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B.Westwański

APPLICATION OF DIAGRAM TECHNIQUE FOR HAMILTONIANS WITH THE COULOMB INTERACTION TO HUBBARD MODEL

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Let us consider the Hubbard Hamiltonian with magnetic field [1]

$$H = \sum_{\substack{\kappa\kappa' \\ \sigma}} t_{\kappa\kappa'} d^{+}_{\kappa\sigma} d_{\kappa'\sigma} + \sum_{\kappa} [U n_{\kappa+} n_{\kappa-} + h(n_{\kappa+} - n_{\kappa-})]. \quad (1)$$

Then define

$$\langle X \rangle = Z^{-1} Tr\{X \exp[-\beta(H-\mu N)]\}, \quad Z = Tr\{\exp[-\beta(-H-\mu N)]\},$$

where X is any operator, N the total number operator, μ - chemical potential. The operator $H-\mu N$ can be rewritten in the form

$$H - \mu N = H_0 + V, \quad (2)$$

where (the "unperturbed Hamiltonian")

$$H_0 = \sum_{\kappa} H_{0\kappa} \; ; \; H_{0\kappa} = \epsilon_{+} n_{\kappa+} + \epsilon_{-} n_{\kappa-} + U n_{\kappa+} n_{\kappa-} \quad (3)$$

and the "interaction"

$$V = \sum_{\substack{\kappa \neq \kappa' \\ \sigma}} t_{\kappa\kappa'} d^{+}_{\kappa\sigma} d_{\kappa'\sigma}, \quad (4)$$

$\epsilon_{\pm} = \epsilon \pm h - \mu$, $\epsilon = t_{\kappa\kappa}$, $n_{\kappa\pm} = d^{+}_{\kappa\pm} d_{\kappa\pm}$ and $d^{+}_{\kappa\pm}$, $d_{\kappa\pm}$

are the Fermi creation and annihilation operators, respectively for an electron with the spin up and down in the atomic state of the κ- th lattice site. This division is very natural because we have separated the one-particle part of the operator (2), which can be diagonalized in

every case. The subsystem Hamiltonian H_{0K} in (3) acts in four dimensional Hilbert space and has eigenvalues: $H'^{1}_{0K} = \epsilon_{+} + \epsilon_{-} + U$, $H'^{2}_{0K} = \epsilon_{-}$, $H'^{3}_{0K} = \epsilon_{+}$, $H'^{4}_{0K} = 0$. To determine the realization of general statistical Wick theorem (GSWT) it is sufficient to find the eigenoperators J^{ij}_{K} of superoperator H^{x}_{0K} [2,3]

$$H^{x}_{0K} J^{ij}_{K} = [H_{0K}, J^{ij}_{K}] = H'^{ij}_{0K} J^{ij}_{K} \; ; \; H'^{ij}_{0K} = H'^{i}_{0K} - H'^{j}_{0K} = \overset{+}{H}{}'^{ji}_{0K} .$$

For H_{0K} in (3) the operators J^{ij}_{K} ($J^{ij}_{K} = \overset{+}{J}{}^{ji}_{K}$) have the form

$$J^{12}_{K} = d_{K+} n_{K-} , \; J^{34}_{K} = d_{K+} (1 - n_{K-}) , \; J^{13}_{K} = n_{K+} d_{K-} ,$$
$$J^{24}_{K} = (1 - n_{K+}) d_{K-} , \tag{5}$$

$$J^{23}_{K} = d^{+}_{K+} d_{K-} , \quad J^{14}_{K} = d_{K+} d_{K-} . \tag{6}$$

In the general case of interaction we have to introduce the following free Green functions: eight free Green functions of the Fermi type corresponding to the pseudo-Fermi operators (5) and four free Green functions of the Bose type corresponding to pseudo-spin operators (6), as well as the following diagonal operators:

$$P^{ij}_{K} = [J^{ij}_{K}, \overset{+}{J}{}^{ij}_{K}]_{-\eta} \; (\eta = \mp 1 \quad \text{for } J^{ij}_{K} \quad \text{from} \binom{5}{6}) \; \text{for } i < j ;$$

$$P^{12}_{K} = n_{K-} , \; P^{34}_{K} = 1 - n_{K-} , \; P^{13}_{K} = n_{K+} , \; P^{24}_{K} = 1 - n_{K+} ,$$
$$P^{23}_{K} = n_{K+} - n_{K-} , \quad P^{14}_{K} = 1 - (n_{K+} + n_{K-}) . \tag{7}$$

