Quasiparticle Anisotropy and Pseudogap Formation from the Weak-Coupling Renormalization Group Point of View

A. A. Katanin[1,2] and A. P. Kampf[1]

[1]*Institut für Physik, Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86135 Augsburg, Germany*

[2]*Institute of Metal Physics, 620219 Ekaterinburg, Russia*

(Received 6 October 2003; published 3 September 2004)

Using the one-loop functional renormalization group technique, we evaluate the self-energy in the weak-coupling regime of the 2D t-t' Hubbard model. At van Hove (vH) band fillings and at low temperatures, the quasiparticle weight along the Fermi surface (FS) continuously vanishes on approaching the $(\pi, 0)$ point where the quasiparticle concept is invalid. Away from vH band fillings the quasiparticle peak is formed inside an anisotropic pseudogap and the self-energy has the conventional Fermi-liquid characteristics near the Fermi level. The spectral weight of the quasiparticle features is reduced on parts of the FS between the near vicinity of hot spots and the FS points closest to $(\pi, 0)$ and $(0, \pi)$.

DOI: 10.1103/PhysRevLett.93.106406 PACS numbers: 71.10.Fd, 71.27.+a, 74.25.Dw

The apparent non-Fermi-liquid (nFL) normal-state features and the intriguing pseudogap structures remain a key issue in the ongoing research activities on high-T_c superconductors. Angle resolved photoemission spectroscopy (ARPES) keeps providing new and increasingly detailed insight into the nature of the correlated electronic states responsible for the unconventional normal-state properties and the superconducting pairing state [1,2]. Refined ARPES data continue to serve as challenging test grounds for theoretical concepts developed for studying correlated lattice electrons in two dimensions.

The pseudogap phenomenon in cuprates manifests itself by the absence of well-defined quasiparticles (qps) near the $(\pi, 0)$ point of the Brillouin zone (BZ) and by the seeming partial disappearance of the Fermi surface (FS) [2]. One direction of recent research has been to seek the origin of these apparent nFL characteristics and pseudogap structures in the competing nature of different ordering tendencies indicative for the existence of quantum critical points in the ground-state phase diagram [3,4].

On the other hand, the vicinity to the transition from a metal to an antiferromagnetic (AF) insulator in doped cuprates demands the understanding of the role of AF spin fluctuations on the evolution of spectral properties on the metallic side of the metal-insulator transition. Anisotropic spectral features naturally arise within the two-dimensional (2D) Hubbard model near its AF instability even in the weak-coupling regime [5]; they were studied within the spin-fermion model [6], fluctuation exchange [7,8], and two-particle self-consistent (TPSC) approximations [9], and more recently in cluster extensions of the dynamical mean-field theory (DMFT) [10] and cluster perturbation theory [11]. Quantum Monte Carlo studies on finite clusters [12] provided valuable insight into the doping evolution of the spectral function on a sparse momentum grid in the strong to intermediate coupling regime, but they were not able to trace the pseudogap formation into the weak-coupling regime. The results of previous studies agree with each other only for the case of perfect nesting [next-nearest neighbor (nnn) hopping $t' = 0$ and half filling] where a pseudogap opens everywhere around the FS upon cooling. The experimentally most relevant case of a non-nested FS remains an issue of debate.

From the apparent necessity for the development of alternative methods for the analysis of correlated electron systems in two dimensions, functional renormalization group (fRG) techniques have proven to be most promising additional tools with an emphasis on the identification of the leading electronic instabilities in the weak-coupling regime of the 2D Hubbard model and its extensions [13–17]. Although the electronic on-shell lifetime, the FS shift, and the approximate qp weight calculated from the imaginary part of the self-energy at the lowest Matsubara frequency were recently considered within the many-patch fRG analysis[18], these quantities alone are only indicative but not sufficient to trace the evolution of the spectral properties in the vicinity of the AF instability.

In this Letter, we use the one-loop fRG scheme for the t-t' weak-coupling Hubbard model to evaluate the self-energy on the real frequency axis. We show that at van Hove (vH) band fillings the qp weight along the FS continuously vanishes from the BZ diagonal towards the $(\pi, 0)$ point where the qp concept is invalid. The qp weight suppression is accompanied by the growth of two additional incoherent peaks in the spectral function, from which an anisotropic pseudogap originates. On moving away from vH band fillings, a qp peak with small weight is formed inside the pseudogap. This peak regains spectral weight from the incoherent pseudogap features on moving towards the BZ diagonal. These results

offer a complementary weak-coupling view of pseudogap formation from the RG perspective with new implications for the doped AF-insulator regime of the Hubbard model.

