Quasiparticle spectrum of the Hubbard model

R. Kishore
Instituto de Pesquisas Espaciais (INPE), Ministério da Ciência e Tecnologia (MCT), 12225 São José dos Campos, São Paulo, Brazil
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We study the quasiparticle spectrum of the Hubbard model by using a projection-operator formalism of the Green's function. In the weak-electron-correlation regime, we obtain the exact results up to second order in the intra-atomic interaction. For strong electron correlations, the quasiparticle spectrum consists of two bands. For each band, the quasiparticle energy is obtained exactly up to the first order in the transfer integral. We also propose a semiclassical approximation which gives the above-mentioned exact results in proper limits.

I. INTRODUCTION

Because of its simplicity and richness, the Hubbard model has been extensively studied to investigate the magnetic ordering and metal-nonmetal transitions in narrow-band systems.[1-9] The exact solutions of the model are of fundamental interest because if we can solve it exactly, we can establish some minimal requirements for the existence of magnetism and metal-nonmetal transitions. The purpose of this paper is to obtain exact results for the quasiparticle spectrum in weak and strong correlation regimes and propose a semiclassical approximation which can give these exact results in proper limits.

We obtain the quasiparticle spectrum by using a projection-operator formalism of the Green's function. This formulation has been developed by Fedro and Wilson[7] for the single-particle Green's function. Here we use its generalized version proposed by Kishore[8] for the many-particle Green's function. The quasiparticle spectrum is analyzed in the limiting case of weak- and strong-electron correlations. For weak correlations, we obtain the quasiparticle spectrum exactly up to second order in the intraatomic interaction. For strong correlations, the quasiparticle spectrum splits up into two bands. The quasiparticle energy in each band has been expanded exactly up to first order in the transfer integral. In addition to these exact results, we propose a semiclassical approximation for the damping part of the quasiparticle energy. This approximation gives the above-mentioned exact results in the proper limits.

In Sec. II we give a brief outline of the projection-operator formalism and describe the Hubbard model.[1] In Sec. III we study the quasiparticle spectrum in the weak- and strong-correlation regimes. In Sec. IV, a semiclassical approximation for the damping part of the quasiparticle energy is proposed. Finally a brief conclusion is given in Sec. V.

II. GENERAL FORMULATION

We first describe the projection operator formalism of the Green's function.[7] Let us consider the retarded Green's function[10]

$$G_{AB}(t)=i\Theta(t)\langle[A,B(t)]_\eta\rangle\ , \tag{1}$$

where $\Theta(t)$ is the Heaviside unit step function, and A and B are any scalar or vector Heisenberg operators. The time dependence of the operator is given by

$$B(t)=e^{iHt}Be^{-iHt}=e^{iLt}B\ , \tag{2}$$

where H is the Hamiltonian of the system, $B\equiv B(t=0)$, and for any arbitrary operator χ the Liouville operator L is defined as

$$L\chi=[H,\chi]_-\ . \tag{3}$$

The square brackets correspond to a commutator for $\eta=-1$ and an anticommutator for $\eta=+1$, the angular brackets denote the ensemble average, and the system of units is chosen such that $\hbar=1$.

For the sake of convenience, we work with the Fourier transform of the Green's function

$$G_{AB}(\omega)=\int_{-\infty}^{\infty}G_{AB}(t)e^{-i\omega t}dt\ , \tag{4}$$

which, after substituting the expressions for $G_{AB}(t)$ and $B(t)$ from Eqs. (1) and (2) and then performing the integration, takes the form

$$G_{AB}(\omega)=\left\langle\left[A,\frac{1}{\omega-L-i\epsilon}B\right]_\eta\right\rangle\ , \tag{5}$$

where $\epsilon\to 0^+$. Just for brevity, hereafter we shall omit ϵ by understanding that $\omega-i\epsilon$ is replaced by ω. If we multiply both sides of Eq. (5) by ω and rewrite $\omega/(\omega-L)$ as $1+[L/(\omega-L)]$, we get

$$\omega G_{AB}(\omega)=\langle[A,B]_\eta\rangle+\left\langle\left[A,\frac{L}{\omega-L}B\right]_\eta\right\rangle\ , \tag{6}$$

which is just the Fourier transform of the equation of motion of the Green's function $G_{AB}(t)$.

