ON A SIMPLE CEPA LIKE APPROACH TO ELECTRON CORRELATIONS IN d-DIMENSIONAL HUBBARD MODEL CLUSTERS*

K. Rościszewski

Institute of Physics, Jagellonian University,
Reymonta 4, 30-059 Kraków, Poland

(Received June 16, 1997)

In this short note a simple quantum chemical type of approach to electron correlations in d-dimensional Hubbard model is proposed. In essence, the method is very closely related to CEPA-0 approximation (also to Gutzwiller approximation and to the Local ansatz) and as such is no novelty. The real aim is to provide unsophisticated and computationally cheap method which allows for an easy treatment of electron correlations in finite cluster models with a simple Hubbard type Hamiltonians.

PACS numbers: 71.10. Fd, 71.15. –m, 31.15. Dv

1. CEPA-0 type approximation

Coupled cluster (CC) expansions are very powerful tools of quantum chemistry [1–3]. They allow for accurate treatment of electron correlations in many electron systems. In contrast to the popular configuration interaction (CI) method [1–3] the CC expansion avoids the problem of size consistency.

The correlated ground state wave function in CC method is customarily written in the form

$$|\Psi_0\rangle = \exp(O_1 + O_2 + \cdots)|\Phi_{\rm scf}\rangle\,, \tag{1.1}$$

where

$$O_1 = \sum_{S,v} \alpha_v^S \omega_v^S\,,$$

$$O_2 = \sum_{S,T;v,w} \alpha_{v,w}^{S,T} \omega_{v,w}^{S,T}\,.$$

* Supported by the Polish State Committee for Scientific Research (KBN) Project No. 2 P03B 144 08.

Here the alpha symbols are the expansion coefficients, $|\Phi_{\rm scf}\rangle$ is the self consistent ground–state wave function, and

$$\omega_v^S = c_S^\dagger c_v;\ \ \omega_{v,w}^{S,T} = c_S^\dagger c_T^\dagger c_v c_w;\ \ \cdots$$

are formed out of the electron creation and annihilation operators. The *capital latin indices* $S, T, \cdots$ denote the virtual (unoccupied) single particle spin-orbitals; the small letter indices $v, w, \cdots$ denote the occupied orbitals. $O_1, O_2, \cdots$ refer to one particle, two particles, $\cdots$ excitations from the occupied orbitals of the self consistent ground–state to the virtual orbitals. We stress that in the CC method the coefficients $\alpha_v^S, \alpha_{v,w}^{S,T}, \cdots$ are not the variational parameters (like in the CI) but has to be fixed in such a way that the state $|\Psi_0\rangle$ represents a true ground state.

For the Hubbard type Hamiltonian H, which consists of one and two particle operators only [1,4,5], it is easy to show [1] that the energy of the ground state is

$$E_0 = E_0^{\rm scf} + \langle H(O_1 + \tfrac{1}{2}O_1^2\rangle + \langle HO_2\rangle\,,$$

where $\langle\cdots\rangle$ denotes the expectation value over the self consistent ground state and $E_0^{\rm scf}$ is self consistent energy of the ground state.

Neglecting O_1 is a common procedure because in most cases this part leads only to a small density changes in presence of two particle correlations [1,2]. The approximate formula for E_0 in such a case is

$$E_0 = E_0^{\rm scf} + \langle HO_2\rangle\,. \tag{1.2}$$

The alpha coefficients are fixed using the condition [1]:

$$\langle(\omega_{v,w}^{S,T})^\dagger\, {\rm e}^{-O_2}\, H\, {\rm e}^{O_2}\rangle = 0\,. \tag{1.3}$$

Neglecting the terms of the order of α^2 (CEPA-0 type approximation — compare [1]) one obtains

$$\langle(\omega_{v,w}^{S,T})^\dagger H\rangle + \sum_{A,U,b,d} \alpha_{b,d}^{A,U} \langle(\omega_{v,w}^{S,T})^\dagger (H - E_0^{\rm scf})\omega_{b,d}^{A,U}\rangle = 0\,. \tag{1.4}$$

The technical task to solve Eq. (1.4) for a many electron system turns out to be very difficult. On the other hand, if we decide to use crude approximation with a single alpha parameter (instead of many), then the solution of the Eq. (1.4) presents no real problem. So the approximation we propose in this paper is

$$O_2^{\rm appr} \approx \frac{\alpha_1}{N} \sum_{S,T,v,w} c_{S\uparrow}^\dagger c_{T\downarrow}^\dagger c_{v\uparrow} c_{w\downarrow} \Delta(S + T - v - w)\,, \tag{1.5}$$

where the spin variable is specified explicitly. For the sake of simplicity only singlet excitations are being considered in (1.5). We remind the reader again that the capital latin indices (they are vector indices in momentum space) denote unoccupied levels above Fermi surface (SCF ground state) while small latin indices denote occupied SCF momentum space orbitals. The capital N denotes the total number of single particle orbitals (for one orientation of the spin) or the number of sites in the cluster if we consider the one band Hubbard model. The Δ function is zero or $\Delta = 1$ but only if the argument value is equal to zero or to any integer translation of reciprocal lattice (umklapp processes). Note that S_2^{appr} is closely related to potential part of the Hubbard Hamiltonian H — *i.e.*, to $V = U_0 \sum_r n_{r\uparrow} n_{r\downarrow}$, where r runs over (real space) lattice sites. Note further that one particle processes present in V were omitted in O_2^{appr} as well as the operators which upon acting on SCF ground state yield zeros. The very close connection of our method to the Gutzwiller approximation and to the Local ansatz [1, 4] is evident.

