Concentration phase transition in the Hubbard model

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The spin-wave-excitation spectrum in the ferromagnetic Hubbard model is calculated with allowance for Fermi-background vacancies. An increase in the number of vacancies causes the principal ferromagnetic state to become unstable with respect to the spin-wave excitations with a maximum wave vector.

Beginning with the landmark paper of Nagaoka,[1] the properties of magnetic materials with collective electrons [e.g., the $3d$ transition metals, narrow-band magnetic semiconductors, solid He^3 (Refs. 2–9)] have been generally described by the Hubbard model with the Hamiltonian

$$H = \sum_{i,\sigma} \left(\frac{U}{2} n_{i\sigma} n_{i-\sigma} - \mu n_{i\sigma} \right) - \sum_{i,j,\sigma} t_{ij} a^{+}_{i\sigma} a_{j\sigma}, \tag{1}$$

where $a_{i\sigma}$ is the operator for annihilation of an electron with spin σ in the ith lattice site ($n_{i\sigma} = a^{+}_{i\sigma} a_{i\sigma}$), μ is the chemical potential, U is the integral of Coulomb repulsion at a single lattice site, and t_{ij} is the integral for the jump of an electron from the jth to the ith lattice site:

$$t_{ij} = \begin{cases} t & \text{for the nearest neighbors} \\ 0 & \text{for all other cases} \end{cases}$$

In spite of the apparent simplicity of Hamiltonian (1), the case of strong electron-electron correlations, $U \gg t$, the most interesting one in this model, has so far been hardly studied. Most of the theoretical studies of the Hubbard model (see Refs. 2–4, for example) have used approximations that do not hold for strong electron-electron correlations. There is no comprehensive solution of this problem even for the limiting case $U > \infty$.

Nagaoka[1] proved a theorem which can be summarized as follows. If the intratomic Coulomb repulsion U is infinitely strong and if the number of electrons N_e in the system differs from the number of lattice sites N by unity, then the principal state of a

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simple cubic lattice and a body-centered-cubic lattice will be ferromagnetic for any sign of t and the principal state of a face-centered-cubic lattice and a hexagonal-close-packed lattice will also be ferromagnetic when $t<0$. In the studies cited above, the cases in which $N_e = N \mp 1$ were investigated in fcc and hcp lattices[6,7] or the magnon spectrum was calculated ignoring the Fermi background of the vacancies.[1,8]

It is of interest, however, to calculate the magnon spectrum when the Fermi background of the vacancies in the system is finite in the thermodynamic limit. We will show below that the amplitude for the scattering of electrons with spin + (in terms of magnetization) by a spin wave has logarithmic features if the Fermi background of the vacancies is taken into account. These vacancies, in turn, lead to the appearance of a soft mode in the spin wave with a finite momentum, whose energy goes down to zero as a certain critical vacancy concentration is reached, $(1-c)_{\text{crit}} \ll 1$; i.e., the principal ferromagnetic state becomes unstable.

Our task, therefore, is to calculate the spin-wave spectrum of Hamiltonian (1) under the assumption that $U \to \infty$ and the vacancy concentration $(1-c) \ll 1$.

We assume, in accordance with Nagaoka's theorem, that ferromagnetic order is the initial principal state: the density of electrons with spin + $n^+ = c$. In the following calculations the Fermi momentum $p_F = [(3/4\pi)(1-c)]^{1/3}$ is the small parameter.

The magnon spectrum is determined by the pole of the Green's function $\langle \hat{T} X^{+-} X^{-+} \rangle$, where X^{+-} and X^{-+} are the Hubbard operators or X operators. To calculate this function, we will make use of the diagram technique for the X operators.[9,10]

Since we are starting with the principal ferromagnetic state, we can assume that the electrons with spin − (opposite the direction of magnetization) are the bound states of electrons with spin + and of magnons. Formally, this approach, which requires that X^{0-} be replaced by $X^{0+}X^{+-}$ in the T products, leads to the fact that two types of lines appear in the diagrams.

Before determining the Green's function for magnons, we will consider the vertex part of $\Gamma(\mathbf{p}, \mathbf{p}', \mathbf{q})$, which describes in the momentum representation the scattering of an electron from the state $\mathbf{p}, \epsilon'$ to the state $\mathbf{p}', \epsilon'$ by a magnon with a momentum $\mathbf{q}-\mathbf{p}$ and frequency $\omega - \epsilon$. In the parquet approximation, we can write for it the system of equations

$$\Gamma(\mathbf{p},\mathbf{p}',\mathbf{q}) = \Gamma_v(\mathbf{p},\mathbf{p}',\mathbf{q}) + \Gamma_h(\mathbf{p},\mathbf{p}',\mathbf{q}), \tag{2a}$$

$$\Gamma_h(\mathbf{p},\mathbf{p}',\mathbf{q}) = -\sum_{k<p_F} \Gamma_v(\mathbf{p},\mathbf{k},\mathbf{q}-\mathbf{p}'+\mathbf{k})\,\Gamma(\mathbf{k},\mathbf{p}',\mathbf{q}-\mathbf{p}+\mathbf{k})(\omega+\mu-t_{\mathbf{k}})^{-1}, \tag{2b}$$

$$\Gamma_v(\mathbf{p},\mathbf{p}',\mathbf{q}) = \Gamma_0(\mathbf{p},\mathbf{p}',\mathbf{q}) - \sum_{\mathbf{k}>p_F} (\Gamma_0(\mathbf{p},\mathbf{k},\mathbf{q}) + \Gamma_h(\mathbf{p},\mathbf{k},\mathbf{q})) \times \Gamma(\mathbf{k},\mathbf{p}',\mathbf{q})(\omega+\mu-t_{\mathbf{k}})^{-1}, \tag{2c}$$

where

$$\Gamma_0(\mathbf{p},\mathbf{p}',\mathbf{q}) = t_{\mathbf{q}-\mathbf{p}-\mathbf{p}'} - t_{\mathbf{p}'}; \quad t_{\mathbf{k}} = t\sum_{\text{n.n.}} e^{i\mathbf{k}\mathbf{R}_{ij}}.$$

In deriving the system of equations (2), we must retain both the regular terms of zeroth order in p_F and the singular terms linear in p_F, which are proportional to $\ln\omega$, and drop the terms of order p_F^3.