The essence of the projection operator formalism is to break up the operator $1/(\omega-L)B$ as

$$\frac{1}{\omega-L}B=P\frac{1}{\omega-L}B+(1-P)\frac{1}{\omega-L}B\ , \tag{7}$$

where P is the projection operator. We define it by

$$P\chi=B\langle[A,B]_\eta\rangle^{-1}\langle[A,\chi]_\eta\rangle\ . \tag{8}$$

It is easy to show that the operator P is a projection operator, namely $P^2=P$. Replacing the operator $1/(\omega-L)B$ in Eq. (6) by Eq. (7), we get

$$\omega G_{AB}(\omega)=\langle[A,B]_\eta\rangle+\Omega_{AB}G_{AB}(\omega)+\left\langle\left[A,L(1-P)\frac{1}{\omega-L}B\right]_\eta\right\rangle\ , \tag{9}$$

where

$$\Omega_{AB}=\langle[A,LB]_\eta\rangle\langle[A,B]_\eta\rangle^{-1}\ . \tag{10}$$

Now we shall try to relate the third term of the right-hand side of Eq. (9) to the Green's function $G_{AB}(\omega)$. It can be done by using the operator identity

$$\frac{1}{\omega-L}=\frac{1}{\omega-(1-P)L}+\frac{1}{\omega-(1-P)L}PL\frac{1}{\omega-L}\ . \tag{11}$$

Multiplying the above identity by the operator $(1-P)$ from the left and by the operator B from the right, we get

$$(1-P)\frac{1}{\omega-L}B=(1-P)\frac{\omega}{\omega-(1-P)L}P\frac{1}{\omega-L}B\ . \tag{12}$$

In obtaining Eq. (12), we have used the relation

$$(1-P)B=0\ , \tag{13}$$

which follows from the definition of the projection operator P. Rewriting $\omega/[\omega-(1-P)L]$ as

$$\left[1+\frac{(1-P)L}{\omega-(1-P)L}\right]$$

and using the property of the projection operator

$$P(1-P)=0\ , \tag{14}$$

Eq. (12) becomes

$$(1-P)\frac{1}{\omega-L}B=\frac{1}{\omega-(1-P)L}(1-P)LP\frac{1}{\omega-L}B\ . \tag{15}$$

Now, by using the definition of the projection operator for $P[1/(\omega-L)]B$, we can relate the right-hand side of Eq. (15) to the Green's function $G_{AB}(\omega)$ as

$$(1-P)\frac{1}{\omega-L}B=\frac{1}{\omega-(1-P)L}(1-P)LB\times\langle[A,B]_\eta\rangle^{-1}G_{AB}(\omega)\ . \tag{16}$$

Substituting Eq. (16) in Eq. (9), we get a closed equation for the Green's function

$$G_{AB}(\omega)=[\omega-\Omega_{AB}-\gamma_{AB}(\omega)]^{-1}\langle[A,B]_\eta\rangle\ , \tag{17}$$

where the damping term $\gamma_{AB}(\omega)$ is given by

$$\gamma_{AB}(\omega)=\left\langle\left[A,L\frac{1}{\omega-(1-P)L}(1-P)LB\right]_\eta\right\rangle\times\langle[A,B]_\eta\rangle^{-1}\ . \tag{18}$$

The above Eq. (17) is the matrix version of the expression for the Green's function obtained earlier by the present author.[9] In deriving this equation, it is implicitly assumed in the definition of the projection operator that the matrix $\langle[A,B]_\eta\rangle$ is not a null matrix. Hereafter, Eq. (17) of the Green's function $G_{AB}(\omega)$ will be our starting point for all further calculations. As a concrete application of this equation, we shall study the quasiparticle spectrum of the Hubbard model, described by the Hamiltonian

$$H=H_\epsilon+H_U\ , \tag{19}$$

where

$$H_\epsilon=\sum_{ij\sigma}\epsilon_{ij}a_{i\sigma}^\dagger a_{j\sigma}\ , \tag{20}$$

and

$$H_U=U\sum_i n_{i\sigma}n_{i-\sigma}\ , \tag{21}$$

$a_{i\sigma}$ and $a_{i\sigma}^\dagger$ are the annihilation and the creation operator of an electron of spin σ at the site i; ϵ_{ij} is the transfer integral associated with the sites i and j; U represents the intraatomic correlation; and $n_{i\sigma}\equiv a_{i\sigma}^\dagger a_{i\sigma}$ is the number operator corresponding to site i and spin σ. We assume that the system described by the Hubbard Hamiltonian (19) is translationally invariant.

