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Спиновая восприимчивость в модели Хаббарда
с зависящим от энергии эффективным взаимодействием

Дана самосогласованная схема расчета спиновой восприимчивости в модели Хаббарда при нулевой температуре. В предположении о локальности двухчастичной вершинной части найдено выражение для статической и однородной парамагнитной восприимчивости. Численные расчеты указывают на возможность ферромагнитной упорядоченности.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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On the Spin Susceptibility for Itinerant Electrons with Energy-Dependent Effective Interaction

A self-consistent scheme is given to calculate the spin susceptibility for the Hubbard model at zero temperature. By assuming a local two-particle vertex a correlation-enhanced expression for the static and uniform paramagnetic susceptibility is found. Numerical results exhibit the possibility of ferromagnetic ordering.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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A possible ferromagnetic ordering in a system of interacting electrons described by the Hubbard model [1] depends on the approximation used ([2] to [6]). Spin susceptibility calculations performed within the Hubbard I approximation [2], Roth's two-pole scheme [3], and the method of spectral moments [4] yield instabilities of the paramagnetic phase towards ferromagnetic ordering; whereas the susceptibility is proved to remain finite in the Hubbard III approximation [5]. On the other hand, by summing up ladder diagrams both non-magnetic and magnetic spectral properties were found [6].

In this paper we calculate the magnetic susceptibility with Green functions dressed by the ladder scheme [6], starting from the Fermi liquid approach [7] to narrow band systems. Then, the longitudinal dynamic susceptibility $\chi(\vec{k},\omega)$ corresponding to the linear response to a space-and time-varying magnetic field $h_i(t) = h_0 e^{i(\vec{k}\vec{R}_i - \omega t)}$ can be expressed in terms of causal Green functions at $T=0$ by

$$\chi(\vec{k},\omega) = \frac{\mu_B^2}{N} \sum_{ij\sigma} \sigma \int \frac{d\bar{E}}{2\pi} G_{ij\sigma}(\bar{E}+\omega) i\Lambda_{j\sigma}(\bar{E}+\omega,\bar{E}) G_{ji\sigma}(\bar{E}) e^{-i\vec{k}\vec{R}_i}, \quad (1a)$$

where μ_B is the Bohr magneton, N is the number of lattice sites, $\vec{R}_i$ is the position vector of site i, σ denotes the spin. The spin vertex Λ following from the two-particle correlation function obeys the integral equation

$$\Lambda_{i\sigma}(E+\omega,E) = \sigma e^{i\vec{k}\vec{R}_i} - \sum_j \int \frac{d\bar{E}}{2\pi} i T_i(E+\bar{E}) \times$$

$$\times G_{ij-\sigma}(\bar{E}+\omega) G_{ji-\sigma}(\bar{E}) \Lambda_{j-\sigma}(\bar{E}+\omega,\bar{E}) +$$

$$+ \sum_j \int \frac{d\bar{E}\, d\bar{\bar{E}}}{(2\pi)^2} G_{ii-\sigma}(\bar{\bar{E}}) G_{ii\sigma}(E+\bar{\bar{E}}-\bar{E}) [T_i(E+\bar{\bar{E}})]^2 \times$$

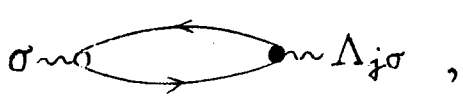
$$\times G_{ij-\sigma}(\bar{E}+\omega) G_{ji-\sigma}(\bar{E}) \Lambda_{j-\sigma}(\bar{E}+\omega,\bar{E}) +$$

$$+ \sum_j \int \frac{d\bar{E}\, d\bar{\bar{E}}}{(2\pi)^2} G_{ii-\sigma}(\bar{\bar{E}}) G_{ii-\sigma}(E+\bar{\bar{E}}-\bar{E}) [T_i(E+\bar{\bar{E}})]^2 \times$$

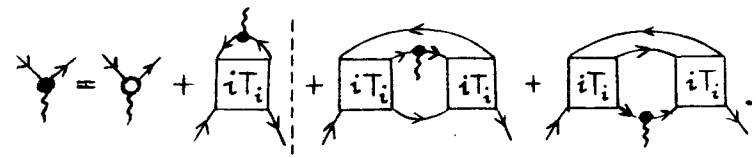
$$\times G_{ij\sigma}(\bar{E}+\omega) G_{ji\sigma}(\bar{E}) \Lambda_{j\sigma}(\bar{E}+\omega,\bar{E}) . \qquad (2a)$$

Formula (2a) involving particle-hole and particle-particle scatterings can be derived self-consistently (reference [7]) on the basis of a local effective two-particle vertex T_i. Note that the indices i in the quantities G_{ii}, T_i (below Σ_{ii}, too) are redundant. Off-diagonal elements of Λ in spin and lattice spaces vanish identically, provided the local T_i is only taken into account.

