Aust. J. Phys., 1989, **42**, 565–71

Correlation Effects of Third-order Perturbation in the Extended Hubbard Model

G. Z. Wei, H. Q. Nie, L. Li and K. Y. Zhang

Department of Physics, Northeast University of Technology, Shenyang, People's Republic of China.

Abstract

Using the local approach, we have performed a third-order perturbation calculation to investigate the effects of intra-atomic electron correlation and electron and spin correlation between nearest neighbour sites in the extended Hubbard model. We found that significant correction of the third order over the second order results and, in comparison with the results of the third-order perturbation where only the intra-atomic electron correlation is included, the influence of the electron and spin correlation between nearest neighbour sites on the correlation energy is non-negligible.

1. Introduction

Recently there has been renewed interest in the study of the Hubbard model and the extended Hubbard model to explain high T_c superconductivity. Many authors have studied electron correlation effects in both models, with the help of functional integration (Albani *et al.* 1973; Ropke *et al.* 1975), cluster expansion (Lorenz 1981; Bartkowiak and Robaszkiewicz 1982), the perturbation method (Robaszkiewicz *et al.* 1981*a*), the Monte Carlo method (Hirsch *et al.* 1982), the Bogoliubov variational method for negative U (Robaszkiewicz *et al.* 1981*b*, 1982) and the Gutzwiller (1963) variational method. Among the various approaches tackling the Hubbard model and the extended Hubbard model, the Gutzwiller method has received most attention (Kotliar and Ruckenstein 1986). In his original work, Gutzwiller considered only the singlet-site operator $O^{(1)} = n_{i\uparrow} n_{i\downarrow}$ and used the quasi-chemical approximation to calculate E_c. The approximation was later generalised and developed into the so-called local approach (Stollhoff and Flude 1977; Horsch and Flude 1979; Oles 1982). In this paper, we consider the singlet-site operator $O^{(1)} = n_{i\uparrow} n_{i\downarrow}$, and the nearest neighbour site operators $O^{(2)} = n_i n_j$ and $O^{(3)} = \boldsymbol{s}_i . \boldsymbol{s}_j$ to calculate the correlation energy and the local moments in paramagnetic phase and to check the accuracy of the second-order perturbation results. The results show that the third-order results differ significantly from the second order, and the correction of the electron and spin correlation between nearest neighbour sites on the correlation effects is non-negligible.

0004-9506/89/050565$03.00

2. Theory and Results

The extended Hubbard model Hamiltonian can be written as

$$H = \sum_{ij\sigma} t_{ij}\, a^{+}_{i\sigma}\, a_{j\sigma} + U \sum_{i} n_{i\uparrow}\, n_{i\downarrow} + \frac{W}{2} \sum\nolimits'_{ij\sigma\sigma'} n_{i\sigma}\, n_{j\sigma'}, \tag{1}$$

where $a^{+}_{i\sigma}$ ($a_{i\sigma}$) is a creation (annihilation) operator with spin σ at the i site, $n_{i\sigma} = a^{+}_{i\sigma}\, a_{i\sigma}$ is the electron density operator, t_{ij} is the hopping integration, U and W represent the effective Coulomb interaction at the same site and between nearest neighbour sites respectively, and the prime sum runs over all nearest neighbour sites.

With the local approach, one first decomposes the Hartree–Fock ground state $|\psi_{\mathrm{HF}}\rangle$ into a linear combination of configurations. The trial function for the ground state $|\psi_{\mathrm{L}}\rangle$ is then constructed by modulating the linear combination as

$$|\psi_{\mathrm{L}}\rangle = \sum_{ijm} (1 - \eta_m O^{(m)}_{ij}) |\psi_{\mathrm{HF}}\rangle, \tag{2}$$

where i, j run over all sites. The variational parameters $\{\eta_m\}$ are determined by minimisation of the ground state energy per site

$$E_{\mathrm{G}} = \langle\psi_{\mathrm{L}}|\tilde{H}|\psi_{\mathrm{L}}\rangle / \langle\psi_{\mathrm{L}}|\psi_{\mathrm{L}}\rangle, \tag{3}$$

where $\tilde{H} = H - \langle H\rangle$. The correlation operators $O^{(m)}$ we use, in general form, can be written as

$$O^{(m)}_{ij} = \begin{cases} O^{(1)} = n_{i\uparrow}\, n_{i\downarrow} \\ O^{(2)} = n_i\, n_j \qquad \text{for} \quad i \neq j \\ O^{(3)} = \boldsymbol{s}_i . \boldsymbol{s}_j \qquad \text{for} \quad i \neq j \end{cases} \tag{4}$$

where operators $O^{(2)}$ and $O^{(3)}$ denote the electron correlation and the spin correlation between nearest neighbour sites.

