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16.Summary/Notes

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QUASI-PARTICLE ENERGY OF THE HUBBARD MODEL IN THE WEAK CORRELATION REGIME

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ABSTRACT

We have investigated the Fedro-Wilson theory to obtain a hierarchy of differential equations for the correlation functions. An approximation is suggested for the truncation of the hierarchy of equations. The result is applied to the weakly correlated Hubbard model to calculate the quasi-particle energy.

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Since 1963 the Hubbard model (Hubbard 1963; Kanomori 1963; Gutzwiller 1963) has been extensively used by many authors to investigate the magnetic ordering and the metal -nonmetal transition in narrow energy band systems. Although the general property of the Hubbard Hamiltonian is of fundamental interest, lots of the works have been devoted to the strong correlation limit where the magnetic and the metal-insulator transitions are expected to occur. This area has been so popular among the solid state physicists in recent years, that it seems not necessary to list the detailed literature references.

On the other hand, the Hubbard model in the weak correlation regime is relatively not much explored. The main reason is the tedious mathematical manipulation encountered in the degenerate perturbation expansion, besides the lack of confidence in the applicability of the Hubbard model to real physical systems if the correlation is not strong. However, recently Friedel and Sayers (1977) have calculated the cohesive energies of the transition metals using the Hubbard model in the weak correlation regime. Their results are quite satisfactory.

In 1975 Fedro and Wilson (1975) had developed a self-consistent many body theory for the single particle Greens function by using a commutation projection operator introduced by Kim and Wilson (1973). When applied to the Hubbard model, their theory yielded a systematic approach to treat the higher order effect. Kishore (1978) has generalized the Fedro-Wilson theory and derived from it an exact microscopic formula for the transverse dynamical susceptibility.

In this letter we will derive a recursion formula for the essential correlation function appeared in the Fedro-Wilson theory.

Then we will pinpoint the condition under which the series expansion of the correlation function derived from the recursion formula can be truncated. Finally, we will use the result to derive the quasi-particle energy for the Hubbard model in the weak correlation limit, not only as an example to demonstrate the usefulness of the analytical result but also for the intrinsic theoretical interest in this weak correlation case which is relevant to the real systems.

We first briefly outline the theory (Fedro and Wilson 1975) reformulated by Kishore (1978). Let $\{A_i\}$ and $\{B_i\}$ be two sets of operators which satisfy the conditions

$$<[A_i,B_j]_\eta> = <[A_i,B_i]>\delta_{i,j} \tag{1}$$

where the angular brackets denote the grand canonical ensemble average, $\eta=-$ corresponds to the commutator and $\eta=+$ corresponds to the anticommutator. The retarted Greens function (Zubarev 1960)

$$G_{ij}(t) = i\theta(t) < [A_i,B_j(t)]_\eta > \tag{2}$$

satisfies the equation of motion

$$-i\frac{\partial}{\partial t} G_{ij}(t)=<[A_i,B_i]_\eta>\delta_{ij}\delta(t)+i\theta(t)<[A_i,LB_j(t)]_\eta> \tag{3}$$

where $B_j(t)$ is the Heisenberg representation of B_j, and the Liouville operator L is defined as

$$L\chi \equiv [H,\chi]_-$$

for arbitrary χ. Here we work in a system of units with $\hbar = 1$.

Following the projection operator formalism of Zwanzig (1960) and of Mori (1965), we define the operator P_j by

$$P_j\chi = B_j\langle [A_j,\chi]_\eta\rangle / \langle [A_j,B_j]_\eta\rangle \quad \text{if} \quad \langle [A_j,B_j]_\eta\rangle \neq 0 \tag{5}$$

$$= 0 \quad \text{if} \quad \langle [A_j,B_j]_\eta\rangle = 0$$

Then it is easy to show that the operator $P = \sum_j P_j$ is a projection operator, namely $P^2 = P$. Substituting the unit operator $\{P + (1-P)\}$ in front of the $B_j(t)$ in Eq. (3), we get

$$-i\frac{\partial}{\partial t}G_{ij}(t) = \langle [A_i,B_i]_\eta\rangle\delta_{ij}\delta(t)+\sum_\ell\Omega_{i\ell}G_{\ell j}(t)+i\theta(t)\langle [A_i,L(1-P)B_j(t)]_\eta\rangle, \tag{6}$$

where

$$\Omega_{i\ell} \equiv \langle [A_i,LB_\ell]_\eta\rangle / \langle [A_\ell,B_\ell]_\eta\rangle. \tag{7}$$

With the help of $(1-P)B_j = 0$, we have

$$\frac{\partial}{\partial t}(1-P)\theta(t)B_j(t)=(1-P)\frac{\partial}{\partial t}\theta(t)B_j(t) = i(1-P)\theta(t)B_j(t). \tag{8}$$

