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Quasi-particle spectrum of the Hubbard model:

Strong - intraatomic - interaction limit

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We have exploited a self consistent many body theory to calculate the quasi-particle spectrum of the Hubbard model, in the limit of strong intraatomic interaction. The quasi-particle energy of each band of the spectrum, consisting of two bands, is calculated exactly up to terms linear in the hopping-integral.

The Hubbard model¹, which has been studied very extensively during last fifteen years², is described by the Hamiltonian

$$H = H_I + H_\epsilon \quad (1)$$

where

$$H_I = \frac{I}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma} \quad (2)$$

and

$$H_\epsilon = \sum_{ij\sigma} \epsilon_{ij} a_{i\sigma}^+ a_{j\sigma} ; \epsilon_{ii} = 0 \quad (3)$$

Here $a_{i\sigma}$ ($a_{i\sigma}^+$) is the Fermion annihilation creation operator for the Wannier State at the lattice site i corresponding to spin σ $n_{i\sigma} = a_{i\sigma}^+ a_{i\sigma}$; I is in the intraatomic interaction, and ϵ_{ij} is the hopping integral between the lattice sites i and j .

Taking H_I as the starting point, Hubbard found that the introduction of the hopping term H_ϵ splits the quasi-particle spectrum into two bands separated by an energy gap. And thus he showed the possibility of the existence of insulating state due to electron correlations for partially filled band. However, some difficulties were associated with his solutions. First, for one electron per atom, the two bands did not contain the same number of states required to obtain insulating state, as argued by Mott³. And second, even for arbitrarily small values of (I/Δ) (where Δ is the bandwidth in the absence of intraatomic interaction), the bands were separated by a finite energy gap. Later on Hubbard improved his approximation⁴ and removed these difficulties. But Edward and Hewson⁵ showed that, in the metallic region, there was no sharp Fermi surface. In 1972 Ikeda et al.⁶ solved the Hubbard model taking H_ϵ as the starting point,

instead of H_I , and removed all the difficulties mentioned above. However, for strong intraatomic interactions ($\frac{I}{\Delta} > 1$) their solutions are not accurate enough to give the ordered magnetic state. In this paper we find that this is due to the fact that the quasi-particle spectrum of the Ikeda et al.⁶ does not contain all the terms linear in the hopping integral. Using a self consistent many body theory, developed by Fedro and Wilson⁷, for the single particle Green's functions and extended by Kishore⁸ for the many particles Green's functions, we obtain the quasi-particle energy of each band of the spectrum, consisting of the two bands, exactly up to the first order in the hopping integral in the limit of strong intra atomic interaction.

A brief outline of the self consistent many body theory is given as follows^{7,8}. An equation of motion for the Green's functions⁹

$$G_{ij}(t) = i \theta(t) \langle [A_i, B_j(t)]_n \rangle ; n = \pm \quad (4)$$

for any two sets of Heisenberg operators, A_i and B_j , obeying the condition

$$[A_i, B_j]_n = [A_i : B_j]_n \delta_{ij} \quad (5)$$

is given as

$$-i \frac{\partial}{\partial t} G_{ij}(t) = \langle [A_i, B_i]_n \rangle \delta_{ij} \delta(t) + i \theta(t) \langle [A_i, LB_j(t)]_n \rangle \quad (6)$$

where for the Hamiltonian H and any arbitrary operator x , the Liouville operator L is defined in the following manner

$$L x \equiv [H, x] \quad (7)$$

Now, the operator $B_j(t)$ is broken into two parts

$$B_j(t) \equiv P B_j(t) + (1 - P) B_j(t), \quad (8)$$

where the projection operator P is chosen as

$$P \equiv \sum_j P_j \quad (9)$$

with

$$P_j x = \frac{B_j \langle [A_j, x]_{\eta} \rangle}{\langle [A_j, B_j]_{\eta} \rangle} \quad (10)$$

