Quantitative Aspects of the Dynamical CPA in Harmonic Approximation
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Magnetic and electronic properties of the Hubbard model on the Bethe and fcc lattices in infinite dimensions have been investigated numerically on the basis of the dynamical coherent potential approximation (CPA) theory combined with the harmonic approximation (HA) in order to clarify the quantitative aspects of the theory. It is shown that the dynamical CPA+HA reproduces well the sublattice magnetization, the magnetizations, susceptibilities, and the Néel temperatures ($T_N$) as well as the Curie temperatures calculated by the Quantum Monte-Carlo (QMC) method. The critical Coulomb interactions ($U_c$) for the metal-insulator (MI) transition are also shown to agree with the QMC results above $T_N$. Below $T_N$, $U_c$ deviate from the QMC values by about 30% at low temperature regime. These results indicate that the dynamical CPA+HA is applicable to the quantitative description of the magnetic properties in high-dimensional systems, but one needs to take into account higher-order dynamical corrections in order to describe the MI transition quantitatively at low temperatures.

KEYWORDS: Dynamical CPA, Curie temperature, Néel temperature, Effective Bohr magneton number, Metal-insulator transition, Excitation spectra, Hubbard model

1. Introduction

The magnetism of correlated electron systems with intermediate Coulomb interaction strength has been one of the long standing problems in the solid-state physics because these systems show the complex properties known as the itinerant vs. localized behaviors.\(^1\)\(^2\) The ground-state magnetizations of Fe, Co, Ni, for example, show the noninteger values in unit of the Bohr magneton number being characteristic of a band model, while their finite-temperature properties such as the magnetization vs. temperature curves and the Curie-Weiss susceptibilities are well explained by a Heisenberg-type localized model. The Hartree-Fock theory and simple perturbation theories could not explain their magnetic properties since these theories overestimate the magnetic energy at finite temperatures.

Because of the difficulty in describing the itinerant vs. localized behavior in the magnetism of transition metals, interpolation theories have been developed by many investigators. Cyrot\(^3\) adopted the functional integral method\(^4\) to the Hubbard model and derived the $P-T$ phase diagram of metal-insulator (MI) phase transition at finite temperatures. Hubbard\(^5\) and Hasegawa\(^6\) independently developed the single-site spin fluctuation theory (SSF) on the basis of the functional integral method. The theory transforms the electron-electron interaction into a time-dependent random potential by introducing the time-dependent charge and exchange random fictitious field variables, and treats the potentials using the coherent potential approximation (CPA).\(^7\) The theory interpolates between the weak and strong Coulomb interaction limits, and explained qualitatively the localized vs. itinerant behaviors of magnetism in transition metals.

The SSF is based on the static approximation (SA) which neglects the time dependence of the fictitious fields. Though the SA is exact in the high temperature limit, it reduces to the Hartree-Fock theory at the ground state. Thus it does not take into account the electron correlations as found at the zero temperature by Gutzwiller,\(^8\) Hubbard,\(^9\) and Kanamori.\(^10\) Kakehashi and Fulde\(^11\) proposed a variational theory at finite temperatures which takes into account the ground-state electron correlations, and showed that the correlations at finite temperatures can reduce the Curie temperatures.

Towards more quantitative theory, Kakehashi\(^12\) proposed the dynamical CPA which completely takes into account electron correlations at finite temperatures within the single-site approximation, and clarified the basic properties of the theory using a Monte-Carlo technique. Later he proposed an analytic theory of the dynamical CPA combined with the harmonic approximation (HA),\(^13\) and examined the dynamical effects on the itinerant ferromagnetism. In the HA,\(^14\) we neglect the mode-mode couplings between the dynamical potentials, and take into account the contributions from the dynamical potentials with the same frequency independently. The HA is known to be exact up to the second order in the weak Coulomb interaction limit, and is known to describe quantitatively the Kondo limit in the strong Coulomb interaction regime.\(^15\) The dynamical CPA has recently been proved\(^2\)\(^16\) to be equivalent to the many-body CPA in the disordered problem,\(^17\) the dynamical mean-field theory in the metal-insulator transition in infinite dimensions,\(^18\) and the projection-operator method CPA for excitations in solids.\(^19\)

More recently, we proposed the first-principles dynamical CPA\(^20\) on the basis of the tight-binding linear muffin tin orbital (TB-LMTO) Hamiltonian\(^21\)\(^22\) with the LDA (Local Density Approximation)+$U$ type in-
traatomic Coulomb interactions,23) and clarified the ferromagnetism of Fe, Co, and Ni,24,25) as well as the systematic change of excitation spectra in 3d transition metal series.26,27)

Although the numerical results of the first-principles dynamical CPA combined with the HA seem to be reasonable and explained well a systematic change of the XPS and BIS data,26) the validity of the dynamical CPA+HA has not yet been examined in details. The purpose of the present paper is to clarify the quantitative aspects of the dynamical CPA+HA from the numerical point of view. For this purpose, we have calculated the antiferromagnetic properties of the half-filled Hubbard model on the Bethe lattice in infinite dimensions18) and the ferromagnetic properties of the non half-filled Hubbard model on the fcc lattice in infinite dimensions28) on the basis of the dynamical CPA+HA. We clarify the validity of the theory by comparing the results of calculations with those of the Quantum Monte-Carlo (QMC) method.29–33) We will conclude that the dynamical CPA approach is useful for the quantitative understanding of the magnetic properties of solids in high dimensions where the single-site approximation works well.

