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# Destruction of Fermi-liquid quasiparticles in two dimensions by critical fluctuations

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**Abstract.** – It is shown that an analytic approach which includes vertex corrections in a paramagnon-like self-energy can quantitatively explain the two-dimensional Hubbard model in the weak-to-intermediate coupling regime. All parameters are determined self-consistently. This approach clearly shows that in two dimensions Fermi-liquid quasiparticles disappear in the finite-temperature paramagnetic state when the antiferromagnetic correlation length becomes larger than the electronic thermal de Broglie wavelength. Quantum Monte Carlo results are used to compare the accuracy of this approach with others.

For almost forty years, the concepts of Fermi-liquid theory have served as a basis to understand interacting fermion systems. Recently, especially in the context of high-temperature superconductors, the universal applicability of Fermi-liquid theory has been challenged. Most studies of the stability of the Fermi liquid have been done at zero temperature. However, in many physically interesting cases, a phase transition at some temperature $T_\mathrm{c}$ trivially precludes a zero-temperature Fermi liquid. Yet the system behaves as a Fermi liquid at finite temperature when $T_\mathrm{c} < T \ll E_\mathrm{F}$. Then the issue of how close to the phase transition one must be to destroy the Fermi liquid quasiparticles arises. This is especially interesting in two dimensions where the transition to a spin-density wave state (SDW) occurs only at exactly zero temperature ($T_\mathrm{c} = T_\mathrm{N} = 0$) but the system enters a renormalized classical regime (RC) at a finite temperature $T_X \ll E_\mathrm{F}$, below which the correlation length grows exponentially.

In this paper, we show for the Hubbard model that the Fermi-liquid quasiparticles are destroyed in two dimensions and replaced by a pseudogap below $T_X$, well before the zero-temperature phase transition. Although Monte Carlo simulations have addressed the issue of the pseudogap on small lattices [1], the thermodynamic limit remains uncertain. Clearly, an analytical approach is necessary to reach a definite conclusion. The development of such an approach for the Hubbard model is a long-standing and challenging problem. Below, we first present a new approach for the weak-to-intermediate coupling regime that compares better with Monte Carlo data than presently available approaches for the Hubbard model [2]-[4]. The important physical advantage of our approach is that it is based on enforcing a number of crucial sum rules instead of diagrammatic perturbative arguments that are not valid for $U > t$.

After formulating the approach, we use it to show that in two dimensions spin fluctuations do destroy Fermi-liquid quasiparticles in the paramagnetic state when the antiferromagnetic correlation length $\xi$ becomes larger than the thermal de Broglie wavelength of electrons $\xi_{\mathrm{th}} = \hbar v_{\mathrm{F}}/(\pi k_{\mathrm{B}} T)$. This situation is always realized for a range of fillings, around $n = 1$, where at $T = 0$ there is long-range order. Indeed, below $T_X > 0$ the exponentially growing correlation length $\xi$ quickly overcomes $\xi_{\mathrm{th}} \sim 1/T$.

*Physical approach.* – Our approach has the straightforward physical interpretation of paramagnon theories [5], [6]. These theories are physically attractive since they describe the effect of low-lying collective modes on single-particle properties in a manner similar to that of phonons. However, contrary to the case of phonons, the effective interactions of electrons with spin and charge excitations are strongly renormalized (no Migdal theorem). We show then how to take this effect into account without adjustable parameter.

We consider the one-band Hubbard model on the square lattice with unit lattice spacing, on-site repulsion $U$ and nearest-neighbour hopping $t$. We work in units where the lattice spacing is unity, $k_{\mathrm{B}} = 1$, $\hbar = 1$ and $t = 1$. The theory has a simple structure that we explain physically below, postponing to a longer paper the formal derivation based on the Baym-Kadanoff technique.

