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Spontaneous breaking of four-fold rotational symmetry in two-dimensional electronic systems explained as a continuous topological transition

M. V. Zverev[+1)], *J. W. Clark*[*], *Z. Nussinov*[*], *V. A. Khodel*[+*1)]

[+]*Russian Research Centre Kurchatov Institute, 123182 Moscow, Russia*

[*]*McDonnell Center for the Space Science and Department of Physics, Washington University, St.Louis, USA*

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The Fermi liquid approach is applied to the problem of spontaneous violation of the C_4 symmetry in strongly correlated two-dimensional electronic systems on a square lattice. The symmetry breaking is traced to the existence of a topological phase transition. This continuous transition is triggered when the Fermi line, driven by the quasiparticle interactions, reaches the van Hove saddle points, where the group velocity vanishes and the density of states becomes singular. An unconventional Fermi liquid emerges beyond the implicated quantum critical point.

The breaking of fundamental symmetries in ground states of strongly correlated two-dimensional (2D) electron systems [1 – 6] remains one of the most intensely debated topics in low-temperature condensed matter physics. Kivelson, Fradkin, and Emery [7] were the first to discuss the case of nematic phase transitions, well before relevant experimental data was obtained. Somewhat later, Yamase and Kohno [8] (within $t - J$ model) and Halboth and Metzner [9] (within the Hubbard model) attributed the breaking of four-fold symmetry to violation of a Pomeranchuk stability condition [10] associated with antiferromagnetic fluctuations.

Subsequently, much theoretical work has been aimed at elucidating salient features of this phenomenon, primarily within mean-field theory [11 – 17]. It is instructive to recognize that the approach taken in these efforts bears a striking resemblance to that employed by Belyaev fifty years ago to describe quadrupole deformation in atomic nuclei [18]. To determine the critical point at which the spherical shape becomes unstable and calculate the nuclear deformation beyond this point, he introduced an effective Hamiltonian with separable quadrupole-quadrupole $\mathbf{Q}_1\mathbf{Q}_2$ interaction. Analogously, for two-dimensional tetragonal electronic systems, a separable interaction $d_2(\mathbf{p}_1)d_2(\mathbf{p}_2)$ with order parameter $d_2(p_x, p_y) = \cos p_x - \cos p_y$ is adopted in the mean-field treatments of the breakdown of C_4 symmetry, momenta being measured in units of the inverse lattice constant. However, such an effective Hamiltonian with separable interaction is appropriate only in the channel where symmetry breaking occurs. Moreover, even in this channel a mean-field approach may be inadequate, as exhibited for example in the prediction of a first-order phase transition in the case of violation of point-group symmetries on a square lattice [19].

Burdened with variety of inconsistencies, the mean-field description of nuclear deformation was superseded many years ago by the more sophisticated Fermi-liquid (FL) approach [20]. Following this successful precedent, we work within the FL framework to obtain a better understanding of C_4-symmetry breaking in electron systems on a 2D square lattice. Intensive numerical calculations assuming a finite-range exchange interaction, supported by complementary analysis of a simplified model, disclose unexpected features of the phenomenon. In contrast to the description given by mean-field theory, we find that the breakdown of C_4 symmetry is associated with a *topological* phase transition that occurs under conditions that allow the Fermi line, *calculated within FL theory*, to reach the van Hove saddle points $(0, \pi), (\pi, 0), (0, -\pi), (-\pi, 0)$.

Consideration of topological transitions dates back to an article by I. M. Lifshitz [21], in which the form of the single-particle spectrum $\epsilon(\mathbf{p})$ was assumed to be known. However, within FL theory $\epsilon(\mathbf{p})$ is itself a functional of the quasiparticle momentum distribution $n(\mathbf{p}) = [1 + \exp((\epsilon(\mathbf{p}) - \mu)/T)]^{-1}$. Accordingly, self-consistent inclusion of the interactions between quasiparticles may lead to unforeseen types of the topological transitions [22 – 33]. We find just such a case in the problem of C_4-symmetry violation.

Stated simply, topological transitions in correlated Fermi systems are signaled (at zero temperature) by a change of the number of roots of equation

[1)] e-mail: zverev@mbslab.kiae.ru, vak@wuphys.wustl.edu

$$\epsilon(\mathbf{p}, n_F) = \mu, \tag{1}$$

where n_F is the Fermi step distribution and μ is the chemical potential. For a thorough development of the concept, see the review by Volovik [30]. Throughout, we adhere to his rigorous quantitative definition of topological phase transitions, as distinguished from looser notions such as transitions between large and small Fermi surfaces that are also prevalent in the literature.