Outline of the present paper is as follows. In §2, we summarize the dynamical CPA combined with the HA and extend the theory to the antiferromagnetic case with the bipartite lattice. In §3.1 we present the results of calculations for the antiferromagnetic states in the half-filled Hubbard model on the Bethe lattice. It is shown that the zeroth approximation to the dynamical CPA, i.e., the SA quantitatively describes the Néel temperatures (TN) as well as the MI boundary above TN. We present in §3.2 the results of calculations for the densities of states (DOS) as well as the MI transition below TN. We will show that the dynamical effects tend to increase the critical Coulomb interaction for the MI transition. The numerical results for the ferromagnetic properties on the fcc lattice in infinite dimensions are presented in §3.3. The Curie temperatures as well as the paramagnetic susceptibilities are shown to be described quantitatively by means of the dynamical CPA+HA in the quarter-filled regime of electron number. In the last §4 we summarize our numerical results. It is emphasized that the dynamical CPA is applicable to the quantitative description of the magnetic properties in high dimensions.

2. Dynamical CPA in the ferro- and antiferromagnetic states

We adopt in the present paper the Hubbard model as follows.

\[ H = \sum_{i,\sigma} \varepsilon_0 n_{i\sigma} + \sum_{i,j,\sigma} t_{ij} a_{i\sigma}^+ a_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow}. \]  \hspace{1cm} (1)

Here \( \varepsilon_0 \) is the atomic energy level, \( t_{ij} \) is the transfer integrals between sites \( i \) and \( j \), and \( U \) is the intraatomic Coulomb interaction energy parameter. \( a_{i\sigma}^+ (a_{i\sigma}) \) denotes the creation (annihilation) operator for an electron with spin \( \sigma \) on site \( i \), and \( n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma} \) is the number operator for the electron.

In the dynamical CPA,13) we transform the two-body interaction \( U_{i\uparrow} n_{i\uparrow} \) in the free energy into a dynamical one-body potential \( v_i \) with time-dependent random spin and charge fields using the Hubbard-Stratonovich transformation.34) Then introducing the site-diagonal effective potential \( \Sigma_i \) (i.e., the coherent potential) into the potential part of the free energy, we expand the correction terms containing \( n_i - \Sigma_i \) with respect to the site. The zeroth term is the coherent term \( \tilde{F}[\Sigma] \) which does not depend on the dynamical potential at all. The next term consists of the single-site terms each of which contains the dynamical potential on the same site. The higher-order terms \( \Delta F \) describe the inter-site spin and charge fluctuations.

In the dynamical CPA, we adopt the single-site approximation which neglects the higher-order inter-site corrections \( \Delta F \). The free energy of the dynamical CPA is then written as follows.

\[ F_{\text{CPA}} = \tilde{F}[\Sigma] - \beta^{-1} \sum_i \ln \int \frac{\beta}{4\pi} d\xi_i e^{-\beta E_i(\xi_i)} . \]  \hspace{1cm} (2)

Here \( \beta \) denotes the inverse temperature, \( \xi_i \) is the static exchange field on site \( i \), and \( E_i(\xi_i) \) is a single-site effective potential projected onto the static field \( \xi_i \). The effective potential \( E_i(\xi_i) \) consists of the static part \( E_{\text{st}}(\xi_i) \) and the dynamical part \( E_{\text{dyn}}(\xi_i) \).

\[ E_i(\xi_i) = E_{\text{st}}(\xi_i) + E_{\text{dyn}}(\xi_i) . \]  \hspace{1cm} (3)

The static potential \( E_{\text{st}}(\xi_i) \) is obtained by neglecting the time-dependence of the field variables and is given by

\[ E_{\text{st}}(\xi_i) = -\frac{1}{\beta} \sum_{l,\sigma} \ln \left[ 1 - (v_{i\sigma}^{(0)}(\xi_i) - \Sigma_{i\sigma}(\omega_l)) F_{i\sigma}(\omega_l) \right] \]  \[ -\frac{1}{4} U (\tilde{n}_i(\xi_i))^2 - \xi_i^2 . \]  \hspace{1cm} (4)

\[ v_{i\sigma}^{(0)}(\xi_i) = \varepsilon_0 - \mu + \frac{1}{2} U \tilde{n}_i(\xi_i) - \frac{1}{2} U \xi_i. \]  \hspace{1cm} (5)

Here \( v_{i\sigma}^{(0)}(\xi_i) \) is the Hartree-Fock type static potential. \( \mu \) denotes the chemical potential. \( \Sigma_{i\sigma}(\omega_l) \) is the frequency representation of a time-dependent coherent potential \( \Sigma_{i\sigma}(\tau) \), \( \tau \) being the imaginary time, \( \omega_l = (2l + 1)\pi/\beta \) denotes the Matsubara frequency. The electron number \( \tilde{n}_i(\xi_i) \) for a given exchange field \( \xi_i \) is defined by

\[ \tilde{n}_i(\xi_i) = \frac{1}{\beta} \sum_{l,\sigma} G_{i\sigma}(\omega_l,\xi_i) . \]  \hspace{1cm} (6)

The Green function \( G_{i\sigma}(\omega_l,\xi_i) \) will be determined later self-consistently (see eq. (16)).