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 we make the approximation that spin and charge susceptibilities $\chi_{\mathrm{sp}}$, $\chi_{\mathrm{ch}}$ are given by RPA-like forms but with two different effective interactions $U_{\mathrm{sp}}$ and $U_{\mathrm{ch}}$ that are then determined self-consistently. The necessity to have two different effective interactions for spin and for charge is dictated by the Pauli exclusion principle $\langle n_\sigma^2 \rangle = \langle n_\sigma \rangle$ which implies that both $\chi_{\mathrm{sp}}$ and $\chi_{\mathrm{ch}}$ are related to only one local pair correlation function $\langle n_\uparrow n_\downarrow \rangle$. Indeed, using the fluctuation-dissipation theorem in Matsubara formalism and the Pauli principle, one can write

$$\frac{1}{\beta N} \sum_q \chi_{\mathrm{ch,sp}}(q) = \frac{1}{\beta N} \sum_q \frac{\chi_0(q)}{1 + \frac{(-1)^\ell}{2} U_{\mathrm{ch,sp}} \chi_0(q)} = n + 2\,(-1)^\ell \langle n_\uparrow n_\downarrow \rangle - (1-\ell)\, n^2\,, \tag{1}$$

where $\ell = 0$ for charge (ch), $\ell = 1$ for spin (sp), $\beta \equiv 1/T$, $n = \langle n_\uparrow \rangle + \langle n_\downarrow \rangle$, $q = (\mathbf{q}, iq_n)$ with $\mathbf{q}$ the wave vectors of an $N$ site lattice, $iq_n$ the Matsubara frequencies and $\chi_0(q)$ the susceptibility for non-interacting electrons. The value of $\langle n_\uparrow n_\downarrow \rangle$ may be obtained self-consistently [7] by adding to the above set of equations the relation $U_{\mathrm{sp}} = g_{\uparrow\downarrow}(0)\, U$, with $g_{\uparrow\downarrow}(0) \equiv \langle n_\uparrow n_\downarrow \rangle / \langle n_\downarrow \rangle \langle n_\uparrow \rangle$. Since the theory has an RPA-like form with *bare* bubble $\chi_0$, it satisfies conservation laws, in particular the condition $\chi_{\mathrm{sp,ch}}(\mathbf{q} = 0, iq_n \neq 0) = 0$. As shown in ref. [7], the above 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. There is, however, a crossover temperature $T_X$ below which the magnetic correlation length $\xi$ grows exponentially. Quantitative agreement with Monte Carlo simulations is obtained [7] 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 [8]

$$\lim_{\tau \to 0^-} \frac{1}{\beta N} \sum_k \Sigma_\sigma(k)\, G_\sigma(k) \exp[-ik_n \tau] = U \langle n_\uparrow n_\downarrow \rangle \tag{2}$$

that 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 eq. (1). Using the Baym-Kadanoff tech-