Substituting equation (2) into (3), then expanding (3) in powers of $\{\eta_m\}$ up to third order, one can obtain the expression for the correlation energy as

$$E_{\mathrm{c}} = -2 \sum_{m} \eta_m A_m + \sum_{mm'} \eta_m\, \eta_{m'}\, B_{mm'} - \tfrac{1}{3} \sum_{mm'm''} \eta_m\, \eta_{m'}\, \eta_{m''}\, C_{mm'm''}, \tag{5}$$

where

$$\begin{aligned} A_m &= \frac{1}{N} \sum_{ij} \langle O^{(m)}_{ij}\, \tilde{H}\rangle, \\ B_{mm'} &= \frac{1}{N} \sum\nolimits'_{ij,i'j'} [\langle O^{(m)}_{ij}\, \tilde{H} O^{(m')}_{i'j'}\rangle + \langle O^{(m)}_{ij}\, O^{(m')}_{i'j'}\, \tilde{H}\rangle], \\ C_{mm'm''} &= \frac{1}{N} \sum\nolimits'_{ij,i'j',i''j''} [3\langle O^{(m)}_{ij}\, O^{(m')}_{i'j'}\, \tilde{H} O^{(m'')}_{i''j''}\rangle + \langle O^{(m)}_{ij}\, O^{(m')}_{i'j'}\, O^{(m'')}_{i''j''}\, \tilde{H}\rangle], \end{aligned} \tag{6}$$

and the prime sum means that the notation set $\{ijm\}$ of operators on the right side of $\tilde{H}$ are not all the same.

Except for the third-order perturbation calculation on a six-atom Hubbard model ring by Horsch (1979) and our work (Wei *et al.* 1987*a*, 1987*b*) in which only the intra-atomic electron correlation is considered, all existing works of local approach are within the scope of second-order perturbation. Horsch discovered that for the Hubbard model, the third-order correction to the correlation energy E_c is not negligibly small compared with the second-order calculation of E_c. Our work has given the same conclusion for both the Hubbard model and the extended Hubbard model when considering the local operator $O^{(1)} = n_{i\uparrow} n_{i\downarrow}$. In this paper we investigate this problem in detail, at first, using the extended Hubbard model to perform a third-order perturbation calculation for the case of electron and spin correlation between nearest neighbour sites added, and then discuss this in detail. For simplifying the discussion, we use the bandwidth D as a unit of energy then H contains the two parameters U and W. If U is positive and W is negative, the number of sites ν which are double occupied by two antiparallel-spin electrons decreases with increasing U and $-W$. If U is negative and W is positive, then ν should increase with $-U$ and W. In this case, antiparallel-spin electrons tend to form local pairs and the ground state of H may be either charge ordered or singlet superconducting (Robaszkiewicz *et al.* 1981*a*; Oles *et al.* 1984). The optimum values of the variational parameter set $\{\eta_m\}$ are determined by the minimisation of the ground state energy, i.e. $\partial E_c/\partial \eta_m = 0$ where $m = 1, 2, 3$. To solve a set of $\{\eta_m\}$, we have to solve the combination of quadratic equations of a set $\{\eta_m\}$ where we could not obtain the analytic solutions of $\{\eta_m\}$.

In order to provide explicit results quantitatively, we consider the paramagnetic phase in a simple cubic lattice with rectangular density of states:

$$\rho(\epsilon) = \begin{cases} 1/D & \text{for } |\epsilon| = D/2 \\ 0 & \text{otherwise.} \end{cases} \tag{7}$$

As mentioned Wei *et al.* (1987*a*), the Hamiltonian has the electron-hole symmetry, and we only need to calculate E_c and a set $\{\eta_m\}$ in the region $0 < n < 1$.