The coherent Green function \( F_{i\sigma}(\omega_l) \) in eq. (4) is defined by

\[ F_{i\sigma}(\omega_l) = \left[ (\omega_l - H_0 - \Sigma_{i\sigma}(\omega_l))^{-1} \right]_{ii} . \]  \hspace{1cm} (7)

Here \( (H_0)_{ij} = (\varepsilon_0 - \mu) \delta_{ij} + t_{ij}(1 - \delta_{ij}) \) is the one-electron Hamiltonian matrix element in eq. (1) and \( (\Sigma_{i\sigma}(\omega_l))_{ij} = \Sigma_{i\sigma}(\omega_l) \delta_{ij} \).

The dynamical potential \( E_{\text{dyn}}^{(i)}(\xi_i) \) in eq. (3) is given in
the harmonic approximation (HA) as

$$E_{\text{dyn}}^{(i)}(\xi) = -\frac{1}{\beta} \ln \left[ 1 + \sum_{\nu=1}^{\infty} \sum_{n=1}^{\infty} D_{\nu}^{(n)} \right], \quad (8)$$

$$D_{\nu}^{(n)} = U^{2n} \left( \frac{i}{2\pi \nu} \right)^{2n} B_{\nu}^{(n)} D_{\nu}^{(n)}.$$  

First few terms of $B_{\nu}^{(n)}$ are given as follows.\(^{13}\)

$$B_{\nu \sigma}^{(1)} = \frac{2\pi i \nu}{\beta} \sum_{l=0}^{\infty} \left( \tilde{g}_{\nu \sigma}(l - \nu) \tilde{g}_{\nu \sigma}(l) + \tilde{g}_{\nu \sigma}(l + \nu) \tilde{g}_{\nu \sigma}(l) \right), \quad (10)$$

$$B_{\nu \sigma}^{(2)} = \left( \frac{2\pi \nu}{\beta} \right)^{2} \left[ 2 \sum_{l=0}^{\infty} \tilde{g}_{\nu \sigma}(l - \nu) \tilde{g}_{\nu \sigma}(l) \times (\tilde{g}_{\nu \sigma}(l - 2\nu) \tilde{g}_{\nu \sigma}(l - \nu) + \tilde{g}_{\nu \sigma}(l - \nu) \tilde{g}_{\nu \sigma}(l)) + \tilde{g}_{\nu \sigma}(l + \nu) \right]^{2} + B_{\nu \sigma}^{(1)}^{2}. \quad (11)$$

Here $\tilde{g}_{\nu \sigma}(l)$ is the static Green function on site $i$, which is defined by

$$\tilde{g}_{\nu \sigma}(l) = [F_{\nu \sigma}(i\omega) - v_{\nu \sigma}^{(0)}(\xi)]^{-1} + \Sigma_{\nu \sigma}(i\omega_l). \quad (12)$$

For the higher-order terms of $B_{\nu \sigma}^{(n)}$, one can adopt the following form of the asymptotic approximation.

$$B_{\nu \sigma}^{(n)} = \sum_{k=0}^{n-1} \frac{1}{k!} \sum_{l=0}^{\infty} B_{\nu \sigma}^{(l)}(k), \quad (13)$$

$$B_{\nu \sigma}^{(l)}(k) = b_{\nu \sigma}^{(l)}(\nu, k) + \sum_{m=0}^{l-1} \frac{(-1)^{l-m}}{(l-m)!} b_{\nu \sigma}^{(l-m)}(-\nu, k) \times b_{\nu \sigma}^{(l-m)}(-\nu, k). \quad (14)$$

The functions $b_{\nu \sigma}^{(l+m)}(\pm \nu, k)$ and $b_{\nu \sigma}^{(l-m)}(\pm \nu, k)$ in the 0-th order and the second order asymptotic approximation are given in Appendix B of Ref.\(^{13}\).

The coherent potential $\Sigma_{\nu \sigma}(i\omega_l)$ is determined so that the higher-order inter-site corrections become minimum. The condition called the CPA equation is given by

$$\langle G_{\nu \sigma}(i\omega_l, \xi) \rangle_{\text{eff}} = F_{\nu \sigma}(i\omega_l). \quad (15)$$

The average $\langle . \rangle_{\text{eff}}$ at the l.h.s. (left-hand-side) of the above equation means taking a classical average with respect to the effective potential $E^{(i)}(\xi)$. The on-site dynamical impurity Green function is given by

$$G_{\nu}^{(i)}(i\omega_l, \xi) = \frac{1}{1 + \sum_{\nu=1}^{\infty} \sum_{n=1}^{\infty} \frac{\delta D_{\nu}^{(n)}}{1 + \sum_{\nu=1}^{\infty} \sum_{n=1}^{\infty} D_{\nu}^{(n)}} \frac{\delta}{\delta \Sigma_{\nu \sigma}(i\omega_l)} \frac{\delta \Sigma_{\nu \sigma}(i\omega_l)}{\delta \Sigma_{\nu \sigma}(i\omega_l)}. \quad (16)$$

Here $\Sigma_{\nu \sigma}(i\omega_l) = 1 - F_{\nu \sigma}(i\omega_l) \delta F_{\nu \sigma}(i\omega_l)/\delta \Sigma_{\nu \sigma}(i\omega_l)$.