The quasiparticle spectrum is obtained from the Fourier transform $G_{\mathbf{k}\sigma}(\omega)$ of the single-particle Green's function

$$G_{ij\sigma}(\omega)\left\langle\left[a_{i\sigma},\frac{1}{\omega-L}a_{j\sigma}^\dagger\right]_+\right\rangle\ . \tag{22}$$

The Fourier transform $F_{\mathbf{k}\sigma}(\omega)$ of any function $F_{ij\sigma}(\omega)$ is defined as

$$F_{ij\sigma}(\omega)=\frac{1}{N}\sum_{\mathbf{k}}e^{i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}F_{\mathbf{k}\sigma}(\omega)\ , \tag{23}$$

where N is the number of lattice sites. The Green's function $G_{ij}(\omega)$ can be obtained from Eq. (17) by choosing $A\equiv\{a_{i\sigma}\}$ and $B\equiv\{a_{j\sigma}^\dagger\}$ as N component vectors. If we denote the projection operator P as P_σ for a fixed σ, the definition (8) of the projection operator P and the Eq. (17) for the Green's function $G_{AB}(\omega)$ can be written as

$$P_\sigma\chi=\sum_j a_{j\sigma}^\dagger\langle[a_{j\sigma},\chi]_+\rangle\ , \tag{24}$$

and

$$\sum_l[\omega\delta_{il}-\Omega_{il\sigma}-\gamma_{il\sigma}(\omega)]G_{lj\sigma}(\omega)=\delta_{ij}\ , \tag{25}$$

where

$$\Omega_{il\sigma}=\langle[a_{i\sigma},La_{l\sigma}^\dagger]_+\rangle\ , \tag{26}$$

and

$$\gamma_{il\sigma}(\omega)=\left\langle \left[a_{i\sigma}, L\frac{1}{1-(1-P_\sigma)L}(1-P_\sigma)La^{\dagger}_{l\sigma}\right]_+\right\rangle . \tag{27}$$

On taking the Fourier transform of Eq. (25), we get

$$G_{\mathbf{k}\sigma}(\omega)=[\omega-\Omega_{\mathbf{k}\sigma}-\gamma_{\mathbf{k}\sigma}(\omega)]^{-1} , \tag{28}$$

where $\Omega_{\mathbf{k}\sigma}$ and $\gamma_{\mathbf{k}\sigma}(\omega)$ are the Fourier transforms of $\Omega_{il\sigma}$ and $\gamma_{il\sigma}(\omega)$, respectively. Equations (26) and (27) can be simplified by using the following identities[7]

$$L_\epsilon a^{\dagger}_{j\sigma}=\sum_l \epsilon_{lj}a^{\dagger}_{\sigma} , \tag{29}$$

$$L_U a^{\dagger}_{j\sigma}=Un_{j-\sigma}a^{\dagger}_{j\sigma} , \tag{30}$$

$$(1-P_\sigma)a^{\dagger}_{j\sigma}=0 , \tag{31}$$

$$\langle [a_{j\sigma},(1-P_\sigma)X]_+\rangle=0 , \tag{32}$$

and for any X and Y

$$\langle [X,LY]_+\rangle=-\langle [LX,Y]_+\rangle . \tag{33}$$

Here L_ϵ and L_U are defined by Eq. (3) for the Hamiltonian H_ϵ and H_U, respectively. By a simple and straightforward algebra, the application of the above identities (29)–(33) in Eqs. (26) and (27) gives us

$$\Omega_{il\sigma}=\epsilon_{il}+U\langle n_{i-\sigma}\rangle\delta_{il} , \tag{34}$$

$$\gamma_{il\sigma}(\omega)=U^2\tilde{\gamma}_{il\sigma}(\omega) , \tag{35}$$

where

$$\tilde{\gamma}_{il\sigma}(\omega)=\left\langle \left[a_{i\sigma}n_{i-\sigma}, \frac{1}{\omega-(1-P_\sigma)L}(1-P_\sigma)n_{l-\sigma}a^{\dagger}_{l\sigma}\right]_+\right\rangle . \tag{36}$$

Since the system is assumed to be translationally invariant, $\langle n_{i-\sigma}\rangle$ must be independent of the site i. Therefore, hereafter we shall write $\langle n_{i-\sigma}\rangle\equiv n_{-\sigma}$. We should note that we could obtain the quantity $\Omega_{il\sigma}$ exactly, but the damping term $\gamma_{il\sigma}(\omega)$ is still written in terms of the quantity $\tilde{\gamma}_{il\sigma}(\omega)$. In general, it is not possible to obtain it exactly. However, in the next section we shall try to obtain it exactly in the limiting cases of weak and strong correlations.

