direction of $\mathbf{r}/r$; the "small diameter" is $\Delta k_2\propto z^{1/2}$.

$$\nu_{an}(R,\alpha)\approx-\frac{4m_\parallel m_\perp{}^2 z}{\pi^4 R^4\sin\alpha}\{[p_0/(2m_\perp)^{1/2}+z^{1/2}\sin\alpha]^{1/2}$$

$$\times\cos[R(p_0\sin\alpha/(2m_\perp)^{1/2}+z^{1/2})]$$

$$+[p_0/(2m_\perp)^{1/2}-z^{1/2}\sin\alpha]^{1/2}\sin[R(p_0\sin\alpha/(2m_\perp)^{1/2}-z^{1/2})]\}^2. \tag{64}$$

The validity range of this expression is:

$$R\gg(z^{1/2}\sin^2\alpha)^{-1}. \tag{65}$$

One of the oscillation wave numbers $\mathfrak{R}(\alpha)$ tends to zero linearly: $\mathfrak{R}(\alpha)\propto\alpha-\alpha_{cr}$, where α_{cr} satisfies the condition

$$\sin\alpha_{cr}=(2m_\perp z)^{1/2}/p_0. \tag{66}$$

We note that for all angles α there exist oscillations with a wave number $\propto 2z^{1/2}$, as is also obvious from Fig. 6.

If the tangency points are parabolic ($\theta=0$), then $\nu_{an}(\mathbf{r})$ decreases as r^{-3} with increasing r, i.e., more slowly than the principal term in (41).

6. STRUCTURE OF RKKY INTERACTION NEAR ETT POINTS

In the preceding sections we found the asymptotic form of the pair correlation function near an ETT point. These results make it possible to calculate the exchange integral within the model of RKKY-interaction between the spins of two atoms located at large distances from each other.

Let the energy of exchange inteaction between a conduction electron and ions or atoms of a magnetic impurity be

$$\mathscr{H}=-(J/\hbar)\sum_i\boldsymbol{\sigma}\mathbf{S}_i\delta(\mathbf{r}-\mathbf{r}_i). \tag{67}$$

Here $\boldsymbol{\sigma}$ are Pauli matrices, and $\mathbf{S}_i$ is the spin of an ion located at site $\mathbf{r}_i$.

Within second-order perturbation theory, the interaction (67) determines the exchange interaction of atomic spins.[23] The Hamiltonian describing this exchange interaction

$$E_{SS}=\sum J_{RKKY}(\mathbf{r}_{ik})\mathbf{S}_i\mathbf{S}_k,\quad \mathbf{r}_{ik}=\mathbf{r}_k-\mathbf{r}_i, \tag{68}$$

is called the RKKY interaction.

The Ruderman-Kittel exchange integral $J_{RKKY}(\mathbf{r})$ is specified by the expression

$$J_{RKKY}(\mathbf{r})=-2\left(\frac{J}{\hbar}\right)^2\int\frac{n_\mathbf{q}(1-n_{\mathbf{q}'})}{\varepsilon(\mathbf{q})-\varepsilon(\mathbf{q}')}$$

$$\times\exp\left[\frac{i}{\hbar}(\mathbf{q}-\mathbf{q}')\mathbf{r}\right]\frac{d^3q\,d^3q'}{(2\pi\hbar)^6}. \tag{69}$$

For rare-earth metals $J\propto(\Theta\varepsilon_F)$, where Θ is the magnetic-transition temperature.[24]

It must be noted that the periodic field of the crystal lattice is not taken into account in the derivation of Eq. (69).[23] Accordingly, the electron wave function is resolved into de Broglie waves, not Bloch waves. Thus, strictly speaking, expression (69) is not applicable to conduction electrons in a metal, but is applicable to a Fermi gas with an arbitrary dispersion relation. It is easy to write down an equation valid for a conduction-electron gas, as was done for the correlation function [see Eq. (3)]. The exchange integral $J_{RKKY}(\mathbf{r}_1,\mathbf{r}_2)$ is then not a function of the difference of its arguments (see Sec. 1), and so on. We will use just expression (69), since it is simpler. However, Eq. (73) (see below), which relates the asymptotic $J_{RKKY}(\mathbf{r})$ to the asymptotic correlation function, and obtained by us for a Fermi gas with an arbitrary dispersion relation, is also valid for conduction electrons.

