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Electron correlations in narrow-band systems at finite temperatures: Gutzwiller-type variational approach

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Abstract. A theory is presented for finite-temperature band magnetism which takes into account the effect of electron correlations using the Gutzwiller-type variational approach. The functional-integral method recently proposed by Kotliar and Ruckenstein is combined with the alloy-analogy approximation to include the effect of local spin fluctuations at finite temperatures. The theory at $T = 0$ K is equivalent to Gutzwiller's approximation for the correlated ground state, while in the high-temperature limit it reduces to the local spin-fluctuation theory developed previously by Hasegawa and Hubbard. Numerical calculations for the half-filled simple-cubic Hubbard model demonstrate that both electron correlations and local spin fluctuations play important roles at finite temperatures. The Brinkman–Rice-type metal–insulator transition is critically discussed on the basis of the model calculation.

1. Introduction

In the last decade we have seen significant progress in the theory of finite-temperature band magnetism (for reviews see Gautier 1982, Capellmann 1987). Various types of approximation theories have been proposed so far. Most of them employ the Stratonovich–Hubbard functional-integral method (Stratonovich 1958, Hubbard 1959), which transforms the two-body Hamiltonian to the effective one-electron Hamiltonian, H_{eff}. Depending on the method of choosing H_{eff}, we can classify the proposed theories into three categories: (i) the fluctuating band theory (Korenman *et al* 1977, Capellmann 1979); (ii) the disordered-local-moment approach (Hubbard 1979, Hasegawa 1979); and (iii) the interpolation theory (Moriya and Takahashi 1978, Haines *et al* 1985). The fluctuating band theory assumes a large short-range magnetic order (SMO) of about 20 Å in Fe and Ni, while the disordered-local-moment approach postulates a vanishing SMO. Interpolating theories assume the form of H_{eff} to interpolate between the weak- and strong-interaction limits and/or between the small- and large-SMO limits. There have been controversies on the validity of the proposed theories, and we have no agreement yet as to which approach among the three provides us with the best description of various observed finite-temperature properties of transition metals. This is because there always exist uncertainties in interpreting experimental data and because it is impossibly difficult to obtain analytically exact solutions for three-dimensional systems.

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Quite recently several attempts have been reported of applying the Monte Carlo (MC) simulation method to the simple-cubic Hubbard model. Hirsch (1986) and Scalettar *et al* (1988) performed MC calculations for clusters of 2^3–10^3 to calculate various quantities such as the susceptibility and the energy as a function of the temperature and the interaction strength. In order to discuss the ground-state properties, Yokoyama and Shiba (1987a, b) proposed the variational Monte Carlo (VMC) method, which exactly calculates the expectation values for the Gutzwiller wavefunctions (Gutzwiller 1965). These 'exact' calculations are very useful to investigate the validity of analytic approximation theories. It has been shown (Kakehashi and Hasegawa 1987, 1988) that the Néel temperature obtained by the MC method is well reproduced in the calculation using the disordered-local-moment theory of Hasegawa (1979, 1980a) and Hubbard (1979). This justifies to a large extent the local spin-fluctuation theory of Hasegawa and Hubbard, which has been successfully applied to various problems (Hasegawa 1980b, 1981, Hubbard 1981, Hasegawa and Pettifor 1980, Kakehashi 1981, 1983, 1985), including the surface-related subjects (Hasegawa 1986a, b, 1987a, b, c, Hasegawa and Herman 1988a, b).

In the Hasegawa–Hubbard (HH) theory, the two-field functional-integral method within the static approximation is combined with the alloy-analogy approximation to include the effect of local spin fluctuations, which is indispensable in discussing magnetic and thermodynamic properties of transition metals at finite temperatures. A single atom of a 'pure' magnetic metal is regarded as an 'impurity' embedded in the host 'multicomponent alloy'. The self-consistency conditions between the impurity and the host determine finite-temperature properties. The alloy-analogy approximation of the HH theory is an extension of Cyrot's binary alloy theory (Cyrot 1972), avoiding his local saddle-point approximation. This generalisation yields a unified description covering weak- and strong-coupling limits. It reduces to the Hartree–Fock approximation in the weak-interaction limit or at $T = 0$ K, and in the strong-coupling limit it is equivalent to the molecular-field theory for the Heisenberg model. The HH theory correctly describes the high-temperature behaviour; for example, it leads to the exact Curie constant. It has been shown that the calculated Curie temperature is much reduced compared with that in the Hartree–Fock or Stoner theory. The observed Curie–Weiss susceptibility and the appreciable magnetic entropy in the paramagnetic state are well explained in the calculations (Hasegawa 1980b, 1983a, b, 1984, Kakehashi 1981, 1983, 1985).

All the theories mentioned above employed the static approximation to the functional-integral method, and most of them reduce, at $T = 0$ K, to the Hartree–Fock approximation. Therefore the correlations among electrons are completely neglected. There are two approaches to include the effect of electron correlations at finite temperatures. The first method is to employ the local-spin-density method combined with the Korringa–Kohn–Rostoker coherent-potential approximation (KKR–CPA). Oguchi *et al* (1983) and Pindor *et al* (1983) applied it to paramagnetic Fe to obtain detailed band structures. This method is, however, valid only for strongly magnetic systems such as Fe, and at the moment no solutions for the ferromagnetic state have been reported except for the ground state, even for Fe. As the second approach, Kakehashi and Fulde (1985, referred to as KF) proposed a variational method based on the Hubbard model to include electron correlations at finite temperatures. Their free energy at $T = 0$ K reduces to the ground-state energy obtained in the local correlation theory of Stollhoff and Fulde (1978). In this theory the Gutzwiller-type wavefunction for the correlated states is constructed with the projection operators onto the Hartree–Fock state. The correction to the Hartree–Fock energy is calculated up to the second order of the projection

operators. This is in contrast with the original Gutzwiller approximation (Gutzwiller 1965), in which the correlated state is projected onto the non-magnetic state to include the effect of electron correlations 'exactly' within the quasi-chemical approximation. Although the local correlation theory of Stollhoff and Fulde (1978) has been proved very useful for atoms, molecules and transition metals, it cannot be applied to strongly correlated systems because it is essentially a perturbation theory (Oles 1981, Stollhoff and Thalmeier 1981, Oles and Stollhoff 1984).

It is a challenging subject to develop a theory that takes into account the effect of electron correlations at finite temperatures along Gutzwiller's original approach. Chao and Berggren (1977) first tried to extend Gutzwiller's scheme to finite temperature. Unfortunately their discussion was confined to the weak-interaction regime because they faced difficulty in calculating the magnetic entropy, which should reduce to ln 2 in the high-temperature limit. Note that, although their theory can yield the entropy of ln 2 at very high temperatures where the fermion degeneracy is removed, the magnetic entropy nearly corresponding to disordered moments is experimentally realised at much lower temperature (but above the Curie temperature). Quite recently, Kotliar and Ruckenstein (1986) proposed a new functional-integral method introducing boson fields. It clarifies the relationship between the Gutzwiller approximation and the slave-boson approach which is now widely employed in connection with the heavy-fermion problem (Coleman 1984, Read and Newns 1983). They showed that its simplest saddle-point approximation leads, at $T = 0$ K, to results obtained in the Gutzwiller approximation. The finite-temperature saddle-point approximation to this functional-integral method is equivalent to the theory of Chao and Berggren (1977), and then it has the same difficulty in calculating magnetic entropy as discussed above. We should remember that, in the disordered-local-moment approach, the appreciable magnetic entropy arises from disordered moments and it becomes ln 2 sufficiently above the Curie temperature. We expect that, if the alloy-analogy approximation of the HH theory is combined with the functional-integral method of Kotliar and Ruckenstein, we may construct a sound theory which can go beyond the HH theory. Such an attempt is the purpose of the present study. Our new theory agrees with Gutzwiller's theory at $T = 0$ K while in the high-temperature limit it reduces to the HH theory. We can show that electron correlations play important roles not only in the ground state but also at finite temperatures.

The outline of this paper is as follows. In the next section (§ 2), we develop the finite-temperature band theory employing the functional-integral method with the alloy-analogy approximation. Numerical calculations are performed for the half-filled simple-cubic Hubbard model, whose results are reported in § 3. The final section (§ 4) is devoted to conclusions and supplementary discussions.

2. Formulation

2.1. Functional-integral method

We adopt the single-band Hubbard model given by

$$H = \sum_{\sigma} \sum_{i,j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U c_{i\uparrow}^{\dagger} c_{i\uparrow} c_{i\downarrow}^{\dagger} c_{i\downarrow} \tag{2.1}$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) is a creation (annihilation) operator of an electron with spin σ at site i, t_{ij} is the hopping matrix and U is the on-site electron interaction. In order to enlarge the

Fock space at each site in analogy with the 'slave-boson' approach (Coleman 1984, Read and Newns 1983), Kotliar and Ruckenstein (1986) introduced a set of four bosons represented by the creation (annihilation) operators, $e_i^\dagger$ (e_i), $p_{i\sigma}^\dagger$ ($p_{i\sigma}$) ($\sigma = \uparrow, \downarrow$) and $d_i^\dagger$ (d_i). The Bose fields, e_i, $p_{i\sigma}$ and d_i, play roles, respectively, as projection operators onto the empty, singly occupied with spin σ and doubly occupied states at each site. Unphysical states in this enlarged Fock space can be eliminated by imposing a set of constraints (Kotliar and Ruckenstein 1986):

$$\sum_\sigma p_{i\sigma}^\dagger p_{i\sigma} + e_i^\dagger e_i + d_i^\dagger d_i = 1 \tag{2.2a}$$

$$c_{i\sigma}^\dagger c_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} + d_i^\dagger d_i. \tag{2.2b}$$