The numerical results for the correlation energy E_c as a function of U for fixed W and n are shown in Fig. 1 for both the second-order and third-order perturbation calculation. The curves are separated into two groups for two values of the electron density $n = 0{\cdot}5$ and 1, each group consisting of five curves which correspond to $W = 0$, $0{\cdot}25$, $0{\cdot}5$, $0{\cdot}75$ and 1. The two groups exhibit similar characteristic features; for example when $n = 1$, $E_c = E_c(U, W)$ as a function of U for fixed W has a maximum value $E_c(W{=}0, U_0) = 0$ or $E_c(W{\neq}0, U_0) < 0$, which differs from the results in Fig. 1 of Wei *et al.* (1987*a*). When E_c has a maximum, we also have a set of optimum values of $\{\eta_m^0\}$ as expected. In the numerical calculation we found that the parameter sets of $\{\eta_m^0\}$ corresponding to maximum E_c for any given $W > 0$ have no certain relation between themselves, but the maximum E_c mainly depends on the parameter η_1^0 near $\eta_1^0 = 0$. This means that the intra-atomic correlation plays a dominant role in E_c. Therefore, the curves of both the second-order and third-order perturbation in Fig. 1 have a similar form to the ones in Fig. 1 of Wei *et al.* (1987*a*) except for the maximum $E_c \neq 0$ for $W > 0$. The results show

that for a given W, the correlation energy E_c increases monotonically with U, when $U < U_0$, and E_c decreases monotonically with U, when $U > U_0$, and the U_0 corresponding to the maximum E_c for given W and n increases with increasing W. Here we cannot draw a hypersurface of a set $\{\eta_m\}$ satisfying $E_c = \max.$ in $n-U-W$ space, but in the analysis we found that, when electron and spin correlation between nearest neighbour sites are added, the number of doubly occupied sites (i.e. antiparallel-spin electrons tend to form local pairs) is increased. In comparison with Fig. 1 of Wei *et al.* (1987*a*), we found that the electron and spin correlation between nearest neighbour sites is non-negligible on the correction of E_c.

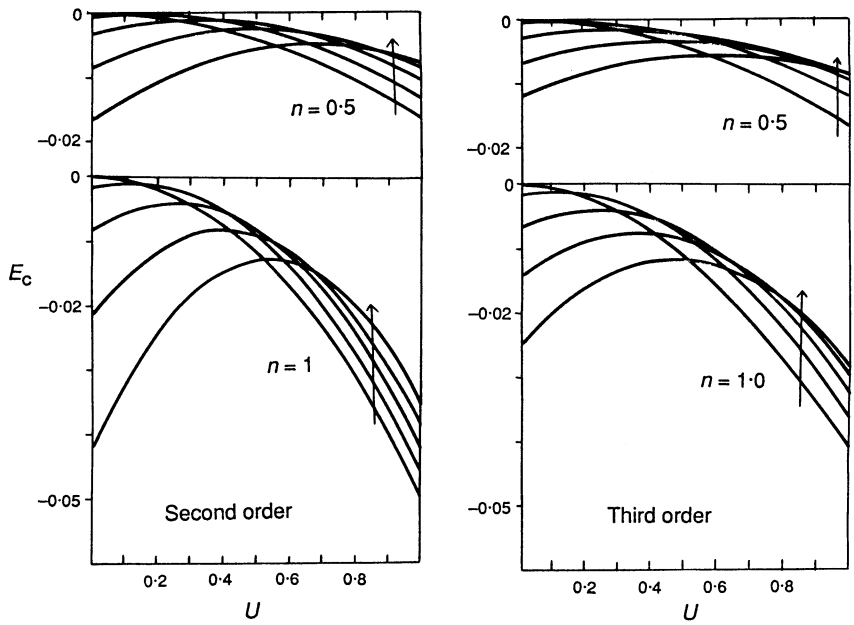

Fig. 1. Second-order and third-order perturbation calculation of the correlation energy E_c for various values of W and n. The arrows indicate increasing W, where $W = 0$, $0{\cdot}25$, $0{\cdot}50$, $0{\cdot}75$ and 1.

These qualitative results on the third-order perturbation significantly differ from the second-order perturbation (as seen in Fig. 1). Although the curves of both second- and third-order perturbation results have similar features, the correlation effects become weaker.

The spin moments S_m and the local polarisation P_L are defined as

$$S_m = \tfrac{3}{4}(n - 2\langle\psi_L \mid n_{i\uparrow} n_{i\downarrow} \mid \psi_L\rangle)/\langle\psi_L \mid \psi_L\rangle, \tag{8}$$

$$P_L = \langle\psi_L \mid n_{i\sigma} n_{j-\sigma} - n_{i\sigma} n_{j\sigma} \mid \psi_L\rangle/\langle\psi_L \mid \psi_L\rangle, \tag{9}$$

where the ith and jth sites are nearest neighbours to each other. One can obtain the expression for the third-order perturbation as