The Fourier transform of $J_{RKKY}(\mathbf{r})$ is

$$J_{RKKY}(\mathbf{k})=-2\left(\frac{J}{\hbar}\right)^2\int\frac{n_\mathbf{q}(1-n_{\mathbf{q}-\hbar\mathbf{k}})}{\varepsilon(\mathbf{q})-\varepsilon(\mathbf{q}-\hbar\mathbf{k})}\frac{d^3q}{(2\pi\hbar)^3}. \tag{70}$$

Integrals of type (70) are often encountered in the study of effects related to the electron-phonon interaction; their behavior has been investigated in detail. They have singularities at vectors $\mathbf{k}$ corresponding to tangency of an FS with its analog shifted by $\hbar\mathbf{k}$. Two types of tangency are distinguished in this case:

1) The electron velocities at the tangency points are antiparallel—the Migdal-Kohn singularity.[4,5]

2) Parallel velocities—Taylor singularities.[7]

Consider initially the first case, and turn to Eq. (69). Let the electron velocity vector $\mathbf{v}_{\mathbf{q}0}$ at some point $\mathbf{q}_0$ on the FS be parallel to the radius-vector $\mathbf{r}$ whose direction is assumed below to be fixed. The asymptotic behavior of the quantity $J_{RKKY}(\mathbf{r})$ is determined at large r by the singularities of its Fourier transforms $J_{RKKY}(\mathbf{k})$ as functions of $k=\mathbf{k}\cdot\mathbf{r}/r$. This singularity corresponds, in particular, to the tangency of the FS to its analog shifted by $2\mathbf{q}_0$ (we assume that $\mathbf{q}=0$ in the symmetry center of the FS). We change variables in (69):

$$\begin{aligned}\mathbf{q}&=\mathbf{q}_0+\mathbf{p}-\boldsymbol{\xi},\\ \mathbf{q}'&=-\mathbf{q}_0+\mathbf{p}-\boldsymbol{\xi}.\end{aligned} \tag{71}$$

Since we are interested only in the asymptote of the integral (69), it is clear we can restrict the integration there to a small neighborhood of the singular point: $p,\xi\ll q_0$. Expanding the denominator of the integrand we have

$$J_{RKKY}(\mathbf{r})\approx-\frac{1}{(2\pi\hbar)^6}\exp\left(2\frac{i}{\hbar}\mathbf{q}_0\mathbf{r}\right)\int\frac{n_{\mathbf{q}_0+\mathbf{p}-\boldsymbol{\xi}}(1-n_{\mathbf{p}-\mathbf{q}_0+\boldsymbol{\xi}})}{\mathbf{v}_{\mathbf{q}0}\mathbf{p}}$$

$$\times d^3p\exp\left(-2\frac{i}{\hbar}\boldsymbol{\xi}\mathbf{r}\right)d^3\xi. \tag{72}$$

We initially integrate over $d^2p_\perp$, where $\mathbf{p}_\perp=\mathbf{p}-p_\parallel\mathbf{n}$ and $p_\parallel=\mathbf{p}\mathbf{n}$, and the unit vector $\mathbf{n}=\mathbf{r}/r$ coincides in direction with the outward normal to the FS at the point $\mathbf{q}_0$. If the point $\mathbf{q}_0$ is elliptic or hyperbolic, it is clear from geometric considerations (see Fig. 7) that we obtain subsequently in the numerator of (72) a difference of areas of intersections of the FS with planes perpendicular to $\mathbf{n}$.[14)] In turn, these areas can be found in this case by differentiating the Fourier-transforms $\nu(\mathbf{k})$ of the correlation function $\nu(\mathbf{r})$ with respect to $\mathbf{k}$ (we recall that the Fourier-transform of the correlation function is the volume of the FS intersection with its shifted analog; it was already noted above that in the present section we consider the model of a Fermi gas with an arbitrary dispersion relation, when $\nu(\mathbf{r}_1,\mathbf{r}_2)=\nu(\mathbf{r}_2-\mathbf{r}_1)$ and $\nu(\mathbf{K},\mathbf{k})$ (7) are independent of $\mathbf{K}$—see Ref. 2). Thus, for the area $S(x_\parallel)$ of the FS intersection with a plane parallel to the plane tangent to the FS at the point $\mathbf{q}_0$ and spaced a distance $x=\mathbf{x}\mathbf{n}$ from it, we obtain

