Non-Fermi-liquid behavior due to short-range order

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An exactly soluble one-dimensional model of electrons interacting with order-parameter fluctuations associated with short-range order is considered. The energy and momentum dependence of the electronic self-energy and spectral function are calculated and found to exhibit non-Fermi-liquid features similar to that seen for the two-dimensional Hubbard model: a pseudogap, shadow bands, anomalies in the self-energy, and breakdown of the quasiparticle picture. Deviations from Fermi-liquid behavior are largest close to the Fermi surface and as the correlation length increases. [S0163-1829(96)52242-3]

The question as to whether the metallic properties of high-T_c superconductors[1] and quasi-one-dimensional materials[2] can be described by the Fermi-liquid picture that works so well in conventional metals has recently received considerable attention. Many theoretical studies have been made of strongly correlated electron models such as the Hubbard and t-J models.[3] The availability of high-quality photoemission data[4–7] has recently focused attention on the electron spectral weight function $A(k,E)$ which is related to the probability of observing an electron with momentum k and energy E.

A consistent picture is gradually emerging from studies of the two-dimensional Hubbard model using quantum Monte Carlo simulations[8–11] and studies using the fluctuation exchange (FLEX) approximation.[12–15] Some common features are observed as the temperature is lowered, the hole doping is decreased, or the Coulomb repulsion U is increased. It has been suggested that these changes have a common origin:[11] they correspond to an increase in ξ, the correlation length associated with short-range antiferromagnetic order.[16]

The common non-Fermi-liquid features observed are the following: (1) As ξ increases a pseudogap develops, i.e., there is a suppression of the density of states near the Fermi energy.[8–11,13,14] (2) As ξ increases peaks in the electron spectral function become smaller and broader.[14] Near the Fermi surface a breakdown of the quasiparticle picture may occur. (3) On the Fermi surface the real part of the self-energy $\Sigma(k,E)$ can develop a positive slope at the Fermi energy.[14] (4) The magnitude of the imaginary part of the self-energy has a local maximum at the Fermi energy.[14] (5) "Shadow bands" exist due to the incipient antiferromagnetic order,[17] i.e., in addition to the peak in the spectral function at the energy E and momentum k there is a much smaller peak at $k+Q$ where $Q=(\pi,\pi)$ is the wave vector associated with antiferromagnetic order (and the nesting vector of the Fermi surface for half filling). This means the spectral function $A(k,E)$ has peaks for $|k|>k_F$ but $E<E_F$. It is estimated that such shadow bands are observable when the correlation length is larger than a couple of lattice spacings.[10] The corresponding photoemission peaks have been observed in metallic $Bi_2Sr_2CaCu_2O_{8+x}$ (Refs. 5 and 7) and insulating $Sr_2CuO_2Cl_2$.[6] (6) The self-energy associated with the shadow bands is singular.[18] As ξ increases the imaginary part of the self-energy is much larger on the shadow Fermi surface than on the regular Fermi surface.[15]

The purpose of this Rapid Communication is to point out that there is a simple one-dimensional model which also has many of the features listed above. It is easy to study because it has an *exact* analytic solution, found by Sadovskii.[19] This solution can be used to test different approximation schemes and methods of analytic continuation used on two-dimensional models. Hopefully, the results presented here will also provide physical insight into how short-range order produces non-Fermi-liquid behavior in two dimensions. The model is directly relevant to the related issues for quasi-one-dimensional materials.[20,21]