The solution of this equation has been obtained by Fedro and Wilson (1975) as

$$(1-P)\theta(t)B_j(t)=i\int_0^t d\tau\; e^{i\tau(1-P)L}(1-P)LP\theta(t)B_j(t-\tau) \tag{9}$$

which on using the projection operator P can be rewritten as

$$(1-P)\theta(t)B_j(t) = \sum_\ell \int_0^t d\tau\; e^{i\tau(1-P)L}(1-P)L\frac{B_\ell}{\langle [A_\ell,B_\ell]_\eta\rangle}G_{\ell j}(t-\tau). \tag{10}$$

Substitution of the above relation into Eq. (6) yields a closed equation for the Greens function as

$$-i\frac{\partial}{\partial t}G_{ij}(t) = \langle [A_i,B_i]_\eta\rangle\delta_{ij}\delta(t)+\sum_\ell\Omega_{i\ell}G_{\ell j}(t)+\sum_\ell\int_{-\infty}^{\infty}\gamma_{i\ell}(\tau)G_{\ell j}(t-\tau)d\tau, \tag{11}$$

where

$$\gamma_{i\ell}(\theta) = i\theta(\tau)<[A_i, Le^{i\tau(1-P)L}(1-P)LB_\ell]_\eta>/<[A_\ell, B_\ell]_\eta>. \tag{12}$$

The Fedro-Wilson theory thus converts the calculation of higher order Greens functions into the calculation of the correlation functions $\gamma_{i\ell}(\tau)$. As was pointed out by Fedro And Wilson, $\gamma_{i\ell}(\tau)$ can be obtained either by the perturbation expansion or by the differential equation approach. In this letter we will investigate in detail the differential equation approach.

Let us define

$$\gamma_{i\ell}(n:t) = -i\theta(t)<[L^n A_i, e^{it(1-P)L}(1-P)LB_\ell]_\eta>/<[A_\ell, B_\ell]_\eta> \tag{13}$$

Since $<[A,LB]_\eta> = -<[LA,B]_\eta>$, we see that $\gamma_{i\ell}(1:t) = \gamma_{i\ell}(t)$. Taking the time derivation of $\gamma_{i\ell}(n:t)$, we get

$$\begin{aligned} -i\frac{\partial}{\partial t}\gamma_{i\ell}(n:t) = &- <[L^n A_i, (1-P)LB_\ell]_\eta>\delta(t)/<[A_\ell, B_\ell]_\eta> \\ &- i\theta(t)<[L^n A_i, Le^{it(1-P)L}(1-P)LB_\ell]_\eta>/<[A_\ell, B_\ell]_\eta> \\ &+ i\theta(t)<[L^n A_i, P\{Le^{it(1-P)L}(1-P)LB_\ell\}]_\eta>/<[A_\ell, B_\ell]_\eta>. \end{aligned}$$

The second term at the right hand side is simply $-\gamma_{i\ell}(n+1:t)$. Applying the projection operator to the curly bracket in the above equation, we have

$$\begin{aligned} -i\frac{\partial}{\partial t}\gamma_{i\ell}(n:t) = &- <[L^n A_i, (1-P)LB_\ell]_\eta>\delta(t)/<[A_\ell, B_\ell]_\eta> - \gamma_{i\ell}(n+1:t) \\ &+ \sum_m (<[L^n A_i, B_m]_\eta>/<[A_m, B_m]_\eta>)\gamma_{m\ell}(1:t) \end{aligned} \tag{14}$$

We can now perform the time Fourier transform and obtain from Eq. (14) the recursion formula

$$\omega\gamma_{i\ell}(n:\omega) = -<[L^n A_i,(1-P)LB_\ell]_\eta>/<[A_\ell,B_\ell]_\eta> - \gamma_{i\ell}(n+1:\omega)$$

$$+ \sum_m (<[L^n A_i,B_m]_\eta>/<[A_m,B_m]_\eta>)\gamma_{m\ell}(1:\omega) \tag{15}$$

If we define

$$S_n(\omega) = \sum_{\nu=1}^{n} (L/\omega)^\nu$$

and use the recursion formula repeatedly, we have

$$\gamma_{i\ell}(1:\omega)+\sum_m(<[A_i,S_n(\omega)B_m]_\eta>/<[A_m,B_m]_\eta>)\gamma_{m\ell}(1:\omega)$$

$$= <[A_i,S_n(\omega)(1-P)LB_\ell]_\eta>/<[A_\ell,B_\ell]_\eta> + (-1)^n\gamma_{i\ell}(n+1:\omega) \tag{17}$$