III. QUASIPARTICLE SPECTRUM IN WEAK- AND STRONG-CORRELATION REGIMES

A. Weak-correlation regime

The quasiparticle spectrum $\omega_{\mathbf{k}\sigma}$ corresponding to the wave vector $\mathbf{k}$ and spin σ, obtained from the poles of the Green's function (28), is given by

$$\omega_{\mathbf{k}\sigma}=\Omega_{\mathbf{k}\sigma}+\gamma_{\mathbf{k}\sigma}(\omega_{\mathbf{k}\sigma}) . \tag{37}$$

Substituting the Fourier transform of $\Omega_{il\sigma}$ and $\gamma_{il\sigma}(\omega)$ from Eqs. (34) and (35), respectively, in Eq. (37), we get

$$\omega_{\mathbf{k}\sigma}=\epsilon_{\mathbf{k}}+Un_{-\sigma}+U^2\tilde{\gamma}_{\mathbf{k}\sigma}(\omega_{\mathbf{k}\sigma}) , \tag{38}$$

where $\epsilon_{\mathbf{k}}$ and $\tilde{\gamma}_{\mathbf{k}\sigma}(\omega_{\mathbf{k}\sigma})$ are the fourier transforms of ϵ_{il} and $\tilde{\gamma}_{il}$, respectively.

The weak-correlation regime can be considered of academic interest because the Hubbard model does not apply to real physical system if the correlation is not strong. In this regime for the extreme limit of zero intraatomic correlation ($U=0$), the quasiparticle spectrum $\omega_{\mathbf{k}\sigma}=\epsilon_{\mathbf{k}}$ and, therefore, the right-hand side of Eq. (38) can be expanded in ascending powers of U. An expression which is exact up to the second order in U is given as

$$\omega_{\mathbf{k}\sigma}=\epsilon_{\mathbf{k}}+Un_{-\sigma}+U^2[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}})]_{U=0} . \tag{39}$$

The quantity $[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}})]_{U=0}$ can be calculated exactly from Eq. (36). It is given by

$$[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_k)]_{U=0}=\sum_{(i-l)}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_l)}\left\langle \left[a_i n_{i-\sigma}, \frac{1}{\epsilon_{\mathbf{k}}-(1-P_\sigma)L_\epsilon}(1-P_\sigma)n_{l-\sigma}a^{\dagger}_{l\sigma}\right]_+\right\rangle . \tag{40}$$

If we transform the operator $a_{i\sigma}$ as

$$a_{i\sigma}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}a_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{R}_i} , \tag{41}$$

Eq. (40) can be rewritten as

$$[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}})]_{U=0}=\frac{1}{N^2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\left\langle \left[a_{\mathbf{k}_1\sigma}a^{\dagger}_{\mathbf{k}_2\sigma}a_{\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1-\sigma}, \frac{1}{\epsilon_{\mathbf{k}}-(1-P_\sigma)L_\epsilon}(1-P_\sigma)a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}a^{\dagger}_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3\sigma}\right]_+\right\rangle . \tag{42}$$

The awkward presence of the opertors P_σ and L_ϵ in Eq. (42) can be destroyed by using the following easily verified identities

$$(1-P_\sigma)a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}a^{\dagger}_{\mathbf{k}-\mathbf{k}_4-\mathbf{k}_3\sigma}=a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}a^{\dagger}_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3\sigma}-\langle a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_3-\sigma}\rangle a^{\dagger}_{\mathbf{k}\sigma}\delta_{\mathbf{k}_3,\mathbf{k}_4} \tag{43}$$

and

$$[(1-P_\sigma)L_\epsilon]^n(1-P_\sigma)a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}a^{\dagger}_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3\sigma}=(\epsilon_{\mathbf{k}_3}-\epsilon_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3}-\epsilon_{\mathbf{k}_4})^n(1-P_\sigma)a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}a^{\dagger}_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3\sigma} . \tag{44}$$

Using the above identities in Eq. (42), we get

$$[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}})]_{U=0}=\frac{1}{N^2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4}\frac{1}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k}_4}-\epsilon_{\mathbf{k}_3}-\epsilon_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3}}\times\langle[a_{\mathbf{k}_1\sigma}a^{\dagger}_{\mathbf{k}_2-\sigma}a_{\mathbf{k}+\mathbf{k}_2-\mathbf{k}_1-\sigma},(a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}-\langle a^{\dagger}_{\mathbf{k}_3-\sigma}a_{\mathbf{k}_4-\sigma}\rangle\delta_{\mathbf{k}_3,\mathbf{k}_4})a^{\dagger}_{\mathbf{k}+\mathbf{k}_4-\mathbf{k}_3\sigma}]_+\rangle \ . \tag{45}$$