On substituting the identity (8) in (6) and using the relation $\langle [x, LY]_{\eta} \rangle = -\langle [LX, Y]_{\eta} \rangle$, obtained from the cyclic invariance of the trace implied in the ensemble average, we get

$$\begin{aligned} -\frac{\partial}{\partial t} G_{ij}(t) &= \langle [A_i, B_i]_{\eta} \rangle \delta_{ij} \delta(t) + \sum_{\ell} \Omega_{i\ell} G_{\ell j}(t) \\ &\quad - i \theta(t) \langle [L A_i, (1 - P) B_j(t)]_{\eta} \rangle \end{aligned} \quad (11)$$

where

$$\Omega_{i\ell} = - \frac{\langle [L A_i, B_{\ell}]_{\eta} \rangle}{\langle [A_{\ell}, B_{\ell}]_{\eta} \rangle} \quad (12)$$

From the solution of the equation of motion of the operator

$(1 - P) \theta(t) B_j(t)$, it can be shown that^{7,8}

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

Substitution of the above equation (13) in (10) gives a closed equation for the Green's function

$$\begin{aligned} -i \frac{\partial}{\partial t} G_{ij}(t) &= \langle [A_i, B_i]_{\eta} \rangle \delta_{ij} \delta(t) + \sum_{\ell} \Omega_{i\ell} G_{\ell j}(t) \\ &+ \sum_{\ell} \int_{-\infty}^{\infty} d\tau \gamma_{i\ell}(t) G_{\ell j}(t - \tau) \end{aligned} \quad (14)$$

where

$$\gamma_{i\ell}(\tau) = \frac{-i \theta(\tau) \langle [L A_i, e^{i\tau(1-P)L} (1-P)L B_{\ell}]_{\eta} \rangle}{\langle [A_{\ell}, B_{\ell}]_{\eta} \rangle} \quad (15)$$

For a special case, where subscripts i, j or ℓ corresponds to lattice sites or Wannier states and the system is spatially homogeneous, Eq. (14) can be Fourier transformed into energy-momentum space by introducing the Fourier transform

$$F_{ij}(t) = \frac{1}{2\pi N} \sum_{\vec{k}} \int_{-\infty}^{\infty} d\omega e^{i\vec{k} \cdot (\vec{R}_i - \vec{R}_j) + i\omega t} F_{\vec{k}}^{\omega} \quad (17)$$

where N is the number of lattice sites and F_{ij} stands for G_{ij} , Ω_{ij} or γ_{ij} . Use of (17) in (14) gives the Dyson equation

$$G_{\vec{k}}(\omega) = \frac{\langle [A_i, B_i]_{\eta} \rangle}{\omega - \Omega_{\vec{k}} - \gamma_{\vec{k}}(\omega)} \quad (18)$$

Now we shall restrict ourselves to the spatially homogeneous systems and Eq. (18) will be the starting point of the present work. By choosing $A_i = a_{i\sigma} n_{i-\sigma}^{\pm}$, where $n_{i-\sigma}^+ \equiv n_{i-\sigma}$ and $n_{i-\sigma}^- \equiv 1 - n_{i-\sigma}$; $B_i = a_{i\sigma}^+$, and $\eta = +$, Eq. (18) gives

$$G_{\vec{k}\sigma}^{\pm}(\omega) = \frac{n_{-\sigma}^{\pm}}{\omega - \Omega_{\vec{k}\sigma}^{\pm} - \gamma_{\vec{k}\sigma}^{\pm}(\omega)} \quad (19)$$

where from (4), (12) and (15) $G_{\vec{k}\sigma}^{\pm}(\omega)$, $\Omega_{\vec{k}\sigma}^{\pm}$ and $\gamma_{\vec{k}\sigma}^{\pm}(\omega)$ are respectively the Fourier transforms of

$$G_{ij\sigma}(t) = i \theta(t) \langle [a_{i\sigma} n_{i-\sigma}^{\pm}, a_{j\sigma}^+(t)]_+ \rangle \quad (20)$$