Specifically, we consider the Hubbard model for N_e electrons on a square lattice:

$$H = -\sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} - (\mu - 4t')N_e, \quad (1)$$

where the hopping amplitude $t_{ij} = t$ for nearest neighbor sites i and j, and $t_{ij} = -t'$ for nnn sites ($t, t' > 0$); for convenience we have shifted the chemical potential μ by $4t'$. We apply the fRG approach for one-particle-irreducible functions with a sharp momentum cutoff [15]. This technique considers the effective action obtained by integrating out modes with energy $|\varepsilon_{\mathbf{k}}| \geq \Lambda$, where $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) + 4t'(\cos k_x \cos k_y + 1) - \mu$ is the electronic dispersion; Λ ($0 < \Lambda < \Lambda_0 = \max|\varepsilon_{\mathbf{k}}|$) is the cutoff parameter. This procedure is used in the weak-coupling regime for small and intermediate $t' \lesssim 0.3t$ when the ferromagnetic instability is absent [16]. In this scheme the flow of the self-energy $\Sigma_\Lambda(\mathbf{k}, i\omega)$ is given by

$$\frac{d\Sigma_\Lambda}{d\Lambda} = V_\Lambda \circ S_\Lambda, \quad (2)$$

where $\circ$ is a short notation for the summation over momentum, frequency, and spin variables; see, e.g., Ref. [15]. The renormalization of the electron-electron interaction vertex V_Λ at one-loop order is given by

$$\frac{dV_\Lambda}{d\Lambda} = V_\Lambda \circ (G_\Lambda \circ S_\Lambda + S_\Lambda \circ G_\Lambda) \circ V_\Lambda. \quad (3)$$

The propagators G_Λ and S_Λ are defined by

$$\left\{ \begin{array}{c} G_\Lambda \\ S_\Lambda \end{array} \right\}(\mathbf{k}, i\omega_n) = \left\{ \begin{array}{c} \theta(|\varepsilon_{\mathbf{k}}| - \Lambda) \\ -\delta(|\varepsilon_{\mathbf{k}}| - \Lambda) \end{array} \right\} \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}}}. \quad (4)$$

We neglect the influence of the self-energy and the FS shift on the RG flow, and therefore the self-energy is not included in the Green functions (4). Equations (2) and (3) have to be solved with the initial conditions $V_{\Lambda_0} = U$ and $\Sigma_{\Lambda_0} = 0$. Since also the frequency dependence of the vertices is neglected, it is convenient to reinsert, following Ref. [18], the vertex from Eq. (3) into Eq. (2) to obtain

$$\frac{d\Sigma_\Lambda}{d\Lambda} = S_\Lambda \circ \int_\Lambda^{\Lambda_0} d\Lambda' [V_{\Lambda'} \circ (G_{\Lambda'} \circ S_{\Lambda'} + S_{\Lambda'} \circ G_{\Lambda'}) \circ V_{\Lambda'}]. \quad (5)$$

To solve Eqs. (3) and (5) numerically, we divide the momentum space into 48 patches with the same patching scheme as in Refs. [15,16]. The self-energy on the real axis is obtained by analytical continuation using Padé approximants [19]. To resolve fine structures close to the Fermi level, we take advantage of Eq. (5) that for frequency-independent vertices the self-energy can be calculated at arbitrary frequencies on the imaginary axis. A sample result for $\mathbf{k}_F$ in the first FS patch closest to the $(\pi, 0)$ point is shown in Fig. 1. Obviously, the imaginary part of the self-energy behaves nonmonotonically at frequencies $\omega < \omega_1 = \pi T$ with $[\partial \mathrm{Im}\Sigma(\mathbf{k}_F, i\omega)/\partial\omega]_{\omega \to 0^+} > 0$. By the Cauchy-Riemann conditions for an analytic function, this necessarily implies $[\partial \mathrm{Re}\Sigma(\mathbf{k}_F, \omega)/\partial\omega]_{\omega \to i0^+} > 0$ and thus the breakdown of the qp concept at this particular value of $\mathbf{k}_F$. Evaluating the self-energy at the Matsubara frequencies $i\omega_n$ only (circles in Fig. 1), this behavior is missed. Therefore, for the analytical continuation we use a dense set of frequencies on the imaginary axis at small $|\omega| \lesssim t$ and a set of $i\omega_n$ for $|\omega| \gg t$. This procedure can be viewed as an analytical continuation first from Matsubara frequencies $i\omega_n$ to some suitably chosen set of points on the imaginary axis and a subsequent continuation to the real axis using Padé approximants. The quality of the approximants was checked by both the analysis of the analyticity in the upper half-plane [19] and by requiring the fulfillment of the sum rule for the resulting Green function.