Equation (2.2*a*) shows that no more and no less than one of four possible states must be occupied at each site, while equation (2.2*b*) denotes the two ways of counting the fermion occupancy of a given spin. We get the new Hamiltonian, which has the same matrix elements as the original one, given by

$$H = \sum_\sigma \sum_{i,j} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} z_{i\sigma}^\dagger z_{j\sigma} + \sum_i U d_i^\dagger d_i \tag{2.3}$$

with

$$z_{i\sigma} = e_i^\dagger p_{i\sigma} + p_{i-\sigma}^\dagger d_i. \tag{2.4}$$

To calculate the partition function, Z, the functional-integral method is applied to equation (2.3) (Popov 1983). We incorporate the constraints given by equations (2.2*a*) and (2.2*b*) by introducing the two Lagrangian multipliers, $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$, to get (Kotliar and Ruckenstein 1986)

$$Z = \int De\, Dp_\sigma\, Dd\, D\lambda^{(1)} D\lambda_\sigma^{(2)} \exp\left(-\int_0^\beta \mathrm{d}\tau\, S(\tau)\right) \tag{2.5}$$

with

$$\begin{aligned} S(\tau) = \sum_i \Big(& e_i^\dagger(\partial\tau + \mathrm{i}\lambda_i^{(1)}) e_i + \sum_\sigma p_{i\sigma}^*(\partial\tau + \mathrm{i}\lambda_i^{(1)} - \mathrm{i}\lambda_{i\sigma}^{(2)}) p_{i\sigma} \\ & + d_i^\dagger(\partial\tau + U + \mathrm{i}\lambda_i^{(1)} - \mathrm{i}\lambda_{i\sigma}^{(2)}) d_i - \lambda_i^{(1)} \\ & + \mathrm{tr}\ \ln[\delta_{ij}(\partial\tau - \sigma h + \mathrm{i}\lambda_{i\sigma}^{(2)}) + z_{i\sigma}^\dagger z_{j\sigma} t_{ij}] \Big) \end{aligned} \tag{2.6}$$

where $De = \Pi_i d(\mathrm{Re}\, e_i) d(\mathrm{Im}\, e_i)$ etc. are Grassman variables (Berezin 1966). There is an ambiguity in choosing the form of $z_{i\sigma}$. If the calculation is performed exactly, this ambiguity presents no difficulties. This is not the case, however, when any approximation is employed. Kotliar and Ruckenstein (1986) showed that if $z_{i\sigma}$ in equation (2.4) is replaced by

$$z_{i\sigma} = (1 - d_i^\dagger d_i - p_{i\sigma}^\dagger p_{i\sigma})^{-1/2} (e_i^\dagger p_{i\sigma} + p_{i-\sigma}^\dagger d_i)(1 - e_i^\dagger e_i - p_{i-\sigma}^\dagger p_{i-\sigma})^{-1/2} \tag{2.7}$$

the simplest saddle-point approximation to equation (2.5) leads to the correct result in both the atomic and vanishing interaction limits, reproducing the Gutzwiller approximation at $T = 0$ K.

Before we apply the alloy-analogy approximation to the functional-integral method mentioned above, we make the expressions for the functional integral into a more transparent and manageable form, by taking the following steps:

(i) the static approximation is used for boson fields, and integrations with respect to their imaginary parts are carried out;

(ii) we adopt the changes of variables defined by

$$p_{i\uparrow}^2 + p_{i\downarrow}^2 + 2d_i^2 = n_i \qquad p_{i\uparrow}^2 - p_{i\downarrow}^2 = m_i \tag{2.8a}$$

$$(\mathrm{i}/2)(\lambda_{\uparrow}^{(2)} + \lambda_{\downarrow}^{(2)}) = \nu_i \qquad (\mathrm{i}/2)(\lambda_{\uparrow}^{(2)} - \lambda_{\downarrow}^{(2)}) = -\xi_i \tag{2.8b}$$

where n_i stands for the electron number, m_i the magnetic moment, and ξ_i and ν_i denote the exchange and charge fields, respectively;

(iii) the saddle point approximation is used for $\lambda^{(1)}$ and the integral over e fields is eliminated.

Then we obtain the expression for Z given by

$$Z = \int D\xi\, Dm\, D\nu\, Dn\, D\delta \exp(-\beta S) \tag{2.9}$$

where

$$\mathrm{e}^{-\beta S} = \exp\left(-\beta \sum_i (U\delta_i + \xi_i m_i - \nu_i n_i)\right) \mathrm{Tr} \exp(-\beta H_{\mathrm{eff}}) \tag{2.10}$$

$$H_{\mathrm{eff}} = \sum_{\sigma} \left(\sum_i (\nu_i - \sigma\xi_i) c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{i,j} (q_{i\sigma} q_{j\sigma})^{1/2} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \right). \tag{2.11}$$

Here $\delta_i = d_i^2$ is the double occupancy, $q_{i\sigma} = z_{i\sigma}^2$ the band-narrowing factor and Tr includes the trace over fermion variables. For integrations with respect to m_i, n_i, ν_i and δ_i, we again adopt the saddle-point approximation to get

$$Z = \int D\xi \exp(-\beta\Psi) \tag{2.12}$$

with

$$\Psi = \sum_i (U\delta_i + \xi_i m_i - \nu_i n_i) + \int \mathrm{d}\varepsilon\, f(\varepsilon)(1/\pi)\, \mathrm{Im}\, \mathrm{Tr} \ln(\varepsilon - H_{\mathrm{eff}}) \tag{2.13}$$

where $f(\varepsilon)$ is the Fermi distribution function. The saddle-point values of m_i, n_i, ν_i and δ_i are determined by the simultaneous equations given by

$$\partial S/\partial m_i = \xi_i + \sum_{\sigma} (\partial q_{i\sigma}/\partial m_i) R_{i\sigma} = 0 \tag{2.14a}$$

$$\partial S/\partial n_i = -\nu_i + \sum_{\sigma} (\partial q_{i\sigma}/\partial n_i) R_{i\sigma} = 0 \tag{2.14b}$$

$$\partial S/\partial \nu_i = -n_i + \sum_{\sigma} \langle c_{i\sigma}^{\dagger} c_{i\sigma} \rangle = 0 \tag{2.14c}$$

$$\partial S/\partial \delta_i = U + \sum_{\sigma} (\partial q_{i\sigma}/\partial \delta_i) R_{i\sigma} = 0. \tag{2.14d}$$

We will shortly evaluate $R_{i\sigma} = \partial S/\partial q_{i\sigma}$ in equations (2.14*a*)–(2.14*d*) by using the single-site coherent-potential approximation (CPA) (see equations (2.26*c*) and (2.26*d*)). The

optimum value of the band-narrowing factor, $q_{i\sigma}$, is obtained with the use of equations (2.2*a*), (2.7) and (2.8) as a function of n_i, m_i and δ_i as

$$q_{i\sigma} \equiv q_{i\sigma}(n_i, m_i, \delta_i) = \frac{2\{[(n_i + \sigma m_i - 2\delta_i)(1 - n_i + \delta_i)]^{1/2} + [\delta_i(n_i - \sigma m_i - 2\delta_i)]^{1/2}\}^2}{(n_i + \sigma m_i)(2 - n_i - \sigma m_i)}. \tag{2.15}$$

2.2. *Alloy-analogy approximation*

We now apply the alloy-analogy approximation (Hubbard 1979, Hasegawa 1979, 1980a) to the functional integral given by equations (2.11)–(2.13). We regard H_{eff} in equation (2.11) as a multi-component alloy with the diagonal (ν_i, ξ_i) and off-diagonal randomness ($q_{i\sigma}$). We employ the single-site approximation, assuming the concentration distribution $C(\{\xi_i\})$ to be given by

$$C(\{\xi_i\}) = \prod_i C(\xi_i). \tag{2.16}$$

The diagonal and off-diagonal randomnesses in H_{eff} are treated by the extended coherent-potential approximation (Shiba 1971).

In order to treat both the ferromagnetic (F) and antiferromagnetic (AF) states on the same footing, we divide the crystal into two sublattices, A and B. The sites belonging to A and B lattices are hereafter specified by indices j and l, respectively. When expressions for equations are common for both sublattice sites, we specify them by the index i ($=j$ and l). We assume that, for the antiferromagnetic wavevector Q, the relation $\varepsilon_{k+Q} = -\varepsilon_k$ is satisfied, ε_k being the Fourier transform of t_{ij} in equation (2.1).

The single-site approximation for the electron free-energy functional leads to (Hasegawa 1980a)

$$F = E - T(S_1 + S_2) \tag{2.17a}$$

with

$$E = \sum_i (\langle U\delta_i \rangle + \langle \xi_i m_i \rangle - \langle \nu_i n_i \rangle) + \int \mathrm{d}\varepsilon f(\varepsilon)\varepsilon \sum_\sigma \sum_i \langle \rho_{i\sigma}(\varepsilon, \xi_i) \rangle \tag{2.17b}$$

$$S_1 = -\int \mathrm{d}\varepsilon \sum_\sigma \sum_i \langle \rho_{i\sigma}(\varepsilon, \xi_i) \rangle [f \ln f + (1 - f) \ln (1 - f)] \tag{2.17c}$$

$$S_2 = -\sum_i \langle \ln C(\xi_i) \rangle \tag{2.17d}$$

$$\rho_{j\sigma}(\varepsilon, \xi_j) = (-1/\pi)\, \mathrm{Im}\{q_{j\sigma}^{-1}[K_{\mathrm{A}\sigma}^{-1} + (X_{j\sigma} - \Xi_{\mathrm{A}\sigma})]^{-1}\} \tag{2.17e}$$

and

$$\rho_{l\sigma}(\varepsilon, \xi_l) = (-1/\pi)\, \mathrm{Im}\{q_{l\sigma}^{-1}[K_{\mathrm{B}\sigma}^{-1} + (X_{l\sigma} - \Xi_{\mathrm{B}\sigma})]^{-1}\}. \tag{2.17f}$$

Here E denotes the internal energy, S_1 the one-electron entropy and S_2 the entropy arising from the fluctuating exchange field. The bracket $\langle\ \rangle$ stands for

$$\langle Q(\xi_i)\rangle = \int \mathrm{d}\xi_i \, C(\xi_i) Q(\xi_i) \tag{2.18a}$$

with

$$C(\xi_i) = \exp[-\beta\psi(\xi_i)] \Big/ \int \mathrm{d}\xi_i \exp[-\beta\psi(\xi_i)] \tag{2.18b}$$

$$\psi(\xi_j) = U\delta_j + \xi_j m_j - \nu_j n_j + \int \mathrm{d}\varepsilon f(\varepsilon)(1/\pi) \sum_{\sigma} \mathrm{Im}\ln[1 + (X_{j\sigma} - \Xi_{\mathrm{A}\sigma})K_{\mathrm{A}\sigma}] \tag{2.18c}$$

and

$$\psi(\xi_l) = U\delta_l + \xi_l m_l - \nu_l n_l + \int \mathrm{d}\varepsilon f(\varepsilon)(1/\pi) \sum_{\sigma} \mathrm{Im}\ln[1 + (X_{l\sigma} - \Xi_{\mathrm{B}\sigma})K_{\mathrm{B}\sigma}]. \tag{2.18d}$$