$$\Omega_{ij\sigma}^{\pm} = - \frac{\langle [L a_{i\sigma} n_{i-\sigma}^{\pm}, a_{j\sigma}^+]_+ \rangle}{n_{-\sigma}^{\pm}} \quad (21)$$

and

$$\gamma_{ij\sigma}^{\pm}(t) = - \frac{i \theta(t) \langle [L a_{i\sigma} n_{i-\sigma}^{\pm}, e^{i\tau(1-p_{\sigma}^{\pm})L} (1-p_{\sigma}^{\pm})L a_{j\sigma}^+]_+ \rangle}{n_{-\sigma}^{\pm}} \quad (22)$$

Because of spatial homogeneity we have replaced $\langle n_{i-\sigma}^{\pm} \rangle$ by $n_{-\sigma}^{\pm}$, as independent of the site i . From (10), the projection operators P_{σ}^{\pm} are defined as

$$p_{\sigma}^{\pm} \equiv \sum_j p_{j\sigma}^{\pm} \quad (23)$$

with

$$p_{j\sigma}^{\pm} x = \frac{a_{j\sigma}^{\pm}}{n_{-\sigma}^{\pm}} < [a_{j\sigma} n_{j-\sigma}^{\pm}, x]_{+} > \quad (24)$$

If we divide the Liouville operator L into two parts

$$L = L_I + L_{\epsilon} \quad (25)$$

where L_I and L_{ϵ} are defined by

$$L_I x = [H_I, x] \quad (26)$$

and

$$L_{\epsilon} x = [H_{\epsilon}, x] \quad (27)$$

then, from (2), (3) and (24), we obtain the following easily verified relations:

$$L_I a_{i\sigma} = -I a_{i\sigma} n_{i-\sigma} \quad (28)$$

$$L_I a_{i\sigma} n_{i-\sigma} = -I a_{i\sigma} n_{i-\sigma} \quad (29)$$

$$L_{\epsilon} a_{i\sigma} = - \sum_j \epsilon_{ij} a_{i\sigma} \quad (30)$$

$$L_{\epsilon} a_{i\sigma} n_{i-\sigma} = \sum_j \left[\epsilon_{ij} (-a_{j\sigma} n_{i-\sigma} + a_{i\sigma} (a_{j-\sigma}^+ a_{i-\sigma} - a_{i-\sigma}^+ a_{j-\sigma})) \right] \quad (31)$$

$$(1 - P^\pm) L_\epsilon a_{j\sigma}^+ = 0 \quad (32)$$

$$\langle [L_I a_{i\sigma} (1 - n_{i-\sigma}), (1 - P^\pm) \chi] \rangle = 0 \quad (33)$$

Use of (28) to (31) in (21) and (32) and (33) in (22),
we get

$$\Omega_{ij\sigma}^\pm = \epsilon_{ij} + \frac{I}{2} \pm \frac{I}{2} \quad (34)$$

and

$$\gamma_{ij\sigma}^\pm(t) = - \frac{i \theta(t)}{n_{-\sigma}^\pm} \langle [L_\epsilon a_{i\sigma} n_{i-\sigma}^\pm, e^{it(1-P_\sigma^\pm)(L_I + L_\epsilon)} (1 - P^\pm) L_I a_{j\sigma}^+] \rangle_+ \quad (35)$$

