Spontaneous Fermi surface symmetry breaking on a square lattice

H. Yamase [a], V. Oganesyan [b], W. Metzner [a]

[a] *Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, D-70569, Stuttgart, Germany*
[b] *Department of Physics, Princeton University, Princeton, NJ 08544, USA*

Abstract

We analyze a forward scattering model on a square lattice, which exhibits spontaneous Fermi surface symmetry breaking with a d-wave order parameter: the Fermi surface expands along the k_x-axis and shrinks along the k_y-axis or vice versa. While the transition is usually first order as a function of chemical potential at low temperature, we find that Fermi surface fluctuations near the transition can be strong. For a particularly favorable but not unphysical choice of parameters, the first order transition is completely suppressed, leading to a quantum critical point.

Key words: Fermi surface, quantum criticality
PACS: 71.18.+y; 71.10.Fd

The Fermi surface (FS) usually respects the point group symmetry of the underlying lattice. Recently, however, the possibility of symmetry breaking of the FS was discussed in the two-dimensional t-J [1] and Hubbard [2] models. In electron systems on a square lattice forward scattering processes can drive a d-wave shaped deformation, where the FS expands along the k_x-axis and shrinks along the k_y-axis or vice versa. A tendency toward such a d-wave Fermi surface deformation (dFSD) may play a role in high-T_c cuprates [1,3] and in $Sr_3Ru_2O_7$ [4].

Here we analyze basic properties of the dFSD as obtained from the following simple forward scattering model [5]:

$$H = \sum_{\mathbf{k}} \epsilon^0_{\mathbf{k}}\, n_{\mathbf{k}} + \frac{1}{2L} \sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k}\mathbf{k}'}\, n_{\mathbf{k}} n_{\mathbf{k}'} \,, \qquad (1)$$

where $n_{\mathbf{k}}$ is the spin-summed number operator of electrons with momentum $\mathbf{k}$, and L is the number of lattice sites; the bare dispersion is given by $\epsilon^0_{\mathbf{k}} = -2[t(\cos k_x + \cos k_y) + 2t' \cos k_x \cos k_y + t''(\cos 2k_x + \cos 2k_y)]$ with t, t', and t'' being nearest, next-nearest, and third-nearest neighbors on a square lattice, respectively. The forward scattering interaction has the form

$$f_{\mathbf{k}\mathbf{k}'} = u - g\, d_{\mathbf{k}} d_{\mathbf{k}'} \,, \qquad (2)$$

where $u \geq 0$, $g > 0$, and $d_{\mathbf{k}} = \cos k_x - \cos k_y$; the first term suppresses the uniform compressibility of the system, which works in favor of a second order phase transition, and the second term drives the dFSD.

We analyze the Hamiltonian (1) in the Hartree approximation

$$H_{\rm MF} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}\, n_{\mathbf{k}} - \frac{1}{2} \sum_{\mathbf{k}} \delta\epsilon_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle \,, \qquad (3)$$

which becomes exact in the thermodynamic limit for the present model. Here $\epsilon_{\mathbf{k}} = \epsilon^0_{\mathbf{k}} + \delta\epsilon_{\mathbf{k}}$, $\delta\epsilon_{\mathbf{k}} = un + \eta d_{\mathbf{k}}$, $n = \frac{1}{L}\sum_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle$, and $\eta = -\frac{g}{L}\sum_{\mathbf{k}} d_{\mathbf{k}} \langle n_{\mathbf{k}} \rangle$. The order parameter of the dFSD η and the density n are determined by minimizing the grand canonical potential.

We first take band parameters, $t'/t = -1/6$ and $t''/t = 0$, for which the bare dispersion has saddle points at $(\pi, 0)$ and $(0, \pi)$, yielding a log-divergence in the density of states at $\epsilon^0_{\rm vH} = -2t/3$. Typical features of the spontaneous dFSD are captured for these parameters. In Fig. 1(a) we show the phase diagram for $g/t = 1$ and $u = 0$. The solid line denotes a second order transition, which turns to a first order one at low T (open circles). The end points of the second order transition are tricritical points (solid circles). Since

Email address: h.yamase@fkf.mpg.de (H. Yamase).

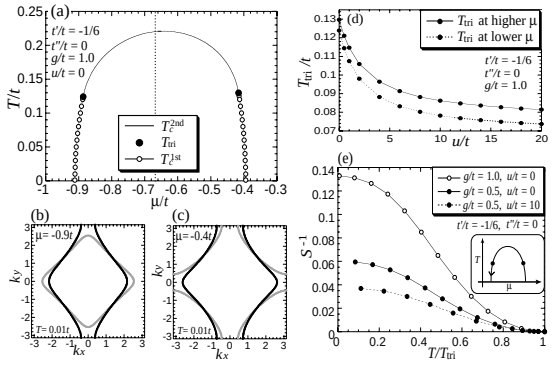

Fig. 1. Results for $t'/t = -1/6$ and $t'' = 0$. (a) μ-T phase diagram for $g/t = 1$ and $u = 0$. The solid line, $T_c^{\rm 2nd}$, is a second order transition line, whose end points, $T_{\rm tri}$, are tricritical points (solid circles); the open circles, $T_c^{\rm 1st}$, denote a first order transition. The dotted line indicates the van Hove energy, $\mu = \epsilon^0_{\rm vH}$. (b) and (c) FS in the symmetry-broken phase near the first order transition; FS for $g = 0$ is also shown by the dotted line. (d) u dependence of $T_{\rm tri}$. (e) The inverse of the Stoner factor for several choices of g and u along the first order line as sketched in the inset by the arrow.

the dFSD is driven by forward scattering of electrons mainly on the (original) FS close to van Hove points [1,2], the maximal $T_c(\mu)$ appears around $\mu = \epsilon^0_{\rm vH} = -2t/3$. The FS in the symmetry-broken phase is shown in Figs. 1(b) and (c). The FS has typically open topology except close to a second order transition.