The average electron number $\langle n_i \rangle$ and the local magnetic moment $\langle m_i \rangle$ are given by

$$\langle n_i \rangle = \langle \tilde{n}(\xi) \rangle_{\text{eff}}, \quad \langle m_i \rangle = \langle \xi \rangle_{\text{eff}}. \quad (17)$$

The double occupation number $\langle n_{i \uparrow n_{i \downarrow}} \rangle$ and the amplitudes of local moment on site $i$ are obtained from the following expressions.\(^{13}\)

$$\langle n_{i \uparrow n_{i \downarrow}} \rangle = \frac{1}{4} \langle \tilde{n}(\xi)_{\text{eff}}^{2} \rangle + \frac{1}{4} \left( \langle \xi \rangle_{\text{eff}}^{2} - \frac{2}{\beta U} \right) + \left[ \left[ \frac{\partial E^{(i)}(\xi)}{\partial U} \right]_{\text{eff}} \right]^2, \quad (19)$$

$$\langle m_i^2 \rangle = \langle n_i \rangle - 2 \langle n_{i \uparrow n_{i \downarrow}} \rangle. \quad (20)$$

Here $\langle . \rangle_{\text{eff}}$ means to take the derivative of a quantity fixing the static potential $v_{\nu \sigma}^{(0)}(\xi)$.

Equations (15) and (17) form a set of self-consistent equations to determine the coherent potential $\{ \Sigma_{\nu \sigma}(i\omega_l) \}$ and the chemical potential $\epsilon_0 - \mu$. However it is time consuming to solve the CPA equation (15) because one has to take the average $\langle . \rangle_{\text{eff}}$ at each frequency $\omega_l$. The following decoupling approximation simplifies the numerical calculations.

$$\sum_{q=\pm 1} \frac{1}{2} \left( 1 + q \langle \xi \rangle_{\text{eff}} \right) G_{\nu}^{(i)}(i\omega_l, q\epsilon) = F_{\nu \sigma}(i\omega_l). \quad (21)$$

Here $\epsilon_i = \sqrt{\langle \xi \rangle_{\text{eff}}^{2}}$. Note that the approximation is correct up to the second moment (i.e., $\langle \xi \rangle_{\text{eff}}$ and $\langle \xi^2 \rangle_{\text{eff}}$).

We assume in this work that each site is crystallographically equivalent to each other. In the para- and ferromagnetic states, we can assume a site-independent coherent potential $\Sigma_{\nu \sigma}(i\omega_l)$. The site-independent coherent Green function $F_{\sigma}(i\omega_l)$ is then obtained by

$$F_{\sigma}(i\omega_l) = \int \frac{\rho(\epsilon) d\epsilon}{i\omega_l - \epsilon_0 + \mu - \Sigma_{\sigma}^{i}(i\omega_l) - \epsilon}. \quad (22)$$

Here $\rho(\epsilon)$ is the density of states (DOS) for the noninteracting Hamiltonian matrix $h_{ij}$.

In the antiferromagnetic state with sublattice magnetization, we have two types of coherent potential: $\Sigma_{\sigma}^{i}(i\omega_l)$ on the up-spin sublattice and $\Sigma_{\sigma}^{i+}(i\omega_l)$ on the down-spin sublattice. Because of the symmetric relation $\Sigma_{\sigma}^{i-}(i\omega_l) = \Sigma_{\sigma}^{i+}(i\omega_l)$, it is enough to require the self-consistency of $\Sigma_{\sigma}^{i+}(i\omega_l)$ on the up-spin sublattice. The corresponding coherent Green function $F_{\sigma}^{i+}(i\omega_l)$ is given
by\(^{35, 36}\)

\[ F_{\sigma}^{(+)}(i\omega_l) = \frac{i\omega_l - \Sigma_+^{(+)}(i\omega_l)}{i\omega_l - \Sigma_0^{(+)}(i\omega_l)} \]

\[
\propto \frac{\rho(\epsilon) d\epsilon}{\sqrt{(i\omega_l - \Sigma_0^{(+)}(i\omega_l))(i\omega_l - \Sigma_+^{(+)}(i\omega_l)) - \epsilon_0 + \mu - \epsilon}}. \quad (23)
\]

We adopted eqs. (22) and (23) in the para- and antiferromagnetic calculations on the Bethe lattice and in the ferromagnetic calculations on the fcc lattice in infinite dimensions. Moreover in the self-consistent calculations with use of the HA, we adopted eqs. (10) and (11) for \( U^2 \) and \( U^4 \) terms and took into account the higher-order terms up to \( U^{16} \) using the asymptotic approximation, i.e. eqs. (13) and (14).

3. Numerical Results

3.1 Antiferromagnetic states on the Bethe lattice

We present in this subsection the numerical results of calculations for the antiferromagnetic states at half filling on the Bethe lattice in infinite dimensions. The DOS for the noninteracting system is given by a semi-elliptical form as

\[
\rho(\epsilon) = \frac{2}{\pi W^2} \sqrt{W^2 - \epsilon^2}. \quad (24)
\]

Here \( 2W \) denotes the band width. In the present and next subsections, we adopt the energy unit to be \( W = 1 \).