The coherent locators, $\Xi_{\mathrm{A}\sigma}$ and $\Xi_{\mathrm{B}\sigma}$, describe the effective medium for σ-spin electrons on the A and B sublattices (Shiba 1971), and they have the following symmetry relations:

$$\Xi_{\mathrm{A}\sigma}(\varepsilon) = \Xi_{\mathrm{B}\sigma}(\varepsilon) \qquad \text{for F state} \tag{2.19a}$$

$$\Xi_{\mathrm{A}\sigma}(\varepsilon) = \Xi_{\mathrm{B}-\sigma}(\varepsilon) \qquad \text{for AF state.} \tag{2.19b}$$

The coherent locators are determined by the CPA conditions, given by

$$K_{\mathrm{A}\sigma}(\varepsilon) = \langle\{K_{\mathrm{A}\sigma}(\varepsilon)^{-1} + [X_{j\sigma}(\varepsilon) - \Xi_{\mathrm{A}\sigma}(\varepsilon)]\}^{-1}\rangle \tag{2.20a}$$

$$K_{\mathrm{B}\sigma}(\varepsilon) = \langle\{K_{\mathrm{B}\sigma}(\varepsilon)^{-1} + [X_{l\sigma}(\varepsilon) - \Xi_{\mathrm{B}\sigma}(\varepsilon)]\}^{-1}\rangle \tag{2.20b}$$

where the locators are given by

$$X_{\mathrm{i}\sigma}(\varepsilon) = (\varepsilon - \nu_i + \sigma\xi_i)/q_{i\sigma}. \tag{2.21}$$

The local Green functions are given by

$$K_{\mathrm{A}\sigma}(\varepsilon) = [\Xi_{\mathrm{B}\sigma}(\varepsilon)/\Xi_{\mathrm{A}\sigma}(\varepsilon)]^{1/2} F^0(\Omega_\sigma) \tag{2.22a}$$

$$K_{\mathrm{B}\sigma}(\varepsilon) = [\Xi_{\mathrm{A}\sigma}(\varepsilon)/\Xi_{\mathrm{B}\sigma}(\varepsilon)]^{1/2} F^0(\Omega_\sigma) \tag{2.22b}$$

with

$$\Omega_\sigma(\varepsilon) = [\Xi_{\mathrm{A}\sigma}(\varepsilon)\Xi_{\mathrm{B}\sigma}(\varepsilon)]^{1/2} \tag{2.23}$$

$$F^0(\varepsilon) = \int \mathrm{d}\varepsilon' \, \rho^0(\varepsilon')/(\varepsilon - \varepsilon') \tag{2.24}$$

$\rho^0(\varepsilon)$ being the unperturbed density of states. Note that for the ferromagnetic state, we get $K_{\mathrm{A}\sigma}(\varepsilon) = K_{\mathrm{B}\sigma}(\varepsilon) = F^0(\Omega_\sigma)$. It is easy to see that the distribution function, $C(\xi_i)$, satisfies the variational condition $\partial F/\partial C(\xi_i) = 0$ (Ducastelle 1975).

Next we examine the self-consistent equations (equations (2.14*a*)–(2.14*d*)) to get the saddle-point values of n_i, m_i and δ_i. A combination of equations (2.14*a*)–(2.14*d*) and the single-site approximation leads to

$$\xi_i = (\tilde{J}_i/2) m_i(\xi_i) \tag{2.25a}$$

$$\nu_i(\xi_i) = (\tilde{U}_i/2) n_i(\xi_i) \tag{2.25b}$$

$$m_i(\xi_i) = \int \mathrm{d}\varepsilon f(\varepsilon) \sum_\sigma \sigma \rho_{i\sigma}(\varepsilon, \xi_i). \tag{2.25c}$$

$$n_i(\xi_i) = \int \mathrm{d}\varepsilon f(\varepsilon) \sum_\sigma \rho_{i\sigma}(\varepsilon, \xi_i) \tag{2.25d}$$

$$U + \sum_\sigma (\partial q_{i\sigma}/\partial \delta_i) R_{i\sigma} = 0 \tag{2.25e}$$

with

$$\tilde{J}_i \equiv \tilde{J}_i(n_i, m_i, \delta_i) = (2U/m_i)\Big(\sum_\sigma (\partial q_{i\sigma}/\partial m_i) R_{i\sigma}\Big) \Big/ \Big(\sum_\sigma (\partial q_{i\sigma}/\partial \delta_i) R_{i\sigma}\Big) \tag{2.26a}$$

$$\tilde{U}_i \equiv \tilde{U}_i(n_i, m_i, \delta_i) = (-2U/n_i)\Big(\sum_\sigma (\partial q_{i\sigma}/\partial n_i) R_{i\sigma}\Big) \Big/ \Big(\sum_\sigma (\partial q_{i\sigma}/\partial \delta_i) R_{i\sigma}\Big) \tag{2.26b}$$

$$R_{j\sigma} = \int \mathrm{d}\varepsilon f(\varepsilon)(-1/\pi)\,\mathrm{Im}\{(X_{j\sigma}/q_{j\sigma})[K_{\mathrm{A}\sigma}^{-1} + (X_{j\sigma} - \Xi_{\mathrm{A}\sigma})]^{-1}\} \tag{2.27a}$$

and

$$R_{l\sigma} = \int \mathrm{d}\varepsilon f(\varepsilon)(-1/\pi)\,\mathrm{Im}\{(X_{l\sigma}/q_{l\sigma})[K_{\mathrm{B}\sigma}^{-1} + (X_{l\sigma} - \Xi_{\mathrm{B}\sigma})]^{-1}\}. \tag{2.27b}$$

The values of $q_{i\sigma}$ and its derivatives are given by equation (2.15) with the saddle-point values to be determined self-consistently. We introduced the effective exchange ($\tilde{J}_i$) and Coulomb ($\tilde{U}_i$) interactions defined by equations (2.26*a*) and (2.26*b*), which are generally reduced compared with the bare U because of the electron correlations. They are very useful when we calculate various physical quantities. For example, the susceptibilities are easily calculated by using the linear-response theory in terms of $\tilde{J}$ and $\tilde{U}$. They also provide us with a clear physical picture in understanding calculated results. We present in appendix 1 supplementary discussions on $q_{i\sigma}$ and $\tilde{J}_i$ for the half-filled band. Calculations of the ground-state susceptibilities by using $\tilde{J}$ and $\tilde{U}$ will be discussed in appendix 2.

The averages of local charge and magnetic moment are obtained as

$$\langle n \rangle = \langle n_i(\xi_i) \rangle \tag{2.28}$$

$$\langle m \rangle = \langle m_i(\xi_i) \rangle \tag{2.29}$$

where $m_i(\xi_i)$ and $n_i(\xi_i)$ are given by equation (2.25*c*) and (2.25d). By using the identity $\langle n_{i\sigma}^2 \rangle = \langle n_{i\sigma} \rangle$, we get the amplitudes of local charge and magnetic moment as

$$\langle m_z^2 \rangle = 2\langle n \rangle - \langle n^2 \rangle = \langle n \rangle - 2\langle \delta \rangle. \tag{2.30}$$

By employing the formalism presented so far, we can discuss electron correlations at finite temperatures. Their effects are essentially included in two quantities: the reduced interactions ($\tilde{J}_i$, $\tilde{U}_i$) and the band-narrowing factor ($q_{i\sigma}$). They represent the main effects of electron correlations, reducing the stability of magnetic long-range order and enhancing the atomic character for the amplitude of local magnetic moments (Gutzwiller 1965, Kanamori 1963, Hubbard 1964). We should note that the arguments (n_i, m_i and δ_i) in $\tilde{J}_i$, $\tilde{U}_i$ and $q_{i\sigma}$, are local quantities. Since the local spin polarisation, namely the local moment, persists even above the Curie (Néel) temperature, we can take into account the electron correlation at finite temperatures as in the ground state.

It should also be noted that, owing to the boson fields introduced in the Kotliar–Ruckenstein functional-integral method, the present theory can take into account the effect of electron correlations even within the static and alloy-analogy approximations; this effect is not included in the static-approximation approaches, such as the HH theory, based on the Stratonovich–Hubbard method.

The most tedious task in performing our program is to solve the CPA equation, equations (2.20*a*)–(2.20*b*). It involves calculations including the average over ξ_i-fields with probability $C(\xi_i)$, which depends on the coherent locator to be determined self-consistently. In order to simplify the CPA equation, we adopt the decoupling approximation employed previously (Hasegawa 1980a) to get

$$\Xi_{A\sigma} = (\varepsilon/\langle q_{j\sigma}\rangle - \langle \nu_j/q_{j\sigma}\rangle + \sigma\langle \xi_j/q_{j\sigma}\rangle) + \{[\Xi_{A\sigma} - (\varepsilon/\langle q_{j\sigma}\rangle - \langle \nu_j/q_{j\sigma}\rangle)]^2 - \langle \xi_j^2/q_{j\sigma}^2\rangle\} K_{A\sigma}. \tag{2.31a}$$

and

$$\Xi_{B\sigma} = (\varepsilon/\langle q_{l\sigma}\rangle - \langle \nu_l/q_{l\sigma}\rangle + \sigma\langle \xi_l/q_{l\sigma}\rangle) + \{[\Xi_{B\sigma} - (\varepsilon/\langle q_{l\sigma}\rangle - \langle \nu_l/q_{l\sigma}\rangle)]^2 - \langle \xi_l^2/q_{l\sigma}^2\rangle\} K_{B\sigma}. \tag{2.31b}$$

Thus the coherent locators are functions of $\langle \xi_i/q_{i\sigma}\rangle$, $\langle \xi_i^2/q_{i\sigma}^2\rangle$ and $\langle q_{i\sigma}\rangle$. The self-consistent equations for $\langle \xi_i/q_{i\sigma}\rangle$, $\langle \xi_i^2/q_{i\sigma}^2\rangle$ and $\langle q_{i\sigma}\rangle$ are implicitly expressed by

$$\langle Q\rangle = \int d\xi_i\, C(\xi_i; \langle \xi_i/q_{i\sigma}\rangle, \langle \xi_i^2/q_{i\sigma}^2\rangle, \langle q_{i\sigma}\rangle)\, Q(\xi_i) \tag{2.32}$$

where Q is $\xi_i/q_{i\sigma}$, $\xi_i^2/q_{i\sigma}^2$ and $q_{i\sigma}$. Note that $C(\xi_i)$ is a function of $\Xi_{A\sigma}$ and $\Xi_{B\sigma}$ (equations (2.18*b*)–(2.18*d*)), which depend on $\langle \xi_i/q_i\rangle$, $\langle \xi_{i\sigma}^2/q_{i\sigma}^2\rangle$ and $\langle q_{i\sigma}\rangle$ as given by equations (2.31*a*)–(2.31*b*). The number of quantities to be determined self-consistently is reduced by the symmetry consideration. Particularly, in the half-filled band $q_{i\sigma}$ becomes spin-independent and we solve the self-consistent equations only for the three quantities $\langle \xi/q\rangle$, $\langle \xi^2/q^2\rangle$ and $\langle q\rangle$ for both the ferromagnetic and antiferromagnetic states.