Analysis of topological phase transitions in fermionic systems is greatly facilitated by the absence of *critical* fluctuations of any order parameter at the transition point and its vicinity, meaning that the Landau-Migdal quasiparticle picture retains its validity. Thus, the physical many-fermion system may be viewed as a system of interacting quasiparticles, and C_4-symmetry violation can be investigated using the fundamental FL relation [34, 35]

$$\frac{\partial \epsilon(\mathbf{p})}{\partial \mathbf{p}} = \frac{\partial \epsilon_0(\mathbf{p})}{\partial \mathbf{p}} + \frac{1}{2}\mathrm{Tr}\int \mathcal{F}_{\alpha\beta,\alpha\beta}(\mathbf{p}, \mathbf{p}_1)\frac{\partial n(\mathbf{p}_1)}{\partial \mathbf{p}_1} d\upsilon_1. \tag{2}$$

In this relation, $d\upsilon = dp_x dp_y/(2\pi)^2$ is the volume element of 2D momentum space, $\epsilon_0(\mathbf{p})$ is the bare single-particle spectrum, and $\mathcal{F}$ is a phenomenological interaction function depending only on the *momenta* $\mathbf{p}$ and $\mathbf{p}_1$ of the colliding quasiparticles.

Our goal is to analyze the impact of antiferromagnetic fluctuations on electron spectra calculated using Eq. (2). Taking account of these fluctuations in the interaction function $\mathcal{F}$ presents little difficulty in the regime *far* from the antiferromagnetic phase transition, since the fluctuation exchange can be treated within the Ornstein-Zernike approximation. The part of $\mathcal{F}$ responsible for the exchange is then given by

$$\mathcal{F}^e_{\alpha\beta\gamma\delta}(\mathbf{p}, \mathbf{p}_1) = \lambda^2 \boldsymbol{\sigma}_{\alpha\beta}\boldsymbol{\sigma}_{\gamma\delta}\left[(\mathbf{p}-\mathbf{p}_1-\mathbf{Q})^2 + \xi^{-2}\right]^{-1}, \tag{3}$$

where the constant λ represents the spin-fluctuation vertex and $\mathbf{Q} = (\pi, \pi)$ the antiferromagnetic wave vector, while ξ denotes the correlation radius. Result (3) relies on the fact that the interaction function $\mathcal{F}$ coincides with a specific static limit of the quasiparticle scattering amplitude whose initial and final energies are on the Fermi surface, such that this quantity is *energy- and frequency-independent* [34, 35].

Inserting Eq. (3) into Eq. (2) and evaluating the spin-fluctuation contribution aided by the identity $2\boldsymbol{\sigma}_{\alpha\beta}\boldsymbol{\sigma}_{\gamma\delta} = 3\delta_{\alpha\delta}\delta_{\gamma\beta} - \boldsymbol{\sigma}_{\alpha\delta}\boldsymbol{\sigma}_{\gamma\beta}$, one arrives at

$$\epsilon(\mathbf{p}) = \epsilon_0(\mathbf{p}) + f_a \int \frac{n(\mathbf{p}_1)}{(\mathbf{p}-\mathbf{p}_1-\mathbf{Q})^2 + \xi^{-2}}\, d\upsilon_1, \tag{4}$$

where $f_a = 3\lambda^2/2$. The chemical potential μ, being constant along the Fermi line, is determined by the normalization condition $\int n(\mathbf{p})\, 2d\upsilon = \rho$, where factor 2 assumes summation over two spin projections.

Numerical solution of the 2D nonlinear integral equation (4) is extremely time-consuming since it is necessary to compute to high precision to rule out spurious signals of broken symmetry.