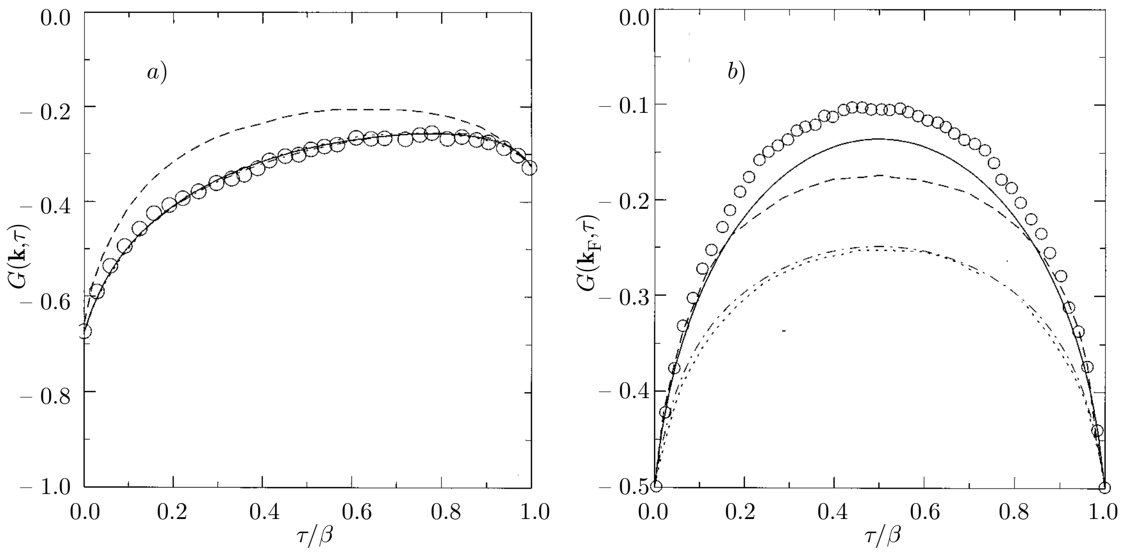


Fig. 1. – Comparison of our results for $G(\mathbf{k},\tau)$ (———) with Monte Carlo data (○), FLEX (– – –), parquet (- - - -), and second-order perturbation theory (– · – · –), all on $8 \times 8$ mesh with $U = 4$, $\mathbf{k}_F = (\pi, 0)$. Monte Carlo data and results for FLEX and parquet are from ref. [4]. *a)* $n = 0.875$, $T = 0.25$; *b)* $n = 1$, $T = 0.17$.

nique [9], we find the following expression for $\Sigma_\sigma(k)$:

$$\Sigma_\sigma(k) = Un_{-\sigma} + \frac{U}{4}\frac{T}{N}\sum_q \left[U_{\rm sp}\chi_{\rm sp}(q) + U_{\rm ch}\chi_{\rm ch}(q)\right] G^0_\sigma(k+q), \tag{3}$$

which satisfies eq. (2) with $G_\sigma$ replaced by $G^0_\sigma$ on the left-hand side. This self-energy expression (3) 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 $U_{\rm sp}$ or $U_{\rm ch}$ depending on the type of fluctuation being exchanged. Equation (3) already gives good agreement with Monte Carlo data but the accuracy can be improved even further by requiring that the consistency condition (2) be satisfied with $G_\sigma$ instead of $G^0_\sigma$. To do so, we replace $U_{\rm sp}$ and $U_{\rm ch}$ on the right-hand side of (3) by $\alpha U_{\rm sp}$ and $\alpha U_{\rm ch}$ with $\alpha$ determined self-consistently by eq. (2). For $U < 4$, we have $\alpha < 1.15$. This concludes the description of the structure of our theory.

It is important to realize that $\Sigma$ given by eq. (3) cannot be substituted back into the calculation of $\chi_{\rm sp,ch}$ by simply replacing $\chi_0 = G_0G_0$ with the dressed bubble $\tilde\chi_0 = GG$. This would violate conservation of spin and charge. In particular, the condition(1) $\chi_{\rm sp,ch}(\mathbf{q}=0, iq_n \neq \neq 0) = 0$ would be violated. In the next order, one is forced to work with frequency-dependent irreducible vertices that offset the unphysical behaviour of $\tilde\chi_0$ at finite frequencies.

*Comparisons with other theories and with quantum Monte Carlo data.* – Figure 1 *a)* shows $G(\mathbf{k},\tau)$ for filling $n = 0.875$, temperature $T = 0.25$ and $U = 4$ for the wave vector on the

(1) In FLEX [2] one does substitute $\Sigma$ back in the RPA-like expression with a *dressed* bubble $\tilde\chi_{\rm RPA} = \tilde\chi_0/(1 - U\tilde\chi_0)$. However, $\tilde\chi_{\rm RPA}$ cannot be interpreted as a physical susceptibility since $\tilde\chi_{\rm RPA}(\mathbf{q} = 0, iq_n \neq 0) \neq 0$. The true conserving $\chi$ in FLEX is different from $\tilde\chi_{\rm RPA}$ and is not substituted back in the calculation of $\Sigma$.

