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DESTRUCTION OF THE FERMI LIQUID BY SPIN FLUCTUATIONS IN TWO DIMENSIONS

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Abstract—It is shown that it is possible to quantitatively explain quantum Monte-Carlo results for the Green's function of the two-dimensional Hubbard model in the weak to intermediate coupling regime. The analytic approach includes vertex corrections in a paramagnon-like self-energy. All parameters are determined self-consistently. This approach clearly shows that in two dimensions Fermi-liquid quasiparticles disappear in the paramagnetic state when the antiferromagnetic correlation length becomes larger than the electronic thermal de Broglie wavelength.

Keywords: Hubbard model, spectral weight, spin fluctuations, vertex corrections, paramagnons, photoemission.

INTRODUCTION

We introduce a simple approach to the Hubbard model which includes vertex corrections, and achieves, for both two-particle and single-particle properties, better quantitative agreement with Monte-Carlo simulations than previous theories [1][2][3]. Our analytical approach allows us to unambiguously interpret the Monte-Carlo data and to show that in two dimensions spin fluctuations destroy the Fermi liquid in the paramagnetic state when the antiferromagnetic correlation length becomes larger than the thermal de Broglie wavelength of electrons. This corresponds to the disappearance of the quasiparticle peak and the appearance of a pseudogap, an issue that has been controversial mostly due to finite-size effects in Monte-Carlo [4].

We consider the one-band Hubbard model on the square lattice with unit lattice spacing, on-site repulsion U and nearest-neighbor hopping t. We work in units where the lattice spacing is unity, $k_B = 1$, $\hbar = 1$ and $t = 1$. The theory has a simple structure that we now explain physically.

The calculation proceeds in two steps: we first obtain spin and charge susceptibilities, then we inject them in the self-energy calculation. In the calculation of susceptibilities, spin and charge susceptibilities χ_{sp}, χ_{ch} are given by RPA-like forms but with two different effective interactions U_{sp} and U_{ch} which are then determined self-consistently, as described in Ref. [5]. This procedure reproduces both Kanamori–Brueckner screening as well as the effect of Mermin–Wagner thermal fluctuations, giving a phase transition only at zero-temperature in two-dimensions [5]. There is however a crossover temperature T_X below which the magnetic correlation length ξ grows exponentially. Quantitative agreement with Monte-Carlo simulations is obtained [5] for all fillings and temperatures in the weak to intermediate coupling regime $U < 8$.

We now turn to the discussion of the single-particle properties. In order, to be consistent with the two-particle correlation functions, the self-energy $\Sigma_\sigma(k)$ must satisfy the sum rule

$$\lim_{\tau\to 0^-} \frac{1}{\beta N} \sum_k \Sigma_\sigma(k)\, G_\sigma(k)\, e^{-ik_n\tau} = U\,\langle n_\uparrow n_\downarrow\rangle, \tag{1}$$

which follows from the definition of $\Sigma_\sigma(k)$. Here, we encounter the same key quantity $\langle n_\uparrow n_\downarrow\rangle$ that appears in the sum rule for the susceptibilities. We find the following expression for $\Sigma_\sigma(k)$

$$\Sigma_\sigma(k) = Un_{-\sigma} + \frac{U}{4}\frac{T}{N} \times \sum_q \left[U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right] G^0_\sigma(k+q), \tag{2}$$

which satisfies Eqn (1) with G_σ replaced by G^0_σ on the left-hand side. This self-energy expression (2) is physically appealing since, as expected from general skeleton diagrams, one of the vertices is the bare one U, while the other vertex is dressed and given by U_{sp} or U_{ch} depending on the type of fluctuation being exchanged. Equation (2) already gives good agreement with Monte-Carlo data but the accuracy can be improved even further by requiring that the consistency condition (1) be satisfied with G_σ instead of G^0_σ. To do so we replace U_{sp} and U_{ch} on the right-hand side of (2) by αU_{sp} and αU_{ch} with α determined self-consistently by Eqn (1). For $U < 4$, we have $\alpha < 1.15$. This concludes the description of the structure of our theory.