Calculations have been performed in the case of an open Fermi surface, assuming a tight-binding spectrum

$$\epsilon_0(\mathbf{p}) = -2\, t_0\, (\cos p_x + \cos p_y) + 4\, t_1\, \cos p_x \cos p_y, \tag{5}$$

with the input parameters t_0, t_1 and the chemical potential μ taken to ensure a rather small distance between the tight-binding Fermi line and the saddle points. A finite-range interaction function

$$f(\mathbf{q}) = f_a\left[(\mathbf{q}-\mathbf{Q})^2 + \xi^{-2}\right]^{-1} \tag{6}$$

is adopted, with $\xi = 30$. Salient results are reported for strategically chosen values $f_a = 1.0$ and 1.5 of the coupling parameter (in units of $2t_0$), and at temperatures $T = 10^{-2}$ and 10^{-4} (also in units of $2t_0$). It is worth noting that the approach based on Eq.(4) is self-consistent provided the dimensionaless parameter $f_a N(0)$ is rather small, $N(0) \simeq 1/(2\pi t_0)$ being the density of states of 2D electron gas on square lattice with the tight-binding spectrum (5).

The numerical calculations, as represented here in Figs.1–3, reveal some remarkable features of the quasiparticle rearrangement responsible for violation of C_4 symmetry. One conspicuous feature, well documented in the figures, is that only those quasiparticles residing in domains close to the saddle points are noticeably affected by the inclusion of antiferromagnetic fluctuations in the FL treatment.

To understand of the onset of symmetry breaking, it is most instructive to track the distance between neighboring points where the Fermi line crosses the border of the Brillouin zone. This distance is found to shrink as the coupling constant f_a is increased toward a critical value lying between 1.0 and 1.5. Breakdown of C_4 symmetry presumably occurs for a critical coupling f_{ac} at which the two crossing points *merge* with one another as they embrace and converge upon the nearby saddle point. As seen in Fig.1, the Fermi line (thick solid / red on-line) calculated at temperature $T = 10^{-4}$ (effectively zero) for a coupling constant $f_a = 1.5$ lying beyond the critical point does indeed violate $x - y$ symmetry; the corresponding Fermi line for $f_a = 1.0$ (long-dashed/green) does not. Another feature worthy of note is the effect of temperature in suppressing the symmetry

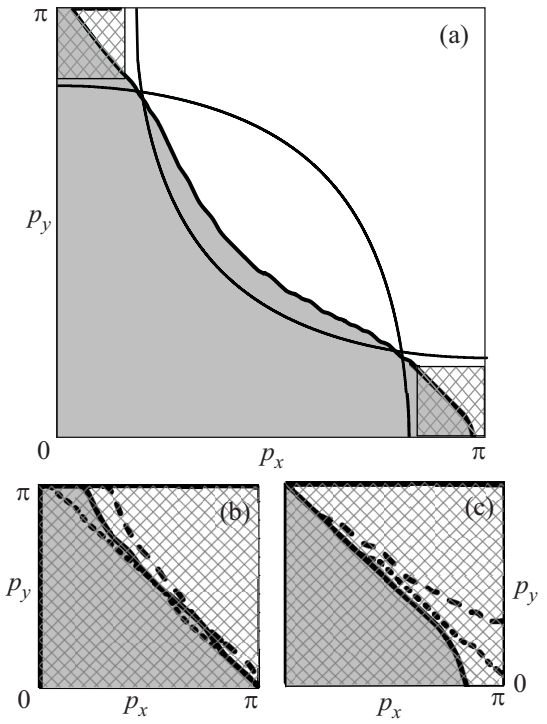

Fig.1. Fermi lines computed for the Fermi-liquid-theory model assuming bare tight-binding spectrum (5) with $t_1/t_0 = 0.45$ and finite range interaction (6) with $\xi = 30$. Panel (a): Results for $f_a = 1.5$ and $T = 10^{-4}$ (both in units of $2t_0$). Thick solid line (red on-line): one of two identical solutions with spontaneously broken C_4 symmetry. Only the first quadrant of the Brillouin zone is drawn, since neither $p_x \to -p_x$ nor $p_y \to -p_y$ reflection symmetry is broken. Thin solid lines: Fermi lines for the bare tight-binding spectrum $\epsilon^0_{\mathbf{p}}$ and its counterpart. Panels (b) and (c): two shaded squares adjacent to the saddle points $(0,\pi)$ and $(\pi,0)$ present in panel (a) are magnified. The Fermi-line solution with broken C_4 symmetry appearing in panel (a) (thick solid/red line) is drawn together with two $x-y$-symmetrical solutions corresponding respectively to $f_a = 1.0$ and $T = 10^{-4}$ (long-dashed/green line), and to $f_a = 1.5$ and $T = 10^{-2}$ (short-dashed/blue line)