We found that the antiferromagnetism is stabilized at half filling with decreasing temperatures. The numerical results of sublattice magnetization vs. temperature curves are presented in Fig. 1 for rather small Coulomb interaction energy parameter \( U = 0.5 \). Calculated Néel temperatures \( T_N \) are 0.017 in the static approximation (SA) and 0.011 in the harmonic approximation (HA), respectively. The dynamical effects reduce the ground-state sublattice magnetization (extrapolated value) by 15% and \( T_N \) by 36%. The calculated Néel temperature with dynamical corrections seems to be in good agreement with the QMC result as shown in Fig. 1. Although the agreement might not be so convincing because of a large error bar in the QMC calculations, quantitative description in the weak Coulomb interaction regime is expected because the HA is exact up to the second order in \( U \) in the weak Coulomb interaction limit. The amplitude of local moment \( \langle m^2 \rangle^{1/2} \) is also enhanced by the dynamical effects because electron correlations suppress the double occupancy of electrons even at finite temperatures.

The results for a strong Coulomb interaction \( U = 3.5 \) are presented in Fig. 2. The sublattice magnetization and Néel temperature are much enhanced as compared with the case of \( U = 0.5 \). The ground-state sublattice magnetization (0.960 \( \mu_B \) for the SA and 0.955 \( \mu_B \) in the HA) is close to the atomic value 1.0 \( \mu_B \). Calculated \( T_N \) are 0.0645 in the SA and 0.0654 in the HA, respectively; the \( T_N \) is slightly increased by the dynamical effects, but is smaller than the QMC value\(^{29}\) by 18%.

We have calculated the Néel temperatures for various Coulomb interaction energy parameters. The results are summarized in Fig. 3. It should be noted that we adopted the decoupling approximation (21) in the calculations of Figs. 1 and 2 in order to reduce the computation time. To clarify the difference between the decoupling approximation (21) and the full self-consistent CPA (15), we performed the full static calculations with use of (15). The calculated \( T_N \) vs. \( U \) curve is shown by solid curve and is compared with those in the decoupling approximation as well as the QMC results. In both the weak and strong Coulomb interaction regimes (i.e., \( U < 1 \) and \( U > 3 \)), calculated \( T_N \) with different approximation schemes yield basically the same result. In the intermediate Coulomb interaction regime (i.e., \( 1 < U < 3 \)), the Néel tempera-
tures in the decoupling approximation deviate from the full static results by several percent. It should be noted that $T_N$ calculated by the full SA quantitatively agree with the QMC results. This indicates that the SA provides us with a good starting point to calculate quantitatively the magnetic properties of electrons especially at high temperatures.

We have estimated the Néel temperatures in the full HA by adding $\Delta T_N = T_N(\text{HA}) - T_N(\text{SA})$ in the decoupling approximation to $T_N$ in the full static one.\(^37\) The results are shown in Fig. 3 by closed squares. We find that the dynamical effects in the harmonic approximation reduce $T_N$ in the weak Coulomb interaction regime ($U < 1$) and slightly increase $T_N$ in the strong Coulomb interaction regime ($U > 2$). Calculated $T_N$ are in agreement with the QMC results in the weak $U$ regime, but are underestimated in the intermediate and strong $U$ regimes ($1 < U < 2$). In particular the present dynamical calculations hardly correct $T_N$ in the SA in the strong $U$ regime ($2 < U$). One of the possible reasons for insufficient corrections is that the decoupling approximation is not suitable at high temperatures; it tends to overestimate the magnetic entropy at high temperatures because the approximation implies to replace a broad distribution $p(\xi) = \exp(-\beta E(\xi)) / \int d\xi \exp(-\beta E(\xi))$ with a two-delta function. The higher order dynamical corrections should also be taken into account in eq. (9) for strong $U$ regime in order to make more reasonable corrections.

3.2 Metal-insulator transition

Single-particle excitation spectra are obtained by means of a numerical analytic continuation\(^3^8\) of the self-energy for temperature Green function, i.e., the coherent potential $\Sigma_{i\sigma}(i\omega_n)$. It should be noted that the coherent potential obtained by solving the CPA equation (21) in the decoupling approximation is an approximate solution to the full equation (15). In order to obtain accurately the DOS as the single-particle excitations, we improved the coherent potential adopting the average $t$-matrix approximation (ATA)\(^7,3^9\) after we solved eq. (21).

$$
\Sigma_{i\sigma}^{\text{ATA}}(i\omega_n) = \Sigma_{i\sigma}(i\omega_n) + \frac{\langle G_{i\sigma}(i\omega_n, \xi) \rangle_{\text{eff}} - F_{i\sigma}(i\omega_n)}{\langle G_{i\sigma}(i\omega_n, \xi) \rangle_{\text{eff}} F_{i\sigma}(i\omega_n)}.
$$

Here the coherent potential in the decoupling approximation was used at the r.h.s. (right-hand-side) of the above equation, but the full average $\langle \rangle_{\text{eff}}$ of the impurity Green function is taken. The ATA is a one-shot correction to the full CPA (15).

