1. Classification *INPE-COM.4/RPE*
C.D.U.: 539.2

2. Period

4. Distribution Criterion

internal ☐

external ☒

3. Key Words (selected by the author)
STANDARD BASIS OPERATORS
MANY BODY THEORY

5. Report No.
INPE-1813-RPE/181

6. Date
July, 1980

7. Revised by
A. Ferreira da Silva

8. Title and Sub-title

ELECTRON CORRELATIONS IN NARROW BANDS

9. Authorized by
Nelson de Jesus Parada
Director

10. Sector *DEE* Code

11. No. of Copies *13*

12. Authorship
KISHORE, R.

13. Signature of first author

14. No. of Pages *07*

15. Price

16. Summary/Notes

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17. Remarks
This paper will be presented at XXXIIa. SBPC meeting.

ABSTRACT

The standard basis operators (SBO) formalism is used to study the problem of electron correlations in narrow bands described by the Hubbard Hamiltonian. Exact Dyson equation in the matrix form for the SBO Green's function is obtained by exploiting the self consistent many body theory developed by Fedro and Wilson, and Kishore. It is found that the present formalism provides a natural extension of the Roth's two poles approximation scheme and reproduces the earlier spin wave results. Some inconsistencies in the Roth's scheme have also been discussed.

Electron correlations play a great role in magnetism and metal-insulator transitions in narrow band materials(C. Hering, 1974). In a narrow nondegenerate band, Hubbard model (J. Hubbard, 1963) has been studied to consider the correlation effects. Hubbard used the standard basis operators (SBO) approach (J. Hubbard, 1965) to study the elementary excitations. The advantage of this approach is that all the single site terms in the Hamiltonian can be considered exactly. Hubbard used an equation of motion method, which although suitable for the elementary excitations, cannot be used to calculate the correlation functions. Recently, a self consistent many body theory (A.J.Fedro and R.S.Wilson,1975) has been developed for the Green's functions which can be used to study both elementary excitations and the correlation functions. This theory gives the Dyson equation for any particle Green's function. In this paper, we apply this theory to obtain SBO Green's functions.

In terms of SBO the Hubbard Hamiltonian (J. Hubbard,1963)

$$H = \sum_{ij\sigma} T_{ij}\, a_{i\sigma}^{+}\, a_{j\sigma} + \frac{I}{2} \sum_{i\sigma} n_{i\sigma}\, n_{i-\sigma} \tag{1}$$

reduces to(J.Hubbard,1965)

$$H = \sum_{i\alpha} \varepsilon_{i\alpha}\, L^{i}_{\alpha\alpha} + \sum_{\substack{ij \\ \alpha\beta\gamma\delta}} T_{ij}^{\alpha\beta\gamma\delta}\, L^{i}_{\alpha\beta}\, L^{j}_{\gamma\delta} \tag{2}$$

where the SBO $L^{i}_{\alpha\beta}$ are defined as

$$L^{i}_{\alpha\beta} = |i\ \alpha\rangle \langle i\ \beta| \tag{3}$$

Here $|i\ \alpha\rangle$ is an eigenstate of the Hamiltonian

$$H_i = \sum_{\sigma} (T_{ii}\, a_{i\sigma}^{+}\, a_{i\sigma} + \frac{I}{2} n_{i\sigma}\, n_{i-\sigma}) \tag{4}$$

with eigenvalue $\varepsilon_{i\alpha}$, and

$$T_{ij}^{\alpha\beta\gamma\delta} = \sum_{\sigma} T_{ij} \langle i\ \alpha|\, a_{i\sigma}^{+}\, |i\ \beta\rangle \langle j\gamma|\, a_{j\sigma}\, |j\delta\rangle \tag{5}$$

The Hamiltonian (4) has four eigenstates $|io\rangle$, $|i\,1_\sigma\rangle$, $|i\,1_{-\sigma}\rangle$ and $|i\,2\rangle$ corresponding to $n_\sigma = n_{-\sigma} = 0$; $n_\sigma = 1$, $n_{-\sigma}=0$; $n_\sigma = 0$, $n_{-\sigma} = 1$ and $n_\sigma = n_{-\sigma} = 1$ respectively. Here, n_σ is the eigenvalue of the operator $n_{i\sigma}$. The eigenvalues $\varepsilon_{i\alpha}$ corresponding to the above four eigenstates are $\varepsilon_{io} = 0, \varepsilon_{i\,1_\sigma} = \varepsilon_{i\,1_{-\sigma}} = T_{ii}$ and $\varepsilon_{i\,2} = 2\,T_{ii} + I$.