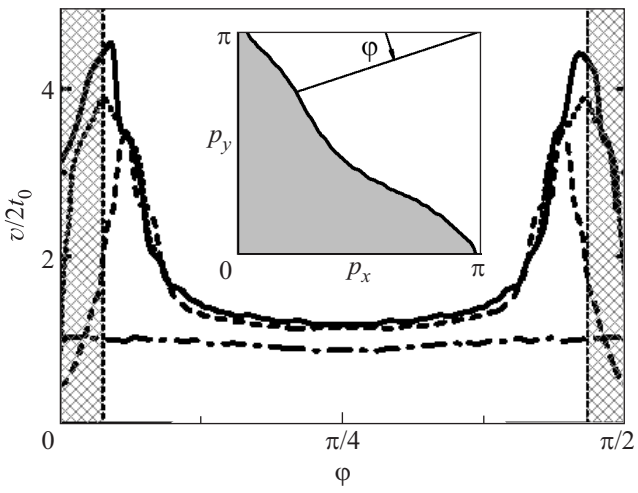

Fig.2. Group-velocity magnitudes $v = |\partial\epsilon(\mathbf{p})/\partial\mathbf{p}|$ (in units of $2t_0$), evaluated along the Fermi line as a function of the angle φ defined in the inset, for different single-particle spectra $\epsilon(\mathbf{p})$. Results are shown for the bare tight-binding model with the same parameter choice as in Fig.1 (dash-dotted/brown line) and for the Fermi-liquid-theory model of Fig.1 at $f_a = 1.0$, $T = 10^{-4}$ (dotted/green line); $f_a = 1.5$, $T = 10^{-4}$ (solid/red line); and $f_a = 1.5$, $T = 10^{-2}$ (dashed/blue line). Broken C_4-symmetry of the solid/red curve with respect to $x-y$ exchange is manifested by its different behavior in the two shaded areas close to the saddle points

breaking phenomenon. Comparison of the deviations of the Fermi line calculated at $f_a = 1.5$ and $T = 10^{-4}$ from the symmetry-preserving Fermi line obtained at $f_a = 1.5$ and $T = 10^{-2}$ (short-dashed/blue) demonstrates that C_4 symmetry can be restored by elevating the temperature.

Results from calculations of the magnitude $v(\mathbf{p}) = |\partial\epsilon(\mathbf{p})/\partial\mathbf{p}|$ of the group velocity along the Fermi line are plotted in Fig.2. These results demonstrate that the impact of antiferromagnetic correlations, as described by Eq. (3), is only significant for quasiparticles in momentum domains adjacent to the saddle points. The small gap between the values for v given by the bare tight-binding model and by the Fermi-liquid-theory treatment, seen in domains away from the saddle points, is due primarily to a shifting of the location of the Fermi line triggered by the antiferromagnetic correlations. On the other hand, the group velocity v evaluated at $f_a = 1.5$ and $T = 10^{-4}$ (solid/red line) is seen to acquire an $x-y$-anisotropic component close to the saddle points.

Fig.3 presents results from calculations of electron spectra at $T = 10^{-4}$ in the direction perpendicular to the Fermi line. Far from the saddle points, the impact of antiferromagnetic fluctuations is again found to be minor, but in their vicinity the effects are very strong. In particular, the particle and hole spectra cease to be alike; the average slope of the hole spectrum noticeably exceeds that of the particle spectrum. One might attribute this difference to the variation of Fermi-line contributions to Eq. (2) associated with a turning point emerging in the trajectory of the Fermi line at the critical point. From all the results discussed above, we infer that the description of the rearrangement of the ground state in terms of a single d_2 parameter is a poor approximation.