We can perform our calculations for a given set of model parameters, U, ε_k, n and T, as follows. We start our calculation with trial values of $\langle \xi_i/q_{i\sigma}\rangle$, $\langle \xi_i^2/q_{i\sigma}^2\rangle$ and $\langle q_{i\sigma}\rangle$, from which $\Xi_{A\sigma}(\varepsilon)$ and $\Xi_{B\sigma}(\varepsilon)$ are obtained by equations (2.31*a*) and (2.31*b*). For the ξ_i-field integration given by equation (2.32), the saddle-point values of m_i, ν_i, n_i and δ_i with $q_{i\sigma}$ are determined for each ξ_i from equations (2.25*a*)–(2.25*d*). By using equations (2.18*b*)–(2.18*d*), we calculate the local energy, $\psi_i(\xi_i)$, and the concentration, $C(\xi_i)$, with which the new averages of $\langle \xi_i/q_{i\sigma}\rangle$, $\langle \xi_{i\sigma}^2/q_{i\sigma}^2\rangle$ and $\langle q_{i\sigma}\rangle$ are obtained by equation (2.32). The iteration is continued until the new results of $\langle \xi_i/q_{i\sigma}\rangle$, $\langle \xi_{i\sigma}^2/q_{i\sigma}^2\rangle$ and $\langle q_{i\sigma}\rangle$ agree with the old ones within an assumed accuracy. Once this convergence is achieved, we can calculate various physical quantities such as $\langle m\rangle$ and $\langle m_z^2\rangle$.

Before showing numerical results, we discuss the interpolating character of our theory.

2.3. *Interpolating character of the theory*

2.3.1. $T = 0$ K. At $T = 0$ K we get from equations (2.31*a*) and (2.31*b*),

$$\Xi_{A\sigma} = X_{j\sigma} \qquad \Xi_{B\sigma} = X_{l\sigma} \tag{2.33}$$

because $\langle \xi_i^2/q_{i\sigma}^2\rangle = \langle \xi_i/q_{i\sigma}\rangle^2$. We can evaluate the functional integral for the ξ_i-field at

the saddle-point values given by equations (2.25*a*)–(2.25*d*). The ground-state values of n, m and q_σ are determined by these saddle-points.

In particular, for the ferromagnetic state, the density of states is given by

$$\rho_\sigma(\varepsilon) = q_\sigma^{-1}\rho^0((\varepsilon - \nu + \sigma\xi)/q_\sigma) \tag{2.34}$$

which denotes the narrowed bands. The free energy is given by

$$F/N_a = U\delta + \sum_\sigma q_\sigma \int_{-\infty}^{x_{F\sigma}} dx\, x\rho^0(x) \tag{2.35}$$

where $x_{F\sigma} = (\mu - \nu + \sigma\xi)/q_\sigma$ and N_a is the number of atoms. This is just the result of Gutzwiller's approximation, as Kotliar and Ruckenstein (1986) showed.

2.3.2. High-temperature limit. At sufficiently high temperatures where the effect of electron correlation becomes unimportant, we get

$$q_{i\sigma} = 1 \qquad \tilde{J}_i = \tilde{U}_i = U_i. \tag{2.36}$$

A combination of equation (2.36) with equation (2.15) yields

$$\delta_i = (\tfrac{1}{4})(n_i^2 - m_i^2). \tag{2.37}$$

From equations (2.18*c*) and (2.37) we get the local energy given by

$$\psi(\xi_j) = U^{-1}[\xi_i^2 - \nu_j^2(\xi_j)] + \int d\varepsilon\, f(\varepsilon)\,(1/\pi)\,\mathrm{Im}\ln[1 + (X_{j\sigma} - \Xi_{A\sigma})K_{A\sigma}] \tag{2.38}$$

where $X_{j\sigma}$, $\Xi_{A\sigma}$ and $K_{A\sigma}$ are given by equations (2.20) and (2.21) but with $q_{j\sigma} = 1.0$. This expression for $\psi(\xi_i)$ agrees with that of the HH theory (Hasegawa 1980a). Thus the present theory in the high-temperature limit reduces to the HH theory, as we expect.

2.3.3. Weak-coupling limit. It is necessary to point out that our Gutzwiller-type theory includes the HH and Hartree–Fock approximations as special cases. The former is given by equations (2.36) and (2.37) as mentioned above. The latter is given when we adopt

$$q_{i\sigma} = 1 \qquad \tilde{J}_i = \tilde{U}_i = U_i \qquad \delta_i = \tfrac{1}{4}(n_i^2 - m_i^2) \tag{2.39a}$$

$$\Xi_\sigma = X_{i\sigma} = [\varepsilon - (U/2)(\langle n\rangle - \sigma\langle m\rangle)] \tag{2.39b}$$

disregarding their optimum values to be determined by equations (2.15), (2.20), (2.25) and (2.26). The expectation values of $\langle m\rangle$ and $\langle n\rangle$ are determined by equations (2.29) and (2.25*c*) with equation (2.39), the integral over the ξ_i-field being evaluated at $\xi_i = (U/2)\langle m\rangle$. In the limit of $U/W \to 0$ (W being the band width), the conditions given by equation (2.39) are satisfied and the present theory reduces to the Hartree–Fock or Stoner theory.

2.3.4. Strong-coupling limit. We consider the case of the half-filled band with infinite U/W. The local moment has the saturated value of $|m_i| = 1$, and then $q_{i\sigma} = 1$ and $\delta_i = 0$ in this limit. The concentration, $C(\xi_i)$, has a structure with distinct double peaks at $\xi_i = \pm\tilde{J}_i/2$. We can evaluate equation (2.32) at these saddle-points to get the Néel temperature (Hasegawa 1980a)

$$T_N = zJ_{sx}/4 = M_2^0/U \tag{2.40}$$

where M_2^0 is the second moment of $\rho^0(\varepsilon)$ and z is the coordination number. This

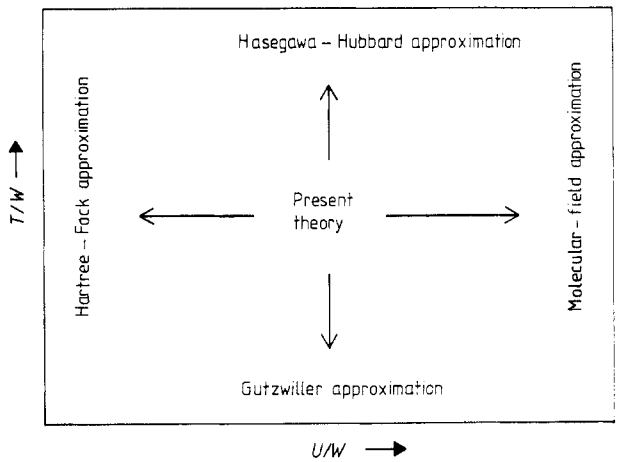

Figure 1. The U–T space showing the interpolation character of the present theory, W being the band width (see text).

expression agrees with the result of the molecular-field theory for the Heisenberg model with $S = \frac{1}{2}$ and the superexchange interaction, J_{sx}.

The interpolation character of the present theory is summarised in figure 1. We expect that our theory yields good results for a wide range of physical parameters.

It is necessary to remark that we cannot prove mathematically that the present theory preserves the variational property with free energy that is an upper bound of the exact one. We should, however, remind ourselves that, although Gutzwiller's approximation is conventionally referred to as a variational theory, it is *not* in the strict sense. In fact, it violates the variational property for a non-half-filled band in the one-dimensional Hubbard model, yielding *lower* energy than the exact VMC method (Yokoyama and Shiba 1987a). In this broad sense that Gutzwiller's approximation is variational, we expect that the present theory would also be variational, at least for the three-dimensional systems, judging from the comparison of the calculated results with those of the MC method (Hirsch 1986, Scalettar *et al* 1988) and VMC method (Yokoyama and Shiba 1987a,b), as will be shown in the next section.

3. Numerical results

3.1. Adopted model

We performed numerical calculations for the simple-cubic Hubbard model with nearest-neighbour hopping t. The input parameters in our calculations are the non-interacting density of states, $\rho^0(\varepsilon)$, the interaction, U, and the electron number, n, which is unity for a half-filled band. We employ the analytic approximate expression for $\rho^0(\varepsilon)$ given by Tonegawa (1974), i.e.

$$\rho^0(\varepsilon) = \begin{cases} A[9 - (\varepsilon/2t)^2]^{1/2} - C[1 - (\varepsilon/2t)^2]^{1/2} & \text{for } |\varepsilon/2t| \leq 1 \\ A[9 - (\varepsilon/2t)^2]^{1/2} - B[1 - (|\varepsilon/2t| - 2)^2]^{1/2} & \text{for } 1 < |\varepsilon/2t| \leq 3 \\ 0 & \text{for } |\varepsilon/2t| > 3 \end{cases} \tag{3.1}$$

where $A/2t = 0.101\,081$, $B/2t = 0.128\,067$ and $C/2t = 0.02$. The energy and the temperature are hereafter measured in units of a half of the total band width, $W = 12t$. The

