# Spontaneous breaking of fourfold rotational symmetry in two-dimensional electron systems as a topological phase transition

M. V. Zverev,<sup>1,2</sup> J. W. Clark,<sup>3</sup> Z. Nussinov,<sup>3</sup> and V. A. Khodel<sup>1,3</sup>

<sup>1</sup>Russian Research Centre, Kurchatov Institute, Moscow 123182, Russia

<sup>2</sup>Moscow Institute of Physics and Technology, Moscow 123098, Russia

<sup>3</sup>McDonnell Center for the Space Sciences and Department of Physics, Washington University, St. Louis, Missouri 63130, USA

(Received 8 June 2010; published 14 September 2010)

Motivated by recent observations of  $C_4$  symmetry breaking in strongly correlated two-dimensional electron systems on a square lattice, we analyze this phenomenon within an extended Fermi-liquid approach. It is found that the symmetry violation is triggered by a continuous topological phase transition associated with exchange of antiferromagnetic fluctuations. In contrast to predictions of mean-field theory, the structure of a part of the single-particle spectrum violating  $C_4$  symmetry is found to be highly anisotropic, with a peak located in the vicinity of saddle points.

DOI: 10.1103/PhysRevB.82.125111

PACS number(s): 71.10.Hf, 71.27.+a, 71.10.Ay

### I. INTRODUCTION

Experimental studies of strongly correlated twodimensional (2D) electron systems have revealed violations of the fundamental symmetries of time reversal and  $C_4$  rotational invariance inherent in the ground states of these systems on a tetragonal lattice.<sup>1-6</sup> Considerable theoretical effort has been aimed at understanding the nature of these phenomena and identifying their underlying mechanisms. In this article, we focus on  $C_4$  symmetry breaking, reserving the analysis of T-invariance violation for the next paper. As regards  $C_4$  symmetry, Kivelson, Fradkin, and Emery<sup>7</sup> were the first to discuss the case of nematic phase transitions, well before relevant experimental data became available. Somewhat later, Yamase and Kohno<sup>8</sup> (within the t-J model) and Halboth and Metzner<sup>9</sup> (within the Hubbard model) attributed the breaking of fourfold symmetry to violation of a Pomeranchuk stability condition<sup>10</sup> associated with antiferromagnetic fluctuations. An analogous result was obtained by Valenzuela and Vozmediano within an extended Hubbard model.11

As a rule, calculations on the ordered side of the implicated second-order phase transition are carried out within the mean-field (MF) approach.<sup>12-17</sup> An effective Hamiltonian containing a separable interaction  $d_2(\mathbf{p})d_2(\mathbf{p}_1)$  with order parameter  $d_2(p_x, p_y) = \cos p_x - \cos p_y$  is adopted to analyze the onset of  $C_4$  symmetry violation and properties of phases arising beyond the critical point. (Momentum components  $p_x, p_y$ are measured in units of the inverse lattice constant.) This approach has the advantages of transparency and analytical accessibility. However, it has noteworthy shortcomings, including sacrifice of translational invariance of the interaction. Furthermore, the structure of the relevant order parameter is always postulated in the MF theory; as a rule the simplest assumption is made consistent with the type of symmetry breaking being considered. However, the structure of the new ground state often turns out to be quite intricate, such that it cannot be properly described in terms of any single order parameter. As will be seen, it is just this situation that emerges in dealing with the  $C_4$  symmetry violation in question.

In the scenario proposed here, the system is considered to be on the *disordered* side of an antiferromagnetic phase transition; hence the corresponding Pomeranchuk stability condition is not violated. With the system situated far from the transition point, the fluctuation exchange is readily analyzed and is too weak to gap out the single-particle spectrum. It will be shown, however, that even if the antiferromagnetic fluctuations are weak, their *momentum dependence* is able to promote a *topological* phase transition associated with disruption of  $C_4$  rotational invariance.

In Sec. II we adopt the Landau-Migdal quasiparticle approach to investigate  $C_4$  symmetry breaking in a 2D electronic system on a square lattice. A simple model with an infinite-range interaction function is employed in Sec. III to analyze a quasiparticle rearrangement due to antiferromagnetic fluctuations. In Sec. IV we present and discuss results of numerical calculations for a more realistic model having a finite-range interaction. Section V is devoted to explanation, within the infinite-range model, of the arc structure of the Fermi line observed in many high- $T_c$  materials. Our findings are summarized in Sec. VI.

