Stability of the split-band solution and energy gap in the narrow-band region of the Hubbard model

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By inserting quasielectron energies ω calculated from the fully renormalized Green's function of the Hubbard model obtained in the preceding paper into the exact expression of Galitskii and Migdal, the ground-state energy, the chemical potential, and the dynamic- and thermodynamic-stability conditions are calculated in the narrow-band region. The results show that as long as the interaction energy I is finite, electrons in the narrow-band region do not obey the Landau theory of Fermi liquids, and a gap appears between the lowest quasielectron energy ω and the chemical potential μ for any occupation n, regardless of whether the lower band is exactly filled or not. This unusual behavior is possible because, when an electron is added to the system of N electrons, the whole system relaxes due to the strong interaction, introducing a relaxation energy difference between the two quantities. We also show that all previous solutions which exhibit the split-band structure, including Hubbard's work, yield the same conclusion that electrons do not behave like Landau quasiparticles. However, the energy gap is calculated to be negative at least for some occupations n, demonstrating the dynamic instability of those solutions. They also exhibit thermodynamic instability for certain occupations, while the fully renormalized solution, having sufficient electron correlations built in, satisfies the dynamic and thermodynamic stability conditions for all occupations. When the lower band is nearly filled, the nature of the solution is shown to change, making the coherent motion of electrons with fixed k values more difficult. In the pathological limit where $I = \infty$, however, the gap vanishes, yielding a metallic state.

I. INTRODUCTION

In the preceding paper (Paper III),[1] we have applied the functional-derivative method of calculating the Green's function developed earlier[2-4] to the Hubbard model and obtained a fully renormalized Green's function. In this paper, we calculate the ground-state energy, chemical potential, and the dynamic- and thermodynamic-stability conditions in the narrow-band region using this fully renormalized solution and compare them with the results obtained from the previous solutions.[5-8]

The results obtained from the fully renormalized solution lead to the conclusions that, as long as the interaction energy I is finite, electrons in the ground state of the Hubbard model do not behave like quasiparticles in the Landau theory of Fermi liquids[9,10] in the narrow-band limit and that there exists a gap between the excitation spectrum and the chemical potential regardless of whether the lower band is completely filled or only partly filled. The physical origin of this gap will be investigated in detail in the following paper (Ref. 11). According to the results, if an electron is added to the system of N electrons, the strong interaction causes the whole system to relax. Therefore, the ground-state energy $E_0(N+1)$ of $N+1$ electrons in the Hubbard model is not given by the sum of the ground-state energy $E_0(N)$ of N electrons and the quasiparticle energy ω of the added electron. Instead, a relaxation energy $\Delta E_0(N)$ appears between the two, yielding

$$E_0(N+1) = E_0(N) + \omega - \Delta E_0(N). \tag{1.1}$$

In order for the system of $N+1$ electrons to be stable, the relaxation energy $\Delta E_0(N)$ must be positive. Our result indeed yields a positive value for $\Delta E_0(N)$ of the order of bandwidth Δ in the partly-filled-lower-band case and of the order of interaction I in the nearly-filled-lower-band case.

We shall also show that all previous results, which include Hubbard I[5] and III,[6] and which yield the split-band structure predicted by Hubbard, lead to the same conclusion that the Hubbard electrons do not behave like quasiparticles, although there is an important and distinct difference between the present solution and all the previous solutions. In the previous solutions, electron correlations are inadequately included and we find the gap $\Delta F_0(N)$ between the lowest excitation energy ω_{k_F} and the chemical potential μ to be negative at least for some occupations n, demonstrating dynamic instability for those occupations. Those solutions also exhibit thermodynamic instability for certain occupations n, suggesting that all of the previous solutions contain serious defects, and some properties such as susceptibility calculated by using those solutions may not be at all reliable. On the other hand, the present solution satisfies the dynamic- and thermodynamic-stability conditions for all occupations n.

In the pathological limit where the interaction en-

ergy I is infinitely large, however, the energy gap $\Delta E_0(N)$ is shown to vanish in agreement with Brinkman and Rice's calculation[12] as we shall discuss in Sec. IV.