A brief summary

The method we propose is summarized by Eqs (1.2), (1.5) and by the equation

$$\langle (\Omega_{v,w}^{S,T})^{\dagger} H \rangle + \alpha_1 \sum_{A,U,b,d} \langle (\Omega_{v,w}^{S,T})^{\dagger} (H - E_0^{\mathrm{scf}}) \omega_{b,d}^{A,U} \rangle \equiv C_1 + \alpha_1 (C_2 - E_0^{\mathrm{scf}} C_0) = 0 \,, \tag{1.6}$$

where

$$\Omega_{v,w}^{S,T} = c_{S\uparrow}^{\dagger} c_{T\downarrow}^{\dagger} c_{v\uparrow} c_{w\downarrow} \,.$$

The spin variables were displayed explicitly. Eq. (1.6) follows logically from Eq. (1.4). The symbols C_0, C_1, C_2 were introduced as aliases to the respective averages.

Now, the technical task to evaluate the C_0, C_1, C_2 coefficients is enormously simplified thanks to the specific form of O_2^{appr}.

2. How the approximation works

The earlier results of computations on correlated ground state in a two dimensional Hubbard model include Refs [5–8] as well as the references cited therein. Here we present the results for 10×10 two dimensional Hubbard cluster (three dimensional clusters can be treated in exactly the same manner).

The Hamiltonian in momentum space representation is represented by the expression

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} - \frac{U_0}{N} \sum_{\mu,\nu,\rho,\tau} c^\dagger_{\mu\uparrow} c^\dagger_{\nu\downarrow} c_{\rho\uparrow} c_{\tau\downarrow} \Delta(\mu + \nu - \rho - \tau)\,, \tag{2.1}$$

where μ, ν, ρ, τ are (vector) momenta for the SCF ground state; for example $\mu = (\mu_x, \mu_y)$. Here we use greek letters (instead of small and capital latin letters) as a convention to indicate in a distinct way that the indices refer to both occupied and unoccupied orbitals. If the lattice constant in two dimensional Hubbard model with square lattice cell is set to unity then $\varepsilon_k = 2t[\cos(k_x) + \cos(k_y)]$ [4,5]. t is the hopping integral and U_0 is on site Coulomb repulsion. The "workhorse" model parameters (two dimensions) are $t = -1$ eV and $U_0 = 4$ eV. These parameters are thought to be the most difficult to treat (by various perturbation expansions) and at the same time they are of interest as they mark a border between different regimens of behaviour on the t, U_0 phase diagram [4,5].

To obtain ground state wave function and ground state energy one has to calculate the averages in (1.6). Thanks to specific form of O_2^{appr} they are very easy to obtain. The resulting formulas are compact and short. We do not present the intermediate results as they are standard. It suffices to say that after the proper factorization of the averages into up and down spin parts one can apply short computer program to perform averages. (Without doubts, this is a practical way to do Wick's theorem if correct signs were assigned to individual terms.) The program was written in PASCAL. It is very simple and short. It manipulates on strings of creation and annihilation operators in an algebraic manner. In each string $c^\dagger_A$ and c_v type operators are commuted to the right side while $c^\dagger_v$ and c_A to the left. The interchange of any two creation or annihilation operators gives rise to an extra average (an extra string with two operators less than the parent string). The strings (averages) with $c^\dagger_A$ and c_v at the rightmost position or $c^\dagger_v$ and c_A at the leftmost position give zero. The most of indices within the averages are clearly assigned: that is, one knows explicitly whether they refer to occupied state or to an unoccupied one. In this respect only 4 indices (greek letters) coming out of potential part of H can be termed "unknown". This is technical reason why the calculation of the averages is simple task. One avoids the nightmarish, pages long, formulas coming out of the evaluation of the averages with many indices which are of the type "unknown". The final result is

$$C_0 = \frac{1}{N^2} S_1\,, \tag{2.2}$$

$$C_1 = -\frac{1}{N^2} S_1 U_0\,, \tag{2.3}$$

$$C_2 = \frac{(S_1 E_0^{\mathrm{scf}} + S_2)}{N^2} + \frac{U_0(S_3 - 2S_4 + S_5)}{N^3}, \tag{2.4}$$

$$\alpha_1 = -\frac{C_1}{(C_2 - E_0^{\mathrm{scf}} C_0)}, \tag{2.5}$$

$$E_0 = E_0^{\mathrm{scf}} + \alpha_1 C_1, \tag{2.6}$$

where N is the total number of sites within the cluster (or the one half of spin-orbitals) and where the sums S are