## II. C<sub>4</sub> SYMMETRY BREAKING WITHIN THE FERMI-LIQUID APPROACH

Adopting the Landau-Migdal quasiparticle picture, in which the physical many-fermion system is viewed as a system of interacting quasiparticles, the genesis of  $C_4$  symmetry breaking can be investigated based on the fundamental relation<sup>18,19</sup>

$$\frac{\partial \boldsymbol{\epsilon}(\mathbf{p})}{\partial \mathbf{p}} = \frac{\partial \boldsymbol{\epsilon}_{\mathbf{p}}^{0}}{\partial \mathbf{p}} + \frac{1}{2} \operatorname{Tr} \int \mathcal{F}_{\alpha\beta,\alpha\beta}(\mathbf{p},\mathbf{p}_{1}) \frac{\partial n(\mathbf{p}_{1})}{\partial \mathbf{p}_{1}} d\nu_{1}, \qquad (1)$$

where  $dv = dp_x dp_y/(2\pi)^2$  is an element of 2D momentum space. This relation connects the quasiparticle spectrum  $\epsilon(\mathbf{p})$ with the quasiparticle momentum distribution  $n(\mathbf{p}) = (1 + \exp\{[\epsilon(\mathbf{p}) - \mu]/T\})^{-1}$  through a phenomenological interaction function  $\mathcal{F}$ . This function, which is defined by a specific static limit of the quasiparticle scattering amplitude with initial and final energies on the Fermi surface,<sup>18,19</sup> depends only on the *momenta* **p**, **p**<sub>1</sub> of the colliding quasiparticles. Of the two particle-hole channels relevant to the scattering amplitude  $\mathcal{F}$ , denoted *t* and *u* in the Mandelstam's terminology, the transverse *t* channel carries vital information in the momentum transfer  $\mathbf{q}=\mathbf{p}-\mathbf{p}_1$ , whereas the longitudinal *u* channel is silent because the corresponding momentum transfer is close to zero.

In homogeneous matter where total momentum is conserved, the first term on the right side of Eq. (1) is just the bare velocity  $\mathbf{p}/M$ , with M the free particle mass.<sup>20</sup> In the presence of a crystal-lattice field, the bare group velocity is multiplied by a quasiparticle effective charge  $e_q(\mathbf{p})$ . However, this modification will be ignored since it reduces merely to a renormalization of phenomenological coefficients  $t_i$  specifying 2D tight-binding electron spectra,

$$\epsilon_{\mathbf{p}}^{0} = -2t_{0}(\cos p_{x} + \cos p_{y}) + 4t_{1}\cos p_{x}\cos p_{y} + \cdots . \quad (2)$$

We are concerned specifically with the impact of antiferromagnetic fluctuations on the electron spectra  $\epsilon(\mathbf{p})$  calculated using Eq. (1). Treatment of the effect of these fluctuations on the interaction  $\mathcal{F}$  does not encounter difficulties far from the attendant antiferromagnetic phase transition. The corresponding fluctuation exchange is adequately addressed within the Ornstein-Zernike approximation, which neglects scattering of fluctuations. The part of  $\mathcal{F}$  responsible for the exchange is then

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

The constant  $\lambda$  represents the spin-fluctuation vertex and **Q** =  $(\pi, \pi)$  is the antiferromagnetic wave vector while  $\xi$  is the correlation radius.

Inserting Eq. (3) into Eq. (1) and evaluating the spinfluctuation contribution aided by the identity  $2\sigma_{\alpha\beta}\sigma_{\gamma\delta}$ = $3\delta_{\alpha\delta}\delta_{\gamma\beta}-\sigma_{\alpha\delta}\sigma_{\gamma\beta}$ , one arrives at

$$\boldsymbol{\epsilon}(\mathbf{p}) = \boldsymbol{\epsilon}_{\mathbf{p}}^{0} + \frac{3\lambda^{2}}{2} \int \frac{n(\mathbf{p}_{1})}{(\mathbf{p} - \mathbf{p}_{1} - \mathbf{Q})^{2} + \boldsymbol{\xi}^{-2}} d\upsilon_{1}.$$
 (4)

The normalization condition  $2 \int n(\mathbf{p}) d\mathbf{v} = \rho$  determines the chemical potential  $\mu$  consistent with density  $\rho$ . This approach to the problem is self-consistent provided the dimensionless parameter fN(0) is rather small, where  $f = (3\lambda^2/4\pi)\ln(1/\xi)$  is a coupling constant and  $N(0) \approx 1/2\pi t_0$  is the density of states of a 2D electron gas on a square lattice having the tight-binding spectrum, Eq. (2).

Direct numerical solution of this 2D nonlinear integral equation is extremely time consuming. If only the component of the interaction, Eq. (3), proportional to  $d_2(\mathbf{p})d_2(\mathbf{p}_1)$  is retained, then beyond the point where the corresponding Pomeranchuk stability condition is violated, one obtains the ordinary mean-field theory equations. However, this approximation is quite poor for the interaction, Eq. (3), which peaks at momentum transfer  $\mathbf{q}=\mathbf{Q}$ . Accordingly, the customary MF scenario must be regarded as vulnerable.