First we consider the results at the vH band filling ($\mu = 0$) for $t' = 0.1t$ and $U = 2t$. The self-energy at temperature $T = 0.17t$ calculated within fRG together with the result in second-order perturbation theory (SOPT) [which is obtained by the replacement $V \to U$ in Eq. (5)] is shown in Fig. 2. Remarkably, in the first patch closest to the vH singularity (vHS) at $(\pi, 0)$, SOPT and fRG results both show a minimum of $\mathrm{Im}\Sigma(\mathbf{k}_F, \omega)$ at the Fermi level $\omega = 0$ instead of a maximum as expected for a FL. Simultaneously, $\mathrm{Re}\Sigma(\mathbf{k}_F, \omega)$ has a positive slope near $\omega = 0$. The dip in $\mathrm{Im}\Sigma$ calculated within fRG is much more pronounced than in SOPT. Moreover, the physical origin of these features is very different. The peculiarities of the SOPT self-energy arise solely from the thermal excitation of electrons near the vHS, and, although they exist at all $T > 0$, they lose their relevance with decreasing T. Instead, the more pronounced anomalies in the fRG self-energy *increase* in size with

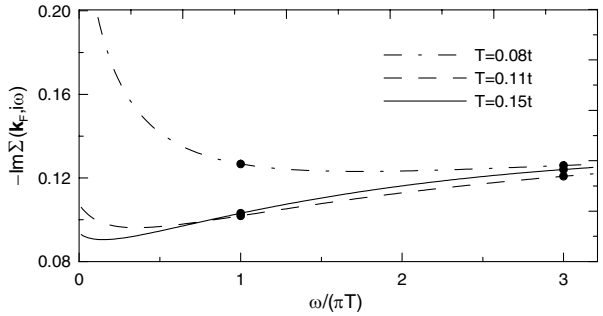

FIG. 1. Imaginary part of the self-energy at imaginary frequencies within the one-loop RG approach at $U = 2t$, $t'/t = 0.1$, and vH band filling $n = 0.92$. $\mathbf{k}_F$ is chosen in the patch closest to the vH point at $(\pi, 0)$. The dots show the positions of the first and second Matsubara frequency.

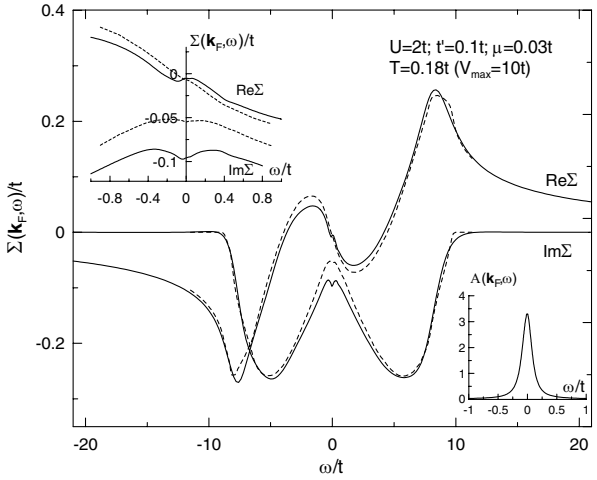

FIG. 2. Self-energy in SOPT (dashed line) and one-loop RG (solid line) at $U = 2t$, $t'/t = 0.1$, and vH band filling $n = 0.92$ at $T = 0.17t$ ($V_{\max} = 10t$). $\mathbf{k}_F^1 = (3.100, 0.003)$ is chosen in the first patch, closest to the vHS. The insets show the self-energy and the spectral function at small frequencies.

decreasing T and reflect the growing AF correlations and the concomitant tendency towards pseudogap formation. Importantly, the single peak in $A(\mathbf{k}_F, \omega) = -\mathrm{Im}G(\mathbf{k}_F, \omega + i0^+)/\pi$ in Fig. 2 is not a qp feature because the low-energy structure of Σ invalidates the qp concept.