Since for $U=0$ the Hamiltonian (19) is quadratic in $\mathbf{k}$ space, we can apply the Wick's theorem[11] for the ensemble averages in Eq. (45) and get

$$[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}})]_{U=0}=\frac{1}{N^2}\sum_{\mathbf{k}_1,\mathbf{k}_2}\frac{n_{\mathbf{k}_1-\sigma}(1-n_{\mathbf{k}_2-\sigma})+(n_{\mathbf{k}_2-\sigma}-n_{\mathbf{k}_1-\sigma})n_{\mathbf{k}+\mathbf{k}_1-\mathbf{k}_2\sigma}}{\epsilon_{\mathbf{k}}+\epsilon_{\mathbf{k}_1}-\epsilon_{\mathbf{k}_2}-\epsilon_{\mathbf{k}+\mathbf{k}_1-\mathbf{k}_2}} \ , \tag{46}$$

where

$$n_{\mathbf{k}\sigma}\equiv a^{\dagger}_{\mathbf{k}\sigma}a_{\mathbf{k}\sigma} \ . \tag{47}$$

It should be mentioned that the expression (39) with expression (46) for $[\tilde{\gamma}_{\mathbf{k}\sigma}(\epsilon_{\mathbf{k}})]_{U=0}$ can be obtained from the quasiparticle spectrum, obtained by Chao *et al.*[9] in weak correlation regime. However, their expression also contains terms of higher than second order in U.

B. Strong-correlation regime

In strong-correlation regime for an extreme case of zero bandwidth ($\epsilon_{\mathbf{k}}=0$), the Hubbard model is exactly soluble.[1] In this case the quasiparticle spectrum consists of two energy levels at $\omega_{\mathbf{k}\sigma}=0$ and $\omega_{\mathbf{k}\sigma}=U$. Because of this two-level structure of the quasiparticle spectrum, it is not possible to apply the expansion procedure of the previous section for small $\epsilon_{\vec{k}}$. We have avoided this difficulty by considering the Green's function $G_{\mathbf{k}\sigma}(\omega)$ as a sum of two Green's functions $G^{-}_{\mathbf{k}\sigma}(\omega)$ and $G^{+}_{\mathbf{k}\sigma}(\omega)$ such that, for zero bandwidth, the quasiparticle spectrum of $G^{-}_{\mathbf{k}\sigma}(\omega)$ and $G^{+}_{\mathbf{k}\sigma}(\omega)$ consists of only one level at $\omega_{\mathbf{k}\sigma}=0$ and $\omega_{\mathbf{k}\sigma}=U$, respectively. This procedure has been first suggested by Hubbard.[12] Following him, we write

$$G_{\mathbf{k}\sigma}(\omega)=G^{-}_{\mathbf{k}\sigma}(\omega)+G^{+}_{\mathbf{k}\sigma}(\omega) \ , \tag{48}$$

where $G^{\pm}_{\mathbf{k}\sigma}(\omega)$ are the Fourier transforms of the Green's functions

$$G^{\pm}_{ij\sigma}(\omega)\left\langle\left[a_{i\sigma}n^{\pm}_{i-\sigma},\frac{1}{\omega-L}a^{\dagger}_{j\sigma}\right]_+\right\rangle \ , \tag{49}$$

with $n^{+}_{i-\sigma}\equiv n_{i-\sigma}$ and $n^{-}_{i-\sigma}=1-n_{i-\sigma}$. If we choose $A\equiv\{a_{i\sigma}n^{\pm}_{i-\sigma}\}$ and $B\equiv\{a^{\dagger}_{j\sigma}\}$ as N component vectors in Eq. (17), the Green's functions $G^{\pm}_{\mathbf{k}\sigma}(\omega)$ become

$$G^{\pm}_{\mathbf{k}\sigma}(\omega)=[\omega-\Omega^{\pm}_{\mathbf{k}\sigma}-\gamma^{\pm}_{\mathbf{k}\sigma}(\omega)]^{-1}n^{\pm}_{-\sigma} \ , \tag{50}$$

where $n^{\pm}_{-\sigma}\equiv\langle n^{\pm}_{i-\sigma}\rangle$, $\Omega^{\pm}_{\mathbf{k}\sigma}$, and $\gamma^{\pm}_{\mathbf{k}\sigma}(\omega)$ are the Fourier transforms of

$$\Omega^{\pm}_{ij\sigma}=\frac{\langle[a_{i\sigma}n^{\pm}_{i-\sigma},La^{\dagger}_{j\sigma}]_+\rangle}{n^{\pm}_{-\sigma}} \ , \tag{51}$$

