Instability of Nagaoka state in the approximation of a self-consistent-kinematic field in the limit $U\to\infty$

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It is shown in the approximation of a kinematic field [E. G. Goryachev and E. V. Kuzmin, Phys. Lett. A **131**, 481 (1988)] that the state of a Nagaoka ferromagnet ($R = n = n^{\sigma}$, $n^{\sigma} = 0$) is unstable at finite hole densities ($p_c \approx 0.2$), in agreement with the rigorous assertion of Shastry *et al.* [Phys. Rev. B **41**, 2375 (1990)].

1. A thermodynamic generalization of Nagaoka's theorem results[3] is presently a most pressing matter, since a solution of this problem can lead to an understanding of the physical nature of the ground state in the Hubbard model. An important step in this direction was recently taken. Shastry *et al.*[2] proved rigorously that the state of a saturated ferromagnet ($R = n = n^{\sigma}$, $n^{\bar{\sigma}} = 0$) with $U = \infty$ is unstable at a certain threshold hole density p_c which depends on the symmetry and dimensionality of the lattice.

2. We have previously shown[1] that the Hubbard model incorporates a regular representation of the eigenenergy part as a power series in the tunneling integral $t(\vec{f}-\vec{f}')$. A one-particle Green's function which arises in first order in $t(\vec{f}-\vec{f}')$ satisfies four exact relations for the spectral moments corresponding to a Kalashnikov–Fradkin linear canonical transformation. The Green's function is thus the best one-particle approximation of the problem in the class of solutions which contain two δ-functions.

Below we examine homogeneous solutions of the problem in the limit $U\to\infty$ ($t>0$). The system of self-consistent equations for these solutions is

$$n^{\bar{\sigma}} = (1-n^{\sigma})\int d\epsilon\rho(\epsilon) f[(1-n^{\sigma})\epsilon + n^{\sigma}\Omega^{I}_{\sigma}(\epsilon)], \tag{1a}$$

$$n^{\bar{\sigma}}(1-n^{\bar{\sigma}})\Omega^{I}_{\sigma}(\epsilon) = \varphi^{\bar{\sigma}}(\epsilon) - \Psi^{\bar{\sigma}}, \tag{1b}$$

$$\Psi^{\bar{\sigma}} = (1-n^{\sigma})\int d\epsilon\rho(\epsilon)\epsilon f[(1-n^{\sigma})\epsilon + n^{\sigma}\Omega^{1} - \Omega^{I}_{\bar{\sigma}}(\epsilon)], \tag{1c}$$

$$\varphi^{\bar{\sigma}}(\vec{k}) = -\frac{\epsilon(\vec{k})}{W^{2}(1-n)}[n^{\bar{\sigma}}_{-}(\Psi^{\bar{\sigma}})^{2} + \Psi^{\sigma}\Psi^{\bar{\sigma}}], \tag{1d}$$

$$\epsilon(\vec{k}) = \sum_{\vec{h}\neq 0} t(h)e^{i\vec{k}\vec{h}},\ \ n^{\bar{\sigma}}_{+} = n^{\bar{\sigma}},\ \ n^{\bar{\sigma}}_{-} = 1-n^{\bar{\sigma}},\ \ n = n^{\bar{\sigma}} + n^{\sigma},\ \ W = |t|z. \tag{1e}$$

Equation (1b) for the field $\Psi^{\bar{\sigma}}$ stems from the kinematic nature of the vacuum transitions which couple the kinetic degree of freedom with the spin configuration on the lattice. This equation follows from a local correlation function

$$\Phi^{\bar{\sigma}} = \sum_{\vec{h}\neq 0} t(\vec{h}) < X_0^{\bar{\sigma}0} X_{\vec{h}}^{0\bar{\sigma}} >, \quad X_f^{\bar{\sigma}0} = n_{f-}^{\sigma} a_{f\bar{\sigma}}^{+} \tag{2}$$

The kinematic field $\Psi^{\bar{\sigma}}$ (Ψ^{σ}) shifts the center of gravity of the spin subbands to a new energy balance between the ferromagnetic and paramagnetic phases. The binary correlation function

$$\varphi^{\bar{\sigma}}(k) = \sum_{h\neq 0} t(h) e^{i\vec{k}\vec{h}} [< n_0^{\bar{\sigma}} n_h^{\bar{\sigma}} > -(n^{\bar{\sigma}})^2 + < X_0^{\bar{\sigma}\sigma} X_{\vec{h}}^{\sigma\bar{\sigma}} >] \tag{3}$$

is quadratic in the kinematic fields in the approximation linear in $t(\vec{h})$ [see (1d)] and determines the correlation narrowing of the spin subbands.[1]

3. We consider the case $T=0$, and we restrict the discussion to a rectangular density of states, $\rho(\epsilon) \equiv \rho = 1/(2W)$. An equation for the magnetization $R(n) = n^{\sigma} - n^{\bar{\sigma}}$ arises under the following conditions:

$$\xi_+ = \xi_- = \xi, \tag{4a}$$

$$\xi_+ \geq \omega_+, \tag{4b}$$

$$\xi_- \geq \omega_-, \tag{4c}$$

where $\xi_{\pm} = \mu_{\pm}/W$ is the dimensionless chemical potential in the spin subbands (+ and −), and $\omega_{\pm}$ is the lower edge of the corresponding subband.[1)]