In Fig. 3 we decrease the temperature to $T = 0.082t$, which is closer to the crossover temperature T^* where the one-loop interaction vertices V tend to diverge [15] as a fingerprint of the nearby AF instability. Although the low-temperature regime where the effective vertices are so large ($V_{\max} = 100t$) is outside the validity region of the

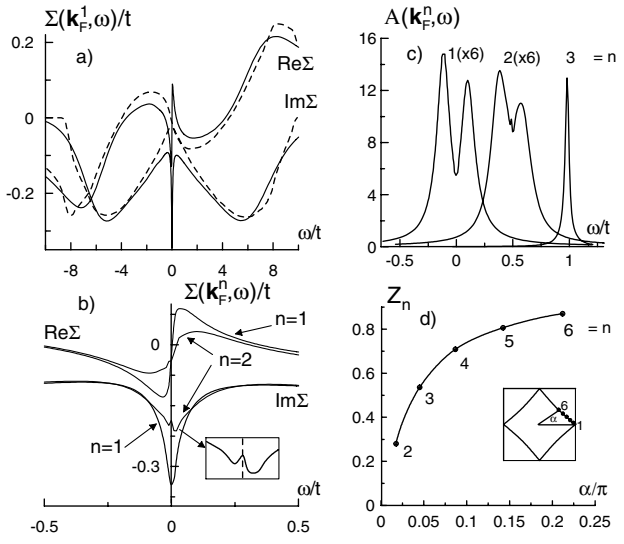

FIG. 3. Same as Fig. 2 for $T = 0.082t$ ($V_{\max} = 100t$). In addition, (c) and (d) show the spectral functions and the qp weights for $\mathbf{k}_F^n$ in different patches around the FS. The spectral functions are shifted by $(n-1)0.5t$ for a better view; for $n = 1, 2$, they are multiplied by 6.

one-loop approach, it proves most useful to clearly identify the structure of the spectral function which originates from the above discussed form of the self-energy. In the first patch a two-peak structure in $A(\mathbf{k}_F, \omega)$ arises with a local minimum at the Fermi energy. Outside the first patch, the real part of the self-energy has a narrow region with negative slope near $\omega = 0$ accompanied by a local maximum of $\mathrm{Im}\Sigma$ [Fig. 3(b)], which leads to the formation of a qp peak inside a pseudogap structure [Fig. 3(c)]. This behavior is in fact reminiscent of the finite temperature DMFT results in the metal to insulator crossover region [20]. For larger $|\omega|$ the behavior is qualitatively similar in all patches. The qp peak quickly merges with the two incoherent peaks of the pseudogap on approaching the BZ diagonal along the FS. The qp weight around the FS [see Fig. 3(d)] gradually vanishes when approaching the $(\pi, 0)$ point. For $t' = 0$ and the corresponding vH band filling $n = 1$, the qp peak is absent in all patches. All spectral functions along the FS show, in this case, a two-peak pseudogap structure at low temperatures similar to the TPSC results [9] and the dynamical cluster approach [10].

In Figs. 4(a) and 4(b) we show the self-energy for $U = 2t$, $t' = 0.1t$ at high and low temperatures, respectively, for $\mu = 0.03t$ ($n = 0.94$) when the Fermi level is slightly above the vHS energy. At higher temperatures only weak anomalies in $\Sigma(\mathbf{k}_F^1, \omega)$ are present near the Fermi level. Upon lowering the temperature towards T^*, a clear maximum of $\mathrm{Im}\Sigma$ develops at the Fermi energy, similar to that in $\mathrm{Im}\Sigma(\mathbf{k}_F^n, \omega)$ for $n > 1$ at vH band fillings. The real part of self-energy has the proper negative slope for a FL in a