The model consists of left- and right-moving electrons, with Fermi velocity v_F, interacting with a static backscattering random potential $\Delta(z)$, with Hamiltonian

$$H=\int dz\Psi^\dagger\left[-iv_F\sigma_3\frac{\partial}{\partial z}+\Delta(z)\sigma_+ +\Delta(z)^*\sigma_-\right]\Psi, \quad (1)$$

where σ_3 and $\sigma_\pm\equiv\frac{1}{2}(\sigma_1\pm i\sigma_2)$ are Pauli matrices. The upper and lower components of the spinor $\Psi(z)$ are left-moving, up-spin and right-moving, down-spin electrons, respectively. The other electrons are described by a similar Hamiltonian. (The form of the Hamiltonian is motivated by considering backward scattering in the Hubbard model.) The random potential has zero mean and finite range Gaussian correlations given by

$$\langle\Delta(z)\Delta(z')^*\rangle=\psi^2\exp(-|z-z'|/\xi). \quad (2)$$

where ψ is the rms fluctuation in the potential at a given point and ξ is the correlation length. ψ defines an energy scale and a length scale $\xi_0\equiv v_F/\psi$. It will be seen below that the ratio of the correlation length to ξ_0 determines to what extent the short-range order causes deviation from Fermi-liquid behavior. For the commensurate case of a half-filled band $\Delta(z)$ is real.

An alternative interpretation of the Hamiltonian is that it represents electrons interacting with spin fluctuations, $S(x)\equiv\Delta(x)/\psi$, with susceptibility

$$\chi(\omega,q)=\delta(\omega)\sum_\pm\frac{\xi^{-1}}{(q\pm 2k_F)^2+\xi^{-2}} \quad (3)$$

and ψ then defines the strength of the coupling of the electrons to the spin fluctuations. In this interpretation we are assuming that the energy scale associated with the spin fluctuations is so much smaller than the electronic energy scale that the spin fluctations can be treated as *static*. Deisz, Hess, and Serene[14] noted that for the two-dimensional Hubbard model at half filling anomalies in the self-energy were always accompanied by a spin fluctuation T-matrix $T_{\sigma\sigma}(q,\omega_n)$ that is strongly peaked near the wave vector $q=Q$ and Matsubura frequency $\omega_n=0$. In this regime there is a natural mapping onto the model considered here. At half filling the Fermi surface is square and has perfect nesting, so is somewhat ''one dimensional.'' The one-dimensional momentum then corresponds to that along the (π,π) direction in the two-dimensional model. ψ^2 corresponds to the weight of the peak in $T_{\sigma\sigma}(q,0)$ within ξ^{-1} of Q [compare Eq. (5) in Ref. 14].

Sadovskii considered the model defined by Eqs. (1) and (2) and found an *exact* solution by summing all the diagrams generated by perturbation theory.[19] The electronic Green function is a continued fraction

$$G(k,E)=\cfrac{1}{E-a_0-\cfrac{\psi^2 c_1}{E-a_1-\cfrac{\psi^2 c_2}{E-a_2-\cdots}}}, \tag{4}$$

where for right-moving electrons

$$a_l=(-1)^l v_F k+\mathrm{sgn}(k)\frac{il}{\xi} \tag{5}$$

and $c_l=l$ for the commensurate case of a half-filled band and for the incommensurate case $c_l=l/2$ for l even and $c_l=(l+1)/2$ for l odd. As far as we are aware this is the only nontrivial electronic model for which there is an exact analytic solution for the continued fraction representation of a correlation function. Since the Lanczos method of exact diagonalization produces such a continued fraction representation of spectral functions[3] this model could provide insights into trends in the continued fraction coefficients and possible termination procedures.[22] In the limit $\xi\rightarrow\infty$ a perturbation expansion for $G(k,E)$ is divergent but Borel summable.[20] We evaluated the continued fraction (4) numerically using the modified Lentz's method.[23] All the results shown here are for the incommensurate case. Qualitatively similar results are obtained for the commensurate case.

Generally we find that as the correlation length increases and the Fermi surface is approached the properties of the self-energy and spectral function deviate significantly from the quasiparticle picture of Fermi-liquid theory. Many of the anomalous features we see are similar to those found for the two-dimensional Hubbard model at half filling treated in the fluctuation-exchange approximation.[14] Figure 1 shows how the spectral function $A(k,E)$ broadens significantly as the electron momentum approaches the Fermi momentum. This happens even for correlation lengths of the order of $\xi_0=v_F/\psi$. This means that for strong coupling, i.e., ψ of the order of the bandwidth, the correlation length ξ can be of the order of a lattice constant. Shadow bands are present and become larger as ξ increases and $|k|$ decreases.