Diagrams representing equations (1a) and (2a) are



, (1b)



(2b)

To evaluate the scattering amplitude T_i we use the local version of the horizontal ladder approximation (reference [6]), i.e., $T_i(E_1+E_2)$ as a shorthand of $T_{\substack{iiii \\ \sigma-\sigma\sigma-\sigma}}(E_1,E_2;E_3,E_1+E_2-E_3)$ must be determined in the self-consistent cycle:

$$T_i(E) = [\frac{1}{U} + \int \frac{d\bar{E}}{2\pi i} G_{ii\sigma}(\bar{E}) G_{ii-\sigma}(E-\bar{E})]^{-1}, \qquad (3)$$

$$\Sigma_{ii\sigma}(E) = \int \frac{d\bar{E}}{2\pi i} G_{ii-\sigma}(\bar{E}) T_i(E+\bar{E}) . \qquad (4)$$

$$(G^{-1}(E))_{ij\sigma} = (G_\Lambda^{-1}(E))_{ij} - \Sigma_{ii\sigma}(E)\delta_{ij}, \qquad (5)$$

$$n = \sum_\sigma \int \frac{d\bar{E}}{2\pi i} G_{ii\sigma}(\bar{E}) . \qquad (6)$$

Here U is the bare intra-atomic Coulomb repulsion in the Hubbard model, G_Λ is the free propagator, $\Sigma_{ii\sigma}$ is the site-diagonal self-energy in the particle-particle channel, and n is the average number of electrons per site.

Going over to the paramagnetic phase ($\Sigma_{ii\sigma} = \Sigma_{ii-\sigma} = \Sigma_{ii}$) and making the ansatz $\Lambda_{i\sigma}(E+\omega,E) = \sigma \Lambda_{\vec{k}}(E+\omega,E) e^{i\vec{k}\vec{R}_i}$ one obtains from equation (1) the paramagnetic susceptibility in terms of $\vec{k}$-transformed Green function as

$$\chi(\vec{k},\omega) = \frac{2\mu_B^2}{N} \sum_{\vec{k}'} \int \frac{d\bar{E}}{2\pi} G_{\vec{k}'+\vec{k}}(\bar{E}+\omega) G_{\vec{k}'}(\bar{E}) i\Lambda_{\vec{k}}(\bar{E}+\omega,\bar{E}) , \qquad (7)$$

where equation (2) (the last two terms cancel each other exactly) now reads

$$\Lambda_{\vec{k}}(E+\omega,E)=1+\int\frac{d\bar{E}}{2\pi}\,i\,T_i(E+\bar{E})\,\frac{1}{N}\sum_{\vec{k}'}G_{\vec{k}+\vec{k}'}(\bar{E}+\omega)\times$$

$$\times G_{\vec{k}'}(\bar{E})\Lambda_{\vec{k}}(\bar{E}+\omega,\bar{E}). \qquad (8)$$

More practically, we approximate the energy dependence in equation (8) by replacing $T_i(E+\bar{E})\longrightarrow\tilde{T}_i(E)=\frac{2\Sigma_{ii}(E)}{n}$. Then, one gets in the so-called $\vec{k}$-limit the static paramagnetic susceptibility

$$\chi(\vec{k}\to 0,\omega=0)=\frac{2\mu_B^2\,i\int\frac{d\bar{E}}{2\pi}(G^2(\bar{E}))_{ii}}{1-\frac{2i}{n}\int\frac{d\bar{E}}{2\pi}(G^2(\bar{E}))_{ii}\,\Sigma_{ii}(\bar{E})}\,. \qquad (9)$$

This correlation-enhanced expression refers to instabilities of the paramagnetic phase towards ferromagnetic ordering, arising from the condition $\chi^{-1}(\vec{k}\to 0,\omega=0)=0$. In the Hartree-Fock approximation there follows from equation (9) the RPA result $\chi^{HF}=2\mu_B^2\rho^{HF}(\mu)/(1-U\rho^{HF}(\mu))$, where $\rho^{HF}(\mu)$ denotes the one-particle density of states at the Fermi level μ.

In the numerical analysis we suppose the simple form $\rho_\Lambda(E)=\frac{2}{\pi\Lambda}(1-(\frac{E}{\Lambda})^2)^{1/2}\theta(\Lambda-|E|)$ (in the following we set the half-band width $\Lambda=1/2$) for the unperturbed density of states to calculate G_Λ analytically.