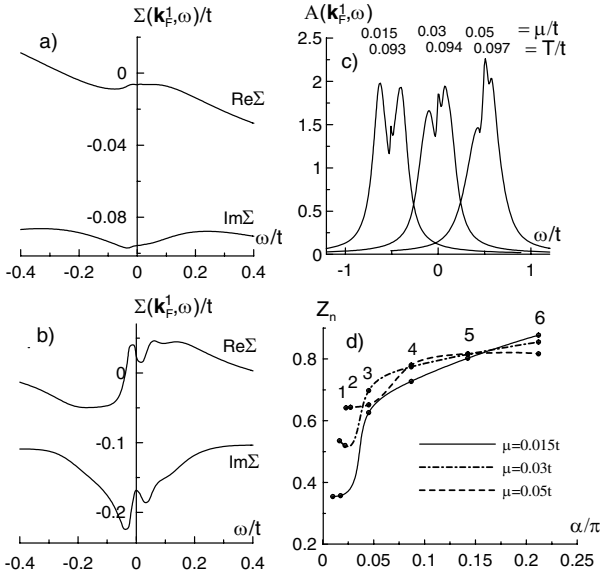

FIG. 4. (a),(b) Self-energy for a patch closest to the vHS at $U = 2t$, $t'/t = 0.1$, $\mu = 0.03t$, $T = 0.18t$ [$V_{\max} = 10t$; (a)] and $T = 0.093t$ [$V_{max} = 100t$; (b)]. (c),(d) The evolution of the spectral function and the qp weight for different chemical potentials; the temperatures are chosen such that $V_{\max} = 100t$. The lines in (c) are shifted by $0.5t$ for a better view.

narrow energy window $|\omega| \lesssim \mu$ around the Fermi level. In the spectral function [see Fig. 4(c)] we observe the split-off of two incoherent peaks near the qp peak at the Fermi level. With increasing μ and with the corresponding increase of temperature which is kept above T^*, the qp peak gains weight from the incoherent pseudogap peaks. For $\mu < 0$ (fillings below vH band filling) the value of T^* rapidly drops with $|\mu|$ for finite t', and we observe a quick crossover to a single-peak structure.

Figure 4(d) shows the anisotropic weight of the qp feature in the three-peak spectral functions of Fig. 4(c) for different chemical potentials $\mu > 0$. Away from the vH band filling the qp weight is finite in the first patch near the $(\pi, 0)$ point, which is now below the Fermi level. Hot spots, i.e., points on the FS which are connected by $\mathbf{Q} = (\pi, \pi)$ and thus most affected by the scattering from AF spin fluctuations, are identified as local shallow minima in the angular dependence of the qp Z factor along the FS line. The central qp peak of the spectral function is suppressed on parts of the FS between the near vicinity of hot spots and the FS points closest to $(\pi, 0)$ and $(\pi, 0)$ and quickly gains spectral weight upon moving towards the BZ diagonal.

In summary, we have investigated the self-energy on the real frequency axis in the 2D t-t' Hubbard model within a one-loop fRG analysis. For vH band fillings the self-energy has a nFL form at the FS points $(\pi, 0)$ and $(0, \pi)$ which are connected by the AF wave vector $\mathbf{Q}$. The qps exist everywhere else on the FS but with anisotropic spectral weight. The RG flow indicates that at low temperatures the continuous decrease of the qp weight along the FS is accompanied by the simultaneous growth of two additional incoherent peaks in the spectral function. Away from vH fillings, a qp peak at $(\pi, 0)$ and $(0, \pi)$ emerges with small spectral weight.

These results provide a complimentary weak-coupling scenario for pseudogap formation and offer implications for the evolution of anisotropic spectral properties at finite temperatures on the metallic side of the transition to an AF insulator. The strong angular dependence of the qp properties in our fRG study is reminiscent of the recent high-resolution ARPES studies on underdoped cuprates [2]. Although the fRG method does not allow one to go below the crossover temperature T^*, and therefore to explore the spectral functions at a fixed temperature in a wide range of dopings, we expect further suppression of the weight of the central peak with decreasing temperature and/or increasing interaction strength, and simultaneously the increase of the doping range near half filling where the pseudogap structures emerge.