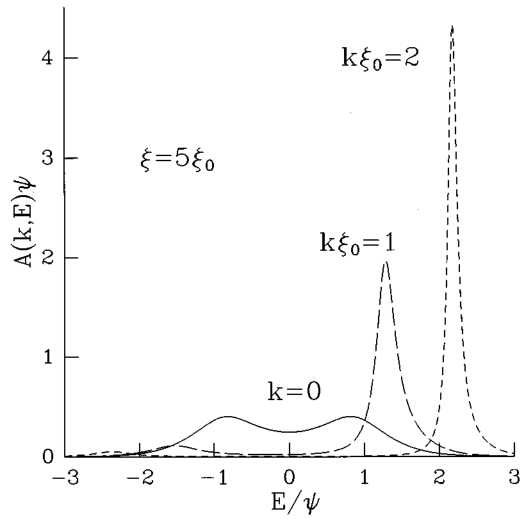

FIG. 1. Shadow bands and the breakdown of the quasiparticle picture near the Fermi surface. The energy dependence of the electron spectral function $A(k,E)$ is shown for three different momenta k. The correlation length associated with the short-range order is equal to $5\xi_0=5v_F/\psi$ where v_F is the Fermi velocity and ψ is a measure of the strength of the coupling of the electrons to the order-parameter fluctuations. Note the presence of ''shadow bands,'' i.e., small peaks in $A(k,E)$ with $E<E_F=0$ and $k>k_F=0$. The spectral function becomes significantly broader as the Fermi surface is approached. Opposite behavior occurs in a Fermi liquid: the quasiparticles are better defined close to the Fermi surface. These results can be compared to those for the two-dimensional Hubbard model at half filling (see Fig. 1 in Ref. 14 and Fig. 2 in Ref. 10).

Figure 2 shows how the quasiparticle picture breaks down as the correlation length ξ increases. As ξ increases from $0.2\xi_0$ to $100\xi_0$ the spectral function on the Fermi surface evolves from a single narrow peak to two broad peaks which are the precursors of conduction and valence bands associated with long-range spin-density-wave order. For similar reasons as the correlation length increases a pseudogap develops in the total density of states (Fig. 2 inset). It should be pointed out that the two-peak structure is *not* seen in FLEX results[14] or quantum Monte Carlo for weak coupling on large lattices.[8] Whether this absence of the two peaks is a real property of the two-dimensional (2D) Hubbard model or a result of the FLEX approximation or not being able to go to low enough temperatures is not clear.

The self-energy has anomalous features similar to those found for the 2D Hubbard model at half filling.[14] At the Fermi energy the real part of the self-energy has a positive slope (Fig. 3). The magnitude of the imaginary part of the self-energy, in a quasiparticle picture, is related to the quasiparticle lifetime and develops a maximum at the Fermi energy (Fig. 3). In contrast, in a Fermi liquid ReΣ has a negative slope and $|\mathrm{Im}\Sigma|$ has a minimum (which goes to zero as the temperature goes to zero) at the Fermi energy. The opposite behavior observed here means that although for our model there is a pole in the spectral function at $E=0$ it is not possible to define a quasiparticle solution there.