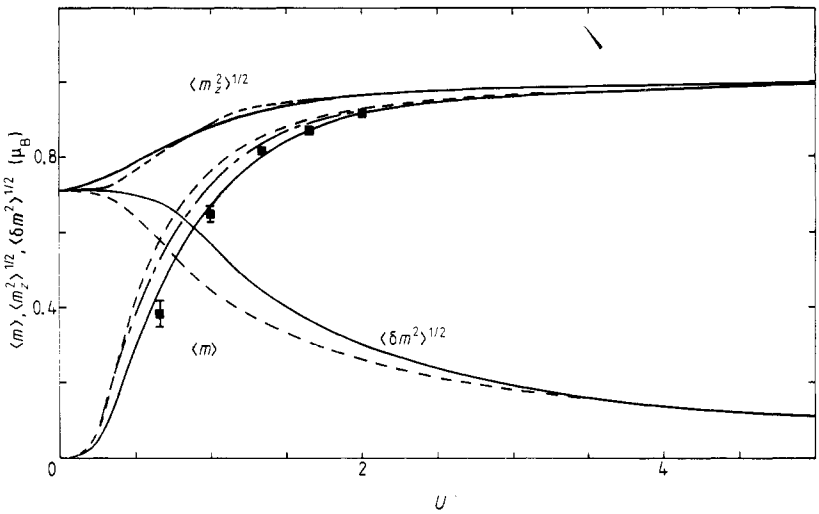

Figure 2. The U-dependence of the sublattice magnetisation, $\langle m\rangle$, RMS values of its amplitude, $\langle m_z^2\rangle$, and fluctuation, $\langle \delta m^2\rangle$, at $T = 0$ K, calculated by the present theory (full curves), the Hartree–Fock approximation (broken curves) and KF theory (Kakehashi and Fulde 1985, Kakehashi and Hasegawa 1987, 1988) (chain curve). Squares denote the result of the VMC calculation (Yokoyama and Shiba 1987b).

ground-state energy for $U = 0$ calculated with the use of equation (3.1) is -0.3349, which is in good agreement with the exact value of -0.3341 (Yokoyama and Shiba 1987a).

The Fermi distribution function is correctly included with the use of the contour integral along the complex axis (Hasegawa 1987b). This method considerably reduces the computational time and makes the CPA calculation much easier than the conventional one along the real axis.

3.2. Ground-state properties

The ground-state sublattice magnetisation, $\langle m\rangle$, is plotted in figure 2 as a function of U. It increases with increasing U, and for infinite U it reaches the saturated value of $\langle m_z\rangle = 1.0\,\mu_B$. Because of the electron correlations, $\langle m_z\rangle$ in our theory is reduced by about 10–20% for $0.5 < U < 1.0$ from the value in the Hartree–Fock theory, to which the HH theory reduces at $T = 0$ K. This is consistent with the VMC result for a cluster of 6^3 (Yokoyama and Shiba 1987b). Qualitatively similar results were obtained in the KF theory (Kakehashi and Fulde 1985, Kakehashi and Samson 1986, Kakehashi and Hasegawa 1987, 1988). There are, however, quantitative differences between the KF and our theories. Even for $U \sim 0.5$, $\langle m\rangle$ in the KF theory is rather larger than that in ours. We note that $\langle m_z\rangle$ for $U = \frac{2}{3}$ in the VMC method is smaller than ours by about 15%. This is considered to be due to the finite-size cluster effect; a similar effect is observed also for the square lattice (see figure 4 in Yokoyama and Shiba 1987b).

We should stress that our theory leads to the antiferromagnetic state even for an infinitesimally small interaction, just as in the Hartree–Fock approximation (Penn 1966). This is in contrast with the previous calculations extending Gutzwiller's approach to antiferromagnetism (Ogawa *et al* 1975, Takano and Uchinami 1975, Florencio and Chao

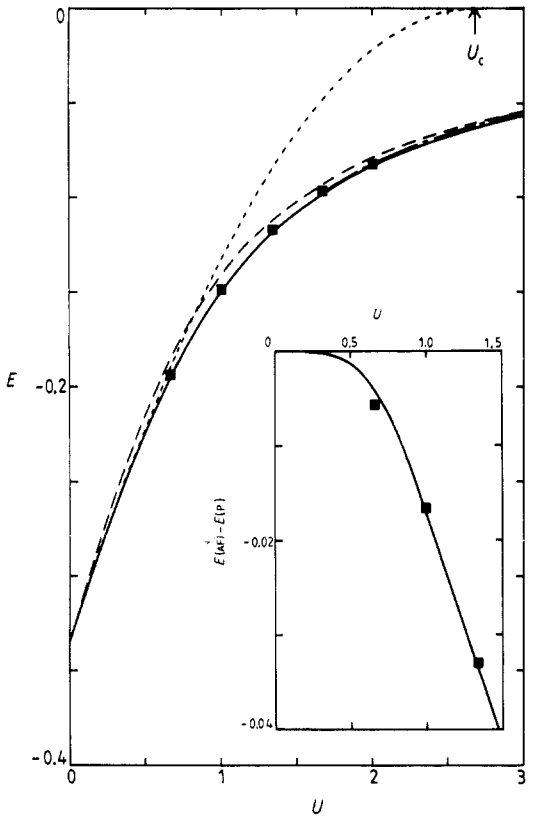

Figure 3. The ground-state energy, E, as a function of the interaction, U. Full, long broken and chain curves express E of the AF state calculated by the present theory, the Hartree–Fock approximation and the KF theory (Kakehashi and Fulde 1985, Kakehashi and Hasegawa 1987, 1988), respectively. The short broken curve denotes E of the P state calculated by Gutzwiller's approximation (Gutzwiller 1965). Squares show the result of the VMC calculation (Yokoyama and Shiba 1987b). The inset shows the energy difference between the AF and P states in our theory (full curve) and the VMC theory (squares) (see text).

1976). They predicted a first-order antiferromagnetic–paramagnetic (AF-P) transition at a finite U-value of $U/U_c = 0.42$ (Ogawa *et al* 1975), 0.35 (Takano and Uchinami 1975) or 0.71 (Florencio and Chao 1976), depending on the adopted models and approximations. Here U_c is defined by

$$U_c = |16 \sum_k \varepsilon_k| \tag{3.2}$$

and it is 2.6792 in our model. In these calculations, the energy of the AF state in their Gutzwiller approximation is *higher* than that in the Hartree–Fock theory. A comparison between the energies of the AF state in the Hartree–Fock theory and the P state in Gutzwiller's approximation leads to a first-order transition. We show in figure 3 the ground-state energies calculated by various methods. The energy of the AF state in the present theory is in good agreement with those of the VMC method. We note that the energy of the P state in Gutzwiller's approximation is lower than that of the AF state in the Hartree–Fock theory for interactions less than $U = 0.82$, which corresponds to

the critical interaction for a first-order transition obtained in previous approximations (Ogawa *et al* 1975, Takano and Uchinami 1975, Florencio and Chao 1976). Our theory leads to the ground-state energy of the AF state which is *lower* than that in the Hartree–Fock theory for all U-values we investigated. The inset of figure 3 shows the energy difference between the AF and P states in the Gutzwiller-type approximations. The energy of the AF state of the VMC method (Yokoyama and Shiba 1987b) is compared with the P-state energy in Gutzwiller's approximation given by (Vollhardt 1984)

$$E/N_a = -(U_c/8)(1 - U/U_c)^2 \qquad \text{for } U < U_c \tag{3.3}$$

where $U_c = 2.6731$ is employed. The results of the VCM calculation shown by squares are in good agreement with ours. The energy difference gradually vanishes on approaching $U = 0$ from above, which shows the *second-order* AF–P transition at $U = 0$. Our conclusion is supported in part by a calculation of the ground-state staggered susceptibility, which diverges for an infinitesimal U because of perfect nesting of the Fermi surface (see appendix 2). The same conclusion was claimed by Kotliar and Ruckenstein (1986), although an explicit result of their energy calculations has not been reported yet.

The chain curve in figure 3 expresses the ground-state energy calculated by Kakehashi and Hasegawa (1987, 1988) using the KF theory. In this local approach matrix elements are evaluated within the single-site or so-called $R = 0$ approximation in the second-order perturbation expansion (Kajzar and Friedel 1978, Treglia *et al* 1980, Stollhoff and Thalmeier 1981, Oles 1981). We note that the agreement between the results of KF theory and the VMC method (or ours) is excellent for $U < 2$ although it becomes worse by degrees for larger U-values, which is inherent in the expansion-type KF theory. This is consistent with the calculations of Stollhoff and Thalmeier (1981) and Oles (1981) showing that the $R = 0$ approximation works quite well for transition metals, in which interactions are expected to be comparable with or less than the d band width.

Solutions of $\langle q \rangle$, $\langle \delta \rangle$ and $\langle \tilde{J} \rangle / U$, in both P and AF states, are shown in figure 4. For the P state we get the analytic solution given by

$$\langle \delta \rangle = \tfrac{1}{4}(1 - U/U_c) \qquad \langle q \rangle = 1 - (U/U_c)^2 \tag{3.4a}$$

$$\langle \tilde{J} \rangle / U = \langle q \rangle (1 + U/2U_c)/(1 + U/U_c)^2. \tag{3.4b}$$

Equations (3.3)–(3.4) show that $\langle \delta \rangle$, $\langle \tilde{J} \rangle$, $\langle q \rangle$ and E vanish at $U = U_c$, which is referred to as the critical interaction for the metal–insulator transition (Brinkman and Rice 1970); related discussion will be given in § 4. When the interaction is increased from the zero value, $\langle q \rangle$, $\langle \delta \rangle$ and $\langle \tilde{J} \rangle / U$ of the AF state gradually depart from those of the P state. The effect of electron correlations is most significant in the intermediate-coupling regime, $0.5 \lesssim U \lesssim 1.5$, where the effective exchange interaction and the band-narrowing factor are $\langle \tilde{J} \rangle / U \sim 0.75$ and $\langle q \rangle \sim 0.95$. For larger U interactions, $\langle \tilde{J} \rangle / U$ and $\langle q \rangle$ are increased again, approaching unity for infinite U. The renormalisation effect of electron correlation on $\langle \tilde{U} \rangle$ is negligibly small in the half-filled case (see appendix 1).