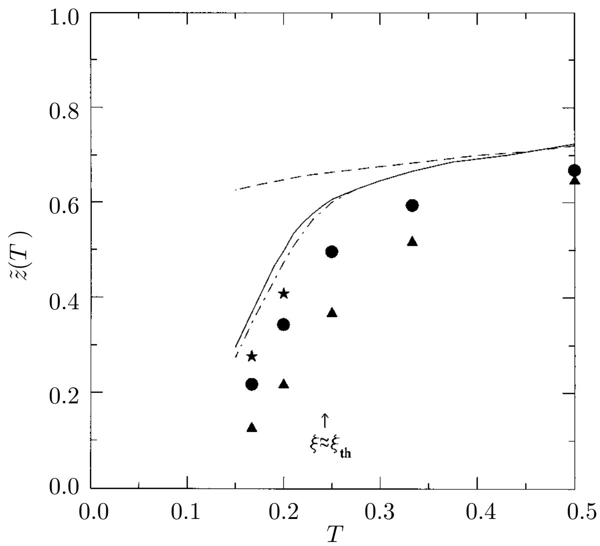


Fig. 2. – Temperature dependence of the generalized renormalization factor $\tilde{z}$ defined in eq. (4). Lines are results of our calculations for infinite lattice (———) and $16\times16$ mesh (–·–·–), and perturbation theory (– – –). Symbols are Monte Carlo data from ref. [1]: ▲ $4\times4$, • $8\times8$, ⋆ $16\times16$.

$8\times8$ lattice which is closest to the Fermi surface, namely $(\pi, 0)$. For these parameters, size effects are negligible. Our theory is in agreement with Monte Carlo data and with the parquet approach but in this regime second-order perturbation theory for the self-energy gives the same result. This surprising performance of perturbation theory (see also [10]) is a consequence of compensation between the renormalized vertices and susceptibilities ($U_{\rm sp} < U$, $\chi_{\rm sp}(q) > \chi_0(q)$; $U_{\rm ch} > U$, $\chi_{\rm ch}(q) < \chi_0(q)$).

Half-filling $n = 1$ is an ideal situation for numerical studies of low-energy phenomena since some of the allowed wave vectors on finite lattices lie exactly on the Fermi surface. Figure 1 *b*) shows $G(\mathbf{k}_{\rm F}, \tau)$ for $\mathbf{k}_{\rm F} = (\pi, 0)$ in a regime where the SDW correlation length is growing exponentially. Our theory shows better agreement with Monte Carlo than previous approaches.

Figure 2 contains our most dramatic numerical results. They address the issue of the influence of critical fluctuations on Fermi-liquid quasiparticles. We plot

$$\tilde{z}\,(T) = -2G\,(\mathbf{k}_{\rm F}, \beta/2) = \int \frac{{\rm d}\omega}{2\pi} \frac{A\,(\mathbf{k}_{\rm F}, \omega)}{\cosh\,(\beta\omega/2)}. \tag{4}$$

This quantity $\tilde{z}\,(T)$ is an average of the single-particle spectral weight $A\,(\mathbf{k}_{\rm F}, \omega)$ 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 since the width of the quasiparticle peak scales as $T^2$ and hence lies within $T$ of the Fermi level. The quantity $\tilde{z}\,(T)$ is the best estimate of $z$ one can get from Monte Carlo data for $G(\mathbf{k}, \tau)$. Moreover $\tilde{z}\,(T)$ gives an estimate of $A\,(\mathbf{k}_{\rm F}, \omega)$ around the Fermi surface even when the Fermi liquid does not exist and $z \neq \tilde{z}\,(T \to 0)$.

One can clearly see from fig. 2 that while second-order perturbation theory exhibits typical Fermi-liquid behaviour 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 [7] $U = 4$, $T_X \approx 0.2$).