To further analyze and interpret the results obtained numerically for the finite-range interaction (6) and bare tight-binding spectrum (5), we simplify the interaction

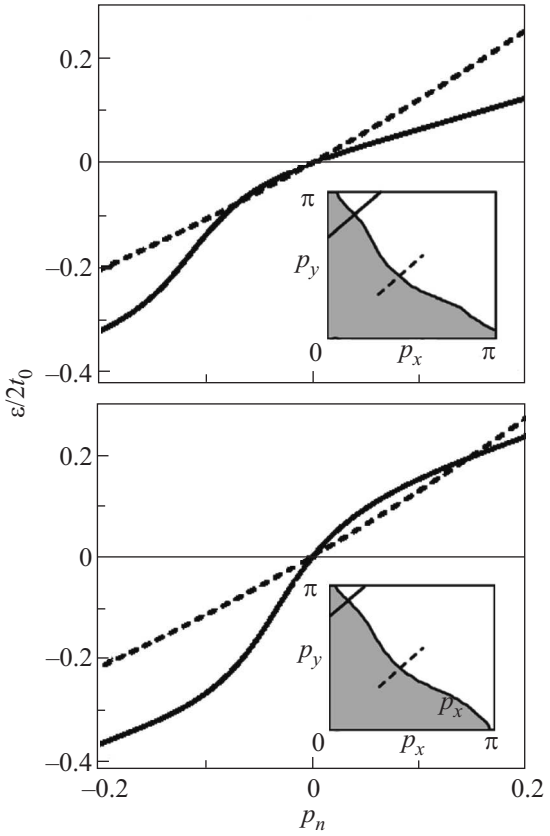

Fig.3. Single-particle spectra $\epsilon(p)$ (in units of $2t_0$) evaluated along two lines in the momentum plane (as indicated with corresponding type/color coding in the insets). The Fermi-liquid theory model used for Fig.1 is applied at $T{=}10^{-4}$ with $f_a{=}1.0$ (upper panel) and $f_a{=}1.5$ (lower panel). Spectral curves are plotted versus the normal component p_n of the momentum, measured with respect to the Fermi line. In the insets, the dashed/blue line coincides with the diagonal of the zone, while the solid/red line crosses the relevant hot line

function in the manner of Ref. [27], replacing the exchange term (3) by an infinite-range form

$$f(\mathbf{q}) = (2\pi)^2 f_0\, \delta(\mathbf{q} - \mathbf{Q}), \tag{7}$$

with coupling constant f_0. Eq. (4) is then replaced by [27]

$$\epsilon(\mathbf{p}, T) = \epsilon_0(\mathbf{p}) + f_0 n(\epsilon(\mathbf{p} + \mathbf{Q}, T)). \tag{8}$$

This treatment is analogous to that adopted by Nozières [24] in a study of non-FL behavior of strongly correlated Fermi systems for the case where forward scattering is dominant. Eq. (8) can be derived within a standard variational procedure based on the formula [27]

$$E = \int \left[\epsilon^0_{\mathbf{p}} n(\mathbf{p}) + \frac{1}{2} f_0 n(\mathbf{p}) n(\mathbf{p} + \mathbf{Q})\right] 2dv \tag{9}$$

for the energy E of the model quasiparticle system. Eq. (8) is conveniently rewritten as a system of two equations

$$\begin{aligned} \epsilon_1 &= \epsilon^0_1 + f_0 n(\epsilon_2), \\ \epsilon_2 &= \epsilon^0_2 + f_0 n(\epsilon_1), \end{aligned} \tag{10}$$

where $\epsilon_1 = \epsilon(\mathbf{p}_1) - \mu$ and $\epsilon_2 = \epsilon(\mathbf{p}_1 + \mathbf{Q}) - \mu$, while $\epsilon^0_1 = \epsilon_0(\mathbf{p})$ and $\epsilon^0_2 = \epsilon_0(\mathbf{p} + \mathbf{Q})$.

In the earlier work [27], a graphical procedure was introduced to solve the set (10) at $T = 0$. Three different solutions were found. One of these corresponds to an exceptional, non-FL state [32] exhibiting a flat single-particle spectrum. In the absence of pairing correlations, this solution turns out to be disfavored energetically relative to the other two solutions, which possess identical FL-like properties.

Focusing on the properties of the latter two solutions, we observe that at $T = 0$ the associated rearrangement of the initial Landau state can occur only in those 2D systems in which hot spots [36] exist–points situated on the Fermi line and connected by the vector $\mathbf{Q}$. In fact, for systems with small quasiparticle filling, the product $n(\mathbf{p})n(\mathbf{p} + \mathbf{Q})$ vanishes for any momentum $\mathbf{p}$; hence the ground-state energy is independent of the coupling constant f_0. The same is true in the case of small quasihole filling.

