Paramagnetic susceptibility and paramagnet-ferromagnet crossover in the ground state of the $U=\infty$ Hubbard model

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The paramagnetic susceptibility $\chi(0,0) = dR(H)/dH$ $(H\to 0, U=\infty)$ of the Hubbard model is calculated in second order in the kinematic interaction. The result found radically changes the conclusion, which follows from the theory of first order in the kinematic field, that there is a paramagnetic instability at $T=0$. The expression for $\chi(0,0)$ agrees with the Pauli susceptibility in the gas limit $(n\to 0)$. It describes a pronounced correlation enhancement (by a factor ≈ 5) at an intermediate filling $(n\approx 0.5)$. It describes a crossover to a ferromagnetic state at the point $n\approx 0.83$ for $\rho(E) = \rho = 1/2W$.

1. The quasiparticle Green's function in second order in $t(f-f')$ for $U=\infty$ is[2,3]

$$G_\sigma(\omega,\mathbf{k}) = \frac{n_-^{\bar\sigma}}{\omega - n_-^{\bar\sigma}E(\mathbf{k}) - \Omega_\sigma(\omega,\mathbf{k})/n_-^{\bar\sigma}}, \tag{1}$$

$$\Omega_\sigma(\omega,\mathbf{k}) = \Omega_\sigma^{\mathrm{I}}(\mathbf{k}) + \Omega_\sigma^{\mathrm{II}}(\omega), \tag{2}$$

where the self-energy part $\Omega_\sigma^{\mathrm{I}}(\mathbf{k})$ incorporates all effects (both local and nonlocal) which are linear[1)] in $t(\mathbf{f}-\mathbf{f}')$:

$$\Omega_\sigma^{\mathrm{I}}(\mathbf{k}) = K_\sigma(\mathbf{h})E(\mathbf{k}) - W\Delta_\sigma(\mathbf{h}), \tag{3}$$

$$\Delta_\sigma(\mathbf{h}) = \langle X_0^{\bar\sigma 0} X_{\mathbf{h}}^{0\bar\sigma} \rangle, \tag{4}$$

$$K_\sigma(\mathbf{h}) = \langle n_0^{\bar\sigma} n_{\mathbf{h}}^{\bar\sigma} \rangle - (n^{\bar\sigma})^2 + \langle X_0^{\bar\sigma\sigma} X_{\mathbf{h}}^{\sigma\bar\sigma} \rangle, \tag{5}$$

$$W = |t|z, \qquad E(\mathbf{k}) = \sum_h t(\mathbf{h})e^{i\mathbf{k}\mathbf{h}}. \tag{6}$$

The system of equations which follows from Ref. 1 for $\Omega_\sigma^{\mathrm{II}}(\omega) = 0$ describes both the Stoner–Nagaoka state (saturated ferromagnetism: $R = n^\sigma$, $n^{\bar\sigma} = 0$) and an instability of this state at finite hole densities.[2–4] It was shown in Ref. 5 that in the special case of the three-body problem (one flipped spin in a Stoner–Nagaoka state) the one-particle Green's function in (1) is the same as the exact solution of the problem.[6]

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2. The Green's function in (1) can easily be generalized to the case of an external magnetic field:

$$G^{\sigma}(\omega, \mathbf{k}, n^{\bar{\sigma}}, H) = G^{\sigma}(\omega + \eta(\sigma)H, \mathbf{k}, n^{\bar{\sigma}}(H), H = 0). \tag{7}$$

The paramagnetic susceptibility $\chi(0,0)$ was calculated in first order in the kinematic field in Ref. 1. The expression derived for $\chi(0,0)$ turned out to be negative in the region $0.7 \geqslant n \geqslant 0$, in which we have $R = n^{\sigma} - n^{\bar{\sigma}} = 0$ according to the equations of the kinematic field[2,3] (i.e., the state is either paramagnetic or singlet). At $n = 0$ and $n \approx 0.7$, the result $\chi(0,0) \to -\infty$ was found (Fig. 1). This result might indicate an instability of the paramagnetic state and the possible existence of a singlet phase in the ground state of the Hubbard model. Now, however, that result looks dubious.