With the help of (5) we obtain for the interaction (4)

$$V = \sum_{K,K'} t_{KK'} [(\overset{+}{J}{}^{12}_{K} + \overset{+}{J}{}^{34}_{K})(J^{12}_{K'} + J^{34}_{K'}) + (\overset{+}{J}{}^{13}_{K} + \overset{+}{J}{}^{24}_{K})(J^{13}_{K'} + J^{24}_{K'})] . \tag{8}$$

We define the transverse Green function G as the matrix 6x6 (and analogously transverse interaction due to (8)) with components

$$G_{ij,lp}(k,n) = \langle\langle J_k^{+ij} ; J_k^{lp} \rangle\rangle \tag{9}$$

being the Fourier transform of $\langle T J_K^{lp}(0) J_K^{+ij}(\tau)\rangle$. The zeroth order result Σ° for the irreducible polarization part Σ /4-6/ of G has the components

$$\Sigma^\circ_{ij,ij}(k,n) = \langle P_K^{ij} \rangle_0 / (i\lambda n + H_{0K}^{+ij})$$

(taking into account (8) it is sufficient to restrict ourselves to $ij = 12, 34, 13, 24$), where

$$\langle P_K^{12}(13) \rangle_0 = [\exp(-\beta H_{0K}^{1}) + \exp(-\beta H_{0K}^{2}(3))] / Z_{0K}, \quad Z_{0K} = \sum_{i=1}^{4} \exp(-\beta H_{0K}^{i}),$$

$i\lambda n$ = imaginary Fermi frequency. In the above approximation for Σ the renormalized components (9) /4-6/ are

$$G^r_{\substack{12,12\\(13,13)}}(k,n) = (1 - \Sigma^\circ_{\substack{34,34\\(24,24)}}) \Sigma^\circ_{\substack{12,12\\(13,13)}} / A_\pm ,$$

$$G^r_{\substack{34,34\\(24,24)}}(k,n) = (1 - \Sigma^\circ_{\substack{12,12\\(13,13)}}) \Sigma^\circ_{\substack{34,34\\(24,24)}} / A_{(\pm)}, \tag{10}$$

$$G^r_{\substack{12,34\\(13,24)}}(k,n) = G^r_{\substack{34,12\\(24,13)}}(k,n) = -\Sigma^\circ_{\substack{12,12\\(13,13)}} \Sigma^\circ_{\substack{34,34\\(24,24)}} t(k) / A_{(\pm)}$$

and the renormalized transverse interaction (effective interaction) $t^r(k,n)$ takes the form

$$t^r_{\substack{12,12\\(13,13)}}(k,n) = t^r_{\substack{12,34\\(13,24)}}(k,n) = t^r_{\substack{34,12\\(24,13)}}(k,n) = t^r_{\substack{34,34\\(24,24)}}(k,n) = -t(k)/A_{(\pm)} .$$

Then the renormalized spectrum follows from $A_\pm = 0$,

$$A_{(\pm)} = (i\lambda n + \epsilon_{(\pm)1})(i\lambda n + \epsilon_{(\pm)2}) / (i\lambda n + H^{+12}_{0K}(13))(i\lambda n + H^{+34}_{0K}(24));$$

$$\epsilon_{(\pm)1} = \epsilon_{(\pm)} + (U + t(k) + \Delta_{(\pm)})/2, \quad \epsilon_{(\pm)2} = \epsilon_{(\pm)} + (U + t(k) - \Delta_{(\pm)})/2.$$

From (10) we obtain two equations

$$\langle n_{(\pm)} \rangle = a_{(\pm)1} f(\epsilon_{(\pm)}) + a_{(\pm)2} f(\epsilon_{(\pm)2}),$$

where

$$a_{(\pm)1} = 1/2 - b_{(\pm)} / \Delta_{(\pm)}, \quad a_{(\pm)2} = 1/2 + b_{(\pm)} / \Delta_{(\pm)},$$

$$\Delta_{(\pm)} = [(U - t(k))^2 + 4 t(k) U \langle n_{(\mp)} \rangle_0]^{1/2},$$

$$b_{(\pm)} = (U - t(k))/2 - U \langle n_{(\mp)} \rangle_0, \quad f(\epsilon) = (\exp(\beta\epsilon) + 1)^{-1}.$$

On the basis of GSWT [2] we have developed the diagram technique for the Hubbard model and have found the expressions for the renormalized spectrum and renormalized transverse interaction. A detailed discussion of realization of GSWT in the case (3), of an analog of GSWT for diagonal operators (7) and diagram technique for some class of interactions will be published elsewhere.

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