In systems having hot spots, the rearrangement occurs due to breaking of quasiparticle pairs occupying single-particle states with momenta $\mathbf{p}$ and $\mathbf{p} + \mathbf{Q}$. The corresponding domain $\mathcal{R}$ (the "reservoir") consists of four quasi-rectangles, each adjacent to one of the van Hove saddle points. Each of the four elements of $\mathcal{R}$ is confined between the border of the Brillouin zone, the *counterpart* of the initial Fermi line, defined by the equation $\epsilon_0(\mathbf{p} + \mathbf{Q}) = \mu$, and two segments of the Fermi line embracing the given saddle point.

In the rearrangement being considered, the quasiparticles move out the domain $\mathcal{R}$ to resettle in a region $\mathcal{L}$ where all pairs of single-particle states connected by the vector $\mathbf{Q}$ are empty. The region $\mathcal{L}$ comprises four "lenses," situated between neighboring hot spots and bounded by the initial Fermi line and its counterpart (see panel (a) of Fig.4). The transfer of one quasiparticle from $\mathcal{R}$ to $\mathcal{L}$ produces a gain in energy which is just the coupling constant f_0 minus the loss τ of kinetic energy. The minimum loss $\tau_{\min}$ occurs when a quasiparticle, vacating a state in $\mathcal{R}$ with momentum $\mathbf{p}$, occupies in $\mathcal{L}$ a state of lowest energy, given by the chemical potential, so that $\tau_{\min} = \mu - \epsilon_0(\mathbf{p})$. Therefore the rearrangement is favorable provided $\epsilon_0(\mathbf{p}) - \mu + f_0 \geq 0$. In the resettlement process, the chemical potential μ, which

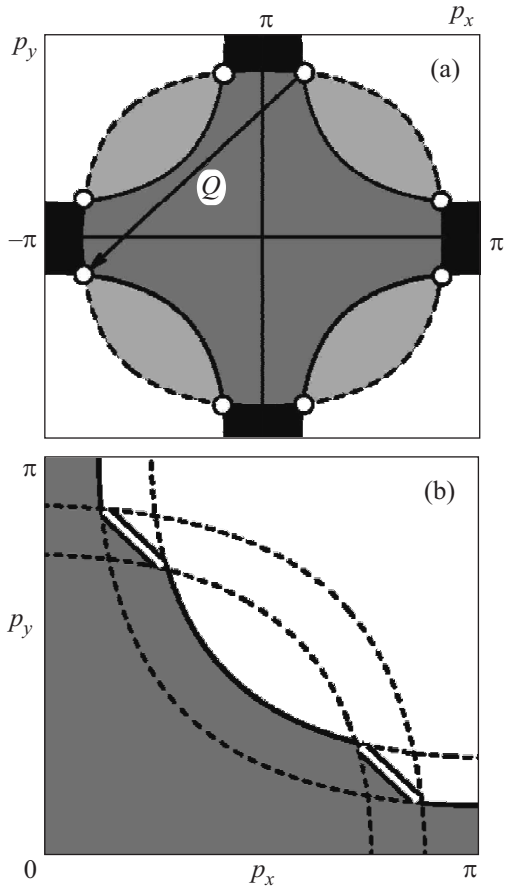

Fig.4. Panel (a): Fermi line (black) and its counterpart (dashed/blue) for the bare tight-binding spectrum of Eq. (5) with $t_1/t_0 = 0.45$. The "reservoirs" $\mathcal{R}$ (see text) are colored in black/green, and the lenses $\mathcal{L}$, in light gray. The hot spots connected with each other by the vector $\mathbf{Q}$ are symbolized by open/red dots. Panel (b): Fermi line for the simplified Fermi-liquid-theory model based on the infinite-range interaction function (7) with f_0=0.4 (in units of $2t_0$). Hot lines are drawn as double line (red on-line). Fermi lines for the bare tight-binding spectrum $\epsilon_0(\mathbf{p})$ and for the same spectrum shifted by $-f_0$ as well as their counterparts are shown as dotted lines (the latter two lines are drawn in blue on-line).

coincides with the maximum quasiparticle energy in occupied states (in particular, in the lens region), evidently increases relative to its initial value μ_i. The quasiparticles that resettle to the lens region then possess almost the same effective mass as the noninteracting electrons. This conclusion is confirmed by the numerical calculations represented in Fig.3.