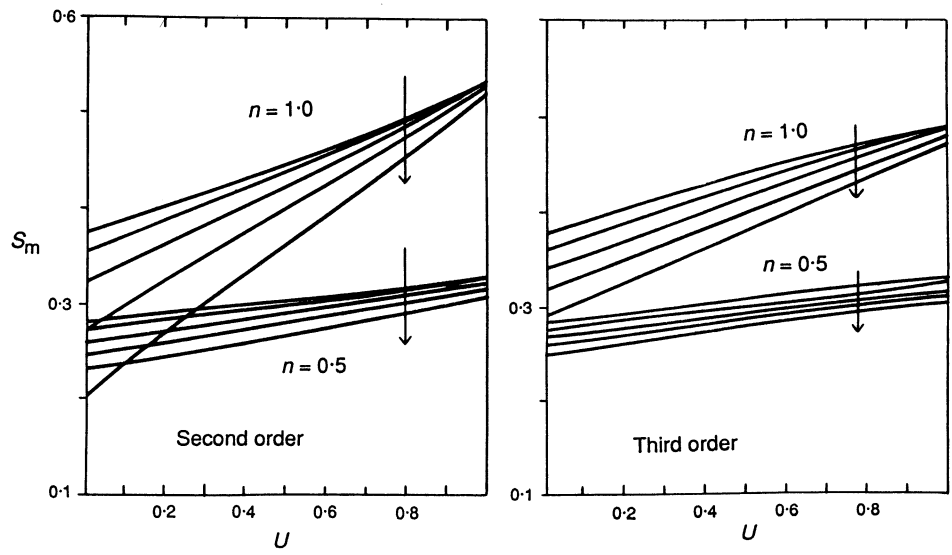

Fig. 2. Spin moments S_m versus U for the second- and third-order perturbation calculation.

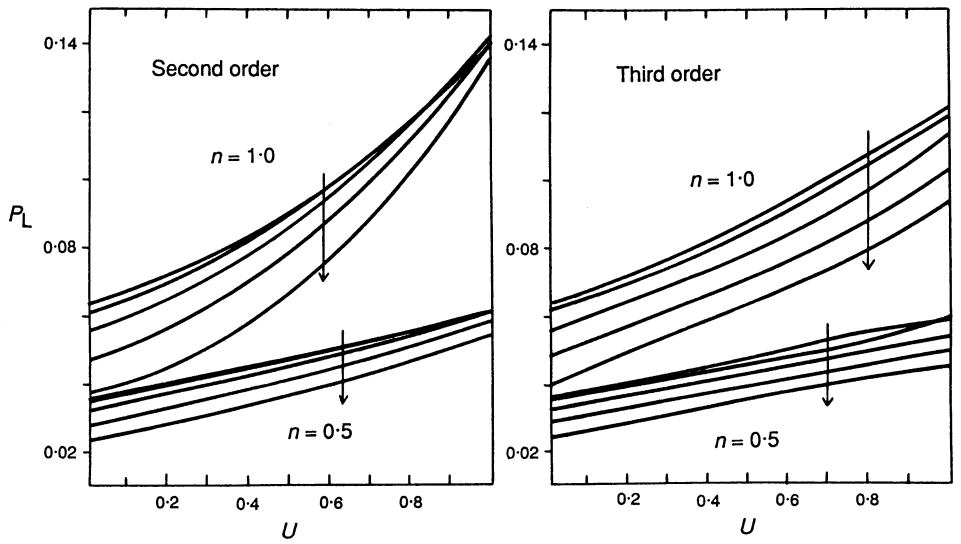

Fig. 3. Local polarisation P_L versus U for the second- and third-order perturbation calculation.

$$S_m = \tfrac{3}{4}\left(n - \frac{n^2}{2} + 4\sum_m \eta_m A_m - 2\sum_{mm'} \eta_m \eta_{m'} B_{mm'} + \tfrac{2}{3}\sum_{mm'm''} \eta_m \eta_{m'} \eta_{m''} C_{mm'm''}\right), \quad (10)$$

$$P_L = a_1 - 2\sum_m \eta_m A'_m + \sum_{mm'} \eta_m \eta_{m'} B'_{mm'} - \tfrac{1}{3}\sum_{mm'm''} \eta_m \eta_{m'} \eta_{m''} C'_{mm'm''}, \quad (11)$$

where $a_1 = \frac{1}{2}n(1 - \frac{1}{2}n)$ and where

$$A'_m = \frac{1}{N}\sum_{ij}\langle\psi_{\rm HF} \mid O_{ij}^{(m)} n_{i\uparrow} n_{i\downarrow} \mid \psi_{\rm HF}\rangle,$$