The root-mean-square (RMS) values of the amplitude of sublattice magnetisation, $\langle m_z^2 \rangle$, and its fluctuations defined by $\langle \delta m^2 \rangle = \langle m_z^2 \rangle - \langle m \rangle^2$ are plotted in figure 2 as a function of U. Although the Hartree–Fock approximation conventionally assumes that $\langle m_z^2 \rangle = \langle m \rangle^2$ and $\langle \delta m^2 \rangle = 0$, we also show, for comparison, the result calculated with the use of equation (2.30) but with δ replaced by $\delta^{HF} = \frac{1}{4}(1 - \langle m \rangle^2)$. Both $\langle m_z^2 \rangle^{1/2}$ and $\langle \delta m^2 \rangle^{1/2}$ have the exact value of $1/\sqrt{2}$ at $U = 0$. With increasing U, $\langle m_z^2 \rangle$ increases, approaching the atomic limit of 1.0 μ_B, while $\langle \delta m^2 \rangle$ decreases. The magnetic-moment

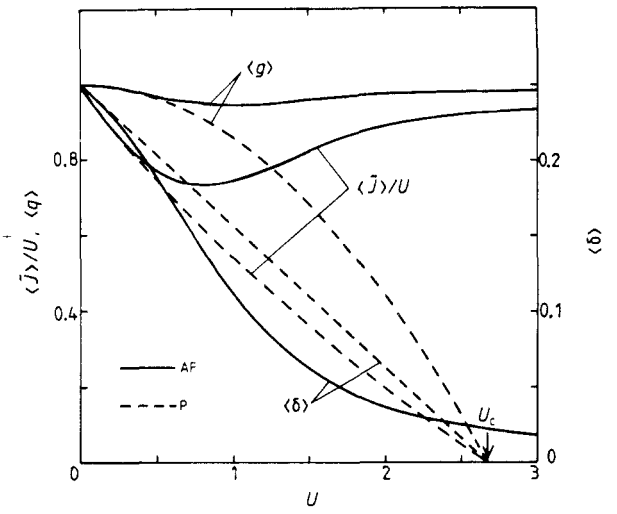

Figure 4. The U-dependence of $\langle\delta\rangle$, $\langle q\rangle$ and $\langle\tilde{J}\rangle/U$ for the AF (full curves) and P (broken curves) states. The arrow denotes U_c defined by equation (3.2).

fluctuation in our theory is larger than that in the above approximation because $\delta < \delta^{HF}$ and $\langle m\rangle < \langle m\rangle^{HF}$ for a given U.

3.3. Finite-temperature properties

The temperature dependence of sublattice magnetisation is plotted in figure 5 for various U-values. The full, broken and chain curves express the results in the present theory, the HH and the KF theories, respectively. For small U, the $\langle m\rangle$ versus T curve deviates downwards from the Brillouin curve for $S = \frac{1}{2}$, while for strong interactions it follows the Brillouin function. The KF theory yields, for $U = 1.0$, a peculiar temperature dependence in $\langle m\rangle$, decreasing rapidly just below the Néel temperature. This was claimed to be due to the effect of electron correlations (Kakehashi and Hasegawa 1987, 1988). Such a temperature dependence is, however, not obtained in our theory. Recent MC calculations (Scalettar *et al* 1988) suggested a weak first-order transition for weak interactions in the model, although further studies are required to clarify this point.

Figure 6 shows the temperature dependence of $\langle q\rangle$, $\langle\delta\rangle$ and $\langle\tilde{J}\rangle/U$. When the temperature is raised from $T = 0$ K, both $\langle q\rangle$ and $\langle\tilde{J}\rangle$ decrease. The effect of electron correlations is significant even at temperatures of the order of T_N, although at the high-temperature limit the effect is expected to diminish. The double occupancy, $\langle\delta\rangle$, for $U = 1.0$ and 1.5 shows little temperature dependence although that of $U = 0.5$ decreases slightly as the temperature is raised. The temperature dependences of $\langle\delta\rangle$ reflect on those of the amplitude of local moments, $\langle m_z^2\rangle$, through the relation given by equation (2.30). The temperature dependence of amplitudes of local magnetic moments is shown in figure 7. When the temperature is raised from $T = 0.0$ to $T = 0.20$, the ground-state values of $\langle m_z^2\rangle^{1/2}$ are increased by 13%, 5% and 3% for $U = 0.5$, 1.0 and 1.5, respectively. We note that $\langle m_z^2\rangle^{1/2}$ has only a small temperature dependence, particularly for large U, with almost the same amplitudes in both the AF and P states. Our result is in fairly good agreement with those of the MC and KF theories, whose results for $U = 1.0$ are plotted for comparison.

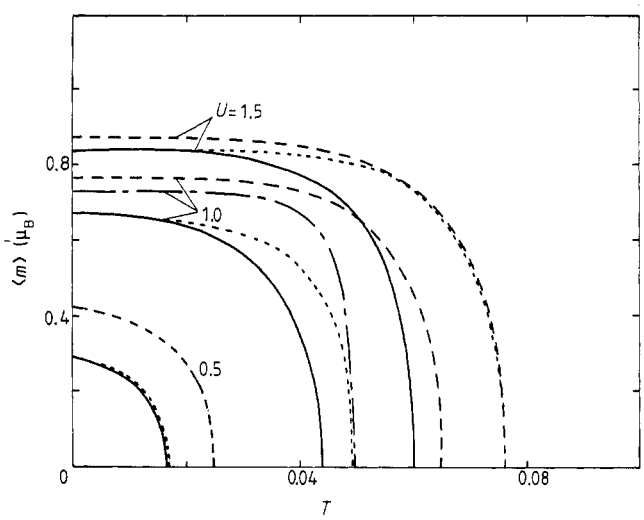

Figure 5. The temperature dependence of sublattice magnetisation, $\langle m \rangle$, for various interactions calculated by the present theory (full curves) and the HH theory (Hasegawa 1979, 1980a, Hubbard 1979) (long broken curves). The chain curve denotes $\langle m \rangle$ for $U = 1.0$ calculated by the KF theory (Kakehashi and Fulde 1985, Kakehashi and Hasegawa 1987, 1988). The short broken curves show $\langle m \rangle$ obtained by the HH theory using the effective interaction (see text).

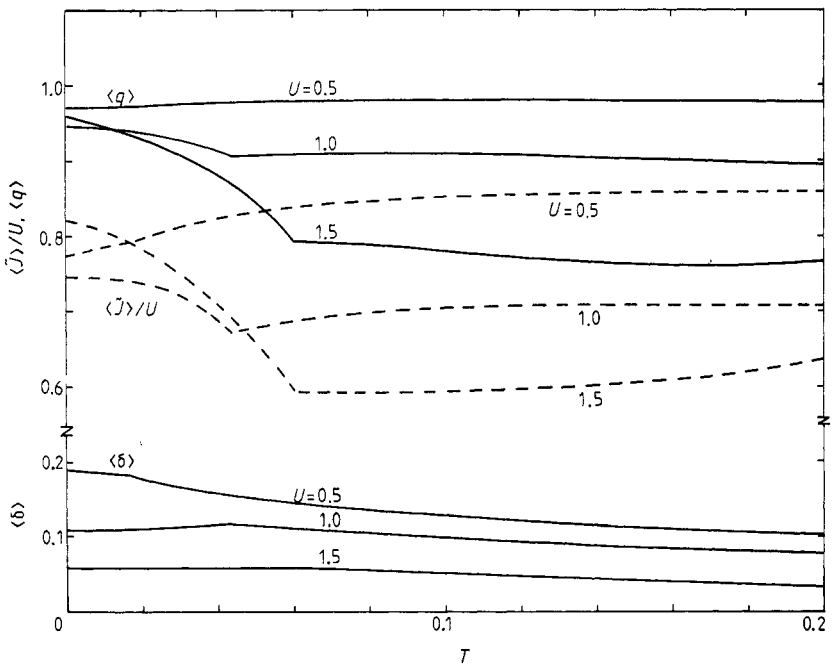

Figure 6. The temperature dependence of $\langle q \rangle$ (upper full curves), $\langle \delta \rangle$ (lower full curves) and $\langle \tilde{J} \rangle / U$ (broken curves).

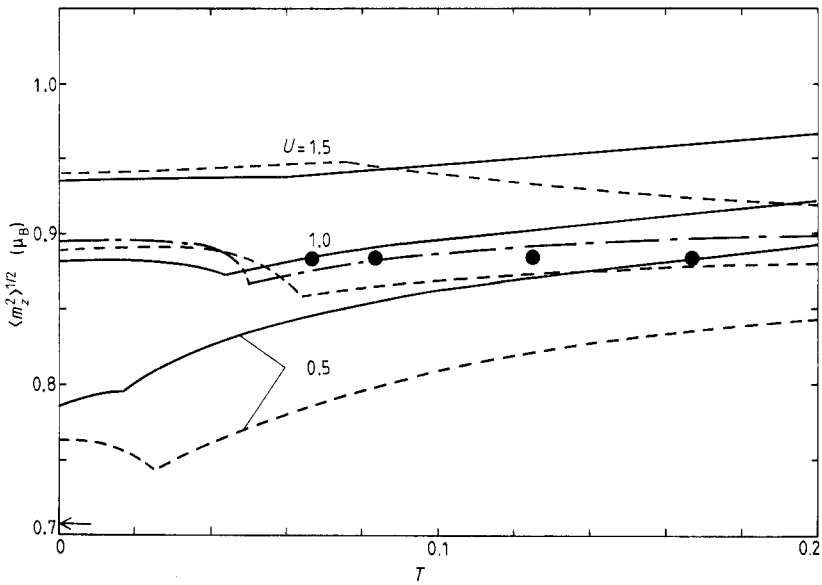

Figure 7. The temperature dependence of the RMS values of amplitude of local moment, $\langle m_z^2 \rangle^{1/2}$. Full and broken curves denote the results of the present theory and the HH theory (Hasegawa 1979, 1980a, Hubbard 1979), respectively. The chain curve and circles show $\langle m_z^2 \rangle^{1/2}$ for $U = 1.0$ in the KF theory (Kakehashi and Fulde 1985, Kakehashi and Hasegawa 1987, 1988) and the MC theory (Hirsch 1986), respectively. The arrow denotes the value $(1/\sqrt{2})$ for non-interacting systems ($U = 0$) at $T = 0$ K.

The U–T phase diagram calculated in our theory is shown in figure 8, where those obtained in other theories are also plotted. The Néel temperature in our theory reduces to those of the Hartree–Fock and molecular-field approximations in the weak- and strong-coupling limits, respectively, as mentioned before. Our T_N curve has a maximum at $U \sim 1.7$ while those of the HH and KF theories are at $U \sim 1.35$ and 1.5, respectively. In the range $0.5 \leqslant U \leqslant 1.5$, our Néel temperature is about 20–30% lower than that of the HH theory. A reduction in T_N from that of the HH theory is realised in our calculation even at $U \gtrsim 1.5$, where the KF theory leads to almost the same T_N as the HH theory.