The self-energy on the Fermi surface $\Sigma(0,E)$ develops a singularity at the Fermi energy $E=0$ as the correlation length increases. Figure 4 shows that $\Sigma(k,E)$ develops similar singular behavior near $E\sim -kv_F$, which corresponds to

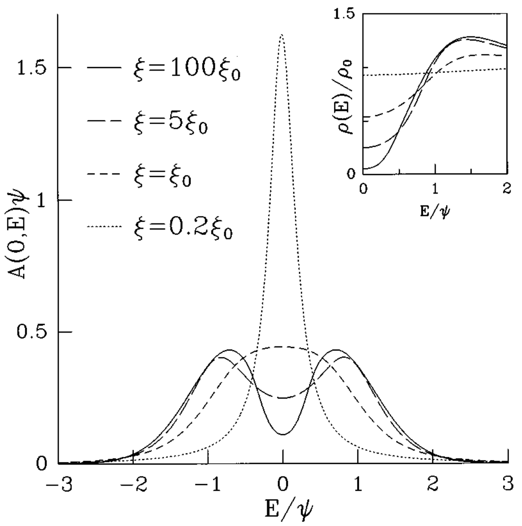

FIG. 2. Breakdown of the quasiparticle picture with increasing correlation length. The energy dependence of the spectral function at the Fermi momentum is shown for several correlation lengths. The spectral function broadens considerably and evolves into two bands as the correlation length increases. These results can be compared to those for the 2D Hubbard model at half filling as the temperature is lowered (see Fig. 1 in Ref. 14). The inset shows how the pseudogap in the total density of states opens up as the correlation length increases. Note that although for $\xi\sim\xi_0$ the pseudogap is rather weak deviations from Fermi-liquid behavior still occur.

the position of the shadow band. In general, the magnitude of the imaginary part of the self-energy (which is related to the scattering rate) is much larger and more singular near $E\sim -kv_F$ than $E\sim +kv_F$. The scattering rate for the shadow band increases with ξ, as is observed for the 2D Hubbard model as the doping or temperature is decreased.[15]

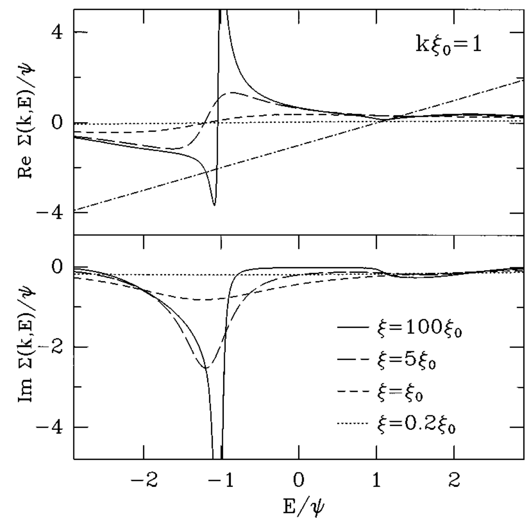

FIG. 4. Singular behavior of the shadow band self-energy. Away from the Fermi surface the self-energy near $E\sim kv_F$ has Fermi-liquid properties. In contrast, near $E\sim -kv_F$, which is associated with the shadow band, the self-energy becomes increasingly singular as the correlation length increases. Intersections of the Re Σ curves with the dot-dashed straight line correspond to poles of the spectral function. Hence, the shadow band is only associated with a pole for very large correlation lengths.

Only for very large correlation lengths does the shadow band feature correspond to a pole of the spectral function, i.e., an energy E_k which satisfies $E_k - kv_F - \mathrm{Re}\Sigma(k,E_k)=0$. Consequently, the shadow band peak is not a replica of the regular quasiparticle peak. These results can be compared to those of Chubukov[18] for a two-dimensional spin-fluctuation model.

Figure 5 shows the spectral function calculated for this model using second-order perturbation theory. This corre-