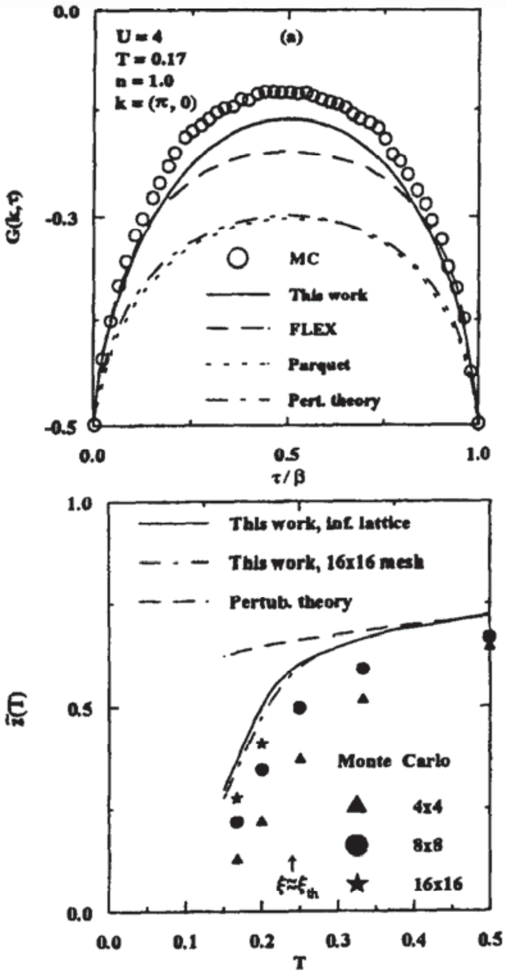

Fig. 1. (a) Comparison of our results for $G(\mathbf{k},\tau)$ with Monte-Carlo data, FLEX, parquet, and second-order pertubation theory, all on 8×8 mesh. Monte-Carlo data and results for FLEX and parquet are from Ref. [3] $n=1$, $T=0.17$. (b) Temperature dependence of the generalized renormalization factor $\tilde{z}$ defined in Eqn (3). Lines are results of our calculations for infinite lattice and 16×16 mesh. Symbols are Monte-Carlo data from Ref. [3]

COMPARISONS WITH OTHER THEORIES AND WITH QUANTUM MONTE-CARLO DATA

Figure 1(a) shows $G(\mathbf{k}_F,\tau)$ for $\mathbf{k}_F=(\pi,0)$ in a regime where the antiferromagnetic correlation length is growing exponentially. Our theory shows better agreement with Monte-Carlo than previous approaches.

Our most dramatic numerical results addressing the issue of the Fermi liquid are shown in Fig. 1(b) where we plot

$$\tilde{z}(T)=-2G(\mathbf{k}_F,\beta/2)=\int\frac{\mathrm{d}\omega}{2\pi}\frac{A(\mathbf{k}_F,\omega)}{\cosh(\beta\omega/2)}. \qquad (3)$$

This quantity $\tilde{z}(T)$ is an average of the single-particle spectral weight $A(\mathbf{k}_F,\omega)$ within $T\equiv 1/\beta$ around the Fermi level ($\omega=0$) and it is a generalization of the usual zero-temperature quasiparticle renormalization factor $z\equiv 1/(1-\partial\Sigma/\partial\omega)$. For non-interacting particles $\tilde{z}(T)$ is unity. For a normal Fermi liquid it becomes equal to a constant less than unity as the temperature decreases. The quantity $\tilde{z}(T)$ gives an estimate of $A(\mathbf{k}_F,\omega)$ around the Fermi surface even when the Fermi liquid does not exist.