Our approach to the problem stems from this observation: collapse of collective degrees of freedom associated with violation of *sufficient* conditions<sup>10</sup> for the stability of the standard Landau Fermi-liquid (FL) state is not the only possible scenario for the breakdown of  $C_4$  symmetry. A viable

alternative is provided by violation of a *necessary* stability condition.<sup>21</sup> This condition requires that an arbitrary admissible variation  $\delta n(\mathbf{p})$  from the FL quasiparticle momentum distribution  $n_F(\mathbf{p})$ , while conserving particle number, must produce a positive change in the ground-state energy  $E_0$ ,

$$\delta E_0 = \int \{ \boldsymbol{\epsilon}[\mathbf{p}; n_F(\mathbf{p})] - \boldsymbol{\mu} \} \delta n(\mathbf{p}) d\boldsymbol{\nu} > 0, \qquad (5)$$

where  $\epsilon(\mathbf{p}; n_F)$  is the spectrum of single-particle excitations and  $\mu$  the chemical potential.

Violation of condition (5) is accompanied by a change in the number of roots of the equation,

$$\boldsymbol{\epsilon}(\mathbf{p}, n_F) = \boldsymbol{\mu},\tag{6}$$

which implies a change in the topology of the Fermi surface. For a thorough development of the concept, see the review by Volovik.<sup>22</sup> 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. It should be emphasized that in contrast to the original Lifshitz description,<sup>23</sup> the topological transition under consideration is triggered by the *interaction between quasiparticles* (see also Refs. 24–31).

# III. QUASIPARTICLE REARRANGEMENT WITHIN A SIMPLIFIED MODEL

To gain insight into the essence of this scenario, we restrict the analysis to zero temperature and simplify the interaction. Replacement of the interaction term, Eq. (3), by an infinite-range form  $\sim \delta(\mathbf{q}-\mathbf{Q})$  leads directly to the explicit version<sup>21</sup>

$$\boldsymbol{\epsilon}(\mathbf{p}) = \boldsymbol{\epsilon}_{\mathbf{p}}^{0} + fn[\boldsymbol{\epsilon}(\mathbf{p} + \mathbf{Q})] \tag{7}$$

of relation (1), where f is the coupling constant identified above. This treatment is analogous to that adopted by Nozières<sup>26</sup> in a study of non-FL behavior of strongly correlated Fermi systems in the case where forward scattering in the *t* channel prevails. Equation (7) can be derived within a standard variational procedure based on the formula<sup>21</sup>

$$E = \int \left[ \epsilon_{\mathbf{p}}^{0} n(\mathbf{p}) + \frac{1}{2} f n(\mathbf{p}) n(\mathbf{p} + \mathbf{Q}) \right] 2 d\nu$$
 (8)

for the energy E of the model quasiparticle system. This form for the energy functional admits a greatly simplified analysis of the problem due to the partial separation of different **p** channels.

To proceed, we observe first of all that at T=0, the posed rearrangement of the initial standard Landau state can occur only in those 2D systems where there exist hot spots,<sup>32</sup> points situated on the Fermi line and connected by the vector **Q**. Indeed, in systems with small quasiparticle filling, the product  $n(\mathbf{p})n(\mathbf{p+Q})$  vanishes for any momentum **p**, so that the ground-state energy is independent of the coupling constant *f*. The same is true in the case of small hole filling.

In systems with hot spots, the rearrangement occurs due to breaking of the quasiparticle pairs occupying single-



FIG. 1. (Color online) Panel (a): Fermi line (black) and its counterpart [blue (gray)] for the bare tight-binding spectrum  $\epsilon_p^0 = -2t_0(\cos p_x + \cos p_y) + 4t_1 \cos p_x \cos p_y$  with  $t_1/t_0 = 0.45$ . The reservoirs  $\mathcal{R}$  are colored in black, and the lenses  $\mathcal{L}$ , in light gray. The hot spots connected with each other by the vector  $\mathbf{Q}$  are symbolized by red (gray) dots. Panel (b): Fermi line for the model assuming the infinite-range interaction function  $f(\mathbf{q}) = (2\pi)^2 f \delta(\mathbf{q} - \mathbf{Q})$ , with fN(0) = 0.13. Hot lines are drawn in red (gray). Fermi lines for the bare tight-binding spectrum  $\epsilon_p^0$  and its counterpart are shown as green (light gray) and blue (gray) lines, respectively.

particle states with momenta **p** and **p**+**Q**. The corresponding domain  $\mathcal{R}$  (the "reservoir") consists of four quasirectangles, each adjacent to one of the saddle points  $(0,\pi)$ ,  $(\pi,0)$ ,  $(0,-\pi)$ ,  $(-\pi,0)$  of the tight-binding spectrum  $\epsilon_p^0$ . Each of the four elements of  $\mathcal{R}$  is confined between (i) the border of the Brillouin zone, (ii) the *counterpart* of the initial Fermi line, defined by the equation  $\epsilon_{p+Q}^0 = \mu$ , and (iii) two segments of the Fermi line embracing the given saddle point.

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. 1]. The transfer of one quasiparticle from  $\mathcal{R}$  to  $\mathcal{L}$  produces a gain in energy which is just the coupling constant f minus the loss  $\tau$  of kinetic energy. Its minimum  $\tau_{\min}$  is attained 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  $\tau_{\min} = \mu - \epsilon_p^0$ . Therefore the rearrangement is favorable provided  $\epsilon_p^0 - \mu + f \ge 0$ .