When the u term in Eq. (2) is introduced, the tricritical points are suppressed in favor of a second order transition. This suppression, however, saturates at a larger u as shown in Fig. 1(d). The first order transition at low T is a robust feature of the dFSD.

However, we find that the d-wave compressibility, which is given exactly by the RPA expression

$$\kappa_d = \frac{N_2}{1 - gN_2}\,, \tag{4}$$

where $N_2 = -\frac{2}{L}\sum_{\mathbf{k}} d_{\mathbf{k}}^2 f'(\epsilon^0_{\mathbf{k}} + un - \mu)$, is typically strongly enhanced by interactions even near the first order transition. The "Stoner factor" $S = (1 - gN_2)^{-1}$ is a dimensionless measure of this enhancement. We calculate S along the first order line as sketched in the inset of Fig. 1(e). The main panel shows that S^{-1} is nearly zero close to $T_{\rm tri}$, as expected. At lower T, S^{-1} becomes finite, but its value is much smaller than one, especially for a smaller g; a finite u reinforces this tendency. We see that the d-wave compressibility is enhanced by a factor of 25 for $g/t = 0.5$ and $u/t = 10$ by interactions. Hence, in the presence of interactions with a small finite momentum transfer (beyond our mean-field model) fluctuations of the dFSD can be strong even near the first order transition at low T. Such fluctuations lead to non-Fermi liquid behavior [3].

Now we consider band parameters that satisfy $\alpha = |\frac{t+2t'}{4t''}| < 1$, setting $t'/t = -1/6$ and $t''/t = 1/5$. The bare dispersion has saddle points at $(\pi \pm \cos^{-1}\alpha,\, 0)$ and $(0,\, \pi \pm \cos^{-1}\alpha)$, and local minima at $(\pi,\, 0)$ and $(0,\, \pi)$. In this case, we can have a quantum critical point (QCP) of the dFSD. In Fig. 2(a), we show the μ-T phase diagram for $g/t = 0.5$ and $u = 0$. We see that qualitative features are the same as in Fig. 1(a), although the transition line is now strongly asymmetric with respect to $\mu = \epsilon^0_{\rm vH} = -13t/9$. This asymmetry is related to a large asymmetry of the bare density of state. When we introduce the u term, the tricritical point at higher μ is suppressed, but saturates to a finite value as in Fig. 1(d). A striking behavior appears on the lower side of μ. As seen in Figs. 2(b) and (c), $T_{\rm tri}$ is substantially suppressed with u and disappears for $u/t \gtrsim 2$, leading to a QCP. It should be noted that if the coupling g is much larger or smaller than the value chosen in Fig. 2, a QCP does not appear even if a large u is introduced.

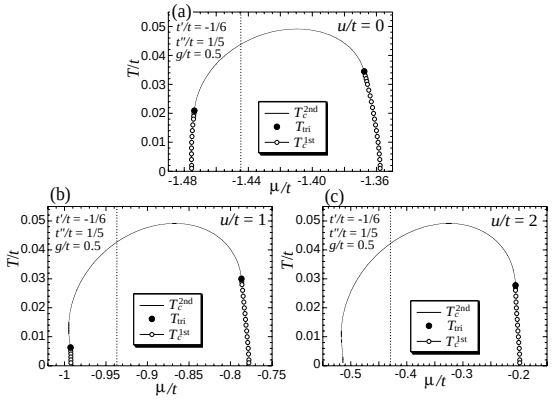

Fig. 2. μ-T phase diagrams for several choices of u for $t'/t = -1/6$, $t''/t = 1/5$, and $g/t = 0.5$. The dotted line indicates the van Hove energy.

The dFSD reduces the symmetry of the FS, which then leads to distinct features in low energy properties of electrons. It will be interesting to further explore theoretical consequences of a dFSD and its fluctuations, and to look for realizations in layered materials.

References

[1] H. Yamase and H. Kohno, J. Phys. Soc. Jpn. **69** (2000) 332; **69** (2000) 2151.

[2] C. J. Halboth and W. Metzner, Phys. Rev. Lett. **85** (2000) 5162.

[3] W. Metzner, D. Rohe, and S. Andergassen, Phys. Rev. Lett. **91** (2003) 066402.

[4] S. A. Grigera *et al.*, Science **306** (2004) 1154.

[5] A comprehensive study is presented in H. Yamase, V. Oganesyan, and W. Metzner, Phys. Rev. B **72**, 035114 (2005); results for $u = 0$ have been published already in I. Khavkine *et al.*, Phys. Rev. B **70**, 155110 (2004).