Since the appearance of an energy gap at the Fermi level for all occupations n under a finite I is a very unusual and rather surprising result, we summarize the basic results of the Green's-function method[13] in Sec. II, while, in Sec. III, the ground-state energy $E_0(N)$, the chemical potential $\mu(N)$, and the dynamic- and thermodynamic-stability conditions are calculated in the narrow-band region for the following approximate solutions: Hubbard I and III, the coherent-potential approximation (CPA) solution of Soven,[14,15] the zeroth order approximate solution of the present method,[3] the Esterling–Lange result,[7] the Fedro–Wilson result,[8] the step-1 solution,[4] and the present fully renormalized solution. In Sec. IV, we summarize the results and discuss the natures of all of those solutions. *The emphasis of the present paper is on obtaining concrete results demonstrating the existence of a gap and testing stability*. Their physical interpretation will be taken up in detail in Ref. 11. For those purposes, we do not need the elaborate functional-derivative techniques developed so far.

II. THE GROUND-STATE ENERGY, CHEMICAL POTENTIAL, AND THE STABILITY CONDITIONS

The ground-state energy $E_0(N)$ can be calculated from the exact expression obtained by Galitskii and Migdal[16]

$$E_0(N_\sigma, N_{\bar\sigma}) = \sum_{k,\sigma} \int_{-\infty}^{\infty} \frac{d\omega}{4\pi} (\epsilon_k + \omega) A_{k\sigma}(\omega) f(\omega), \tag{2.1}$$

where the spectral function $A_{k\sigma}(\omega)$ with real ω is given by

$$A_{k\sigma}(\omega) = \lim_{\eta \to 0} i [G_{k\sigma}(\omega + i\eta) - G_{k\sigma}(\omega - i\eta)]. \tag{2.2}$$

In the cases we shall be considering, the continuations of $G(\omega)$ onto the unphysical sheets [we call them the advanced and retarded Green's functions $G^{(A)}$ and $G^{(R)}$ (Ref. 12)] have several poles so that the spectral weight function can be replaced by a sum of Lorentzians with width $\Gamma_{k\sigma}^{(1)}$, $\Gamma_{k\sigma}^{(2)}$, etc., centered at $\tilde\omega_{k\sigma}^{(1)}$, $\tilde\omega_{k\sigma}^{(2)}$, etc. The ground-state energy is then given by

$$E_0(N_\sigma, N_{\bar\sigma}) = \sum_{k,\sigma} \sum_{\alpha} \int_{-\infty}^{\infty} \frac{d\omega}{4\pi} (\epsilon_k + \omega) \frac{2\Gamma_{k\sigma}^{(\alpha)} Z(\tilde\omega_{k\sigma}^{(\alpha)})}{(\omega - \tilde\omega_{k\sigma}^{(\alpha)})^2 + (\Gamma_{k\sigma}^{(\alpha)})^2} f(\omega), \tag{2.3}$$

where the weight $Z(\omega)$ involved in

$$A_{k\sigma}^{(\alpha)}(\omega) = \frac{2\Gamma_{k\sigma}^{(\alpha)} Z(\tilde\omega_{k\sigma}^{(\alpha)})}{(\omega - \tilde\omega_{k\sigma}^{(\alpha)})^2 + (\Gamma_{k\sigma}^{(\alpha)})^2}, \qquad A_{k\sigma}(\omega) = \sum_{\alpha} A_{k\sigma}^{(\alpha)}(\omega), \tag{2.4}$$

is determined from Eq. (2.2).

The chemical potential $\mu(N)$ in the nonmagnetic case ($N_\sigma = N_{\bar\sigma}$) is calculated from

$$\mu(N) = \mu_\sigma(N_\sigma, N_{\bar\sigma}) = E_0(N_\sigma + 1, N_{\bar\sigma}) - E_0(N_\sigma, N_{\bar\sigma}) = \delta E_0(N_\sigma, N_{\bar\sigma})/\delta N_\sigma \tag{2.5}$$

for $n_0 = n_{\bar\sigma} = \frac{1}{2} n$ under the condition that

$$N_{\sigma'} = \sum_k \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_{k\sigma'}(\omega) f(\omega) \tag{2.6}$$

for $\sigma' = \sigma$ and $\bar\sigma$. From Eq. (2.5), we find that the ground-state energy of $N+1$ electrons is given by

$$E_0(N_\sigma + 1, N_{\bar\sigma}) = E_0(N_\sigma, N_{\bar\sigma}) + \mu(N_\sigma, N_{\bar\sigma}), \tag{2.7}$$

where $n_\sigma = n_{\bar\sigma} = \frac{1}{2} n$. The requirement that the thermodynamic potential is minimum yields the following thermodynamic stability conditions:

$$\frac{\delta^2 E_0(N_\sigma, N_{\bar\sigma})}{\delta N_\sigma^2} > 0, \quad \frac{\delta^2 E_0(N_\sigma, N_{\bar\sigma})}{\delta N_{\bar\sigma}^2} > 0, \tag{2.8}$$

$$\frac{\delta^2 E_0(N_\sigma, N_{\bar\sigma})}{\delta N_\sigma^2} \frac{\delta^2 E_0(N_\sigma, N_{\bar\sigma})}{\delta N_{\bar\sigma}^2} > \left(\frac{\delta^2 E_0(N_\sigma, N_{\bar\sigma})}{\delta N_\sigma \delta N_{\bar\sigma}} \right)^2.$$