The rapid decrease of $\tilde{z}\,(T)$ clearly suggests non–Fermi-liquid behaviour. We checked also that our theory reproduces the Monte Carlo size dependence. The $16 \times 16$ mesh on the figure gives practically the same result as the thermodynamic limit (solid line).

*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 the disappearance of the Fermi-liquid quasiparticle and to the opening of a pseudogap. For simplicity, we give asymptotics for $n = 1$ at the Fermi wave vector, where $\varepsilon(\mathbf{k}_\mathrm{F}) = 0$, but similar results apply for $n \neq 1$ as long as there is long-range order at $T = 0$.

The spin susceptibility $\chi_\mathrm{sp}\,(\mathbf{q}, 0)$ below $T_X$ is almost singular at the antiferromagnetic wave vector $\mathbf{Q} = (\pi, \pi)$ because the energy scale $\delta U \equiv U_\mathrm{mf,c} - U_\mathrm{sp}$ ($U_\mathrm{mf,c} \equiv 2/\chi_0\,(\mathbf{Q}, 0)$) associated with the proximity to the SDW becomes exponentially small [7]. This small energy scale, $\delta U \ll T$, leads to the so-called renormalized classical regime for the fluctuations. Then, the main contribution to $\Sigma$ in eq. (3) comes from $iq_n = 0$ and wave vectors $(\mathbf{q} - \mathbf{Q})^2 \le \xi^{-2}$ near $\mathbf{Q}$. Approximating $\chi_\mathrm{sp}\big(\mathbf{q}, 0\big)$ in eqs. (1) and (3) by its asymptotic form $\chi_\mathrm{sp}\,(\mathbf{q}, 0) \approx \approx 2\left[U_\mathrm{sp}\xi_0^2(\xi^{-2} + (\mathbf{q} - \mathbf{Q})^2)\right]^{-1}$, where $\xi_0^2 \equiv \frac{-1}{2\chi_0(Q)}\frac{\partial^2\chi_0(Q)}{\partial q_x^2}$ and $\xi \equiv \xi_0(U_\mathrm{sp}/\delta U)^{1/2}$, we obtain

$$\tilde{\sigma}^2 = \frac{2T}{U_\mathrm{sp}\xi_0^2}\int \frac{\mathrm{d}^2 q}{(2\pi)^2}\frac{1}{q^2 + \xi^{-2}}\,, \tag{5}$$

while the *correction* to Hartree-Fock is

$$\Sigma\,(\mathbf{k}_\mathrm{F}, ik_n) \cong \frac{UT}{2\xi_0^2}\int \frac{\mathrm{d}^2 q}{(2\pi)^2}\frac{1}{q^2 + \xi^{-2}}\frac{1}{ik_n - \mathbf{q}\cdot\mathbf{v}_\mathrm{F}}\,, \tag{6}$$

where $\tilde{\sigma}^2 \equiv n - 2\langle n_\uparrow n_\downarrow\rangle - C < 1$ is the right-hand side of eq. (1) minus corrections $C$ that come from the sum over non-zero Matsubara frequencies (quantum effects) and from $(\mathbf{q} - \mathbf{Q})^2 \gg \xi^{-2}$.