An alternative process involves transfer of the quasiparticle counterpart, which has momentum $\mathbf{p}+\mathbf{Q}$. In this case, the rearrangement occurs provided $\epsilon_0(\mathbf{p}+\mathbf{Q}) - \mu + f \geq 0$. The choice between the two options is decided by comparison of the corresponding energies. The boundary at which one behavior gives way to the other is defined by the relation $\epsilon_0(\mathbf{p}) = \epsilon_0(\mathbf{p}+\mathbf{Q})$. Since the straight line so defined is part of the *new* Fermi line, we infer that the rearrangement has converted the original, isolated hot spot into a *continuous line of hot spots* (see panel (b) of Fig.4).

The results obtained imply that quasiparticles are swept from a certain subdomain $\mathcal{S}$ of $\mathcal{R}$ consisting of eight approximately trapezoidal strips. The boundaries of a given strip are traced on three sides by (respectively) the initial Fermi line, the border of the Brillouin zone, and a line geometrically similar to the initial Fermi line but shifted into the domain $\mathcal{R}$ (see Fig.4). The strip's fourth side (double/red line) is just the *hot line*. The solution derived is self-consistent: any single-particle state with momentum $\mathbf{p} \in \mathcal{S}$ has its counterpart, with momentum $\mathbf{p}+\mathbf{Q}$, located outside $\mathcal{S}$, and this state is occupied, so that Eq. (8) is fulfilled. Transparently, in this non-critical scenario, the new momentum distribution *does not* violate C_4 symmetry.

In the situation where C_4 symmetry is violated in the rearrangement, the symmetry breaking occurs for a critical value f_c of f_0, at which two segments of the Fermi line crossing the same boundary of the Brillouin zone *merge* at the saddle point. When this happens, the number of solutions of Eq. (1) certainly drops, signaling a *topological phase transition* which, as readily seen, entails the breakdown of C_4 symmetry.

Suppose on the contrary that C_4 symmetry is preserved at $f_0 > f_c$. Then all the saddle points must be emptied simultaneously, implying that every rearranged saddle point energy ϵ_s *exceeds* the chemical potential μ. But according to Eq. (8), the interaction contribution to ϵ_s vanishes when all the saddle points are emptied. Consequently, at $f_0 > f_c$, the saddle-point energy ϵ_s must coincide with the corresponding bare value ϵ_s^0, which is *lower* than the initial chemical potential μ_i. Thus, a contradiction is encountered.

We are driven to the conclusion that the critical situation giving rise to violation of C_4 symmetry is one in which the Fermi line, calculated within FL theory, attains a saddle point. Since both components of the quasiparticle group velocity $\mathbf{v}(\mathbf{p}_s)$ vanish at this critical point, the corresponding density of states must acquire a singularity, which implies that we are dealing with a *quantum critical point* (QCP).

The contradiction is resolved beyond the QCP if only *one* of two neighboring saddle points is emptied, with the second remaining occupied–thereby breaking C_4 symmetry. As a point where the Fermi line crosses the p_x axis moves away from the affected saddle point, its counterpart, shifted by the vector $\mathbf{Q}$, slides along the border of

the Brillouin zone, determining the boundary of the new filling. These conclusions drawn from analysis of the simple infinite-range model are in agreement the findings of the numerical calculations based on the more elaborate model based on Eqs. (4)–(6).

To summarize: in addressing the problem of C_4-symmetry violation, we have taken account of antiferromagnetic fluctuations within a self-consistent Fermi liquid approach, employing an interaction function that is more realistic than the separable approximation assumed in mean-field treatments. We have demonstrated that inclusion of the exchange interaction drives the calculated single-particle spectrum so as to shrink the distance between saddle points and the Fermi line. When merging occurs, the electron group velocity vanishes at the points of mergence, because these points coincide with the saddle points. A quantum critical point (QCP) of a new type is thereby revealed, at which a topological phase transition triggers the violation of C_4 symmetry. Significantly, the transition is found to be *continuous*, in contrast to the first-order phase transition obtained in mean-field theory, where the corresponding QCP does not exist. Beyond the transition point, the group velocity becomes finite again. Thus, on one side of the QCP, the system behaves as conventional Landau Fermi liquid. On the other side, the electron liquid becomes an unconventional Fermi liquid because of the loss of four-fold symmetry.

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