The double-dot chain curve in figure 8 shows the U–T phase diagram calculated using Moriya's 'unified' theory (Moriya and Takahashi 1978, Moriya and Hasegawa 1980), which belongs to the interpolation approaches discussed in the introduction. The Moriya–Takahashi (MT) theory employed the vector-field, static functional-integral method and it reduces, in the strong-U limit, to the spherical model. We note that T_N in the MT theory is one-fifth to one-sixth of that of the HH theory (Kakehashi and Hasegawa 1987, 1988). This large difference is mainly attributed to a neglect of quantum fluctuations in the vector-field (static) functional-integral method, which cannot lead to exact results either in the atomic limit or in the weak-coupling limit. In the former limit, it yields $T_N \propto S^2$ instead of $S(S + 1)$.

The Néel temperature calculated by Hirsch (1986) and Scalettar *et al* (1988) with the MC simulations are shown by open and filled circles, respectively, in figure 8. Kakehashi and Hasegawa (1987, 1988) pointed out that Hirsch's calculation using a cluster of 4^3 greatly overestimated T_N partly due to a finite-size effect and partly due to an improper mean-field boundary condition that he adopted. The recent MC calculation made by

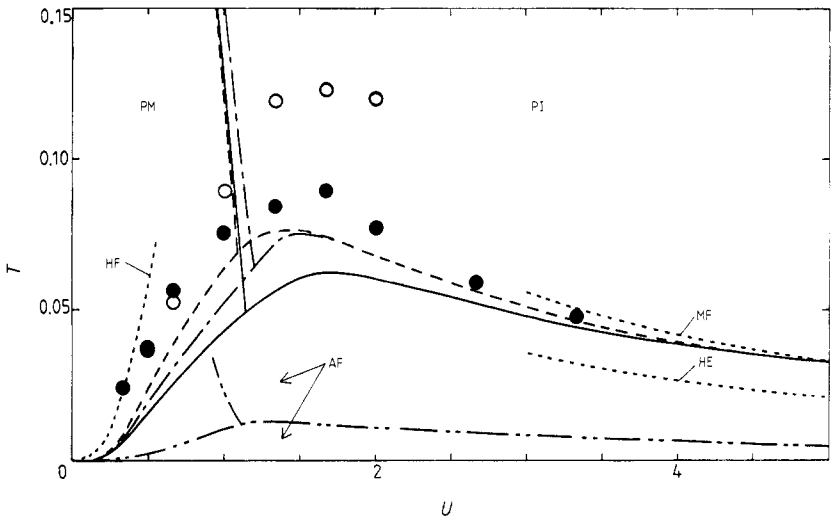

Figure 8. The U–T phase diagram showing the antiferromagnetic (AF) state, paramagnetic metal (PM) and paramagnetic insulator (PI), calculated by using the present theory (full curves), the HH theory (Hasegawa 1979, 1980a, Hubbard 1979) (long broken curves), the KF theory (Kakehashi and Fulde 1985, Kakehashi and Hasegawa 1987, 1988) (chain curves) and the MT theory (Moriya and Takahashi 1978) (double-dot chain curves). Open and filled circles show the MC results obtained by Hirsch (1986) and Scalettar *et al* (1988), respectively. Short broken curves denote T_N in the Hartree–Fock (HF) theory and molecular-field (MF) and high-temperature (HE) expansion approximations for the Heisenberg model.

Scalettar *et al* (1988) for larger clusters of 4^3–10^3 yielded T_N about 30–40% less than those of Hirsch for $U < 1$. The Néel temperature calculated by the HH and KF theories are in good agreement with that of the MC method of Scalettar *et al* (1988). Our theory, however, leads to T_N about 30% smaller than their MC result. We expect that the Néel temperature of Scalettar *et al* (1988) is still overestimated for the following reasons. Scalettar *et al* (1988) estimated T_N from the χ_s versus V plot for temperatures, where χ_s denotes the staggered susceptibility and V the volume of the cluster. When χ_s appears to increase with V for a given temperature, they regarded it as the Néel temperature. As an alternative, we plotted the χ_s^{-1} versus T curve, from which we estimated the Weiss constant, Θ, defined by $\chi_s^{-1} \sim (T - \Theta)$ at $T \gg T_N$. We got $\Theta = 0.043$ and 0.075 for $U = \frac{2}{3}$ and 1, respectively, while Scalettar *et al* (1988) obtained $T_N = 0.055$ and 0.075 from their analysis. This shows that their T_N is nothing but Θ and that their T_N is still overestimated; note that $\Theta/T_N = 6.00/3.83$ in the strong-interaction limit. Indeed, the Néel temperature of their MC calculation reduces, in the strong limit, not to the exact T_N of the high-temperature expansion theory but to a higher one of the molecular-field approximation. For more precise determination of T_N from MC data, it is necessary to establish and adopt a finite-size scaling relation.

4. Conclusions and discussion

We have discussed the finite-temperature band theory, which takes into account effects of both electron correlations and local spin fluctuations, by combining the Kotliar–

Ruckenstein functional-integral method (Kotliar and Ruckenstein 1986) with the alloy-analogy approximation (Hubbard 1979, Hasegawa 1979, 1980a). Our unified theory has the interpolation character describing sensible cross-overs between the low- and high-temperature limits and between the weak- and strong-coupling limits (figure 1). In the course of this development, we have reformulated Gutzwiller's approximation by introducing the effective interactions ($\tilde{J}$, $\tilde{U}$) with the Green function method. This helps us to calculate various quantities easily and to interpret the calculated results physically.

We have established the extension of Gutzwiller's approximation to antiferromagnetism. It has been shown from the calculations of the energy (figure 3) and the susceptibility (appendix 2) that the antiferromagnetic state is stabilised at $T = 0$ K for an infinitesimal interaction in the simple-cubic lattice. This conclusion is in agreement with those of Kotliar and Ruckenstein (1986) and the VMC method (Yokoyama and Shiba 1987b). It is, however, in contrast with previous results (Ogawa *et al* 1975, Takano and Uchinami 1975, Florencio and Chao 1976), which yielded a first-order P–AF transition at finite U-values. It is suggested that, although the VMC calculations (Yokoyama and Shiba 1987a, b) are generally in good agreement with our ground-state results, the VMC sublattice moment for $2U/W = \frac{2}{3}$ may be underestimated due to a finite-size cluster effect.

Our finite-temperature calculations (figures 5–8) have demonstrated that the effect of electron correlations is considerable even at temperatures of the order of T_N. The KF theory (Kakehashi and Fulde 1985) for electron correlations at finite temperatures yields qualitatively similar results as the present theory. Their results are, however, *quantitatively* rather different from ours, even for $2U/W \sim 0.5$. This is not unexpected because the KF theory is based on the second-order perturbation method (Stollhoff and Fulde 1978) with respect to the projection operator, which is, roughly speaking, proportional to the interaction U. We have pointed out that the Néel temperature obtained by the recent MC calculation (Scalettar *et al* 1988) is still overestimated though their T_N is much reduced compared with Hirsch's (1986) result.

We should remember that the effect of local spin fluctuations plays essential roles to reconcile the localised and itinerant-electron models (Hubbard 1979, Hasegawa 1979). In fact, if we neglect this effect in the present approach, it reduces to the theory of Chao and Berggren (1977), which has a serious difficulty in calculating the entropy stemming from local moments, as discussed in the introduction. The HH theory, which takes into account the effect of local spin fluctuations but neglects the electron correlations, has so far been applied to various problems of transition-metal magnetism. In these calculations the interaction is chosen such as to reproduce the ground-state moment observed experimentally or obtained by detailed band calculations. In order to check the validity of this approach, we repeated calculations for the simple-cubic model by using the HH theory. We adopted the interaction U, which is chosen to reproduce $\langle m \rangle$ at $T = 0$ K obtained in our new theory. This approximation is expected to be a good one if $\tilde{J}$, $\tilde{U}$ and q_σ have only a small temperature dependence. Unfortunately it is not the case in general, as figure 6 shows. Nevertheless, the calculated results shown by short broken curves in figure 5 are in semi-quantitative agreement with those in the present theory. This justifies the previous calculations based on the HH theory. By using our newly developed theory, we can discuss magnetic and thermodynamic properties of transition metals in more detail.

It would be interesting to compare the present alloy-analogy theory with Hubbard's on electron correlations (Hubbard 1964). By using the Green function decoupling approximation, Hubbard took into account the scattering and resonance broadening

corrections. The former has an analogue with disorder scattering in an alloy and the latter describes the dynamic effect of motion of $(-\sigma)$-spin electrons on the propagation of σ-spin electrons. If we include only the scattering correction, the medium for σ-spin electrons is regarded as a binary alloy in which two species of atoms have random potentials of $U/2$ and $-U/2$ with concentration $\langle n_{-\sigma}\rangle$ and $1-\langle n_{-\sigma}\rangle$, respectively. In this case Hubbard's approximation is equivalent to the CPA and the site-diagonal Green function is given by equations (2.20*a*)–(2.24) but with the concentration and the locator replaced by

$$C(\xi_i) = \sum_{\tau=\pm} c^\tau \delta(\xi_i - \xi^\tau) \tag{4.1a}$$

$$X_\sigma^\tau(\varepsilon) = (\varepsilon - \sigma\xi^\tau)/q_\sigma^\tau \tag{4.1b}$$

with

$$c^+ = 1 - c^- = \langle n_{-\sigma}\rangle \qquad \xi^\tau = \tau(U/2) \qquad q_\sigma^\tau = 1. \tag{4.2}$$

Here the index τ $(=\pm)$ expresses species of atoms in the binary alloy. On the other hand, our alloy-analogy theory regards the system as a multi-component alloy, which is characterised by the continuous distribution of the ξ_i-field. This leads to a unified description covering the weak- and strong-U limits. Applying the local saddle-point approximation to an integral over the ξ_i-field, we can treat the system as a binary alloy in which the concentration and the locator are given by equations (4.1*a*) and (4.1*b*) with

$$\begin{aligned} &c^+ = 1 - c^- = 1/[1 + \exp(-\beta\Delta\psi)] \\ &\xi^\tau = [\tilde{J}^\tau(n^\tau, m^\tau, \delta^\tau)/2]m^\tau \qquad q_\sigma^\tau = q_\sigma^\tau(n^\tau, m^\tau, \delta^\tau). \end{aligned} \tag{4.3}$$

Here $\tilde{J}^\tau$ and q_σ^τ $(\tau = \pm)$ are functions of the saddle-point values of n^τ, m^τ and δ^τ as given by equations (2.15) and (2.26*a*), and $\Delta\psi = \psi(\xi^-) - \psi(\xi^+)$ stands for the difference between local energies at the two saddle-points of $\xi^\pm$ (see equation (2.18*c*)). When we compare equation (4.2) with equation (4.3), we note some differences in these expressions. The concentration in our theory depends explicitly on the temperature, though its temperature dependence in Hubbard's theory arises implicitly through $\langle n_\sigma\rangle$. The renormalised $\tilde{J}$ and q_σ are used in our theory while Hubbard employed their bare values in equation (4.2). Despite these ostensive differences, however, the two binary-alloy approximations have similar physical ingredients. It is expected that the band narrowing represented by q_σ in our theory mimics, to some extent, the motional narrowing due to the resonance broadening discussed in Hubbard's theory. The present theory has the advantage of being free from the well known defect in Hubbard's theory that each sub-band does not exactly contain one state per atom for the case of a half-filled band.