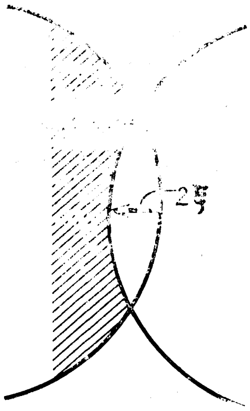


FIG. 7. The region in which the integrand expression in Eq. (72) is nonvanishing is shaded (the case of an elliptic tangency point).

$$S(x_\parallel)=i\frac{\bar{n}}{2}\mathbf{n}(2\pi\hbar)^3\int \mathbf{r}\nu(\mathbf{r})\exp\left[-2\frac{i}{\hbar}(\mathbf{q}_0+\mathbf{x})\mathbf{r}\right]dV, \quad (73)$$

where the vector $\mathbf{x}_\perp = \mathbf{x} - x_\parallel \mathbf{n}$ can, obviously, be assumed to be arbitrary: the relative shift of the FS and of its analog shifted by $2\mathbf{q}_0 - \mathbf{n}x_\parallel$ in a direction perpendicular to $\mathbf{n}$ adds, obviously, a higher-order correction to Eq. (73). Substituting (73) into (72), we find

$$J_{\mathrm{RKKY}}(\mathbf{r})=-\frac{i}{2\hbar(2\pi\hbar)^3}\frac{J^2}{\bar{n}}\exp\left(2\frac{i}{\hbar}\mathbf{q}_0\mathbf{r}\right)$$
$$\times\frac{\mathbf{n}}{v_{\mathbf{q}_0}}\int\left\{\mathbf{r}'\nu(\mathbf{r}')\int\left[\exp\left(-2\frac{i}{\hbar}\mathbf{q}_0\mathbf{r}'+2\frac{i}{\hbar}\boldsymbol{\xi}\mathbf{r}'\right)\right.\right.$$
$$\times\int\frac{1}{p_\parallel}\left[\exp\left(-\frac{i}{\hbar}p_\parallel r\right)-\exp\left(\frac{i}{\hbar}p_\parallel r\right)\right]$$
$$\left.\left.\times dp_\parallel\exp\left(-2\frac{i}{\hbar}\boldsymbol{\xi}\mathbf{r}\right)\right]d^3\xi\right\}dV'. \quad (74)$$

The integration over p is carried out from $-\infty$ to 0, and the integral over ξ reduces to $\delta(\mathbf{r}-\mathbf{r}')$. We finally have

$$J^{(2q_0)}_{\mathrm{RKKY}}(\mathbf{r})\approx-\frac{\pi J^2}{2v_{\mathbf{q}_0}\bar{n}\hbar}r\nu^{(2q_0)}(\mathbf{r}). \quad (75)$$

Here $J^{(2q_0)}{}_{\mathrm{RKKY}}(\mathbf{r})$ and $\nu^{(2q_0)}(\mathbf{r})$ are the terms in the asymptotes of the Ruderman-Kittel integral and of the correlation function, and oscillate with a period $\hbar/(2\mathbf{q}_0\mathbf{n})$.[15]

We apply Eq. (75) to the case of an ETT resulting from broken symmetry of an FS bridge [see Sec. 4 above, Eq. (47)]. Using the expressions (see the Appendix) for $\nu_{\mathrm{an}}(\mathbf{r})$, and calculating the velocity $v_{\mathbf{q}0}$ at the tangency points, we find the anomalous part $J^{(\mathrm{an})}{}_{\mathrm{RKKY}}(\mathbf{r})$ of the Ruderman-Kittel exchange integral (as mentioned above, the form of J_{RKKY} is more complicated in the transition to conduction electrons; the anomalous part can be separated in exactly the same manner as in Sec. 3 for the correlation function). Thus, for $z<0$, $1-\tan\alpha \gg |\beta z|^{1/2}$ or $z>0$, $\tan\alpha - 1 \gg |\beta z|^{1/2}$ [using the notation of Eqs. (50)–(52)] we obtain[16]

$$J^{(an)}_{\mathrm{RKKY}}(R,\alpha)\approx\left(\frac{J}{\bar{n}}\right)^2\frac{m_\perp{}^2 m_\parallel}{2\pi^3}\left|\frac{z}{\cos^3 2\alpha}\right|^{1/2}$$
$$\times R^{-3}\cos(2R|z\cos 2\alpha|^{1/2}). \quad (76)$$

It is seen that when the sign of z is reversed $J^{(\mathrm{an})}_{\mathrm{RKKY}}(R,\alpha)$ behaves as if it were rotated through an angle $\pi/2$.