and

$$\gamma^{\pm}_{ij\sigma}(\omega)=\frac{\left\langle\left[a_{i\sigma}n^{\pm}_{i-\sigma},\frac{L}{\omega-(1-P^{\pm}_{\sigma})L}(1-P^{\pm}_{\sigma})La^{\dagger}_{j\sigma}\right]_+\right\rangle}{n^{\pm}_{-\sigma}} \ , \tag{52}$$

respectively. In Eq. (52), the projection operators $P^{\pm}_{\sigma}$ are defined as

$$P^{\pm}_{\sigma}X=\frac{1}{n^{\pm}_{-\sigma}}\sum_j a^{\dagger}_{j\sigma}\langle[a_{j\sigma}n^{\pm}_{j-\sigma},X]_+\rangle \ . \tag{53}$$

Eq. (50) shows that the quasiparticle spectrum consists of two types of elementary excitations whose spectrum is given by

$$\omega^{\pm}_{\mathbf{k}\sigma}=\Omega^{\pm}_{\mathbf{k}\sigma}+\gamma^{\pm}_{\mathbf{k}\sigma}(\omega^{\pm}_{\mathbf{k}\sigma}) \ . \tag{54}$$

The quantities $\Omega^{\pm}_{\mathbf{k}\sigma}$ and $\gamma^{\pm}_{\mathbf{k}\sigma}(\omega^{\pm}_{\mathbf{k}\sigma})$ can be calculated from Eqs. (51) and (52). Using the identities (29) and (30) in Eq. (51), it is easy to see that

$$\Omega^{\pm}_{\mathbf{k}\sigma}=\frac{U}{2}(1\pm1)+\epsilon_{\vec{k}} \ . \tag{55}$$

To calculate the damping terms $\gamma^{\pm}_{\mathbf{k}\sigma}(\omega^{\pm}_{\mathbf{k}\sigma})$, we use the following identities

$$(1-P^{\pm}_{\sigma})L_{\epsilon}a^{\dagger}_{j\sigma}=0 \tag{56}$$

and

$$\langle[L_U a_{i\sigma}n^{\pm}_{i-\sigma},(1-P^{\pm}_{\sigma})X]_+\rangle=0 \tag{57}$$

in Eq. (52) and get

$$\gamma^{\pm}_{\mathbf{k}\sigma}(\omega^{\pm}_{\mathbf{k}\sigma})=\sum_{(i-j)}e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\frac{\left\langle\left[L_{\epsilon}a_{i\sigma}n^{\pm}_{i-\sigma},\frac{1}{\omega^{\pm}_{\mathbf{k}\sigma}-(1-P^{\pm}_{\sigma})L}(1-P^{\pm}_{\sigma})L_U a^{\dagger}_{j\sigma}\right]_+\right\rangle}{n^{\pm}_{-\sigma}} \ . \tag{58}$$

Further simplification of $\gamma^{\pm}_{\mathbf{k}\sigma}(\omega^{\pm}_{\mathbf{k}\sigma})$ is difficult because of the presence of the operator $(1-P^{\pm}_{\sigma})L$ in the denominator of the right-hand side of Eq. (58).

Now, to calculate the spectrum $\omega^{\pm}_{k\sigma}$, we substitute Eqs. (55) and (58) in Eq. (54) and observe that, in extreme limit of strong correlation ($\epsilon_k=0$), $\omega^{\pm}_{k\sigma}=(U/2)(1\pm1)$. It shows that the spectrum of each elementary excitation can be expanded in power of the Fourier transform of the transfer integral ϵ_k. Up to first order in ϵ_k, we get

$$\omega^{\pm}_{k\sigma}=\frac{U}{2}(1\pm1)+\epsilon_k+\tilde{\gamma}^{\pm}_{k\sigma} , \tag{59}$$

where

$$\tilde{\gamma}^{\pm}_{k\sigma}=-\frac{1}{n^{\pm}_{-\sigma}}\sum_{(i-j)} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\left\langle \left[L_\epsilon a_{i\sigma}n^{\pm}_{i-\sigma}, \frac{1}{\frac{U}{2}(1\pm1)-(1-P^{\pm}_{\sigma})L_U}(1-P^{\pm}_{\sigma})L_U a^{\dagger}_{j\sigma}\right]_{+}\right\rangle . \tag{60}$$

By using the identities

$$(1-P^{\pm}_{\sigma})L_U a^{\dagger}_{j\sigma}=U[n_{j-\sigma}-\tfrac{1}{2}(1\pm1)]a^{\dagger}_{j\sigma} \tag{61}$$

and

$$[(1-P^{\pm}_{\sigma})L_U]^n(1-P^{\pm}_{\sigma})L_U a^{\dagger}_{j\sigma}=\frac{U^n}{2}(1\mp1)(1-P^{\pm}_{\sigma})L_U a^{\dagger}_{j\sigma} , \tag{62}$$