Figure 1 shows the one-electron density of states per site per spin defined in terms of the retarded ("r") Green function by $\rho_\sigma(E)=-\frac{1}{\pi}\,\mathrm{Im}\,G^r_{ii\sigma}(E)$ and calculated numerically

from equations (3) to (6). It is demonstrated the transition from paramagnetic via ferromagnetic to saturated ferromagnetic solutions with increasing U at fixed n.

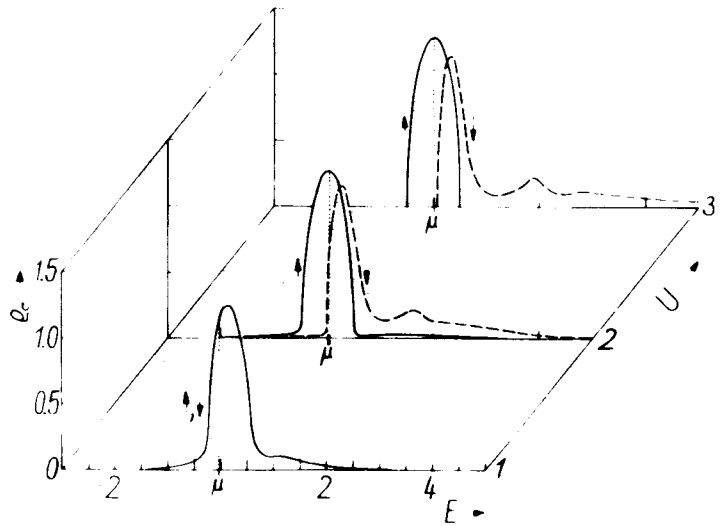


Fig. 1. Spin-dependent electron densities of states $\rho_\sigma(E)$ for different values of the intra-atomic Coulomb repulsion U at the electron concentration $n=0.5$. μ is the Fermi energy.

Results for the static paramagnetic susceptibility $\chi=\chi(\vec{k}\longrightarrow 0,\omega=0)$ at zero temperature computed from equation (9) on the basis of equations (3) to (6) are represented in Fig. 2. χ becoming infinite suggests the possibility of ferromagnetism with increasing n at fixed U (Fig. 2a) or increasing U at fixed n (Fig. 2b), respectively. For comparison, the phase diagram (Fig. 2c) indicated by the susceptibility results confirms the picture of reference /6/; some quantitative

differences may arise by including particle-hole processes. In our treatment an explicit criterion for ferromagnetism can be gi-

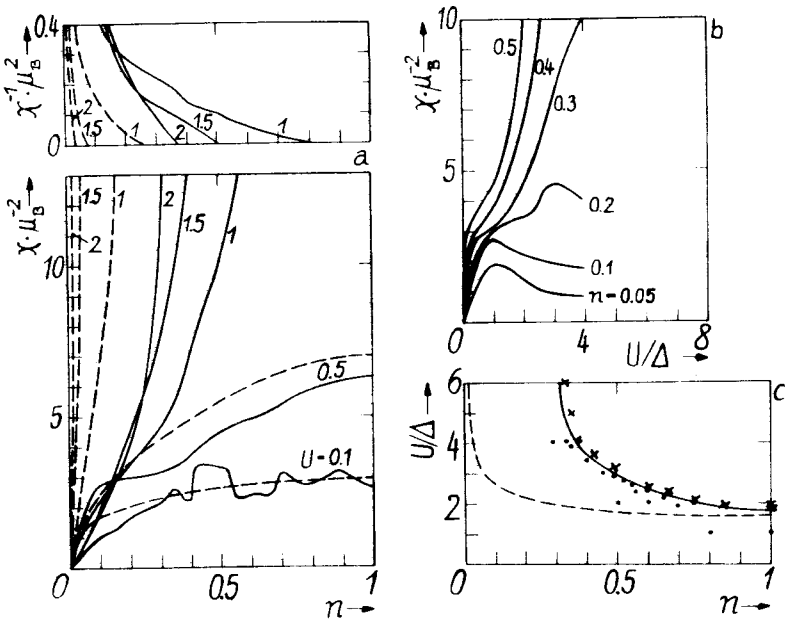


Fig.2. Static paramagnetic susceptibility χ (full lines) at T=0K compared with Hartree-Fock results (dashed lines) in dependence on U and n, see a), b); c) dividing line between paramagnetism(•) and ferromagnetism (×).

ven by the zeros of the denominator of equation (9). As a consequence of the gapless single-particle spectrum (see Fig.1) only one zero of χ^{-1} can appear for $n \leq 1$ (unlike references [3] and [4]). It seems that some artifices of decoupling methods are avoided in the present approach.

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