An alternative process involves transfer of the quasiparticle counterpart, which has momentum  $\mathbf{p} + \mathbf{Q}$ . In this case, the rearrangement occurs provided  $\epsilon_{\mathbf{p}+\mathbf{Q}}^0 - \mu + f \ge 0$ . The choice between the two options is decided by comparing the corresponding energies. The boundary at which one behavior gives way to the other is determined by the relation  $\epsilon_{\mathbf{p}}^0 = \epsilon_{\mathbf{p}+\mathbf{Q}}^0$ . 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 straight line* of hot spots, i.e., a hot line (HL) [see panel (b), Fig. 1].

These results imply that quasiparticles are swept from a certain subdomain 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. 1). The strip's fourth side drawn in red (gray) is just the hot line. This solution is self-consistent: any single-particle state with momentum  $\mathbf{p} \in S$  has its counterpart, with momentum  $\mathbf{p}+\mathbf{Q}$ , located outside S, and this state is occupied, so that Eq. (7) is fulfilled. Transparently, the new momentum distribution *does not* violate  $C_4$  symmetry.

Defining the strip energy width  $W_s$  of the region S as the maximum of the initial hole energy  $|\epsilon_{\mathbf{p}}^0 - \mu_i|$  consistent with the rearrangement, one has  $W_s = D_i - D_f$ , where  $2D_i$  (respectively,  $2D_f$  is the minimum energy distance between the segments of the initial (final) Fermi line situated in different half planes. On the other hand, one finds  $W_s = f - (\mu - \mu_i)$ , where  $\mu_i$  is the initial chemical potential. To estimate the strip width  $W_s$  and the difference  $\mu - \mu_i$ , both proportional to f, we (i) approximate the Fermi velocity  $\mathbf{v}^{0}(\mathbf{p}) = (\partial \boldsymbol{\epsilon}_{\mathbf{p}}^{0} / \partial \mathbf{p})_{0}$  on the Fermi line in terms of two parameters, namely, its average magnitudes  $v_l^0$  and  $v_s^0$  in the lens and strip regions, respectively, and (ii) invoke the coincidence of the chemical potential with the Fermi energy that is intrinsic to Landau theory. In the lens region  $\mathcal{L}$  one then has  $\mu - \mu_i = v_i^0 w_i$ , where  $w_l$  is the momentum width of the lens filling. In the domain S, one obtains the analogous formula  $W_s \equiv f - (\mu - \mu_i)$  $= w_s v_s^0$ . Particle-number conservation implies that  $w_l l_l$  $=2w_s(l_s-w_s/2)$ , where  $l_s$  is the strip length,  $l_l$  is the lens length, and  $w_s = W_s / v_s^0$  is the momentum width of the strip.

Upon elimination of  $w_s$  and  $w_l$  from these relations, we arrive finally at

$$\mu - \mu_i = \frac{2fv_l^0 l_s}{2v_l^0 l_s + v_s^0 l_l},\tag{9}$$

for small  $w_s$ .

As long as all the saddle points remain occupied,  $C_4$  symmetry is preserved. However, as the electron density  $\rho$  decreases, the distance between the new Fermi line and the saddle points shrinks. At a critical density  $\rho_c$ , or equivalently, at the critical constant  $f_c$  where two segments of the Fermi line that cross the same boundary of the Brillouin zone *merge* at the saddle point, the number of solutions of Eq. (6) certainly drops, thereby signaling a *topological phase transition*. In the critical situation one has  $D_f=0$ , or equivalently  $W_s=D_i$ . The trapezoidal shape S then becomes triangular, and we have

$$D_{i} = \frac{f_{c}l_{l}}{v_{l}^{0}l_{s} + v_{s}^{0}l_{l}} \simeq f_{c}.$$
 (10)

Using this result, the critical value  $F_c$  of the dimensionless constant F=fN(0) is given by  $F_c=D/2\pi t_0$ . Assuming the ratio  $D/t_0$  to be small, we thus have  $F_c \ll 1$ , which implies that the derivative  $\partial \Sigma(\mathbf{p}, \varepsilon)/\partial \varepsilon$  remains small, i.e., that the  $\varepsilon$ dependence of the mass operator  $\Sigma(\mathbf{p}, \varepsilon)$  is moderate.<sup>31</sup> Un-



FIG. 2. (Color online) Fermi lines for the model assuming the finite-range interaction function  $f(\mathbf{q})=f_a/[(\mathbf{q}-\mathbf{Q})^2+\xi^{-2}]$ , with  $\xi = 30$ . Panel (a):  $f_aN(0)=0.32$ ;  $C_4$  symmetry is not broken. Panel (b):  $f_aN(0)=0.48$ ; one of the two solutions with spontaneously broken  $C_4$  symmetry is shown. Only the first quadrant of the Brillouin zone is drawn since neither  $p_x \rightarrow -p_x$  nor  $p_y \rightarrow -p_y$  reflection symmetry is broken. Fermi lines for the bare tight-binding spectrum  $\epsilon_p^0$  and its counterpart are shown as green (light gray) and blue (gray) lines, respectively.

der these conditions, the generation of new branches of the single-particle spectrum  $\epsilon(\mathbf{p})$ , such as the small pockets of the Fermi surface suggested to explain magnetic oscillations in the pseudogap regime,<sup>33</sup> is questionable.