Eq. (60) can be further simplified to

$$\tilde{\gamma}^{\pm}_{k\sigma}=\mp\frac{1}{n^{\pm}_{-\sigma}}\sum_{i-j} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle \{L_\epsilon a_{i\sigma}n^{\pm}_{i-\sigma},[n_{j-\sigma}-\tfrac{1}{2}(1\pm1)]a^{\dagger}_{j\sigma}\}_{+}\rangle . \tag{63}$$

With the help of a little lengthy but straightforward algebra, we can rewrite Eq. (63) in a more recognized form

$$\tilde{\gamma}^{\pm}_{k\sigma}=-n^{\mp}_{-\sigma}\epsilon_k-\frac{B_{k\sigma}}{n^{\pm}_{-\sigma}} , \tag{64}$$

where

$$B_{k\sigma}=\sum_{(i-j)} e^{-i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)}\langle [L_\epsilon a_{i\sigma}n_{i-\sigma},(1-P_\sigma)n_{j-\sigma}a^{\dagger}_{j\sigma}]_{+}\rangle . \tag{65}$$

A detail form of $B_{k\sigma}$ is given by Fedro and Wilson.[7] Substituting Eq. (64) in Eq. (59) we get the spectrum $\omega^{\pm}_{k\sigma}$ as

$$\omega^{\pm}_{k\sigma}=\frac{U}{2}(1\pm1)+n^{\pm}_{-\sigma}\epsilon_{\vec{k}}-\frac{B_{k\sigma}}{n^{\pm}_{-\sigma}} . \tag{66}$$

Thus we see that in strong-correlation regime, the quasiparticle spectrum consists of two bands of elementary excitations. The quasiparticle energy of each band, given by Eq. (66), is exact up to first order in the transfer integral. This form of the quasiparticle energies of the bands represents the Esterling-Lange-type[5] result in its more complete form.

IV. SEMICLASSICAL APPROXIMATION

An approximation, which can be applied throughout the range of electron correlations with reasonable confidence, is of a great value in absence of an exact solution. The reliability of the approximation depends on how well it reproduces the rigorous results in the limiting cases. In this section we propose a semiclassical approximation for the damping term $\gamma_{k\sigma}(\omega)$ of the quasiparticle spectrum. In calculating this damping term we assume that the Hamiltonians H_ϵ and H_U commute each other, i.e.,

$$[H_\epsilon,H_U]=0 . \tag{67}$$

We shall call it semiclassical approximation in the sense that in classical mechanics H_ϵ and H_U commute each other.

The calculation of the commutator of Eq. (67) shows that this semiclassical approximation is equivalent to the condition

$$\frac{U}{N}\sum_{kq}(\epsilon_k-\epsilon_{k+q})a^{\dagger}_{k+q\sigma}a_{k\sigma}\hat{n}_{q-\sigma}=0 , \tag{68}$$

where

$$\hat{n}_{q-\sigma}=\sum_i n_{i-\sigma}e^{i\mathbf{q}\cdot\mathbf{R}_i} . \tag{69}$$

Equation (68) shows that this approximation can be expected to give reliable results for narrow bands $[(\epsilon_k-\epsilon_{k+q})\sim0]$ and weak-correlation regime $(U\sim0)$. In addition to this it can be a good approximation for para and ferromagnetic states, where $\langle\hat{n}_q\rangle=\langle\hat{n}_0\rangle\delta_{q\cdot0}$ and $(\hat{n}_q-\langle\hat{n}_q\rangle)\sim0$.

The assumption (67) can also be written as

$$[L_U,L_\epsilon]\chi=0 , \tag{70}$$

which in turn gives

$$\langle [A,L_\epsilon B]_\eta\rangle=-\langle [L_\epsilon A,B]_\eta\rangle \tag{71}$$

and

$$\langle [A,L_U B]_\eta\rangle=-\langle [L_U A,B]_\eta\rangle . \tag{72}$$

Equations (71) and (72) follow from the cyclic invariance of the trace implied in the ensemble averages. For $\chi=a^{\dagger}_{k\sigma}$, Eq. (70) gives us

$$[L_U, L_\epsilon]a^\dagger_{\vec{k}\sigma} = (\epsilon_{\vec{k}} - L_\epsilon)L_U a^\dagger_{\vec{k}\sigma} = 0 \ ,$$