Since $\gamma_{i\ell}(t)=\gamma_{i\ell}(1:t)$, if we know $\gamma_{i\ell}(1:\omega)$ from Eq. (17), we can obtain $G_{ij}(\omega)$ from Eq. (11) by taking a time Fourier transform. Hence, the applicability of the Fedro-Wilson theory lies in the possibility of deriving a close from of $\gamma_{i\ell}(n:\omega)$ for finite values n. We should point out that the sets of operator $\{A_i\}$ and $\{B_i\}$ are arbitrary, provided Eq. (1) is satisfied. Therefore, if the sets $\{A_i\}$ and $\{B_i\}$ are so chosen that

$$L(1-P)LB_\ell = \alpha_\ell LB_\ell \tag{18}$$

for all ℓ, where α_ℓ is a constant, then from Eq. (13) we get

$$\gamma_{i\ell}(n+1:t) = -i\theta(t)\, e^{i\alpha_\ell t} <[L^{n+1}A_i,(1-P)LB_\ell]_\eta>/<[A_\ell,B_\ell]_\eta>. \tag{19}$$

So a close form of $\gamma_{i\ell}(n+1:\omega)$ is derived. However, usually it is extremely difficult to construct $\{A_i\}$ and $\{B_i\}$ to satisfy Eq. (19), and therefore the exact solution of $\gamma_{i\ell}(t)$ can not be obtained. On the other hand, if the Hamiltonian H can be separated into an unperturbed part H_o and a perturbation H_1, often it is not difficult to choose $\{A_i\}$ and $\{B_i\}$ such that

$$L_o(1-P)LB_\ell = \alpha_{o\ell}\, LB_\ell, \tag{20}$$

where L_o is defined through $L_o\chi \equiv [H_o,\chi]$. Consequently $\gamma_{i\ell}(n+1:t)$ can be approximated as

$$\gamma_{i\ell}(n+1:t) \simeq -i\theta(t)e^{i\alpha_{o\ell}t} <[L^{n+1}A_i,(1-P)LB_\ell]_\eta>/<[A_\ell,B_\ell]_\eta>,$$

and the Greens function can be solved approximately accordingly.

By now it is clear the similarity between the present approach and the standard Greens function method. For the latter one truncates the hierarchy of the equation of motion for the Greens function by decoupling the higher order Greens function, while for the former one terminates the hierarchy of the differential equation for the correlation function, namely Eq. (14) by approximating the higher order correlation function. In both methods, at which order to truncate the hierarchy of equation depends solely on the solvability of the time independent correlation functions involved.

We will apply the above developed analysis to the weakly correlated Hubbard Hamiltonian

$$H = H_b + H_u, \tag{22}$$

where

$$H_b = \sum_{k\sigma} \varepsilon(k) a^\dagger_{k\sigma} a_{k\sigma} \tag{23}$$

and

$$H_u = \frac{U}{N} \sum_{qkk'} a^\dagger_{k+q\uparrow}\, a_{k\uparrow}\, a^\dagger_{k'-q\downarrow}\, a_{k'\downarrow}. \tag{24}$$

We choose $\{A_i\} = \{a_{k\sigma}\}$ and $\{B_i\} = \{a^\dagger_{k\sigma}\}$ with fixed σ, and define the projection operator and the Greens function as

$$P^\sigma \chi = \sum_k <[a_{k\sigma}, \chi]_+ > a^\dagger_{k\sigma}, \tag{25}$$

$$G^\sigma_{k_1k_2}(t) = i\theta(t) <[a_{k_1\sigma}, a^\dagger_{k_2\sigma}(t)]_+>. \tag{26}$$

So Eq. (11) becomes

$$-i\frac{\partial}{\partial t} G^\sigma_{k_1k_3}(t) = \delta_{k_1k_3}\delta(t) + \sum_{k_2}\left[\Omega^\sigma_{k_1k_2} G^\sigma_{k_2k_3}(t) + \int_{-\infty}^{\infty} \gamma^\sigma_{k_1k_2}(\tau) G^\sigma_{k_2k_3}(t-\tau)d\tau\right], \tag{27}$$

where

$$\Omega^\sigma_{k_1k_2} = <[a_{k,\sigma}, La^\dagger_{k_2\sigma}]_+> = [\varepsilon(k_1) + n_{-\sigma} U]\delta_{k_1k_2} \tag{28}$$

and

$$\gamma^\sigma_{k_1k_2}(t) = i\theta(t) < [a_{k_1\sigma}, Le^{i(i-P^\sigma)L}(1-P^\sigma)La^\dagger_{k_2\sigma}]_+>. \tag{29}$$