Beyond the transition point (e.g., at  $\rho < \rho_c$ ),  $C_4$  symmetry is necessarily broken. Suppose, conversely, that it is preserved. Then all the saddle points must then be emptied simultaneously, implying that every rearranged saddle point energy  $\epsilon_s(\rho)$  exceeds the chemical potential  $\mu(\rho)$ . But according to Eq. (7), the interaction contribution to  $\epsilon_s$  vanishes when all the saddle points are emptied. Hence the saddlepoint energy  $\epsilon_s(\rho)$  must coincide with the corresponding bare value  $\epsilon_s^0(\rho)$ , implying that  $\epsilon_s^0(\rho) > \mu(\rho)$ . However, if the difference  $\rho_c - \rho$  is small, then without fail  $\epsilon_s^0(\rho) < \mu_i(\rho)$ . Thus a contradiction is encountered, since it follows from Eq. (9) that  $\mu_i(\rho) < \mu(\rho)$ . This deadlock is resolved if, beyond the critical point, only one of two neighboring saddle points is emptied, with the second remaining occupied. Such a solution is indeed consistent with Eq. (7).

### IV. NUMERICAL RESULTS WITH REALISTIC INTERACTION

The results we have derived for the simple model based on an infinite range interaction  $\sim \delta(\mathbf{q}-\mathbf{Q})$  are in agreement with those obtained from numerical calculations performed for the more realistic interaction, Eq. (3), and displayed in Fig. 2 and Eq. (3). Some complications associated with the



FIG. 3. (Color online) Fermi-velocity magnitudes  $v_F = |\partial \epsilon(\mathbf{p})/\partial \mathbf{p}|$  (in units of  $2t_0$ ), evaluated along the Fermi line as a function of the angle  $\varphi$  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 [brown (dark gray) line] and for the Fermi-liquid-theory model of Fig. 2 at  $f_a N(0) = 0.32$ ,  $T = 10^{-4}$  [green (light gray) line];  $f_a N(0) = 0.48$ ,  $T = 10^{-4}$  [red (black) line]; and  $f_a N(0) = 0.48$ ,  $T = 10^{-2}$  [blue (gray) 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.

finite correlation radius of the interaction, Eq. (3), will be considered below, but first we examine the results of the extended Fermi-liquid theory in comparison with corresponding predictions of MF theory. The MF single-particle spectrum coincides with a bare spectrum before the transition point is reached, while beyond the transition it receives a correction  $\delta \epsilon_{\rm MF}(\mathbf{p}) = \eta (\cos p_x - \cos p_y)$ , with the order parameter  $\eta$  taking the same value throughout the Brillouin zone. The Fermi line calculated within the extended FL approach deviates substantially from that predicted by MF theory. In particular, upon comparing the upper and lower panels of Fig. 2, we see that in the lens domain the location of the Fermi line remains almost unchanged as the system passes through the transition point. Indeed, this behavior also prevails over a significant portion of the HL region away from the saddle points. In other words, beyond the point where  $C_4$  symmetry is lost, the associated rearrangement of the Fermi surface occurs only in the immediate vicinity of the saddle points-in a sharp contrast to what is found in MF theory.

Analogous conclusions follow from a study of Fig. 3, where the Fermi velocity calculated on the basis of Eq. (1) is plotted. It is seen that the correction to the bare Fermi velocity  $v_F^0$  stemming from antiferromagnetic correlations as described by Eq. (3) remains smooth and small except in the HL region, where it soars upward.

Such behavior of the Fermi velocity  $v_F$ , which persists through the transition point, can be elucidated by analyzing the Landau relation (1). First, we observe that the overwhelming contributions to the integral in this relation come from the HL region; otherwise there is no appreciable overlap between the peak in the interaction function and the  $\delta$ peak in the derivative  $\partial n(\mathbf{p})/\partial \mathbf{p}$ . To proceed further, we introduce a new set of orthogonal momentum coordinates  $p_t, p_n$ , with the axis  $p_t$  directed along the HL and the axis  $p_n$ perpendicular to it. In the HL region we then have  $dp_x dp_y$   $=dp_ndp_t$  and  $dn(\mathbf{p})/dp_n = \pm \delta(p_n)$ , the sign of the derivative being positive in the left half plane and negative otherwise. This alternate sign is responsible for the vanishing of the group velocity at the saddle points, through interference of the contributions to the integral term in Eq. (1) from neighboring segments of the Fermi line situated in the two half planes. The distance between these segments (as defined in Sec. III) is  $2D_f$ . If the inverse correlation radius  $\xi^{-1}$ , which measures the radius of the spin-interaction term, Eq. (3), in momentum space, turns out to be so small that  $\xi^{-1} \leq D_f$ , then the two contributions cease to interfere, and the elevation of the HL value of the Fermi velocity is readily estimated as

$$v_F(p_t) \simeq (2\pi)^{-2} \xi^{-1}.$$
 (11)