Hubbard (1964) discussed the metal–insulator transition in his paper on electron correlations. He showed that there is a critical ratio of the interaction to the band width such that when it is exceeded the system behaves as an insulator with a vanishing density of states at the Fermi level. We plot the almost vertical lines in figure 8 as those along which we get $\rho(\varepsilon_F) = 0$, ε_F being the Fermi level. Regarding these lines as the metal–insulator boundary, after Hubbard (1964), we constructed the phase diagram showing the antiferromagnetic insulator (AF), paramagnetic insulator (PI) and paramagnetic metal (PM). This type of phase diagram is widely observed in many materials such as V_2O_3(McWhan and Remeika 1971). On the contrary, Brinkman and Rice (1970) proposed an alternative mechanism for the metal–insulator transition in a half-filled

non-magnetic band by using Gutzwiller's approximation. They showed that it takes place at $U = U_c$, beyond which the double occupancy, $\langle\delta\rangle$, and the band-narrowing parameter, $\langle q\rangle$, vanish, yielding the localisation of electrons, U_c being defined by equation (3.2). Extending this idea to the finite-temperature case, Kotliar and Ruckenstein (1986) suggested that a first-order metal–insulator transition occurs at a temperature of order W^2/U where $\langle q\rangle$ vanishes. These speculations are, however, not realised in the present calculations. At $T = 0$ K, the antiferromagnetic state is stabilised at $U < U_c$ and $\langle q\rangle$ in the antiferromagnetic state does not vanish even at $U > U_c$, as figure 4 shows. This is consistent with earlier suggestions (Florencio and Chao 1976). Recent investigations (Kaplan *et al* 1982, Yokoyama and Shiba 1987a) showed that the Brinkman–Rice-type metal–insulator transition does not occur even in the non-magnetic state of one- and two-dimensional systems when the calculation is performed exactly with the use of Gutzwiller's wavefunctions. Our calculation in figure 6 shows that $\langle q\rangle$ does not vanish also at finite temperatures, although it decreases from its zero-temperature value. Rather we expect that $\langle q\rangle$ increases to approach unity at higher temperatures where the effect of electron correlation becomes unimportant. We may conclude from these considerations that the Brinkman–Rice-type metal–insulator transition characterised by $\langle q\rangle = \langle\delta\rangle = 0$ is not realised either in the ground state or at finite temperatures in the half-filled simple-cubic model. The condition $\rho(\varepsilon_F) = 0$ is expected to provide us with a more reasonable criterion for its metal–insulator transition.

We expect that the present theory has wide applicability to a variety of problems, such as magnetism and superconductivity, in which electron correlations play important roles. The effect of electron correlations on magnetism in alloys, surfaces and thin films may be discussed by using the present formalism in which the self-consistent equations are expressed in terms of local quantities. The result reported in the present paper is relevant to the properties of superconductivity described by the Hubbard model with the attractive interaction ($U < 0$) (Nozieres and Schmit-Rink 1985). The U-dependence of the Néel temperature shown in figure 8 may be interpreted as that of the superconducting critical temperature, T_c, whose maximum value is shown to be $2T_c/W \sim 0.06$. In recent years, much attention has been paid to two-dimensional Hubbard antiferromagnets, stimulated by the discovery of high-T_c superconductors. The mechanism leading to superconductivity in the nearly half-filled Hubbard model with purely repulsive interactions has been investigated by various methods. We hope that the present theory is useful and meaningful for these subjects.

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Appendix 1

In the half-filled band, the band-narrowing factor, $q_{i\sigma}$, given by equation (2.15) is spin-independent and becomes

$$q = q(n = 1, m, \delta) = 2\delta[(1 + m - 2\delta)^{1/2} + (1 - m - 2\delta)^{1/2}]^2/(1 - m^2) \qquad \text{(A1.1)}$$

where the index i is suppressed for simplicity. The m- and δ-dependences of q are shown

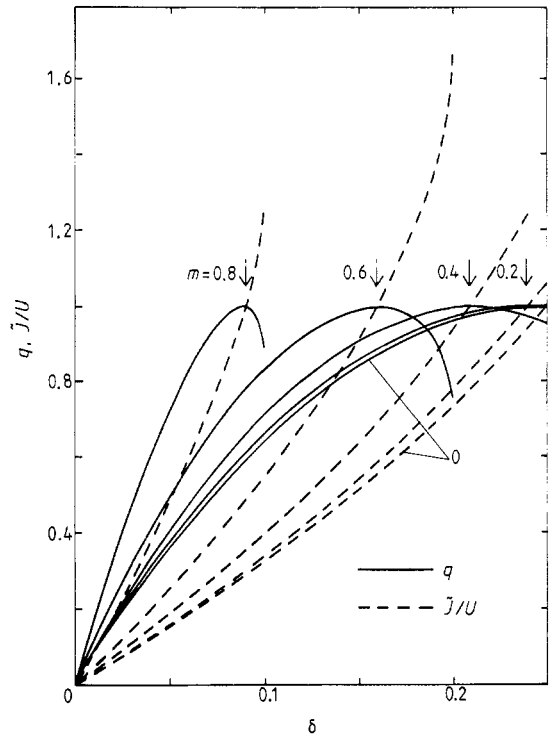

Figure A1. The m- and δ-dependences of q (full curves) and $\tilde{J}/U$ (broken curves) in the half-filled band. The relevant δ-value is less than $\delta_c = \frac{1}{4}(1 - m^2)$ shown by arrows, for which $\tilde{J}/U < 1$ and $\partial q/\partial\delta > 0$ (see text).

in figure A1, where we also plot $\tilde{J}$ calculated by equations (2.26*a*). When $m = 0$, $\tilde{J}$ is given by

$$\tilde{J}/U = \delta(3 - 4\delta)/(1 - 2\delta). \tag{A1.2}$$

The effective exchange interaction, $\tilde{J}$, is always reduced by the effect of electron correlations. Figure A1 shows that we get $\tilde{J}/U > 1$ for $\delta > \delta_c \equiv \frac{1}{4}(1 - m^2)$, δ_c being shown by arrows. This is, however, never realised because the self-consistent equation (2.25*d*) has no solutions for $\delta > \delta_c$ where $\partial q/\partial\delta < 0$; note that $R_{i\sigma} < 0$. The effect of electron correlations on $\tilde{U}$ is negligibly small for the half-filled band. In particular we get $\tilde{U}/U = 1.0$ regardless of U when $m = 0$.

Appendix 2

We will show the calculation of the ground-state susceptibilities in terms of the effective exchange ($\tilde{J}$) and Coulomb ($\tilde{U}$) interactions defined by equations (2.26*a*)–(2.26*b*).

When an infinitesimal uniform or staggered magnetic field h_α (α = u or s) is applied to the non-magnetic system at $T = 0$ K, an induced magnetic moment, m_α, is given by

$$m_\alpha = 2\bar{\chi}_\alpha(h_\alpha + \xi_\alpha) \tag{A2.1}$$

where $\bar{\chi}_u$ ($\bar{\chi}_s$) is the irreducible uniform (staggered) susceptibility. The form of the

molecular field, ξ_α, depends on the approximation to be adopted. In the Hartree–Fock approximation, we have

$$\xi_\alpha^{\mathrm{HF}} = (U/2)m_\alpha \qquad \bar{\chi}_\alpha = \chi_\alpha^0 \tag{A2.2}$$

which yields the well known result

$$\chi_\alpha^{\mathrm{HF}} = 2\chi_\alpha^0/(1 - U\chi_\alpha^0) \tag{A2.3}$$

χ_α^0 being the non-interacting susceptibility. In our Gutzwiller-type theory, the molecular field is given by equation (2.25*a*), namely,

$$\xi_\alpha = [\tilde{J}(n, m = 0, \delta)/2]m_\alpha. \tag{A2.4}$$

A simple calculation leads to the irreducible susceptibility given by

$$\bar{\chi}_\alpha = \chi_\alpha^0/q(n, m = 0, \delta) \tag{A2.5}$$

from which we get

$$\chi_\alpha = (2\chi_\alpha^0/q)/(1 - \tilde{J}\chi_\alpha^0/q). \tag{A2.6}$$

In the case of the half-filled band, we get the susceptibilities with the use of equations (3.4), (A1.2) and (A2.6) as

$$\chi_\alpha = (2\chi_\alpha^0/q)[1 - U\chi_\alpha^0(1 + U/2U_c)/(1 + U/U_c)^2]^{-1} \tag{A2.7}$$

where U_c is given by equation (3.2). The uniform susceptibility (α = u) given by equation (A2.7) is the same as Brinkman and Rice (1970) obtained by calculating the second-order energy shift due to an applied field. Equation (A2.7) shows that the staggered susceptibility (α = s) for the half-filled simple-cubic model in our approximation diverges for an infinitesimal interaction because of the singularity in χ_s^0 just as in the Hartree–Fock approximation (Penn 1966).

A calculation of the charge susceptibility goes along parallel lines when we use the effective Coulomb interaction, $\tilde{U}$, defined by equation (2.26*b*).

The susceptibility at finite temperatures can be calculated by using $\tilde{J}$ and $\tilde{U}$ along the HH theory (Hasegawa 1980a); details will be reported in a separate paper.

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