which is possible only if

$$L_U a^\dagger_{\mathbf{k}\sigma} = f_{\mathbf{k}\sigma} a^\dagger_{\mathbf{k}\sigma} \ , \tag{73}$$

where $f_{\mathbf{k}\sigma}$ is a real constant because the Hamiltonian H_U is a Hermitian operator. By using the above relations (70)–(73) and the definition (24) of the projection operator P_σ, it is straightforward to show that

$$[(1-P_\sigma)L_U, (1-P_\sigma)L_\epsilon]\chi = 0 \ . \tag{74}$$

This commutativity of the operators $(1-P_\sigma)L_U$ and $(1-P_\sigma)L_\epsilon$ enables us to calculate $\gamma_{\mathbf{k}\sigma}(\omega)$. In addition to Eq. (74), if we use the following identities

$$(1-P_\sigma)n_{l\sigma}a^\dagger_{l\sigma} = (n_{l-\sigma} - \langle n_{l-\sigma}\rangle)a^\dagger_{l\sigma} \tag{75}$$

and

$$[(1-P_\sigma)L_U]^n(1-P_\sigma)n_{l-\sigma}a^\dagger_{l\sigma} = [U(1-n_{-\sigma})]^n(1-P_\sigma)n_{l-\sigma}a^\dagger_{l\sigma} \tag{76}$$

in Eqs. (35) and (36), we get

$$\gamma_{il\sigma}(\omega) = U^2\left\langle \left[a_{i\sigma}n_{i-\sigma}, \frac{1}{\omega - U(1-n_{-\sigma}) - (1-P_\sigma)L_\epsilon} \times (1-P_\sigma)n_{l-\sigma}a^\dagger_{l\sigma} \right]_+ \right\rangle \ . \tag{77}$$

The Fourier transform $\gamma_{\mathbf{k}\sigma}(\omega)$ of Eq. (77) can be directly obtained by the procedure used to calculate $[\gamma_{\mathbf{k}\sigma}(\epsilon_\mathbf{k})]_{U=0}$ in Sec. III A. We simply need to replace $\epsilon_{\vec{k}}$ in Eq. (40) by $\omega - U(1-n_{-\sigma})$. It also immediately shows that this approximation reduces to exact results of Sec. III A in weak correlation regime because $[\gamma_{\mathbf{k}\sigma}(\epsilon_\mathbf{k})]_{U=0}$ obtained from Eq. (77) is exactly equivalent to that of Sec. III A.

For strong correlations, if we expand the term

$$\frac{1}{\omega - U(1-n_{-\sigma}) - (1-P_\sigma)L_\epsilon}$$

as a power of $(1-P_\sigma)L_\epsilon$ and retain only the terms up to the first order in L_ϵ, we get

$$\gamma_{il\sigma}(\omega) = \frac{U^2\langle [a_{i\sigma}n_{l-\sigma}, (1-P_\sigma)n_{l-\sigma}a^\dagger_{l\sigma}]_+\rangle}{\omega - U(1-n_{-\sigma})} + \frac{U^2\langle [L_\epsilon L_U a_{i\sigma}, (1-P_\sigma)L_U a^\dagger_{l\sigma}]_+\rangle}{[\omega - U(1-n_{-\sigma})]2} \ . \tag{78}$$

In deriving Eq. (78) we have used the relation (71) and the identity

$$P_\sigma L_\epsilon (1-P_\sigma)L_U a^\dagger_{l\sigma} = 0 \ . \tag{79}$$

Substituting Eq. (78) in Eq. (38), the quasiparticle spectrum is given by

$$\omega(\omega - U) = \{\omega - U(1-n_{-\sigma})\}\epsilon_\mathbf{k} + \frac{\sum_{(i-j)} e^{-i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}\langle [L_\epsilon L_U a_{i\sigma}, (1-P_\sigma)L_U a^\dagger_{l\sigma}]_+\rangle}{\omega - U(1-n_{-\sigma})} \ , \tag{80}$$

which up to first order in $\epsilon_\mathbf{k}$ gives two roots $\omega^\pm_{\mathbf{k}\sigma}$ given by Eq. (66). Thus we see that the present approximation reduces to the exact results in both weak and strong correlation regimes.

V. CONCLUSION

We obtained the rigorous results for the quasiparticle spectrum in weak- and strong-correlation regimes and proposed a semiclassical approximation for its damping part. We have not analyzed the full implications of this approximation. But it does contain the promise of a reasonable solution of the Hubbard model throughout the range of electron correlations. We hope that a detailed analysis of this approximation should tell us how the Hubbard model would really behave.

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