As indicated in Sec. 4, when $\beta z > 0$ and $\Delta\alpha = \Delta\alpha_p$ [see Eq. (53)] the tangency points become parabolic; when the tangency points approach a parabolic point, long-wave terms are generated in $\nu_{\mathrm{an}}(\mathbf{r})$, whose period becomes infinite when $\Delta\alpha = \Delta\alpha_p$. It is seen from Table I that these terms correspond to Taylor singularities. To write down the corresponding terms in J_{RKKY} it is initially necessary to find an equation relating $J^{(\delta q)}_{\mathrm{RKKY}}(\mathbf{r})$ with $\nu^{(\delta q)}(\mathbf{r})$ in the case of a Taylor singularity.

Instead of (71) we make the following change of variables in the integral (69):

$$\mathbf{q}=\mathbf{q}_0+\mathbf{p}-\boldsymbol{\xi},$$
$$\mathbf{q}'=\mathbf{q}_0-\delta\mathbf{q}+\mathbf{p}+\boldsymbol{\xi}. \quad (77)$$

Here $\delta\mathbf{q}$ is a vector joining the corresponding tangency points:

$$\mathbf{v}_{\mathbf{q}_0}=\mathbf{v}_{\mathbf{q}_0-\delta\mathbf{q}}. \quad (78)$$

Expanding in the denominator of the integrand, we obtain[17]

$$J^{(\delta q)}_{\mathrm{RKKY}}(\mathbf{r})=\left(\frac{J}{\bar{n}}\right)^2\exp\left(\frac{i}{\hbar}\mathbf{r}\delta\mathbf{q}\right)\int\frac{n_{\mathbf{q}_0+\mathbf{p}-\boldsymbol{\xi}}(1-n_{\mathbf{q}_0-\delta\mathbf{q}+\mathbf{p}+\boldsymbol{\xi}})}{v_{\mathbf{q}_0}\xi_\parallel}$$
$$\times\exp\left(-2\frac{i}{\hbar}\boldsymbol{\xi}\mathbf{r}\right)\frac{d^3p\,d^3\xi}{(2\pi\hbar)^6}, \quad (79)$$

where $\xi_\parallel = \xi\mathbf{r}/r$. Multiplying both sides of Eq. (79) by $\exp(-i\mathbf{r}\cdot\delta\mathbf{q}/\hbar)$ and differentiating with respect to r for a constant dierction of $\mathbf{r}/r$, we find

$$\frac{\partial}{\partial r}\left[J^{(\delta q)}_{\mathrm{RKKY}}(\mathbf{r})\exp\left(-\frac{i}{\hbar}\mathbf{r}\delta\mathbf{q}\right)\right]$$
$$=-\frac{2i}{\hbar v_{\mathbf{q}_0}}\left(\frac{J}{\bar{n}}\right)^2\int n_{\mathbf{q}_0+\mathbf{p}-\boldsymbol{\xi}}(1-n_{\mathbf{q}_0-\delta\mathbf{q}+\mathbf{p}+\boldsymbol{\xi}})$$
$$\times\exp\left(-2\frac{i}{\hbar}\boldsymbol{\xi}\mathbf{r}\right)\frac{d^3p\,d^3\xi}{(2\pi\hbar)^6}. \quad (80)$$

Following integration over $\mathbf{p}$, the first term in the integrand in the right hand side of Eq. (80) is independent of ξ, and thus does not contribute to the asymptote of $J_{\mathrm{RKKY}}(\mathbf{r})$ at large $|r|$. Following integration over $\mathbf{p}$ and $\boldsymbol{\xi}$, the second term is proportional to $\exp(-ir\delta\mathbf{q}/\hbar)\nu^{(\delta q)}(\mathbf{r})$. Assuming that $r\gg\hbar/(\mathbf{n}\delta\mathbf{q})$, we obtain following integration over r the required equation:

$$J^{(\delta q)}_{\mathrm{RKKY}}(\mathbf{r})=-\frac{i}{2\hbar v_{\mathbf{q}_0}}\frac{J^2}{\bar{n}}\int\nu^{(\delta q)}(\mathbf{r})dr=\frac{i}{2\hbar v_{\mathbf{q}_0}}\frac{J^2}{\bar{n}}\frac{r}{L-1}\nu^{(\delta q)}(\mathbf{r}), \quad (81)$$

where L is the power of r and determines the damping of oscillations of the correlation function as $r\to\infty$:

$$\nu^{(\delta q)}(\mathbf{r})\propto\frac{1}{r^L}\exp\left(\frac{i}{\hbar}\mathbf{r}\delta\mathbf{q}\right).$$