The retarded self-energy $\Sigma_\mathrm{R}\big(\mathbf{k}_\mathrm{F}, \omega\big)$ is obtained from eq. (6) by analytical continuation $ik_n \to \omega + i0$. The key point in what follows is that the 2D integrals in eqs. (5) and (6) are divergent at small $q$ for $\xi = \infty$. This is qualitatively different from higher dimensions where similar integrals are finite. This results in two effects below $T_X$, namely: *a*) $\xi$ grows exponentially, $\xi \sim \exp[\pi\tilde{\sigma}^2\xi_0^2 U_\mathrm{sp}/T]$ and quickly becomes larger then $\xi_\mathrm{th}$. *b*) The imaginary part of the self-energy at the Fermi surface $\Sigma''_\mathrm{R}(\mathbf{k}_\mathrm{F}, 0) \propto T\int d^{d-1}q_\perp(q_\perp^2 + \xi^{-2})^{-1}$ is proportional to $\xi$ in $d = 2$ and hence is very large $\Sigma''_\mathrm{R}(\mathbf{k}_\mathrm{F}, 0) \approx -U\xi/(\xi_\mathrm{th}\xi_0^2) > 1$, when $\xi > \xi_\mathrm{th}$. By contrast, for $d = 3$, $\Sigma''_\mathrm{R}(\mathbf{k}_\mathrm{F}, 0) \sim -U\,(\ln\xi)\,/\,\big(\xi_0^2\xi_\mathrm{th}\big)$ , so that the Fermi-liquid is destroyed only in a very narrow temperature range close the Néel temperature $T_\mathrm{N}$. One can check that the large $\Sigma''_\mathrm{R}(\mathbf{k}_\mathrm{F}, 0)$ in two dimensions (for $T < T_X$) leads to a *minimum* at $\omega = 0$ in the spectral weight $A\,(\mathbf{k}_F, \omega) \equiv -2\,\mathrm{Im}\,G_\mathrm{R}\,(\mathbf{k}_\mathrm{F}, \omega)$ instead of the maximum obtained in Fermi liquids. For $v_\mathrm{F}/\xi < |\omega| < T$, we have

$$A\,(\mathbf{k}_\mathrm{F}, \omega) \cong \frac{2\,|\omega|\,UT/(8\xi_0^2)}{[\omega^2 - UU_\mathrm{sp}\tilde{\sigma}^2/4]^2 + [UT/(8\xi_0^2)]^2}\,. \tag{7}$$

This function has two maxima(²) that correspond to precursors of the zero-temperature antiferromagnetic bands (shadow bands [6]).

(²) The precise location of the maxima of $A\big(\mathbf{k}_\mathrm{F}, \omega\big)$ can be found only numerically since eq. (7) was obtained for $|\omega| < T < T_X < \sqrt{UU_\mathrm{sp}}\tilde{\sigma}/2$. Also, since we start from Fermi-liquid quasiparticles, our analysis of the critical regime is restricted to $T_X - T \ll T_X$ .

The above analysis shows by contradiction that in the paramagnetic state below $T_X$ there is no Fermi-liquid quasiparticle at $k_{\rm F}$. Indeed, starting from quasiparticles $\left(G_\sigma^{(0)}\right)$ we found that as temperature decreases $\Sigma''_{\rm R}(\mathbf{k}_{\rm F},0)$ *increases* indefinitely instead of *decreasing*, in direct contradiction with the starting hypothesis. By contrast, a self-consistent treatment where we use in eq. (3) the full $G_\sigma$ with a large $\Sigma''_{\rm R}(\mathbf{k}_{\rm F},0)$ shows that, for $T < T_X$ , $\Sigma''_{\rm R}(\mathbf{k}_{\rm F},0)$ remains large in $d = 2$ and does not vanish as $T \to 0$, again confirming that the system is not a Fermi-liquid in this regime. These conclusions persist away from half-filling as long as $T_X(n) > 0$. In particular, we do not find a quasiparticle peak in the pseudogap when $\xi > \xi_{\rm th}$. This is different from the results inferred from a phenomenological zero-temperature calculation [6] $\left(\xi_{\rm th} = \infty\right)$ that physically corresponds to $1 \ll \xi \ll \xi_{\rm th}$.

*Experimental prediction.* – We predict that the exponential growth of the magnetic correlation length $\xi$ below $T_X$ will be accompanied by the appearance of precursors of SDW bands in $A(\mathbf{k}_{\rm F},\omega)$ with no quasiparticle peak between them. By contrast with isotropic materials, in quasi–two-dimensional materials like the cuprates, this effect should exist in a wide temperature range, from $T_X$ ($T_X \ll U \lesssim E_{\rm F}$) to the Néel temperature $T_{\rm N}$ ($T_X - T_{\rm N} \sim 10^2$ K).

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