$$S_1 = \sum_{S,T,w,v} \Delta(S+T-w-v), \tag{2.7}$$

$$S_2 = \sum_{S,T,w,v} \Delta(S+T-w-v)(\varepsilon_S + \varepsilon_T - \varepsilon_w + \varepsilon_v), \tag{2.8}$$

$$S_3 = \sum_{S,T,A,U,w,v} \Delta(S+T-v-w)\Delta(A+U-v-w) \times \Delta(A+U-S-T), \tag{2.9}$$

$$S_4 = \sum_{S,T,U,w,v,b} \Delta(S+T-v-w)\Delta(S+U-v-b) \times \Delta(U-T+w-b)), \tag{2.10}$$

$$S_5 = \sum_{S,T,w,v,b,d} \Delta(S+T-v-w)\Delta(S+T-d-b) \times \Delta(w+v-b-d)). \tag{2.11}$$

We remind again that the subscripts are vector indices (momentum space, no spin) and that the capital letters correspond to empty states above the Fermi level and small letters correspond to occupied states below and at the Fermi level. These formulas were derived under assumption that SCF ground state is a single Slater determinant, *i.e.*, they correspond to closed shell case. Each SCF energy shell for the Hubbard cluster being considered must be either empty or entirely filled. The generalization to open shell case is simple but the formulas one could obtain would loose such short and compact form as the ones presented above. This is because open shell SCF wave function is the sum of many individual wave functions. The number of this functions equals the number of different allocations of electrons within the last partially filled SCF energy shell (the deeper energy shells are completely filled) [9].

Some remarks are now in order. First of all the evaluation of $S_1, S_2, \cdots$ is trivial and quick even for relatively large clusters. It can be done on a cheap personal computer. Second remark is about umklapp processes. If they are ignored, the Δ functions reduce to normal Kronecker deltas and the evaluation of $S_1, S_2, \cdots$ is even simpler; instead of computer code one

deals mostly with analytic results for the sums. Neglecting the umklapp processes seems, however, too serious a mistake.

To conclude, we present some results and compare them with practically exact Quantum Monte Carlo calculations [8] for various fillings $f = n_{\mathrm{el}}/(2N)$, where n_{el} is the total number of electrons in the cluster (equal numbers of up and down electrons). To allow for direct comparison with the results of Ref. [8] instead of E_0 we show the values of $\bar{E}_0 = E_0 + U_0 N(0.25 - f)$. This corresponds to a different reference level on the energy scale.

TABLE I

Ground state energy $\bar{E}_0$ [eV] per site for 10×10 Hubbard cluster calculated for various fillings f ($U_0 = 4$ eV, $t = -1$ eV).

f	$\bar{E}_0^{\mathrm{scf}}$	$\bar{E}_0$	
		this work	Ref. [8]
0.25	-1.0567	-1.1280	-1.1355
0.29	-1.2286	-1.3211	-1.3344
0.37	-1.4974	-1.6277	-1.6483
0.41	-1.5631	-1.7101	-1.7376

Taking into account a minimal amount of work needed to get the entries from the third column one concludes that the method presented in this work can be crude, but still it is useful. We presented the simplest version so the formulas are short and look nice. The generalizations of the method are, however, easy and present no problem. In particular, one can extend O_2^{appr} in spirit of Local Ansatz [1] and still the method will remain simple and easy to implement in concrete computations.

The author would like to thank Prof. A.M. Oleś and Prof. J. Spałek for valuable discussions and a critical reading of the manuscript.

REFERENCES

[1] P. Fulde, *Electron Correlations in Molecules and Solids, Springer Series in Solid-State Sciences*, Vol. 100, Springer-Verlag, Berlin, Heidelberg, New York, 1993.

[2] I.N. Levine, *Quantum Chemistry*, Prentice-Hall, Inc., New Jersey 1991.

[3] W. Hehre, L. Radom, P.v.R. Schleyer, J.A. Pople, *Ab Initio Molecular Theory*, J. Wiley-Interscience Pub., New York 1986.

[4] A.P. Balachandran, E. Ercolessi, G. Morandi, A.M. Srivastava, *Hubbard Model and Anyon Superconductivity, Lecture Notes in Physics*, Vol. 38, World Scientific, Singapore, New Jersey, London 1990.

[5] D.J. Scalapino, *Does the Hubbard Model Have the Right Stuff*, in Proceedings of the International School of Physics "Enrico Fermi", Course CXXI, edited by R.A. Broglia, J.R. Scrieffer, P.F. Bortignon, *Perspectives in Many-Particle Physics Series*, North-Holland, Amsterdam, Oxford, New York 1994.

[6] M. Imada, Y. Hatsugi, *J. Phys. Soc. Jap.* **58**, 3752 (1989).

[7] D.J. Scalapino, *Physica* **C 185–189**, 104 (1991).

[8] N. Furukawa, M. Imada, *J. Phys. Soc. Jap.* **61**, 3331 (1992).

[9] C.C.J. Roothaan, *Rev. Mod. Phys.* **23**, 69 (1951); *Rev. Mod. Phys.* **32**, 179 (1960) .