Making use of the Padé numerical analytic continuation,\(^3^8\) we obtained $\Sigma_{i\sigma}^{\text{ATA}}(\omega + i\delta)$. Here $\omega$ is an energy variable on the real axis and $\delta$ is an infinitesimal positive number. Using the self-energy, we obtained the coherent Green function $F_{\sigma}^{(+)}(\omega + i\delta)$, and calculated the DOS via the relation,

$$
\rho_{\sigma}(\omega) = -\frac{1}{\pi} \text{Im} F_{\sigma}^{(+)}(\omega + i\delta).
$$

\(^{\text{Fig. 3.}}\) Néel temperatures ($T_N$) in the SA with decoupling approximation (dotted curve), the full SA (solid curve), the HA with dynamical corrections (closed squares), and the QMC method (closed circles).\(^{2^9,3^0}\) The open squares around $U = 3.0$ above $T_N$ indicate the metal-insulator crossover points in the full SA. Below $T_N$, the antiferromagnetic state (AF) is stabilized, while above $T_N$ the paramagnetic metal (PM) and the paramagnetic insulator (PI) are realized.

\(^{\text{Fig. 4.}}\) Density of states (DOS) for $U = 1.7$ and $T = 0.06$ in the SA (dashed curve), and in the HA with dynamical corrections (solid curve).

\(^{\text{Fig. 5.}}\) DOS for $U = 2.2$ and $T = 0.06$ in the SA (dashed curve), and in the HA with dynamical corrections (solid curve).
The system changes from metal to insulator with the formation of a gap on the Fermi level with increasing Coulomb interaction. In the full SA, the gap is gradually formed above the Neél temperatures. The crossover points are shown in Fig. 3 by open squares. When we assume the paramagnetic state below $T_N$, the formation of a gap becomes clearer at lower temperatures, indicating the metal-insulator (MI) transition.

Figure 4 shows the DOS in the metallic state near the MI transition. We find the upper and lower Hubbard bands. A gap is almost opened on the Fermi level in the SA, while the quasiparticle peak remain in the dynamical calculations. When the Coulomb interaction energy $U$ is increased, a gap is opened as shown in Fig. 5. The dynamical effects shift the spectral weight to the lower energy region.

The metal-insulator transition is accompanied by a localization of electrons. We show in Fig. 6 an example of double occupation number $\langle n_\uparrow n_\downarrow \rangle$ vs $U$ curve at low temperatures. The Hartree-Fock approximation yields the constant value 0.25 irrespective of $U$ because of no on-site correlations. The double occupation number in the SA reduces to the Hartree-Fock value in the weak Coulomb interaction limit. It rapidly decreases near the MI transition, and gives the alloy-analogy results of the Hubbard theory$^9$ in the strong $U$ limit. The dynamical effects based on the HA reduce further the double occupancy in the weak $U$ regime and enhance it in the strong $U$ regime as shown in Fig. 6.

There are no QMC calculations on the double occupation number at $T = 0.02$. We plotted in Fig. 6 the QMC results$^{18}$ at $T = 0.031$ for qualitative or semi-quantitative comparison with the present results. The QMC value at $U = 0.25$ indicates that the dynamical CPA+HA yields the quantitative result in the weak Coulomb interaction. The QMC result at $U = 1.0$ suggests that the HA is not sufficient to reduce the double occupancy in the intermediate regime of the Coulomb interaction. It should be noted that the critical Coulomb interaction in the QMC is $U_c = 2.4$ so that the data in $2.0 < U < 2.4$ are for metallic region. Thus, they are not directly compared with the present results in the insulator regime. The dynamical CPA+HA result at $U = 2.4$ agrees with the QMC result. These results suggest that the HA gives the quantitative results of $\langle n_\uparrow n_\downarrow \rangle$ in both the weak ($U < 1.0$) and strong ($U > 2.4$) Coulomb interaction regimes. In the intermediate Coulomb interaction regime ($1.0 \lesssim U \lesssim 2.3$), we need to take into account more dynamical effects to obtain $\langle n_\uparrow n_\downarrow \rangle$ quantitatively at low temperatures.

We have plotted in Fig. 7 the MI transition points below $T_N$ being obtained from the gap formation in the DOS. The critical Coulomb interactions $U_c$ for gap formation in the full SA increase with increasing temperature, and merge into the QMC results$^{31}$ around $T \approx 0.06$. Since the full SA is exact in the high temperature limit, this indicates that the full SA quantitatively describes $U_c$ at $T > 0.06$. It should be noted that these data are smoothly connected to the data points above $T_N$ for a gap formation in Fig. 3. Below $T = 0.06$, the $U_c$ in the SA deviate from the QMC results, and reduces to $U_c = 1.0$ in the Hubbard alloy-analogy approximation$^9$ at $T = 0$.