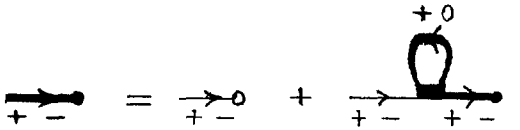
The "horizontal ladder" in (2b), we might note, has only the singular part, while the "vertical ladder" in (2c) has both the regular and the singular parts. Isolating the regular part in the vertical ladder, we obtain the following equation for it:

$$\Gamma_r(\mathbf{p}, \mathbf{p}', \mathbf{q}) = t_{\mathbf{q}-\mathbf{p}-\mathbf{p}'} - t_{\mathbf{p}'} - \sum_{\mathbf{k}} \Gamma_r(\mathbf{k}, \mathbf{p}', \mathbf{q})(t_{\mathbf{q}-\mathbf{p}-\mathbf{k}} - t_{\mathbf{k}})(\omega + \mu - t_{\mathbf{k}})^{-1}. \tag{3}$$

Since the kernel of integral equation (3) is degenerate, this equation can be solved exactly for a particular lattice.[8] Renormalizing the seed vertex part, we find the regular system of "parquet" equations for the total vertex part. Summing the "parquet" in a standard fashion,[11] we find

$$\Gamma(\mathbf{q}) = \Gamma_r(\mathbf{q})\left(1 - 2\Gamma_r(\mathbf{q}) \sum_{k<p_F} (\omega + \mu - t_{\mathbf{k}})^{-1}\right)^{-1}, \tag{4}$$

where $\Gamma_r(\mathbf{q}) = \Gamma_r(0, 0, \mathbf{q})$. In the parquet approximation, the magnon Green's function is determined by Dyson's equation



(5)

The pole of this function gives us the magnon spectrum:

$$E_{\mathbf{q}} = \sum_{\mathbf{p}<p_F} \Gamma_r(\mathbf{q})\left(1 - 2\Gamma_r(\mathbf{q}) \sum_{\mathbf{k}<p_F} (t_{\mathbf{p}} - t_{\mathbf{k}})^{-1}\right)^{-1} = \int \frac{p^2\, dp\, \Gamma_r(\mathbf{q})}{1 + \frac{\pi}{2}\Gamma_r(\mathbf{q}) p_F \ln\left|\frac{p - p_F}{p + p_F}\right|}. \tag{6}$$

For extremely small p_F we have $p_F E_{\mathbf{q}} = \Sigma_{\mathbf{p}<p_F} \Gamma_r(\mathbf{q})$, and the result agrees with the magnon spectrum found in Refs. 1 and 8. For finite p_F we find, after integration,

$$E_{\mathbf{q}} = 2p_F^2 (\exp(-d)\, Ei(d) - 2\exp(-2d)\, Ei(2d) + \exp(-3d)\, Ei(3d)),$$

where

$$d = 2(\pi \Gamma_r(\mathbf{q}) p_F)^{-1}; \quad Ei(x) = \ln(x) + \sum_{n=1}^{\infty} x^n (n \cdot n!)^{-1}. \tag{7}$$

The calculation of $E_{\mathbf{q}}$ on a computer shows that for $d_{\text{crit}} = 1.56$ we have $E_{\mathbf{q}} = 0$. It is important to note that for values of d approximately equal to d_{crit}, we cannot represent the spin-wave energy $E_{\mathbf{q}}$ as a series in powers of p_F. It is also important to note that E_q vanishes at $d = d_{\text{crit}}$ not because of the cancellation of the first term and the following term in the expansion of $E_{\mathbf{q}}$ in powers of p_F, but because the integrand on the right side of Eq. (6) has a singular structure whose sign changes. The permissible error in the calculation of the critical value of p_F below is linked to the accuracy of the calculation of the real value of $\Gamma_r(\mathbf{q})$, which, as we have already mentioned, was determined to

within terms of order p_F^3. We easily see that the minimum value of p_F, at which $E_{\mathbf{q}} = 0$, is reached when $\Gamma_r(\mathbf{q})$ is maximum. The maximum value of $\Gamma_r(\mathbf{q})$, which is realized when $\mathbf{q} = (1, 1, 1)$ is maximum, is equal to 3.35 for a simple cubic lattice. The critical value of p_F, at which the principal ferromagnetic state becomes unstable, will then correspond to the vacancy concentration $1 - c = 0.045$. The condition $1 - c \ll 1$ thus holds, and the parquet approximation is valid.

The loss of stability applies principally to the reciprocal-lattice vector that links the nearest neighbors. This shows that the system is unstable with respect to the formation of an antiferromagnetic structure.

We note in conclusion that the magnon-dispersion law disappears because of the logarithmic singularity of the amplitude for the scattering of magnons by electrons. This singularity is analogous to the logarithmic singularity of the scattering of conduction electrons by an impurity in the Kondo model.

Finally, the theory offered by us can be used to interpret experimental data on concentration magnetic transitions in $Fe(Pt_x Pd_{1-x})_3$ alloys,[12] whose magnetic electrons are collective electrons. The transition in this case occurs from the ferromagnetic phase to the antiferromagnetic phase as the platinum concentration is increased.

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