One can clearly see from Fig. 1(b) that while second-order perturbation theory exhibits typical Fermi-liquid behavior for $\tilde{z}(T)$, both Monte-Carlo data and a numerical evaluation of our expression for the self-energy lead to a rapid fall-off of $\tilde{z}(T)$ below T_X (for $U=4$, $T_X\approx 0.2$ [5]). The physical origin of this effect is that the quasi-particles of the *two-dimensional* paramagnetic state become overdamped when the energy scale associated with the proximity to antiferromagnetism $\delta U\equiv U_{mf,c}-U_{sp}$ ($U_{mf,c}\equiv 2/\chi_0(\mathbf{Q},0)$) becomes exponentially small.

PSEUDOGAP

While size effects and statistical errors make continuation of the Monte-Carlo data to real frequencies particularly difficult, in our approach we can make this continuation analytically to show that the above effect corresponds to a pseudogap.

Since the spin susceptibility $\chi_{sp}(\mathbf{q},0)$ below T_X is almost singular at the antiferromagnetic wave vector $\mathbf{Q}=(\pi,\pi)$, the main contribution to Σ in Eqn (2) comes from $iq_n=0$ and wave vectors $(\mathbf{q}-\mathbf{Q})^2\leq\xi^{-2}$ near $\mathbf{Q}$. Approximating $\chi_{sp}(\mathbf{q},0)$ in by its asymptotic form $\chi_{sp}(\mathbf{q},0)\approx 2\left[U_{sp}\xi_0^2(\xi^{-2}+(\mathbf{q}-\mathbf{Q})^2)\right]^{-1}$ where $\xi_0^2\equiv\frac{-1}{2\chi_0(Q)}\frac{\partial^2\chi_0(Q)}{\partial q_x^2}$ and $\xi\equiv\xi_0(U_{sp}/\delta U)^{1/2}\sim\exp\left(\pi\tilde{\sigma}^2\xi_0^2\frac{U_{sp}}{T}\right)$, the integrals over $\mathbf{q}$ can be done to obtain the low-frequency asymptotic results

$$\Sigma^R(\mathbf{k}_F,\omega)=\frac{U}{2}+\frac{UT}{8\pi\xi_0^2\sqrt{\omega^2+v_F^2\xi^{-2}}}\times\left[\ln\left|\frac{\omega+\sqrt{\omega^2+v_F^2\xi^{-2}}}{\omega-\sqrt{\omega^2+v_F^2\xi^{-2}}}\right|-i\pi\right] \qquad (4)$$

Exactly at the Fermi surface ($\omega=0$) the imaginary part of the self-energy for $\xi>\xi_{th}$ increases exponentially when the temperature decreases, $\Sigma''(\mathbf{k}_F,0)\sim U\xi/(\xi_{th}\xi_0^2)\sim\exp(\pi\tilde{\sigma}^2\xi_0^2U_{sp}/T)$, ($\xi_{th}\equiv v_F/\pi T$). This corresponds to a pseudogap: instead of a quasiparticle peak, the spectral weight has a minimum at the Fermi level and two symmetrically located maxima away from it. Clearly this is not a Fermi liquid, yet the symmetry of the system remains unbroken at any finite T. By contrast * with $3D$, in $2D$ this effect exists in a wide temperature range $T<T_X$. These conclusions persist slightly away from half-filling. In particular, we do not find a quasiparticle peak in the pseudogap close to half-filling when $\xi\gg\xi_{th}$. This is different from the results inferred from a phenomenological zero-temperature

* In the isotropic $3D$ case $\Sigma''(\mathbf{k}_F,\omega)\sim(\ln\xi)/\xi_{th}$ and hence the pseudogap exists only in a very narrow temperature range.

calculation[6] ($\xi_{th} = \infty$) which physically corresponds to $1 \ll \xi \ll \xi_{th}$.

In photoemission experiments on real quasi two-dimensional materials we predict a rapid decrease of the spectral weight and density of states at the Fermi level in a wide temperature range, from T_X to the Néel temperature T_N ($T_X - T_N \sim 10^2$ K).

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