The dynamical results of $U_c$ in Fig. 7 are obtained by adding the dynamical correction $\Delta U_c = U_c(HA) - U_c(SA)$ in the decoupling approximation to $U_c(SA)$ in the full SA.$^{37}$ It is known that there are two critical Coulomb interactions at $T = 0$, $U_{c1}$ for the gap formation and $U_{c2}$ for the disappearance of the quasiparticle state.$^{18}$ But we did not find numerically two solutions near $U_c$ at finite temperatures ($T > 0.01$). The critical
3.3 Ferromagnetism on the fcc lattice in infinite dimensions

We have investigated the ferromagnetic properties of the fcc lattice in infinite dimensions by means of the dynamical CPA+HA in order to examine the quantitative aspects of the theory. The fcc lattice in d dimensions is defined as a lattice with 2d(d−1) nearest neighbors expressed by $R = \pm e_i \pm e_j$ with two different cubic unit vectors $e_i$ and $e_j$ $(i, j = 1, 2, \cdots , d)$. In infinite dimensions the noninteracting DOS is given by

$$\rho(\epsilon) = \frac{e}{\sqrt{\pi(1+\sqrt{2}\epsilon)}}. \quad (27)$$

Here the energy unit is chosen so that the bottom of band edge is given by $-1/\sqrt{2}$.

Note that the DOS (27) monotonically increases with decreasing energy $\epsilon$ and diverges at the band edge $\epsilon = -1/\sqrt{2}$. Therefore the DOS is expected to be favorable for the ferromagnetism in the low density region. Since the numerator in the DOS is reduced by a factor of $1/e$ at $\epsilon = 1/\sqrt{2}$, we may regard $W = \sqrt{2}$ as a characteristic band width of this system. The coherent Green function $F_\sigma(\omega l)$ was calculated from eq. (22) via numerical integration with respect to energy $\epsilon$.

Figure 8 shows an example of calculated magnetization vs temperature curves in various approximations for electron number $n = 0.58$ and Coulomb interaction $U = 4.0$. Extrapolated ground-state magnetizations are almost saturated in both calculations. The magnetization vs. temperature curves considerably deviate downwards from the Brillouin curve. The SA overestimates the Curie temperature ($T_C = 0.0800$) as compared with the QMC ($T_C = 0.0512$). The dynamical effects based on the HA reduces $T_C$ by 30% and results in $T_C = 0.0559$. The result agrees with the QMC ($T_C = 0.0512$) within 9% error. We have also calculated the paramagnetic susceptibilities above $T_C$ by adding the infinitesimal magnetic field. Calculated susceptibilities follow the Curie-Weiss law: $\chi = m_{\text{eff}}^2/(T - T_C)$. Here $m_{\text{eff}}$ is a constant called effective Bohr magneton number. Calculated effective Bohr magneton numbers are 1.00 $\mu_B$ in the SA, 1.13 $\mu_B$ in the HA, and 1.18 $\mu_B$ in the QMC, respectively. We find a good agreement between the dynamical CPA+HA results and the QMC ones.

We have calculated $T_C$ as a function of electron number $n$ by extrapolating the inverse susceptibilities to lower temperatures at various $n$. The results are presented in Figs. 9 and 10 for an intermediate Coulomb interaction strength $U = 2$ and a strong Coulomb interaction $U = 4$, respectively. In the SA, we obtain a finite value of $T_C$ for infinitesimal electron number $n$. The $T_C$ increases linearly with increasing $n$, and shows a maximum $T_C = 0.053$ (0.083) at $n_{\text{max}} = 0.60$ (0.70) for $U = 2$ ($U = 4$). When electron number $n$ approaches to one, $T_C$ vanishes again at $n = 0.93$ (0.98) for $U = 2$ ($U = 4$). The dynamical effects reduce $T_C$, for example, by 35% (25%) at $n_{\text{max}} = 0.60$ (0.70) for $U = 2$ ($U = 4$). As shown in Figs. 9 and 10, the dynamical results quantitatively agree with the QMC results around the quarter filled electron number (i.e., $0.4 \leq n \leq 0.6$) for both $U = 2$ and $U = 4$. However, the $T_C$ vs $n$ curves shift to the higher density region by about $\Delta n = 0.1$; calculated $T_C$ in the low density regime ($0 < n \lesssim 0.3$) are underestimated, and those in the half-filled regime ($0.7 \lesssim n < 1$) are overestimated.

The behavior of $T_C$ for small $n$ is sensitive to the approximation. In the Hartree-Fock approximation, $T_C$ should be finite for infinitesimal number of electron according to the Stoner condition $\rho(0)U > 1$ because the noninteracting DOS diverge at $n = 0$. This holds true even in the static approximation because the SA reduces to the Hartree-Fock approximation in the weak Coulomb interaction limit. The QMC results suggest that $T_C$ vanish at finite electron number in the low density region. There is no exact analysis on the low-density behavior of $T_C$ for this system as far as we know. The present calculations indicate that $T_C$ vanishes at $n = 0.2$ for $U = 2$, and at $n = 0.3$ for $U = 4$.