3. Let us calculate $\chi(0,0)$ in second order in the kinematic field. The self-energy part $\Omega_{\sigma}^{\text{II}}(\omega)$ for $U = \infty$ is[2]

$$\Omega_{\sigma}^{\text{II}}(\omega) = \left\{ \frac{1}{N} \sum_{\mathbf{k}} E^2(\mathbf{k}) \frac{(n_{-}^{\bar{\sigma}})^2 - [(n_{-}^{\bar{\sigma}})^2 + K_{\sigma}]^2}{(n_{-}^{\bar{\sigma}})^2} - \frac{(W\Delta_{\sigma})^2}{(n_{-}^{\bar{\sigma}})^2} \right\} \frac{1}{N} \sum_{\mathbf{k}'} G^{\sigma}(\omega, \mathbf{k}').$$

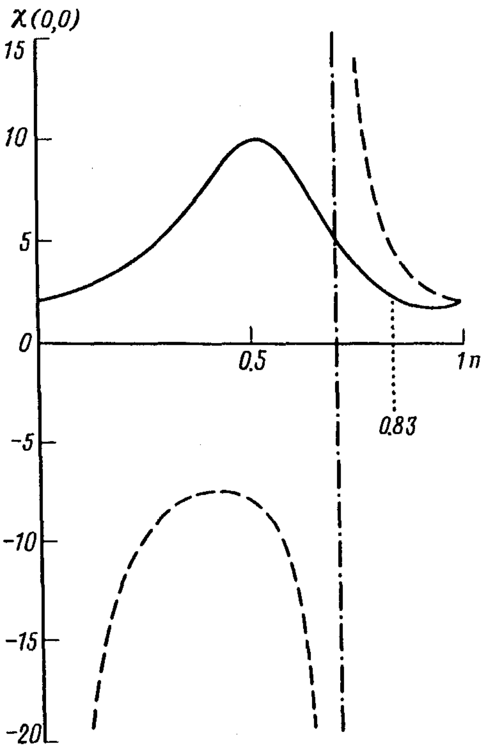

FIG. 1. Uniform static paramagnetic susceptibility as a function of the density in the $U = \infty$ Hubbard model for a density of states $\rho(E) = \rho = 1/2W$. Solid line—$\chi(0,0)$ as calculated in second order in the kinematic field; dashed line—in first order (the result of Ref. 1).

We find $\Omega_\sigma^{II}(\omega)$ in the pole approximation, i.e., with $\Omega_\sigma^{II}(\omega=\omega^I)$, where ω^I is the pole of the Green's function in the theory linear in $t(\mathbf{f}-\mathbf{f}')$. This approach conserves the symmetry of the first-order equations[1] for $\chi(0,0)$,

$$n^+ = (1-n_-)\frac{1}{2\alpha_-}[\xi_+ + \alpha_- - \Delta_-], \tag{9}$$

$$n^- = (1-n_+)\frac{1}{2\alpha_+}[\xi_- + \alpha_+ - \Delta_+], \tag{10}$$

but it substantially changes the constituent terms[2)]: $\xi_\pm(R,n,H)$, $\alpha_\pm(R,n)$, and $\Delta_\pm(R,n)$. These radical differences can easily be seen by comparing the poles of the Green's function in the first- and second-order theories (ω^I and ω^{II}, respectively) in the gas limit ($n\to 0$):

$$\omega^I = E(\mathbf{k})\left[1-\frac{n}{2}-\frac{n^2}{2}\right]+\frac{Wn}{2}-\frac{R}{2}\left[W\left(1-\frac{n^2}{4}\right)-E(\mathbf{k})\left(1+n-\frac{n^2}{4}\right)\right], \tag{11}$$

$$\omega^{II} = E(\mathbf{k})\left[1-\frac{5n^2}{8}\right]+\frac{Wn}{2}-\frac{R}{2}\left[W\left(1-\frac{n^2}{4}\right)-E(\mathbf{k})\left(\frac{5n}{2}-\frac{n^2}{8}\right)\right]. \tag{12}$$