We are interested in calculating the single particle
Green's function

$$G_{ij\sigma}(t) = i \theta(t) \langle [a_{i\sigma}, a_{j\sigma}^+(t)] \rangle_+ \quad (36)$$

which is equal to the sum of the Green's functions $G_{ij\sigma}^+(t)$ and
 $G_{ij\sigma}^-(t)$. From (19) its Fourier transform

$$G_{k\sigma}^{\rightarrow}(\omega) = G_{k\sigma}^{+}(\omega) + G_{k\sigma}^{-}(\omega) \quad (37)$$

is given as

$$G_{k\sigma}^{\rightarrow}(\omega) = \frac{n - \sigma}{\omega - \Omega_{k\sigma}^{+} - \gamma_{k\sigma}^{+}(\omega)} + \frac{1 - n_{-\sigma}}{\omega - \Omega_{k\sigma}^{-} - \gamma_{k\sigma}^{-}(\omega)} \quad (38)$$

where, from (17), (34) and (35)

$$\Omega_{k\sigma}^{\pm} = \frac{I}{2} \pm \frac{I}{2} + \epsilon_k \quad (39)$$

and

$$\gamma_{k\sigma}^{\pm}(\omega_k^{\pm}) = - \frac{1}{n_{-\sigma}^{\pm}} \sum_{i,j} \int_{-\infty}^{\infty} dt e^{-i \vec{k} \cdot (\vec{R}_i - \vec{R}_j) - i \omega t} \times$$

$$\times \langle [L_{\epsilon} a_{i\sigma} n_{i-\sigma}^{\pm}, e^{i + (1 - p_{\sigma}^{\pm}) (L_I + L_{\epsilon}) / (1 - p_{\sigma}^{\pm}) L_I} a_{j\sigma}^{\pm}]_+ \rangle$$

(40)

It should be noted that (38) is an exact expression for the single particle Green's function, $G_{k\sigma}^{\pm}(\omega)$, and is appearing for the first time in the literature, as far as we know. It shows that quasi-particle spectrum consists of two bands

$$\omega_{k\sigma}^{\pm} = \Omega_{k\sigma}^{\pm} + \gamma_{k\sigma}^{\pm}(\omega_{k\sigma}^{\pm}) \quad (41)$$

and

$$\omega_{k\sigma}^{\pm} = \Omega_{k\sigma}^{\pm} + \gamma_{k\sigma}^{\pm}(\omega_{k\sigma}^{\pm}) \quad (42)$$

with density of states $n_{-\sigma}$ and $1 - n_{-\sigma}$ respectively. The terms $\gamma_{k\sigma}^{\pm}(\omega_{k\sigma}^{\pm})$ give the shift and width of the quasi-particle energies $\Omega_{k\sigma}^{\pm}$. If they are neglected, one gets the quasi-particle spectrum and also the single particle Green's function of Ikeda et al.⁶. For zero bandwidth ($\epsilon_k^{\pm} = 0$) and zero intraatomic interaction ($I=0$), $\gamma_{k\sigma}^{\pm}(\omega_{k\sigma}^{\pm})$ are zero. Thus, in principle, $\gamma_{k\sigma}^{\pm}(\omega_{k\sigma}^{\pm})$ can be expanded perturbationally for small bandwidth (strong intraatomic interaction) and small intraatomic interaction (large bandwidth). We develop a perturbation expansion for

strong intraatomic interaction, and calculate the quasi-particle energies exactly up to terms linear in the hopping integral, by an iterative procedure. For small intraatomic interactions, this perturbation procedure is not valid for a part of Brillouin zone where $|\epsilon_{\vec{k}}| > I$. We shall not consider this case. However, recently, for small intraatomic interaction, quasi-particle energies are calculated¹⁰ up to second order in the intraatomic interaction, by using a method similar to that of Fedro and Wilson⁷.

By using the operator identity

$$e^{it(A+B)} = e^{itA} + i \int_0^t d\tau e^{i\tau A} B e^{i(t-\tau)(A+B)} \\ = e^{itA} + i \int_0^t d\tau e^{i\tau A} B e^{i(t-\tau)A} + \dots \quad (43)$$

for the exponential factor $e^{it(1-P_{\sigma}^{\pm})(L_I + L_{\epsilon})}$ with $A = (1 - P_{\sigma}^{\pm}) L_I$ and $B = (1 - P_{\sigma}^{\pm}) L_{\epsilon}$ in Eq. (46) we get a perturbation expansion of $\gamma_{\vec{k}\sigma}^{\pm}(\omega_{\vec{k}\sigma}^{\pm})$ in terms of hopping integral as