Equation (4a), along with the solution $R(n)=0$, leads to the following result:

$$R^2 = (1+p)^2 - 8p\sqrt{1+p-p^2/3}\cos[(\pi-\varphi)/3],$$

$$\varphi = \arccos[(1+p)(1+p-p^2/3)], \quad p = 1-n. \tag{5}$$

Equation (5) describes a state of an unsaturated ferromagnetic metal with a ferromagnet–paramagnet transition at the density[1] $p_c \approx 0.3$. Using (5), we find the self-consistent values ξ, $\omega_{\pm}$ (Fig. 1). It can be seen from Fig. 1 that at hole densities $0 \leqslant p \lesssim 0.2$ inequality (4c) does not hold, so there are two solutions in this region:

$$R = 0; \qquad R = n^+ = n \qquad (n^- = 0). \tag{6}$$

In the density interval $0.2 < p < 0.3$, solution (5) and $R=0$ hold. In the interval $0.3 \lesssim p \leqslant 1$, there is one solution, $R=0$, which corresponds to a paramagnetic state.

Which of these solutions has the lowest energy in the corresponding intervals of the hole density? Using an expression for the one-particle Green's function[1]

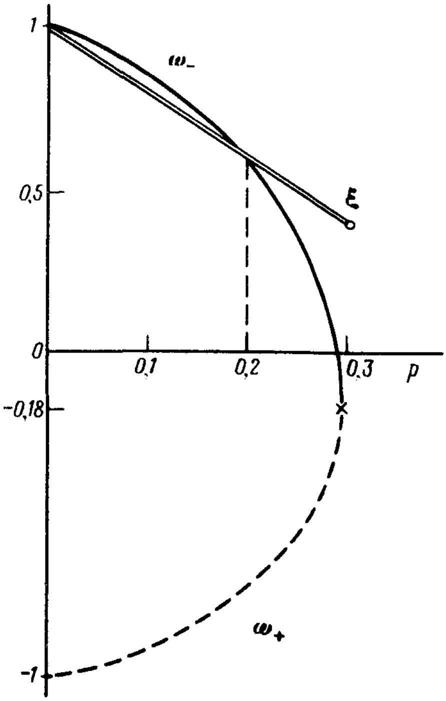

FIG. 1. Self-consistent dependence of the chemical potential $\xi = \mu / W$ of the lower edge of the spin subbands, $\omega_{|}$ and $\omega_{.}$, versus the hole density p.

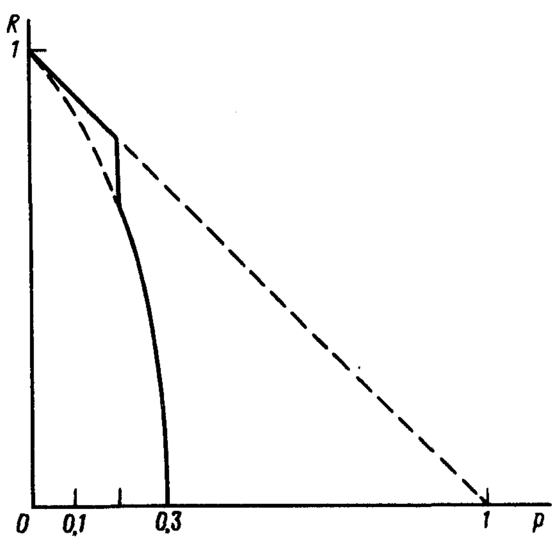

FIG. 2. Self-consistent dependence of the ferromagnetic moment $R = n^{\prime} - n$ on the hole density $p = 1 - n$ in the Hubbard model in the limit $U \to \infty, t > 0$, with a rectangular density of states, $\rho(\epsilon) \equiv \rho = 1/(2W)$.

$G_k^\sigma(\omega + i\delta)$ and an expression for the energy of this system[2)] (Ref. 4),

$$E_0 = \sum_{\vec{k}\sigma} \int \frac{1}{2}(\omega + \epsilon(\vec{k})) f(\omega)(-\frac{1}{\pi}\mathrm{Im}) G_{\vec{k}}^\sigma(\omega + i\delta) d\omega, \tag{7}$$

we can show that we have

$$E_0(R = n) \le E_0(R = 0), \qquad 0 \le p \lesssim 0.2; \tag{8}$$

$$E_0(R < n) \le E_0(R = 0), \qquad 0.2 \lesssim p \lesssim 0.3, \tag{9}$$

where $E_0(R = n)$ is the energy of the saturated ferromagnet, $E_0(R = 0)$ is the energy of the paramagnetic phase, and $E_0(R < n)$ is the energy of the unsaturated ferromagnetic state described by expression (5).

Figure 2 shows a plot of $R(n)$. Our theory predicts an instability of the first kind of the Nagaoka state, again in agreement with the conclusions of Ref. 2.

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[1)] Conditions (4b) and (4c) were omitted from Ref. 1.
[2)] The limit $U \to \infty$ is taken after the integration in (7).

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[2]B. S. Shastry, H. R. Krishnamurthy, and P. W. Anderson, Phys. Rev. B **41**, 2375 (1990).
[3]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[4]P. Martin and J. Schwinger, *Theory of Many-Particle Systems* [Russian translation], IIL, Moscow, 1962, p. 167.

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