The main change of the low-energy physics upon moving from the weak- to the strong-coupling regime is expected in the redistribution of spectral weight from the vicinity of the Fermi energy to the developing lower and upper Hubbard subbands. These subbands should form *in addition* to the low-energy structures we have elucidated in our fRG analysis. This conjecture finds indeed support from recent results of the dynamical cluster approximation [10] and cluster perturbation theory [11].

The observed features are distinctly different from the previously found low-temperature crossover to a nFL form of the self-energy at half filling [7,9] as well as from the proposed hole pocket picture and the partial destruction of the FS in strong-coupling Hubbard or t-J models [21]. The fRG results thereby offer a valid alternative for the interpretation of experimental data from photoemission spectroscopy on cuprates.

This work was supported by the Deutsche Forschungsgemeinschaft through SFB 484 and by Grant No. 747.2003.2 (Support of Scientific Schools) from the Russian Basic Research Foundation.

[1] A. Damascelli *et al.*, Rev. Mod. Phys. **75**, 473 (2003).
[2] T. Yoshida *et al.*, Phys. Rev. Lett. **91**, 027001 (2003); A. Kaminski *et al.*, cond-mat/0404385.
[3] C. M. Varma, Phys. Rev. B **55**, 14 554 (1997).
[4] J. L. Tallon and J. W. Loram, Physica (Amsterdam) **349C**, 53 (2001).
[5] A. P. Kampf and J. R. Schrieffer, Phys. Rev. B **41**, 6399 (1990); *ibid.* **42**, 7967 (1990).
[6] J. Schmalian *et al.*, Phys. Rev. Lett. **80**, 3839 (1998); Phys. Rev. B **60**, 667 (1999); A. V. Chubukov and J. Schmalian, *ibid.* **57**, R11085 (1998); Ar. Abanov *et al.*, Adv. Phys. **52**, 119 (2003).
[7] J. Deisz *et al.*, Phys. Rev. Lett. **76**, 1312 (1996).
[8] J. Altmann *et al.*, Eur. Phys. J. B **18**, 429 (2000).
[9] J. Vilk and A.-M. S. Tremblay, J. Phys. I (France) **7**, 1309 (1997); B. Kyung, Phys. Rev. B **58**, 16 032 (1998); S. Moukouri *et al.*, *ibid.* **61**, 7887 (2000).
[10] C. Huscroft *et al.*, Phys. Rev. Lett. **86**, 139 (2001).
[11] D. Sénéchal and A.-M. S. Tremblay, Phys. Rev. Lett. **92**, 126401 (2004).
[12] S. R. White, Phys. Rev. B **44**, 4670 (1991); M. Vekic and S. R. White, *ibid.* **47**, 1160 (1993); N. Bulut *et al.*, Phys. Rev. Lett. **72**, 705 (1994).
[13] D. Zanchi and H. J. Schulz, Phys. Rev. B **54**, 9509 (1996); *ibid.* **61**, 13 609 (2000).
[14] C. J. Halboth and W. Metzner, Phys. Rev. B **61**, 7364 (2000); Phys. Rev. Lett. **85**, 5162 (2000).
[15] C. Honerkamp *et al.*, Phys. Rev. B **63**, 035109 (2001); M. Salmhofer and C. Honerkamp, Prog. Theor. Phys. **105**, 1 (2001).
[16] C. Honerkamp and M. Salmhofer, Phys. Rev. Lett. **87**, 187004 (2001); Phys. Rev. B **64**, 184516 (2001).
[17] A. P. Kampf and A. A. Katanin, Phys. Rev. B **67**, 125104 (2003).
[18] C. Honerkamp, Eur. Phys. J. B **21**, 81 (2001); C. Honerkamp *et al.*, Phys. Rev. B **67**, 174504 (2003).
[19] H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. **29**, 179 (1977).
[20] R. Bulla, T. Costi, and D. Vollhardt, Phys. Rev. B **64**, 045103 (2001).
[21] X.-G. Wen and P. A. Lee, Phys. Rev. Lett. **76**, 503 (1996); Z. Y. Weng *et al.*, *ibid.* **80**, 5401 (1998); A. V. Chubukov and D. K. Morr, Phys. Rep. **288**, 355 (1997).