$$\gamma_{\vec{k}\sigma}^{\pm}(\omega_{\vec{k}\sigma}^{\pm}) = \pm I \frac{n_{-\sigma}^{\pm} \epsilon_{\vec{k}} + \frac{B_{\vec{k}\sigma}}{n_{-\sigma}^{\pm}}}{\omega - \frac{I}{2} \pm \frac{I}{2}}$$

$$\begin{aligned}
 & - \frac{I}{n_{-\sigma}^{\pm}} \sum_{i,j} \int_{-\infty}^{\infty} dt e^{-i\vec{k} \cdot (\vec{R}_i - \vec{R}_j) - i(\omega - \frac{I}{2} \pm \frac{I}{2})t} \times \\
 & \times \langle [L_{\epsilon} a_{i\sigma} n_{i-\sigma}^{\pm}, e^{it(1-P_{\sigma}^{\pm})L_I} (1-P_{\sigma}^{\pm})L_{\epsilon} n_{j-\sigma}^{\pm} a_{j-\sigma}^{\pm}]_+ \rangle \\
 & + \dots \dots \dots
 \end{aligned} \tag{44}$$

where

$$B_{\vec{k}\sigma}^{\pm} = - \frac{1}{I^2} \langle [L_{\epsilon} L_I a_{i\sigma}, (1 - \sum_{\ell} P_{\ell\sigma}) L_I a_{j\sigma}^{\pm}]_+ \rangle \tag{45}$$

and the projection operators $P_{\ell\sigma}$ are defined as

$$P_{\ell\sigma} \chi = a_{\ell\sigma}^{\pm} \langle [a_{\ell\sigma}, \chi]_+ \rangle \tag{46}$$

And explicit form of $B_{\vec{k}\sigma}^{\pm}$ in terms of correlation functions is given by Fedro and Wilson⁷. First term of (44) is calculated by performing the time integral and using the identity

$$e^{it(1-P_{\sigma}^{\pm})L_I} (1-P_{\sigma}^{\pm})L_I a_{j\sigma}^{\pm} = I e^{it(\frac{I}{2} \pm \frac{I}{2})} n_{j-\sigma}^{\pm} a_{j\sigma}^{\pm} \tag{47}$$

which is obtained by the use of (29) and the definition of the projection operator, P_{σ}^{\pm} , given by (23) and (24). Now we substitute (44) in (41) and (42) and use the iterative procedure with starting quasi-particle energy, $\omega_{\vec{k}\sigma}^{\pm}$. For strong intraatomic interaction ($|\epsilon_{\vec{k}}|/I < 1$), by retaining the terms linear in the hopping integral, we set

$$\omega_{\vec{k}\sigma}^{\pm} = I + n_{-\sigma} \epsilon_{\vec{k}} - \frac{B_{\vec{k}\sigma}^{\pm}}{n_{-\sigma}} \tag{48}$$

$$\omega_{\vec{k}\sigma} = (1 - n_{-\sigma}) \varepsilon_n - \frac{B_{k\sigma}}{1 - n_{-\sigma}} \quad (49)$$

Thus, each band of Ikeda et al.⁶ is shifted and narrowed. This shifting and narrowing gives rise to ordered magnetic state¹¹, not obtained by the solutions of Ikeda et al.⁶. The quasi-particle spectrum (48) and (49) is the same as that of Esterling and Lange¹² including terms of the two site and three sites variety which they neglected.⁷ However, their quasi-particle self-energy is not exact up to terms linear in the hopping integral, as shown by Esterling.¹³ Recently Arai et al.¹⁴ have obtained the self-energy exactly up to terms linear in the hopping integral, but it is not possible to calculate the quasi-particle spectrum correctly through terms linear in the hopping integral since their equation $G_{\vec{k}}^{-1}(\omega) = 0$ is polynomial in ω .