These conclusions are in agreement with the results for the model with finite-range interaction presented in Fig. 3. At the same time, the estimate, Eq. (11), is in agreement with the jump of the single-particle spectrum  $\epsilon(\mathbf{p})$  on crossing the HL, found for the simple model with  $\delta(\mathbf{q}-\mathbf{Q})$  interaction and implying an infinite value of the model's HL group velocity. The above considerations demonstrate that the FL rearrangement of the ground state leading to the phenomenon of  $C_4$  symmetry violation has little in common with the rearrangement predicted by conventional MF theory based on the single order parameter  $d_2$ .

The analysis can be made more informative by focusing on the difference  $D(p_x, p_y) = \epsilon(p_x, p_y) - \epsilon(p_y, p_x)$  and its integral *D* over the intermediate momenta  $p_x, p_y$ . Both quantities vanish on the disordered side of the phase transition and beyond the transition point it is straightforward to evaluate *D* by means of Eq. (4). For  $D \rightarrow 0$ , one can make use of the formula  $n(p_x, p_y) - n(p_y, p_x) = [dn(\mathbf{p}/d\epsilon(\mathbf{p})D(p_x, p_y)$  to recast this equation in a form

$$D(\mathbf{p}) = -\int \mathcal{F}(\mathbf{p}, \mathbf{p}_1) \frac{\partial n(\mathbf{p}_1)}{\partial \epsilon(\mathbf{p}_1)} D(\mathbf{p}_1) \frac{d^2 p_1}{(2\pi)^2}$$
(12)

equivalent to the Pomeranchuk stability condition, whose violation is a prerequisite for the MF description of  $C_4$  symmetry breaking. From the preceding discussion, we infer that if a nontrivial solution of Eq. (12) exists, it must be anisotropic, with a peak located in the HL domain and having a width of order  $\xi^{-1}$ . Such a structure of the order-parameter function  $D(\mathbf{p})$  is quite unlike that adopted in conventional MF theory of the observed *x*-*y* symmetry violation. In evaluating the integral in Eq. (12) we employ the relation  $\partial n(\mathbf{p}) / \partial \epsilon(\mathbf{p}) = [dn(p_n)/dp_n]/v_F$ . Referring to the above derivation of the estimate, Eq. (11), it is seen that the relevant value of the group velocity is  $v_F \simeq \xi$ , as long as  $\xi \ge (D_i - W_s)^{-1}$ . The  $\xi$  dependence of the integral is then effectively nullified, precluding nontrivial solutions of Eq. (12).

Nontrivial solutions of Eq. (12) can in fact emerge before the two neighboring pieces of the Fermi line meet each other at the saddle point, provided  $\xi \leq (D_i - W_s)^{-1}$ . In this case, the characteristic value of the Fermi velocity drops somewhat, thereby enhancing the integral. Whether this enhancement is sufficient for the violation of the Pomeranchuk stability condition will be decided in a more intensive round of numerical calculations.

It is worth emphasizing that the situation underlying the violation of  $C_4$  symmetry in systems in which the Fermi surface comes close to Van Hove points is not specific to either the MF treatment or our analysis. In fact, the effective Stoner factor, which determines the enhancement of the effective field acting on a particle in matter, is proportional to the product of the interaction strength and the density of states. The latter diverges at a Van Hove point, and hence the corresponding Stoner factor diverges as well, independently of the shape of the order parameter. The crucial point of distinction is as follows. In MF theory, which reasonably exploits the enhancement of the density of states near the Van Hove points and an order parameter  $d_2(\mathbf{p})$  having the needed symmetry, the effective field stretches over the whole Brillouin zone in accordance with the chosen shape of the order parameter. In our approach based on exchange of antiferromagnetic fluctuations between electrons, it is instead the shape of the exchange interaction that governs the behavior of the effective field. Since this field dies out at rather small distances from the saddle points, the topological rearrangement of the Fermi surface violating  $C_4$  symmetry occurs only in the regions close to these points.

Let us now identify inherent properties of the interaction function  $\mathcal{F}$  responsible for violation of  $C_4$  symmetry and more generally for topological transitions. In homogeneous matter, it is well understood that topological phase transitions are characterized by a change in the number of sheets of the Fermi surface.<sup>30</sup> In 2D electron systems on a square lattice, topological transitions are of much the same character. The salient common feature here is that no symmetry is violated, provided that a local rearrangement of the quasiparticle momentum distribution leads to dominance of forward scattering in the t channel referred to the momentum transfer **q** specifying  $\mathcal{F}(\mathbf{q})$ . On the other hand, in the case of antiferromagnetic fluctuations backward scattering prevails. Then, at the transition point, quasiparticles leaving the vicinity of one saddle point may move into the vicinity of a neighboring saddle point. Thus the sheet number remains unchanged; instead, the symmetry of the ground state is violated.