In the case of an ETT resulting from a broken symmetric FS bridge, when the tangency point comes close to parabolic, we obtain from Eqs. (81) and (A3) (see the Appendix) for the long-wave term in $J^{(\mathrm{an})}_{\mathrm{RKKY}}(R,\alpha)$ at $z<0$ and $\beta<0$:

$$J_{\mathrm{RKKY}}^{(an)}(R,\alpha)=\frac{2^{3/2}}{9\pi^4}\frac{m_\perp^2 m_\|}{|\beta|}\left(\frac{J}{\bar n}\right)^2\left(\frac{3\beta}{z}\right)^{1/4}(\varphi^2-1)^{-1/2}R^{-3}$$

$$\times\cos\left[2|\beta|\left(\frac{z}{3\beta}\right)^{3/4}|\varphi+1|^{3/2}R\right],\qquad \varphi=\frac{\mathrm{tg}\,\alpha-1}{(3\beta z)^{1/2}},$$

$$\varphi<-1,\quad |\varphi+1|\ll 1. \tag{82}$$

Since the denominator of (81) contains the small quantity v_{q0}, expression (82) contains the factor $|z|^{-1/4}$.

If the tangency point coincides with the parabolic point itself,[18)] it is not sufficient to restrict oneself to the first expansion term in the denominator of the integrand of Eq. (69). Evidently, it can be stated that [in analogy with Eqs. (75) and (81)] that the damping of the oscillations of the corresponding term in $J_{\mathrm{RKKY}}^{(an)}(\mathbf{r})$ is determined in this case by the factor $r^{-8/3}$.

It is well known[14,24] that the magnetic ordering resulting from the RKKY interaction is intimately connected with the FS geometry. In particular, it was noted that the period of the helicoid is determined by one of the small extremal diameters of the FS.[24] The results suggest that ETT can be accompanied by major changes in the magnetic state.

7. CONCLUSIONS

1. As noted in the Introduction, the treatment above does not include temperature effects and the influence of finite lifetimes of electron states. It can be shown[2,3] that both lead to similar results: exponential decay of the correlation function as $r\to\infty$. In other words, all equations derived above for the asymptotes of $\nu(\mathbf{r})$ must contain an additional factor of the order of $\exp(-r/l_{\mathrm{eff}})$, where $l_{\mathrm{eff}}\approx v_F\tau_{\mathrm{eff}}$ and $\hbar/\tau_{\mathrm{eff}}\sim T+\hbar/\tau$, with τ the mean free path time, T the temperature, and v_F the electron velocity at the FS. It is hence clear that, to observe long-period oscillations of $\nu(\mathbf{r})$ it is required to use quite perfect single crystals at very low temperatures. Besides, one must keep in mind that without taking into account the finite temperature ($T\neq 0$) and the finite electron-state lifetimes ($\tau\neq\infty$), one cannot "reach" the ETT arbitrarily closely. All equations containing the transition parameter z (describing the proximity to ETT) are valid for $|z|\gg\hbar/\tau_{\mathrm{eff}}$.

2. The whole treatment was done within the gas approximation (without accounting for the electron-electron interaction). Since electrons at and near the FS participate in all the effects investigated, we assume that a transition to a Fermi-fluid description will not change the results qualitatively, and will apparently only lead to renormalization of the coefficients in the equations obtained (for comparison see §23, 25 of Ref. 8 and Ref. 26).

3. Elucidation of the connection between the structure of the correlation function and the FS geometry has led to detection of long-period oscillations, as well as to establishment of a dependence of the asymptotic behavior on the local FS structure. To be sure, one must keep in mind that the nature of the decrease of $\nu(\mathbf{r})$ as $r\to\infty$ (aasuming that $l_{\mathrm{eff}}=\infty$) depends weakly on the FS geometry. Indeed, in the "best" case of a toroidal FS $\nu(r)\propto r^{-3}$, as against $\nu(r)\propto r^{-4}$ in the standard case (see Secs. 2 and 5).

4. Knowledge of the correlation function of conduction electrons in a metal is necessary for the construction and understanding of the theory of various effects in metals: alloying, screening,[27] exchange magnetism, and others. We have provided one example showing how an asymptote of the Ruderman-Kittel exchange integral is expressed in terms of an asymptote of the correlation function.