The foregoing relations are all exact except for Eqs. (2.3) and (2.4). Let us now adopt the conventional interpretation that the poles of the single-electron Green's function yield the quasiparticle energies, that is, the energy $\omega_{k\sigma}^{(\alpha)}(N)$ of an electron added to the ground state of N electrons. The energy $E_k^{(\alpha)}(N_\sigma + 1, N_{\bar\sigma})$ of the resulting $N+1$ electrons is then given by

$$E_k^{(\alpha)}(N_\sigma + 1, N_{\bar\sigma}) = E_0(N_\sigma, N_{\bar\sigma}) + \omega_{k\sigma}^{(\alpha)}(N). \tag{2.9}$$

Since this energy $E_k^{(\alpha)}$ cannot be lower than the ground-state energy $E_0(N_\sigma + 1, N_{\bar\sigma})$ of $N+1$ electrons, we obtain the dynamic-stability condition

$$\omega_{k\sigma}^{(\alpha)}(N) - \mu(N) \equiv \Delta E_\sigma(N) \geq 0. \tag{2.10}$$

If the above inequality is violated, it implies the existence of a state having a lower energy than the "ground"-state energy, and hence the putative ground state is dynamically unstable.

If the system is a normal Fermi liquid with a singly peaked spectrum, the index α is deleted.

The lowest excitation energy $\omega_{k_F\sigma}(N)$ (which is the energy of an electron at the Fermi level k_F) is equal to the chemical potential $\mu(N)$,

$$\omega_{k_F\sigma}(N)=\mu(N), \tag{2.11}$$

(unless the valence band is exactly filled and the conduction band empty with a finite gap between them). For a Fermi liquid, furthermore, the energy $\omega_{k\sigma}(N)$ of an electron removed from the system of N electrons can also be calculated from

$$\omega_{k\sigma}(N)=\delta E_0(N_\sigma,N_{\bar\sigma})/\delta N_{k\sigma}, \tag{2.12}$$

under the condition (2.6) and for k near k_F.

The calculations in Sec. III will show that all existing nonmagnetic solutions of the Hubbard model do not satisfy Eqs. (2.11) and (2.12) in the narrow-band regime, demonstrating that the electrons of the Hubbard model do not obey the Landau theory of Fermi liquids. However, only the fully renormalized solution satisfies the thermodynamic- and dynamic-stability condition. In the following, we shall again limit our calculation to the case where the lower band is partly or completely filled but the upper band is empty. The case where the upper band is partly filled may be treated in exactly the same manner by reversing the roles of electrons and holes.

III. EXAMINATION OF VARIOUS EXISTING SOLUTIONS

Let us now calculate the ground-state energy $E_0(N_\sigma,N_{\bar\sigma})$ and the chemical potential $\mu(N)$ by using the various approximate solutions available and test whether these solutions are dynamically stable via Eq. (2.10). We also examine whether these solutions satisfy the thermodynamic-stability condition (2.8). Whenever feasible, the calculation has been carried out correctly through terms linear in ϵ/I. Except for the Hubbard-I case, however, we shall show only the leading terms in the following.[17]

A. Hubbard-I approximation[5]

The inverse Green's function is given by

$$2\pi G^{-1}_{k\sigma}(\omega)=\omega-\epsilon_k-\frac{n_{\bar\sigma}I\omega}{\omega-(1-n_{\bar\sigma})I}. \tag{3.1}$$

The poles $\omega^{(\alpha)}_{k\sigma}$ may be expanded in powers of ϵ_k/I as follows:

$$\begin{aligned}\omega^{(1)}_{k\sigma}&=(1-n_{\bar\sigma})\epsilon_k-n_{\bar\sigma}(1-n_{\bar\sigma})(\epsilon_k^2/I)+\cdots,\\ \omega^{(2)}_{k\sigma}&=I+n_{\bar\sigma}\epsilon_k+n_{\bar\sigma}(1-n_{\bar\sigma})(\epsilon_k^2/I)-\cdots,\end{aligned} \tag{3.2}$$

while the spectral weights $A^{(\alpha)}_{k\sigma}$ are given by

$$A^{(1)}_{k\sigma}=1-n_{\bar\sigma}+\cdots,\quad A^{(2)}_{k\sigma}=n_{\bar\sigma}+\cdots. \tag{3.3}$$

