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FUNCTIONAL INTEGRAL METHOD IN ITINERANT ELECTRON MAGNETISM

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Abstract. – Feynman's variational method and the arbitrariness of the Stratonovich-Hubbard transformation in the functional integral method are investigated. By making use of their results the dynamical spin susceptibility is given in the Gaussian approximation and it is applied to the calculation of the paramagnetic susceptibility of Ni.

Functional integral formalism has been extensively used in the study of itinerant electron magnetism and it has brought us many fruitful results. However, some difficulties lie behind this technique. The interaction term of the Hubbard Hamiltonian is rewritten as follows

$$U\sum_i n_{i+}n_{i-} = -\sum_i \left(\frac{J}{4}\sigma_i^2 + \frac{K}{4}n_i^2 - Wn_i\right), \quad (1)$$

with $J = \lambda (U/3)$, $K = (\lambda - 2) U$ and $W = (\lambda - 1) U$, where σ_i is the Pauli spin operator, n_i is the electron number operator and λ is an arbitrary parameter. Through the stratonovich-Hubbard transformation the partition function is expressed in a functional integral form over fluctuating fields conjugate to spin and charge operators σ_i and n_i, respectively. We then introduce an approximate treatment, for example, the Gaussian approximation (GA) [1] or the coherent potential approximation (CPA) [2-3]. However, final results obtained in both methods depend on λ and they do not always give the results obtained in the random phase approximation (RPA) in the lowest order of U. Critical studies in this respect were given by Castellani and Castro [4] and Macedo *et al.* [5]. However, this subject is related to the quantum effect of spin fluctuations and is not yet solved.

Now, we have the following exact relation with respect to the correlation of fluctuating fields ξ :

$$\left\langle \xi_{i-}(u)\,\xi_{j+}(u')\right\rangle_c = \\ = \frac{J}{2\beta}\delta_{ij}\delta\left(u-u'\right) + \frac{J^2}{2\beta}\chi_{ij-+}\left(u,\, u'\right), \quad (2)$$

where $\xi_{i\pm}(u) = \xi_{ix}(u) \pm i\xi_{iy}(u)$, $\beta = 1/(k_BT)$, u is the imaginary time and $\chi_{ij-+}\left(u,\, u'\right)$ is the generalized transverse susceptibility. In equation (2) the first term is purely local in space and time. On the contrary, the second term, which originates from the correlation of fluctuating fields, is rather non-local both in space and time. In the so-called static approximation equation (2) is approximated as

$$\left\langle \xi_{i-}(u)\,\xi_{j+}(u')\right\rangle_c \simeq \frac{J}{2\beta}\delta_{ij} + \frac{J^2}{2\beta}\overline{\chi_{ij-+}(u,\, u')},$$

where $\overline{A(u)}$ means the time average of $A(u)$. This approximation is proper to the second term but quite improper to the first term. This difference has been disregarded in usual spin fluctuation theories [1-3].

On the above considerations we have obtained the dynamical spin susceptibilities in the GA [6]. The transverse component is given as follows,

$$\chi_{-+}(\mathbf{q},\, \omega) = \frac{\tilde{\chi}_{-+}(\mathbf{q},\, \omega)}{1 - U\tilde{\chi}_{-+}(\mathbf{q},\, \omega)}. \quad (3)$$

Here, $\tilde{\chi}_{-+}(\mathbf{q},\, \omega)$ is the Gaussian-averaged dynamical susceptibility of the non-interacting electron system in the presence of the spontaneous field and fluctuating field $\delta\eta_i(u)$ with variance, for example, as

$$\left\langle \delta\eta_{i-}(u)\,\delta\eta_{j+}\left(u'\right)\right\rangle = J^2/(2\beta)\,\chi_{ij-+}\left(u,\, u'\right).$$

Here, $\delta\eta_i(u)$ represents the pure exchange-field which originates from the spin fluctuations. The so-called static approximation is applicable without difficulty in this stage. As an example we have improved the spin fluctuation theory of Hertz and Klenin [1] and extended it to the ferromagnetic state [7]. Then, the exchange field $\delta\eta_i(u)$ is treated as constant in space and time. In the paramagnetic state $\tilde{\chi}_{-+}(\mathbf{q},\, \omega)$ is given as.

$$\tilde{\chi}_{-+}(\mathbf{q},\, \omega) = \\ = \frac{1}{3}\left(\chi_{0-+}(\mathbf{q},\, \omega) + \chi_{0+-}(\mathbf{q},\, \omega) + \chi_{0z}(\mathbf{q},\, \omega)\right)$$

with variance

$$\left\langle \delta\eta^2\right\rangle = \frac{J^2}{2\beta}\sum_{\mathbf{q},\,\omega}\chi_{-+}(\mathbf{q},\, \omega), \quad (4)$$

where $\chi_{0-+}(\mathbf{q},\, \omega)$, $\chi_{0+-}(\mathbf{q},\, \omega)$ and $\chi_{0z}(\mathbf{q},\, \omega)$ are the transverse and longitudinal spin susceptibilities, respectively, of the non-interacting system with uniform and static fluctuating field $\delta\eta$ and $\langle ... \rangle$ means taking the Gaussian average with variance $\langle \delta\eta^2 \rangle$.