5. Metallic crystals are traditionally described in two "supplementary" spaces:

a) coordinate $\mathbf{r}$-space, where most attention is paid to the structure of the crystal cell, to the electron density distribution, and so on;

b) momentum $\mathbf{p}$-space, where the main role is played by the Fermi surface.

The correlation function of conduction electrons clearly shows the connection between the $\mathbf{r}$- and $\mathbf{p}$-spaces: the characteristic singularities of the correlation function are a consequence of the FS geometry. This is clearly manifested in the ETT. We recall that the ETT in $\mathbf{p}$-space is a local "event": at one point $\mathbf{p}=\mathbf{p}_{\mathrm{cr}}$ there appears a new infinitesimal FS cavity, or—again at one point—an FS bridge occurs (or is broken). Major restructuring of the correlation function occurs then in $\mathbf{r}$-space. This alone has seemed to us a worthy topic of discussion.

We are grateful to M. Yu. Kagan and L. P. Pitaevskiĭ for their interest in our study and for stimulating discussions, as well as to O. V. Tapatun for assistance in preparing this manuscript for publication.

APPENDIX

We present expressions for the anomalous parts of the correlation function near ETT points. In that case we use the notation of (50)–(52) in a system of units in which $\hbar=1$. The validity conditions for all expressions written below for $\nu_{\mathrm{an}}(R,\alpha)$ are written in the form $rk_{\min}(\alpha,z)\gg 1$ (cf. Sec. 4).

We consider initially the case of a broken symmetric FS bridge [see Eqs. (47), (49)]. We introduce the notation

$$\varphi=\frac{\mathrm{tg}\,\alpha-1}{(3|\beta z|)^{1/2}}. \tag{A1}$$

1. Let $z<0$. For $\varphi<0$ and $|\varphi|\gg 1$ we then have

$$\nu_{an}(R,\alpha)=-\frac{4m_\perp^2 m_\|}{\pi^4\bar n}\frac{|z|}{R^4\cos^2 2\alpha}\cos^2[R(|z|\cos 2\alpha)^{1/2}], \tag{A2}$$

for $\beta<0$, $\varphi<-1$, and $|\varphi+1|\ll 1$ we obtain[19)]

$$\nu_{an}(R,\alpha)=\frac{8m_\perp^2 m_\|}{3\pi^4\bar n|\beta|}(\varphi^2-1)^{-1/2}R^{-4}$$

$$\times\left[\sin\left(2|\beta|\left|\frac{z}{3\beta}\right|^{3/4}|\varphi+1|^{3/2}R\right)+\varphi\right], \tag{A3}$$

for $\beta<0$ and $\varphi=-1$ (parabolic tangency point):

$$\nu_{an}(R,\alpha)=-\frac{16m_\perp^2 m_\|}{\pi^6\bar n}6^{1/6}\left(\frac{z}{3\beta}\right)^{1/4}|3\beta|^{-2/3}R^{-11/3}$$

$$\times\left[\mathscr{K}\left(\sin\frac{\pi}{12}\right)\Gamma(5/6)\right]^2\cos^2\left[2|\beta|\left(\frac{z}{3\beta}\right)^{3/4}R-\frac{\pi}{4}\right] \tag{A4}$$

and for $\beta>0$ and $|\varphi|\lesssim 1$:

$$\nu_{an}(R,\alpha)=-\frac{8m_\perp^2 m_\|}{3\pi^4\bar n\beta}\frac{(\varphi^2+1)^{1/2}+\varphi}{(\varphi^2+1)^{1/2}}R^{-4}$$

$$\times\cos^2\left\{2^{1/2}\beta\left|\frac{z}{3\beta}\right|^{3/4}\frac{|1-\varphi(\varphi^2-1)^{1/2}-\varphi^2|}{[(\varphi^2+1)^{1/2}+\varphi]^{1/2}}R\right\}. \tag{A5}$$