In this letter we will calculate the quasi-particle energy to the second order U^2 in perturbation. Hence we only need to approximate the L operator in the exponential in Eq. (29) by L_b. After computing $(1-P^\sigma)La^\dagger_{k_2\sigma}$, we can rewrite $\gamma^\sigma_{k_1k_2}(t)$ as

$$\gamma^\sigma_{k_1k_2}(t) = \frac{U}{N} \sum_{qk'} \gamma^\sigma_{k_1k_2:k'q}(t) \tag{30}$$

where

$$\gamma^\sigma_{k_1k_2:k'q}(t) = -i\theta(t) <[La_{k_1\sigma}, \; e^{it(1-p^\sigma)L} \times$$

$$\times (a^\dagger_{k'+q,-\sigma} a_{k',-\sigma} - <a^\dagger_{k'+q,-\sigma} a_{k',-\sigma}>) a^\dagger_{k_2-q,\sigma}]_+>. \tag{31}$$

Since

$$(1-P^{\sigma})L_b(a^{\dagger}_{k'+q,-\sigma}a_{k',-\sigma}-\langle a^{\dagger}_{k+q,-\sigma}a_{k',-\sigma}\rangle)a^{\dagger}_{k_2-q,\sigma},$$

$$=\{\varepsilon(k'+q)+\varepsilon(k_2-q)-\varepsilon(k')\}(a^{\dagger}_{k'+q,-\sigma}a_{k',-\sigma}-\langle a^{\dagger}_{k'+q,-\sigma}a_{k',\sigma}\rangle)\,a^{\dagger}_{k_2-q,\sigma},$$

when we approximate the L in the exponential of Eq. (31) by L_b, we get

$$\gamma^{\sigma}_{k_1k_2:k'q}(t)\simeq-\frac{U}{N}i\theta(t)\,e^{it\{\varepsilon(k'+q)+\varepsilon(k_2-q)-\varepsilon(k')\}}\times \tag{32}$$

$$\times\{(\langle n_{k'-\sigma}\rangle-\langle n_{k'+q,-\sigma}\rangle)\langle n_{k_2-q,\sigma}\rangle-\langle n_{k',-\sigma}\rangle(1-\langle n_{k'+q,-\sigma}\rangle)\}_{k_1k_2}.$$

Substituting Eqs. (28) and (32) into Eq. (27) and taking the time Fourier transform, we have

$$G^{\sigma}_{k}(\omega)=\{\omega-\varepsilon(k)-Un_{-\sigma}-U^2\,\gamma^{\sigma}_{k}(\omega)\}^{-1}, \tag{33}$$

where

$$\gamma^{\sigma}_{k}(\omega)=\left(\frac{1}{N}\right)^2\sum_{k_1k_2}\frac{(\langle n_{k_2-\sigma}\rangle-\langle n_{k_1+k_2,-\sigma}\rangle)\langle n_{k-k_1,\sigma}\rangle-\langle n_{k_2,-\sigma}\rangle(1-\langle n_{k_1+k_2-\sigma}\rangle)}{\omega-\{\varepsilon(k_1+k_2)+\varepsilon(k-k_1)-\varepsilon(k_2)\}} \tag{34}$$

The quasi-particle energy $\omega(k)$ is then obtained simply from

$$\omega(k)-\varepsilon(k)-Un_{-\sigma}-U^2\,\gamma^{\sigma}_{k}\{\omega(k)\}=0. \tag{35}$$

For weak correlation, i.e., small U, $\omega(k)$ can be well approximated as

$$\omega(k)=\varepsilon(k)+Un_{-\sigma}+U^2\,\gamma^{\sigma}_{k}\{\varepsilon(k)+Un_{-\sigma}\}. \tag{36}$$

From Eq. (34), we see that the second order correction term $\gamma^{\sigma}_{k}\{\varepsilon(k)+Un_{-\sigma}\}$ contains $\varepsilon(k)+\varepsilon(k_2)-\varepsilon(k-k_1)-\varepsilon(k_2+k_1)-Un_{-\sigma}$ as the energy denominator. Physically, this energy denominator is associated to the scattering of two electrons from the k- and the k_2-Bloch states into the $(k-k_1)$- and the (k_2+k_1)-Bloch states due to the intraatomic interaction of strength U. Therefore, large contribution to the second order energy comes from the scattering processes for which the initial and the final energies differ by an amount $Un_{-\sigma}$. Since U is small, the self-energy $\omega(k)-\varepsilon(k)$ is specially important for those electrons in the vicinity of the Fermi surface of H_o, as one would expect.

We must point out that not all the second order corrections are included in Eq. (35). This is the intrinsic drawback of the differential equation approach for the correlation function $\gamma_{i\ell}(t)$. As was pointed out by Fedro and Wilson (1975), one can also solve Eq. (29) with a perturbation expansion of the exponential term. If one does so, the calculation of the second order correction energy becomes very complicated and involves the almost impossible task of solving for the time independent three-particle correlation functions.

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