There remains ambiguity in the determination of the value of λ. Exact thermodynamic potential Ω in the functional integral form should be independent of λ. However, a trial thermodynamic potential Ω_t in Feynman's variational method [8] is dependent on λ. Because of the Feynman's inequality $\Omega < \Omega_t(\lambda)$ it is natural that we use the variational principle for λ, namely, the minimization of $\Omega_t(\lambda)$ by λ. We obtain from $\partial\Omega_t/\partial\lambda = 0$ a self-consistent equation to determine λ. We have the inequality $1.5 > \lambda > 0$ in the GA [6]. The λ renormalizes the coupling constant $J = \lambda(U/3)$ between electron and spin fluctuations.

Equations (3) and (4) have been applied to investigate the ferromagnetism of Ni in [9]. However, the agreement with experiment [10] is not enough for the calculated results of the paramagnetic susceptibility. In the calculation of equation (4) we have used the dynamical susceptibility of the RPA theory with the energy spectrum of electron gas. Then the mode-mode coupling of spin fluctuations is not at all considered, so that the amplitude of spin fluctuations is overestimated. So we have introduced the reduction parameter α of $\langle \delta\eta^2 \rangle$ as

$$\alpha = \lambda^2 \sum_{\mathbf{q},\,\omega} \chi(\mathbf{q},\,\omega) \Big/ \sum_{\mathbf{q},\,\omega} \chi^{\mathrm{RPA}}(\mathbf{q},\,\omega)$$

In [9] α has been treated as the adjustable parameter together with U as $\alpha = 0.25$ and $U = 3.44$ eV to give T_c=630 K and the spontaneous moment $M_0 = 0.12\,\mu_B$ (per atom and per band) at $T = 0$. However, not only the reduction of $\chi(\mathbf{q},\,\omega)$ by the mode-mode coupling but also the reduction of λ as shown in [6] becomes more remarkable near T_c. So we assume

$$\alpha = \alpha_0 + (1-\alpha_0)\{1 - U\tilde{\chi}(0,\,0)\}^{\mu}$$

for simplicity. This form of α is devised to give $1 > \alpha > \alpha_0$, $\alpha = \alpha_0$ at $T = T_c$ and $\alpha = 1$ for $U\tilde{\chi}(0,\,0) = 0$. We conjecture $1 > \mu > 0$ from the behaviour of λ in [6]. Below $\mu = 1/2$ is used. In the solid curve of figure 1 $\alpha_0 = 0.25$, $U = 3.44$ eV and $\mu = 1/2$ are adopted and the paramagnetic susceptibility is given by $\chi = \chi(0,\,0) + \chi_{\mathrm{orb}}$, where χ_{orb} is the orbital susceptibility, which is expected to be almost temperature-independent and we use a theretical value of $\chi_{\mathrm{orb}} = 0.44\times10^{-4}$ (emu/mole) [11].

The full self-consistent calculation, including the renormalization of the dynamical susceptibility and the coupling constant J, will give a better agreement with experiment.

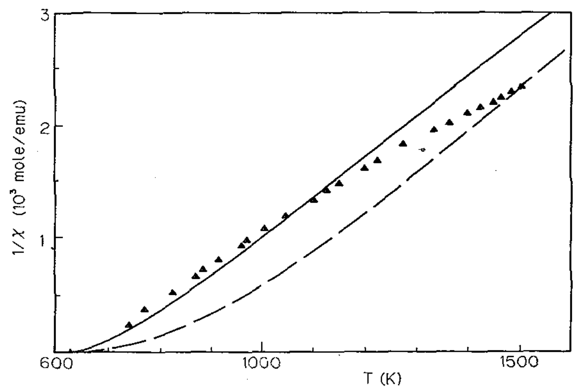

Fig. 1. – Calculated results (solid curve: present work, broken curve: [9]) and the observed ones ((Δ) [10]) of the temperature dependences of the paramagnetic susceptibility in Ni.

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