2. Let now $z>0$. For $\psi \gg 1$ we obtain

$$\nu_{an}(R,\alpha)=-\frac{4m_\perp{}^2m_\parallel}{\pi^4\bar{n}}\frac{z}{R^4\cos^2 2\alpha}\sin^2[R(z|\cos 2\alpha|)^{1/2}], \tag{A6}$$

for $\beta<0$ and $|\varphi|\lesssim 1$:

$$\nu_{an}(R,\alpha)=-\frac{8m_\perp{}^2m_\parallel}{3\pi^4\bar{n}|\beta|}\frac{(\varphi^2+1)^{1/2}-\varphi}{(\varphi^2+1)^{1/2}}R^{-4}$$
$$\times\sin^2\left\{2^{1/2}\beta\left|\frac{z}{3\beta}\right|^{3/4}\frac{|1+\varphi(\varphi^2-1)^{1/2}-\varphi^2|}{[(\varphi^2+1)^{1/2}-\varphi]^{1/2}}R\right\}, \tag{A7}$$

for $\beta>0$ and $\varphi=1$: (parabolic tangency point):

$$\nu_{an}(R,\alpha)=-\frac{16m_\perp{}^2m_\parallel}{\pi^6\bar{n}}6^{1/6}\left(\frac{z}{3\beta}\right)^{1/4}(3\beta)^{-2/3}R^{-11/3}$$
$$\times\left(\mathcal{K}\left(\sin\frac{\pi}{12}\right)\Gamma(5/6)\right)^2\cos^2\left[2\beta\left(\frac{z}{3\beta}\right)^{3/4}R+\frac{\pi}{4}\right] \tag{A8}$$

and for $\beta>0$, $\varphi>1$, and $\varphi-1\ll 1$:

$$\nu_{an}(R,\alpha)=-\frac{8m_\perp{}^2m_\parallel}{3\pi^4\bar{n}\beta}(\varphi^2-1)^{-1/2}R^{-4}$$
$$\times\left\{\sin\left[2\beta\left(\frac{z}{3\beta}\right)^{3/4}|\varphi-1|^{3/2}R\right]+\varphi\right\}. \tag{A9}$$

We turn now to the case of breaking a nonsymmetric FS bridge [see Eqs. (56) and (57)]. We introduce the notation:

$$\psi=\frac{2}{3}\frac{\operatorname{tg}\alpha-1}{(z\gamma^2)^{1/3}}. \tag{A10}$$

Regardless of the signs of z and γ, we then obtain for $\psi>1$ and $|\psi-1|\ll 1$

$$\nu_{an}(R,\alpha)=-\frac{2^{1/2}m_\perp{}^2m_\parallel}{3\bar{n}\pi^4R^4}\left|\frac{z}{\gamma^4}\right|^{1/3}\left\{\frac{1}{3}+\frac{4}{(\psi-1)^{1/2}}\right.$$
$$\left.-\frac{4}{(\psi-1)^{1/2}}\sin[2^{-1/2}|\gamma z^2|^{1/3}(\psi-1)^{3/2}R]\right\}. \tag{A11}$$

This result has been averaged over $\Delta R\sim|\gamma z^2|^{-1/3}$.

For $\psi=1$ (parabolic and elliptic or parabolic and hyperbolic tangency points) we have

$$\nu_{an}(R,\alpha)=-\frac{m_\perp{}^2m_\parallel}{\bar{n}\pi^6}\left\{\frac{2^{1/2}\pi^2}{9}\left|\frac{z}{\gamma^4}\right|^{1/3}R^{-4}\right.$$
$$+\frac{4\cdot 2^{2/3}}{3^{1/2}}\left[\mathcal{K}\left(\sin\frac{\pi}{12}\right)\Gamma\left(\frac{5}{6}\right)\right]^2|\gamma|^{-11/9}|z|^{5/9}R^{-11/3}$$
$$+4\cdot 2^{7/12}\cdot 3^{-5/4}\pi\left|\frac{z}{\gamma}\right|^{4/9}|\gamma|^{-5/6}\mathcal{K}\left(\sin\frac{\pi}{12}\right)$$
$$\left.\times\Gamma\left(\frac{5}{6}\right)R^{-23/6}\cos\left[\frac{27}{8\cdot 2^{1/2}}(|\gamma|z^2)^{1/3}R+\frac{3\pi}{4}\right]\right\}. \tag{A12}$$

For $\psi<1$ it seems that near the point $\mathbf{q}_{cr}$ there exists only one plane tangent to the FS and perpendicular to the vector $\mathbf{r}$. As a result $\nu_{an}(R,\alpha)$ is a monotonically decreasing function of R:

$$\nu_{an}(R,\alpha)=-\frac{2^{1/2}m_\perp{}^2m_\parallel}{9\bar{n}\pi^4}\left|\frac{z}{\gamma^4}\right|^{1/3}R^{-4}. \tag{A13}$$

This equation is valid for $1-\psi\ll 1$ and $R\gg|\gamma z^2|^{-1/3}$.