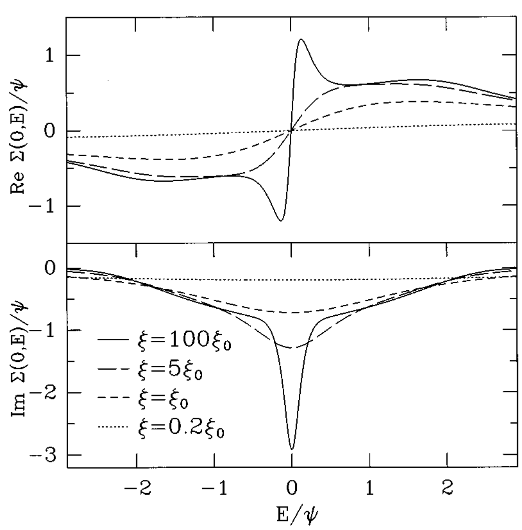

FIG. 3. Anomalous behavior of the self-energy. The real part of the self-energy at the Fermi momentum, $\mathrm{Re}\Sigma(0,E)$, has a positive slope at the Fermi energy ($E=0$). This means that a quasiparticle weight cannot be defined. As the correlation length increases a maximum at $E=0$ develops in the magnitude of the imaginary part of the self-energy at the Fermi momentum $|\mathrm{Im}\Sigma(0,E)|$. (Compare Fig. 2 in Ref. 14.)

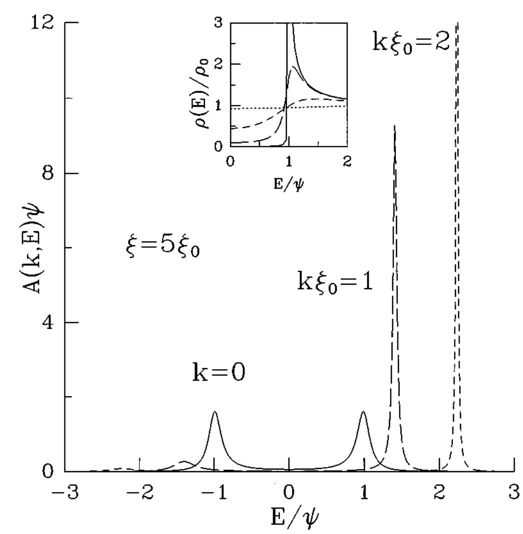

FIG. 5. Second-order perturbation theory is unreliable near the Fermi surface. The spectral function is calculated for the same parameter values as in Fig. 1. (Note the vertical scale is three times larger here.) The discrepancy with the exact results is large for $|k|<1/\xi_0$ and becomes larger as ξ increases. The inset shows the total density of states for the same parameter values as in Fig. 2. (Note the vertical scale is two times larger here.)

sponds to termination of the continued fraction at $l=1$. Such a perturbative form for the Green's function has been used in calculations concerning the role of order-parameter fluctuations in quasi-one-dimensional materials.[24] However, the discrepancy with the exact results shown in Fig. 1 shows this is quite unreliable for $|E|<\psi$ when $|k-k_F|<\psi/v_F$ and $\xi>v_F/\psi$. In particular perturbation theory greatly underestimates the width of the spectral function. The inset of Fig. 5 shows how perturbation theory gives unreliable results for the total density of states if $\xi>\xi_0$.

In conclusion, the simple model considered here has many features similar to those seen for the two-dimensional Hubbard model and provides insight into how short-range order can produce non-Fermi-liquid behavior. Of particular interest are the following: (a) The ratio of the correlation length to $\xi_0=v_F/\psi$ determines deviations from Fermi-liquid behavior. (b) Non-Fermi-liquid behavior occurs even when the correlation length is sufficiently short that there is only a weak pseudogap. (c) The ''shadow band'' is associated with singularities in the self-energy and only corresponds to poles in the spectral function for very large correlation lengths. (d) Perturbation theory gives unreliable results in the non-Fermi-liquid regime.

Note added in proof. Recent angle-resolved photoemission measurements [H. Ding *et al.*, Nature (London) **382**, 51 (1996); A. G. Loeser *et al.*, Science **273**, 325 (1996)] have measured a pseudogap in the normal state of $Bi_2Sr_2CaCu_2O_{8+x}$. The observed opening up of the pseudogap with decreasing doping and decreasing temperature are qualitatively similar to how the pseudogap considered here opens up with increasing correlation length (Fig. 2 inset).

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