$$A''_m = \frac{1}{N}\sum_{ij}\langle\psi_{\rm HF} \mid O_{ij}^{(m)} n_{i\sigma} n_{j-\sigma} - n_{i\sigma} n_{j\sigma} \mid \psi_{\rm HF}\rangle,$$

$$B'_{mm'} = \frac{1}{N}\sum_{ij,i'j'}[\langle\psi_{\rm HF} \mid O_{ij}^{(m)} n_{i\uparrow} n_{i\downarrow} O_{i'j'}^{(m')} \mid \psi_{\rm HF}\rangle + \langle\psi_{\rm HF} \mid O_{ij}^{(m)} O_{i'j'}^{(m')} n_{i\uparrow} n_{i\downarrow} \mid \psi_{\rm HF}\rangle],$$

$$B''_{mm'} = \frac{1}{N}\sum_{ij,i'j'}[\langle\psi_{\rm HF} \mid O_{ij}^{(m)}(n_{i\sigma} n_{j-\sigma} - n_{i\sigma} n_{j\sigma}) O_{i'j'}^{(m')} \mid \psi_{\rm HF}\rangle$$
$$+\langle\psi_{\rm HF} \mid O_{ij}^{(m)} O_{i'j'}^{(m')}(n_{i\sigma} n_{j-\sigma} - n_{i\sigma} n_{j\sigma}) \mid \psi_{\rm HF}\rangle],$$

$$C'_{mm'm''} = \frac{1}{N}\sum_{ij,i'j',i''j''}[3\langle\psi_{\rm HF} \mid O_{ij}^{(m)} O_{i'j'}^{(m')} n_{i\uparrow} n_{i\downarrow} O_{i''j''}^{(m'')} \mid \psi_{\rm HF}\rangle$$
$$+\langle\psi_{\rm HF} O_{ij}^{(m)} O_{i'j'}^{(m')} O_{i''j''}^{(m'')} n_{i\uparrow} n_{i\downarrow} \mid \psi_{\rm HF}\rangle],$$

$$C''_{mm'm''} = \frac{1}{N}\sum_{ij,i'j',i''j''}[3\langle\psi_{\rm HF} \mid O_{ij}^{(m)} O_{i'j'}^{(m')}(n_{i\sigma} n_{j-\sigma} - n_{i\sigma} n_{j\sigma}) O_{i''j''}^{(m'')} \mid \psi_{\rm HF}\rangle$$
$$+\langle\psi_{\rm HF} \mid O_{ij}^{(m)} O_{i'j''}^{(m')} O_{i''j''}^{(m'')}(n_{i\sigma} n_{j-\sigma} - n_{i\sigma} n_{j\sigma}) \mid \psi_{\rm HF}\rangle.$$

The coefficients of $A'_{m'}$, A''_m, $B'_{mm'}$, $B''_{mm'}$, $C'_{mm'm''}$ and $C''_{mm'm''}$ can be calculated in a similar procedure to A_m, $B_{mm'}$ and $C_{mm'm''}$ in (6). The numerical results for $S_{\rm m}$ and $P_{\rm L}$ as a function of U for fixed W and n are shown in Figs 2 and 3 respectively. The arrangement of both is similar to Fig. 1. At first, comparing the results of the third-order perturbation with those of the second order, we found that the features of the curves are similar, but the correlation effects become weaker, and the correction of the third-order perturbation over the second order is non-negligible. On other hand, comparing the results with those for the third order in Figs 3 and 4 of Wei *et al.* (1987*a*), we found that the correlation effects are also weaker than in Wei *et al.* This means that when electron and spin correlation between nearest neighbour sites is added, it leads to an enhancement of the double occupancy of electrons, and a reduction in the local moments, and then the hetero-point disappears for $U < 1$. Fig. 3 shows $P_{\rm L} > P_{\rm HF}$ for $U < 1$, where the polarisation is always antiferromagnetic and the system tends to order antiferromagnetically.

3. Conclusions

In summary we have considered both the intra-atomic electron correlation and the electron and spin correlation between nearest neighbour sites in paramagnetic phase up to a third-order perturbation calculation. The results show that quantitively the third-order differs significantly from the second order, and that the second-order perturbation results are not accurate enough. On other hand, we emphasize that the electron and spin correlation between nearest neighbour sites is a non-negligible correction to the ground state energy in a perturbation calculation to any order.

Acknowledgment

We would like to thank Prof. K. A. Chao for many helpful discussions.

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Manuscript received 14 April, accepted 19 June 1989