Finally, for $z<0$ and $1-\tan\alpha\gg|z\gamma^2|$, or for $z>0$ and $\tan\alpha-1\gg(z\gamma^2)^{1/3}(\tan\alpha)^{1/3}$ one may neglect the cubic term in Eq. (56); expression (A2) or (A6), respectively, is obtained for $\nu_{an}(R,\alpha)$.

1) Moscow State University.

2) To avoid misunderstandings we emphasize that the FS, consisting of one cavity when only the first Brillouin zone is used, is a surface having an infinite number of cavities, each in its own unit cell of reciprocal space. The integration over $\mathbf{q}$ is always performed in the first Brillouin zone (see below).

3) In the present section we find it more convenient to treat the singularities of the correlation function, rather than the singularities of its Fourier-components, which were discussed in Sec. 1. The two approaches are, naturally, equivalent, but the treatment of $\nu(\mathbf{r}_1,\mathbf{r}_2)$ (10) itself is simpler, since it requires the study of tangency to the FS by a plane (see below), and not by its shifted analog (see Sec. 1). This approach is possible because, according to Eq. (10), the function $\nu(\mathbf{r}_1,\mathbf{r}_2)$ can be expressed in terms of the square of the absolute value of the integral (11).

4) If the FS sizes are determined by a single scale, the Fermi momentum hk_F, then obviously $|A|\sim|B|\sim k_F^{-1}$. Similarly, the total nth order derivative of ξ_3 is in this case $\sim k_F^{1-n}$.

5) In that case we must construct those terms, whose asymptotes at $r\delta\gg 1$ contain $e^{\pm ir\delta}$. These terms are obviously unrelated to the singularity considered, and do not appear in the asymptotic integral (11).

6) If $B<0$, one obtains instead of Eq. (31) the complex conjugate of this quantity with the opposite sign: $-I_p^*(r)$.

7) In this section it is assumed that the points $\mathbf{k}_j$ are located in the first Brillouin zone.

8) This expression is:

$$\nu_{is}(r)\approx\frac{3\hbar}{2\pi^2p_Fr^4}\cos^2\frac{p_Fr}{\hbar},\quad r\gg\hbar/p_F,$$

where p_F is the Fermi momentum. The FS cavities are in general ellipsoids, leading naturally to the appearance of angular dependence of the correlation function.

9) Note that for $\beta=0$ and $\tan\theta=\pm(m_\parallel/m_\perp)^{1/2}$ the tangency point goes off to infinity. It is precisely this nonphysical singularity which leads to the necessity of including fourth-order terms in (46).

10) Similar results can be obtained from Table I for the case $\beta>0$, replacing α by $\pi/2-\alpha$ and z by $-z$ (see below).

11) It turns out that the monotonic term in $\nu_{an}(\mathbf{r})$ is always of the same order as the oscillation amplitude (see the Appendix).

12) As $\Delta\alpha\to\Delta\alpha_0$ the wave number of the $\nu_{an}(\mathbf{r})$ oscillations vanishes linearly with $|\Delta\alpha-\Delta\alpha_0|$ as a function of r.

13) When $p_0\sin d\pm(2m_\perp z)^{1/2}\sim k_F$ the tangency points are separated into two groups far from each other, and expression (64) must be averaged over $\Delta R\sim m_\perp^{1/2}/k_F$.

14) This is always the case if the intersection of the FS with its shifted analog is a planar curve. In that case one of the surfaces is inside the other on either side of the plane containing this curve. Thus, the difference of areas in the numerator of Eq. (72) is also obtained if $\mathbf{q}_0$ is the flattening point due to crater formation on the FS (see Sec. 2) or a parabolic point on a toroidal FS cavity (Sec. 5). This is not case, for example, for a parabolic point of general type (Sec. 2).

15) We note that, generally speaking, J_{RKKY} does not contain monotonic terms.[23]

16) It is seen from the figures in Table I that we have here a Migdal-Kohn singularity.

17) Here and below we denote by $J_{\mathrm{RKKY}}^{(\delta q)}(\mathbf{r})$ and $\nu^{(\delta q)}(\mathbf{r})$ the terms containing the factor $\exp(i\mathbf{r}\cdot\delta\mathbf{q}/h)$ in the asymptotes of the Ruderman-Kittel integral and correlation function, respectively.

18) With an ensuing Migdal-Kohn singularity (see Table I).

19) An averaging over $\Delta R\sim(\beta/z)^{3/4}/|\beta|$ has been carried out in Eqs. (A3) and (A9) (see below).

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