#### V. ARC STRUCTURE OF THE FERMI LINE

The model we have developed may also have a bearing on the emergence of the arc structure of the Fermi line observed in many high- $T_c$  materials. If we consider pairing based on the interaction, Eq. (3), then Eq. (8) must be supplemented by a pairing term  $(f/2)\kappa(\mathbf{p})\kappa(\mathbf{p}+\mathbf{Q})$ ,<sup>26</sup> where  $\kappa(\mathbf{p}) = \langle a^+(\mathbf{p})a^+(-\mathbf{p})\rangle$  is a superfluid density. With this modification, Eq. (7) as written remains unchanged, but the quasiparticle occupation number  $n(\mathbf{p})$  acquires the BCS form  $n(\mathbf{p}) = 1/2 - \epsilon(\mathbf{p})/2E(\mathbf{p})$ , with quasiparticle energy  $E(\mathbf{p}) = [\epsilon^2(\mathbf{p}) + \Delta^2(\mathbf{p})]^{1/2}$ . The additional equation

$$\Delta(\mathbf{p}) = -f \frac{\tanh[E(\mathbf{p} + \mathbf{Q})/2T]}{2E(\mathbf{p} + \mathbf{Q})} \Delta(\mathbf{p} + \mathbf{Q})$$
(13)

determines the gap function  $\Delta(\mathbf{p})$ . In advance of the topological phase transition, where  $C_4$  symmetry is preserved, a standard nonzero solution of Eq. (13) has the property  $\Delta(\mathbf{p})=-\Delta(\mathbf{p}+\mathbf{Q})$  exhibited by *D* pairing, and we find

$$\frac{E(\mathbf{p})E(\mathbf{p}+\mathbf{Q})}{\tanh[E(\mathbf{p})/2T]\tanh[E(\mathbf{p}+\mathbf{Q})/2T]} = \frac{f^2}{4}.$$
 (14)

As seen from Eq. (14), the associated gap  $E_{\min}$  in the singleparticle spectrum is suppressed near the diagonals of the Brillouin zone, where

$$E_{\min}(T=0) \sim \frac{f^2}{4W_l},$$
 (15)

 $W_l$  being the total-energy lens width. On moving along the Fermi line toward the hot line where one has  $E(\mathbf{p})=E(\mathbf{p}+\mathbf{Q})$ , the gap soars upward, with Eq. (14) yielding

$$E(\mathbf{p}, T=0) \simeq \frac{f}{2}.$$
 (16)

It is important to note that in the HL region itself, the gap value is markedly suppressed, because Eq. (7) tells us that  $|\epsilon(\mathbf{p})| \simeq f$  in a significant part of this region, which is incompatible with Eq. (16). This indicates that pairing has little impact on the violation of  $C_4$  symmetry, which primarily involves the immediate vicinities of the hot lines.

### VI. CONCLUSION

In summary, we have addressed the problem of  $C_4$ -symmetry violation in electron systems on a square lattice

within a self-consistent Fermi-liquid approach, assuming that the Landau interaction describes the exchange of antiferromagnetic fluctuations, which is treated within the Ornstein-Zernike approximation. We have demonstrated that as the strength of this interaction builds up, the distance between saddle points and the Fermi line shrinks, eventually generating a quantum critical point of a new type, at which a *continuous* topological phase transition triggers the violation of  $C_4$  symmetry. The group velocity becomes finite again once the transition point is passed. Thus, the properties of the electron system are governed by Fermi-liquid theory throughout the vicinity of the proposed quantum critical point, implying that magnetic oscillations should be observed on both the sides of the topological transition, in agreement with recent measurements.<sup>34</sup>

#### **ACKNOWLEDGMENTS**

We express our gratitude to V. Yakovenko and H. Yamase for comprehensive discussion of key points and also thank A. S. Alexandrov, A. Balatsky, E. Fradkin, A. Mackenzie, and V. Shaginyan for fruitful discussions. This research was supported by the McDonnell Center for the Space Sciences, by Grants No. 2.1.1/4540 and No. NS-7235-2010.2 from the Russian Ministry of Education and Science, and by Grant No. 09-02-01284 from the Russian Foundation for Basic Research.