The SBO $L^i_{\alpha\beta}$ cause the transitions from the state $|i\beta\rangle$ to the state $|i\alpha\rangle$ and satisfy the multiplication rules

$$L^i_{\alpha\beta}\ L_{\gamma\delta} = \delta_{\beta\gamma}\ L^i_{\alpha\beta} \tag{6}$$

Any operator O_i can be written in terms of SBO according to

$$O_i = \sum_{\alpha\beta} \langle i\alpha|\ O_i|\ i\beta|\ L^i_{\alpha\beta} \tag{7}$$

From (7) the creation operators for the single particle excitations and spin waves can be written in terms of SBO as

$$a^+_{i\sigma} = L^i_{1_\sigma 0} + \sigma\ L^i_{2\ 1_{-\sigma}} \tag{8}$$

and

$$a^+_{i\sigma}\ a_{i-\sigma} = L^i_{1_\sigma\ 1_{-\sigma}} \tag{9}$$

Now, we consider the Green's function (A.J. Fedro and R.S. Wilson, 1975; D.N. Zubarev, 1960)

$$G^{\alpha\beta}_{ij}(\omega) = \langle\langle L^i_{\alpha\alpha'}\ ;\ L^j_{\beta'\beta}\rangle\rangle\,\omega\,, \tag{10}$$

Where $L^i_{\alpha\alpha'}$ and $L^j_{\beta'\beta}$ are the members of the sets $\{L^i_{\alpha\alpha'}\}$ and $\{L^j_{\beta'\beta}\}$ corresponding to a particular type of excitation. For example for single particle excitations corresponding to spin σ

$$\{L^i_{\alpha\alpha}\} \equiv \{L^i_{0\,1_\sigma}, L^i_{1_{-\sigma}2}\} \tag{11}$$

$$\{L^j_{\beta'\beta}\} \equiv \{L^j_{1_\sigma 0}, L^i_{2\,1_{-\sigma}}\}$$

and for spin waves

$$\{L^i_{\alpha\alpha}\} \equiv \{L^i_{1_{-\sigma}1_\sigma}\}$$

$$\{L^j_{\beta'\beta}\} \equiv \{L^j_{1_\sigma\, 1_{-\sigma}}\} \tag{12}$$

Now by applying the self consistent many body theory (A.J.Fedro and R.S. Wilson, 1975), one obtains a matrix Dyson equation for the fourier transform of the Green's function (10) as

$$[\omega\, I - B_{\vec{k}}\,(\omega)\; 1\,]\; G_{\vec{k}}\,(\omega) = A, \tag{13}$$

where I is the unit matrix, and the matrix elements of A and $B_{\vec{k}}\,(\omega)$ are

$$A^{\alpha\beta} = (\langle L^i_{\alpha\alpha}\rangle \;-\; \langle L^i_{\alpha'\alpha'}\rangle\;)\;\delta_{\alpha\beta} \tag{14}$$

and

$$B^{\alpha\beta}_{\vec{k}}\,(\omega) = \Omega^{\alpha\beta}_{\vec{k}} \;+\; \gamma^{\alpha\beta}_{\vec{k}}\;(\omega) \tag{15}$$

$\Omega^{\alpha\beta}_{\vec{k}}$ and $\gamma^{\alpha\beta}_{\vec{k}}$ (ω) are the fourier transform of

$$\Omega^{\alpha\beta}_{ij} = \frac{\langle [L^i_{\alpha\alpha'}, L\, L^j_{\beta'\beta}]_\eta\rangle}{\langle [L^j_{\beta\beta}\;, L^j_{\beta'\beta}\;\;]_\eta\rangle} \tag{16}$$

and

$$\gamma^{\alpha\beta}_{ij}(t) = \frac{-i\Theta(t)\;\langle [L\; L^i_{\alpha\alpha'}, e^{it(1-P)L}(1-P)L\; L^j_{\beta'\beta}]_\eta\rangle}{\langle [L^J_{\beta\beta'}\;,\; L^J_{\beta'\beta}]_\eta\rangle} \tag{17}$$

where $\eta = +1$ for the single particle excitation and $\eta = -1$ for the spin waves. The Liouville operator L and the projection operator P are defined according to

$$L\,X \equiv [H,X]_- \tag{18}$$

and

$$P \equiv \sum_{i\alpha} P_{i\alpha} \tag{19}$$

with

$$P_{i\alpha X} = \frac{L^{i}_{\alpha'\alpha} < [L^{i}_{\alpha\alpha'}, X]_{\eta} >}{< [L^{i}_{\alpha\alpha'}, L^{i}_{\alpha'\alpha}]_{\eta} >} \tag{20}$$

The Dyson equation (13) can be used to obtain the single particle excitations and the spin waves. For spin waves, it is possible to solve it exactly for the stiffness constant. It gives the same results as already obtained by the author (R.Kishore, 1979) without using SBO.For single particle excitations, it is necessary to make approximations. If we assume $\gamma_k^{\alpha\beta}(\omega) = 0$, the results of two poles approximation of Roth (L.M.Roth, 1969) are recovered. It is found that when one obtains correlation functions from the Green's functions, the Roth's approximation does not satisfay the multiplication rules (6). This difficulty can be removed if we assume that $\gamma_k^{\alpha\beta}(\omega)$ are approximated in such a way that $B_{\vec{k}}^{\alpha\beta}(\omega)=0$ for $\alpha \neq \beta$ and $\gamma_{\vec{k}}^{\alpha\beta}(\omega) = 0$ for $\alpha = \beta$. Within this approximation, our results reduce to that of Ikeda et al (1972). Recently, Ikeda et al(1972) theory has been applied to the dopped semiconductors to calculate the specific heat (A. Ferreira da Silva et al). It gives a very good agreement with the experiment.

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