A complete cancellation of the leading virial coefficients in (12) in the dispersive part of the equation leads to the following result for $\chi(0,0)$ in the gas limit:

$$\chi_{n\Rightarrow 0}(0,0) = \frac{2-n}{-\xi\left(1-\frac{5n}{2}+\frac{11n^2}{8}\right)+n-\frac{13n^2}{8}},$$
$$\xi = \frac{\mu}{W} = -1+\frac{3n}{2}+\frac{7n^2}{8}. \tag{13}$$

The complete expression for $\chi(0,0)$, which holds for all n in the region $R=0$, is

$$\chi(0,0) = \frac{2-n}{\alpha-\left\{(\xi-\Delta)\left[1-\frac{\alpha'(2-n)}{\alpha}\right]+\Delta'(2-n)\right\}}, \tag{14}$$

$$\xi = -\alpha+\Delta+\frac{2\alpha n}{(2-n)}, \tag{14a}$$

$$\alpha = \frac{2-n}{2}-\frac{2m}{2-n}+\frac{2c}{2-n}\frac{a_1-a_2}{a_1+a_2}; \qquad \Delta = \frac{2s}{2-n} \tag{14b}$$

$$\alpha' = \frac{1}{2}+\beta+\frac{2m}{(2-n)^2}-\frac{2p}{2-n}; \qquad \Delta' = \frac{2}{2-n}\left[Q+\frac{s}{2-n}\right]; \tag{14c}$$

$$\beta = \frac{2}{2-n}\left[\frac{a_2b_1-b_2a_1}{(a_1+a_2)^2}c+\frac{a_1-a_2}{a_1+a_2}\left(d-\frac{c}{2-n}\right)\right]; \tag{14d}$$

$$s=\frac{n(1-n)}{2-n};\quad m=\frac{n^2(1-n)(4-n)}{2(2-n)^2};\quad Q=\frac{2(1-n)^2}{(2-n)^2};\tag{14e}$$

$$a_1=\frac{(2-n)^2}{4}-4s^2;\quad a_2=c^2;\quad b_1=(2-n)+16sQ;\quad b_2=4cd,\tag{14f}$$

$$p=\frac{n(1-n)(5n-4)}{2(2-n)^2};\quad c=\frac{(2-n)^2}{4}-m;\quad d=\frac{2-n}{2}-p.\tag{14g}$$

Figure 1 shows the susceptibility in (14) as a function of n. The minimum value $\chi_{\min}(0,0)=2$, which corresponds to the Pauli value for a given density of states $\rho=1/2W$, is reached at the points[3)] $n=0$, $n=0.83$, and $n=1$. This result obviously makes the density dependence of $\chi(0,0)$ radically different from that which follows from the first-order theory (the dashed line in Fig. 1). The value $n=0.83$ is evidence of a paramagnetic instability of this system, which shifts to densities above $n\approx0.7$ $[\Omega^{11}_{\sigma}(\omega)\equiv0]$. The transition from a highly correlated paramagnetic phase to an ordered ferromagnetic state is not accompanied by the appearance of discontinuities in the function $\chi(0,0)$, so it is a crossover transition.

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[1)]All definitions are the same as in Refs. 1–3.

[2)]It can be shown that the component due to the incoherent part is $\mathrm{Im}\Omega^{11}_{\sigma}(\omega=\omega')\leqslant\mathrm{Re}\Omega^{11}_{\sigma}(\omega=\omega')$, but there is a dangerous proximity near $n\approx0.5$.

[3)]For $\rho(E)\sim\sqrt{W^2-E^2}$ this would be $\chi_{\min}(0,0)=0$.

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