- <sup>1</sup>A. Kaminski, S. Rosenkranz, H. W. Fretwell, J. C. Campuzano, Z. Li, H. Raffy, W. G. Cullen, H. You, C. M. Varma, and H. H. Hoehst, Nature (London) **416**, 610 (2002).
- <sup>2</sup>Y. Ando, K. Segawa, S. Komiya, and A. N. Lavrov, Phys. Rev. Lett. 88, 137005 (2002).
- <sup>3</sup>J. Xia, E. Schemm, G. Deutscher, S. A. Kivelson, D. A. Bonn, W. N. Hardy, R. Liang, W. Siemons, G. Koster, M. M. Fejer, and A. Kapitulnik, Phys. Rev. Lett. **100**, 127002 (2008).
- <sup>4</sup>V. Hinkov, D. Haug, B. Fauque, P. Bourges, Y. Sidis, A. Ivanov, C. Bernhard, C. T. Lin, and B. Keimer, Science **319**, 597 (2008).
- <sup>5</sup>H. A. Mook, Y. Sidis, B. Fauque, V. Baledent, and P. Bourges, Phys. Rev. B **78**, 020506(R) (2008).
- <sup>6</sup>K. Daou, J. Chang, D. LeBoeuf, O. Cyr-Choiniere, F. Laliberte, N. Doiron-Leyraud, B. J. Ramshaw, R. Liang, D. A. Bonn, W. N. Hardy, and L. Taillefer, Nature (London) **463**, 519 (2010).
- <sup>7</sup>S. A. Kivelson, E. Fradkin, and V. J. Emery, Nature (London)
  **393**, 550 (1998).
- <sup>8</sup>H. Yamase and H. Kohno, J. Phys. Soc. Jpn. **69**, 2151 (2000).
- <sup>9</sup>C. J. Halboth and W. Metzner, Phys. Rev. Lett. 85, 5162 (2000).
- <sup>10</sup>I. Ya. Pomeranchuk, Sov. Phys. JETP **8**, 361 (1958).
- <sup>11</sup>B. Valenzuela and M. A. H. Vozmediano, Phys. Rev. B **63**, 153103 (2001).
- <sup>12</sup> V. Oganesyan, S. A. Kivelson, and E. Fradkin, Phys. Rev. B 64, 195109 (2001).
- <sup>13</sup>A. P. Kampf and A. A. Katanin, Phys. Rev. B 67, 125104 (2003).
- <sup>14</sup>I. Khavkine, C. H. Chung, V. Oganesyan, and H. Y. Kee, Phys.

Rev. B 70, 155110 (2004).

- <sup>15</sup>A. Neumayr and W. Metzner, Phys. Rev. B **67**, 035112 (2003).
- <sup>16</sup>H. Y. Kee, E. H. Kim, and C. H. Chung, Phys. Rev. B **68**, 245109 (2003).
- <sup>17</sup>E. Fradkin, S. Kivelson, M. Lawler, J. Eisenstein, and A. Mackenzie, Annual Reviews of Condensed Matter Physics 1, 153 (2010).
- <sup>18</sup>L. D. Landau, Sov. Phys. JETP **3**, 920 (1957); **8**, 70 (1959).
- <sup>19</sup>L. D. Landau and E. M. Lifshitz, *Statistical Physics*, Course of Theoretical Physics Vol. 5, 3rd ed. (Nauka, Moscow, 1976); *Statistical Physics*, Course of Theoretical Physics (Addison-Wesley, Reading, MA, 1970).
- <sup>20</sup>L. P. Pitaevskii, Sov. Phys. JETP **10**, 1267 (1960).
- <sup>21</sup>M. V. Zverev, V. A. Khodel, and J. W. Clark, JETP Lett. **74**, 46 (2001).
- <sup>22</sup>G. E. Volovik, Lect. Notes Phys. 718, 31 (2007).
- <sup>23</sup>I. M. Lifshitz, Sov. Phys. JETP **11**, 1130 (1960).
- <sup>24</sup>V. A. Khodel and V. R. Shaginyan, JETP Lett. **51**, 553 (1990).
- <sup>25</sup>G. E. Volovik, JETP Lett. **53**, 222 (1991).
- <sup>26</sup>P. Nozières, J. Phys. I **2**, 443 (1992).
- <sup>27</sup> M. V. Zverev and M. Baldo, Sov. Phys. JETP **87**, 1129 (1998); J.
  Phys.: Condens. Matter **11**, 2059 (1999).
- <sup>28</sup>S. A. Artamonov, V. R. Shaginyan, and Yu. G. Pogorelov, JETP Lett. **68**, 942 (1998).
- <sup>29</sup>J. Quintanilla and A. J. Schofield, Phys. Rev. B 74, 115126 (2006).
- <sup>30</sup>V. A. Khodel, J. W. Clark, and M. V. Zverev, Phys. Rev. B **78**, 075120 (2008), and references cited therein.

- <sup>31</sup>V. A. Khodel, J. W. Clark, and M. V. Zverev, JETP Lett. **90**, 628 (2009).
- <sup>32</sup>D. Pines, Physica C **282-287**, 273 (1997); A. V. Chubukov, Europhys. Lett. **44**, 655 (1998).
- <sup>33</sup>Y. Qi and S. Sachdev, Phys. Rev. B **81**, 115129 (2010); M.

Khodas and A. M. Tsvelik, *ibid.* **81**, 155102 (2010).

<sup>34</sup>J.-F. Mercure, S. K. Goh, E. C. T. O'Farrell, R. S. Perry, M. L. Sutherland, A. W. Rost, S. A. Grigera, R. A. Borzi, P. Gegenwart, and A. P. Mackenzie, Phys. Rev. Lett. **103**, 176401 (2009).