Magnetic properties at the high temperatures above $T_C$ are expected to be described well by the dynamical CPA+HA. We present in Figs. 11 and 12 calculated effective Bohr magneton number ($m_{\text{eff}}$) and amplitude of local moment $\langle m^2 \rangle^{1/2}$ as a function of electron number $n$. Note that $\langle m^2 \rangle^{1/2} = \sqrt{3} \langle m^2 \rangle^{1/2}$ where $\langle m^2 \rangle^{1/2}$ is the...
amplitude of local moment for \( z \) component given by eq. (20). These quantities were obtained at high temperatures \((T \approx 0.09)\). In the case of \( U = 2 \), the effective Bohr magneton number monotonically increases with increasing electron number from 0 to 1, and shows the maximum \( 1.64 \mu_B \) at half-filling. Although \( m_{\text{eff}} \) agrees with the amplitude \( \langle m^2 \rangle^{1/2} \) in the atomic limit, it is in general smaller than the latter in the metallic state. At half-filling, the difference is small; \( m_{\text{eff}} \approx \langle m^2 \rangle^{1/2} \) because of considerable suppression of charge fluctuations. By comparing the effective Bohr magneton numbers in the HA with those in the SA, we find that the dynamical effects enhance the effective Bohr magneton number, though the SA describes \( m_{\text{eff}} \) quantitatively at half-filling.

For larger value of \( U = 4 \), we find similar behavior of \( m_{\text{eff}} \) as a function of \( n \), but the effective Bohr magneton number shows a maximum at \( n \approx 0.95 \), and jumps from 1.3 \( \mu_B \) to 1.6 \( \mu_B \) at \( n = 1 \). Sudden jump to the value 1.6 \( \mu_B \) being close to the atomic value \( \sqrt{3} \) is associated with the formation of an insulator at half-filling. Calculated effective Bohr magneton number at \( n = 0.58 \) quantitatively agrees with the QMC result as shown in Fig. 12.

4. Summary

In the present paper we have investigated magnetic and electronic properties of the Hubbard model in infinite dimensions on the basis of the dynamical CPA combined with the harmonic approximation (HA) in order to clarify the accuracy of the theory at finite temperatures.

In the dynamical CPA, we transform the interacting electron system into an independent electron system coupled with the time-dependent random charge and exchange fictitious fields on the basis of the functional integral method. Introducing the coherent potential, we made a single-site approximation in the free energy. The coherent potential is self-consistently determined by the condition that the average of dynamical impurity Green function embedded in the effective medium (i.e., the coherent potential) should be equal to the coherent Green function for the uniform medium. The former Green
function is calculated by means of the HA. The dynamical CPA+HA becomes exact in the high-temperature limit, leads to the free energy being exact up to the second order in the weak $U$ limit, and yields the exact result in the strong $U$ limit in infinite dimensions.

We have performed the numerical calculations with use of the dynamical CPA+HA in which the dynamical corrections have been taken into account up to the 4th order in $U$ exactly and the higher-order corrections up to the 16th order in $U$ have been taken into account with use of the second order asymptotic approximation.

In the present calculations for the half-filled band Hubbard model on the Bethe lattice in infinite dimensions we found that the Néel temperatures $T_N$ are well described by the zeroth approximation to the dynamical CPA, i.e., the static approximation (SA). The dynamical corrections based on the HA reduce further $T_N$ in the weak Coulomb interaction regime, leading to a quantitative agreement with the QMC results. In the intermediate Coulomb interaction regime, the dynamical corrections in the present approximation tend to underestimate $T_N$ by about 10%. In the strong Coulomb interaction regime we found that the dynamical corrections slightly increase $T_N$. These results suggest that the dynamical CPA+HA can describe $T_N$ within 10% error in infinite dimensions.

We have also verified using the same model at half filling that the SA quantitatively describes the MI crossover above $T_D$. It however underestimates the critical Coulomb interaction $U_c$ at low temperatures. The dynamical corrections based on the HA enhance $U_c$. But the corrections in the present version are not enough to reproduce quantitatively the critical $U_c$ obtained by the QMC; the present theory leads to $U_c$ smaller than those of the QMC by 30% at low temperatures ($T \sim 0.02$).

We have investigated the ferromagnetic properties on the fcc lattice in infinite dimensions. In this case, the SA overestimates the Curie temperatures $T_C$ more than 30% irrespective of electron number. The dynamical CPA+HA reduces $T_C$ in the SA, and quantitatively describes the Curie temperatures as well as the susceptibilities in the quarter-filled regime ($0.4 \lesssim n \lesssim 0.6$). However the $T_C$ vs $n$ curves tend to shift to the higher density region by about $\Delta n = 0.1$ as compared with those in the QMC calculations, so that $T_C$ in the low density region ($0 < n \lesssim 0.3$) are somewhat underestimated and those in the half-filled regime ($0.7 \lesssim n < 1$) are overestimated. We found that the effective Bohr magneton number $m_{\text{eff}}$ is smaller than the amplitude $\langle m^2 \rangle^{1/2}$ in itinerant electron system except at half-filling where electrons tend to localize due to electron correlations for the intermediate Coulomb interaction strength. The dynamical effects enhance $m_{\text{eff}}$ for non half-filled bands, while the corrections are negligible at half-filling.

We have to perform the full CPA calculations without decoupling approximation (21) in order to obtain more solid conclusions. Nevertheless, the present results of calculations indicate that the dynamical CPA combined with the HA is suitable for the quantitative calculations of magnetic properties at finite temperatures as well as the MI transition at high temperature region.

It is not enough for the quantitative description of the MI transition at low temperatures and for the quantitative description of the ferromagnetism in the low-density regime as well as in the half-filled regime. For more quantitative description in the intermediate Coulomb interaction and low-temperature regime, one has to treat more seriously the higher-order dynamical corrections. The improvement is left for future work.

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