As long as the lower band $\omega^{(1)}_{k\sigma}$ is partly or completely filled but the upper band is empty, the ground-state energy $E_0(N_\sigma,N_{\bar\sigma})\equiv E_0(N)$ and the chemical potential $\mu(N)$ can be calculated by inserting $\omega^{(1)}_{k\sigma}$ and $A^{(1)}_{k\sigma}$ obtained above into Eqs. (2.1) and (2.5). We then find that

$$\begin{aligned}\mu(N)=&(1-\tfrac{1}{2}n_{\bar\sigma})\epsilon_{k_F\sigma}+(1-\tfrac{1}{2}n_\sigma)n_{\bar\sigma}(1-n_\sigma)^{-1}\epsilon_{k_F\bar\sigma}\\&-(\tfrac{3}{2}-n_\sigma)N_a^{-1}\sum_k\epsilon_k f_{k\bar\sigma},\end{aligned} \tag{3.4}$$

where $f_{k\sigma}$ is shorthand for $f(\omega^{(1)}_{k\sigma})$ and $\epsilon_{k_F\sigma}$ is the band energy of an electron with spin σ at the Fermi level. Note here that the chemical potential $\mu(N)$ is not equal to the quasiparticle energy, $\omega^{(1)}_{k_F\sigma}=(1-n_{\bar\sigma})\epsilon_{k_F\sigma}+\cdots$, at the Fermi level thus violating Eq. (2.11). In the nonmagnetic case where $n_\sigma=n_{\bar\sigma}=\frac{1}{2}n$, the difference $\Delta E_0(N)$ between $\omega^{(1)}_{k_F\sigma}$ and $\mu(N)$ is calculated to be

$$\Delta E_0(N)=-\frac{n(3-n)}{2(2-n)}\epsilon_{k_F}+\tfrac{1}{2}(3-n)\frac{1}{N_a}\sum_k\epsilon_k f_{k\sigma}. \tag{3.5}$$

The average energy of the occupied states defined by

$$\bar\epsilon=\sum_k\epsilon_k f_{k\sigma}\Big/\sum_k f_{k\sigma} \tag{3.6}$$

is negative and less than ϵ_{k_F}, that is

$$\bar\epsilon<0,\quad \bar\epsilon<\epsilon_{k_F}. \tag{3.7}$$

By inserting Eq. (3.6) into Eq. (3.5), we find

$$\Delta E_0(N)=\frac{n(3-n)}{2(2-n)}(\bar\epsilon-\epsilon_{k_F})<0 \tag{3.8}$$

for all values of $n(\leq 1)$, proving that the inequality (2.10) is never satisfied. Therefore, the Hubbard-I solution is dynamically unstable for all occupations n.

By differentiating Eq. (3.4), the second derivative can be calculated. In the nonmagnetic case ($n_\sigma=n_{\bar\sigma}=\frac{1}{2}n$), the result is reduced to

$$\begin{aligned}N_a\frac{\delta^2E_0(N_\sigma,N_{\bar\sigma})}{\delta N_\sigma^2}=&\frac{4-n}{2(2-n)}N_a\frac{\delta\epsilon_{k_F}}{\delta N_\sigma}\\&+\frac{n}{2-n}(\bar\epsilon-\epsilon_{k_F}),\end{aligned} \tag{3.9}$$

where $\bar\epsilon<\epsilon_{k_F}$. When the lower band is nearly empty ($n\approx 0$, $k\approx 0$) or nearly filled ($n\approx 1$), $\delta\epsilon_{k_F}/\delta N_\sigma$ vanishes, making the expression on the right-hand side of Eq. (3.9) negative. Hence the Hubbard-I solution is thermodynamically unstable in these limits.

The foregoing results follow exactly from Eq. (3.1) in the narrow-band limit ($\Delta\ll I$) and are rather surprising. The Hubbard-I solution, being dynamically unstable, cannot be used for calculating thermodynamic properties of the Hubbard model. This solution is also thermodynamically unstable in the half-filled case, even though it is most often applied for that case.

B. Hubbard-III approximation[6]

The inverse Green's function may be written as

$$2\pi G_{k\sigma}^{-1}(\omega)=\omega-\epsilon_k-\frac{n_{\bar\sigma}I\omega}{\omega-(1-n_{\bar\sigma})I}-\frac{n_{\bar\sigma}(1-n_{\bar\sigma})I^2\Omega_\sigma(\omega)}{[\omega-(1-n_{\bar\sigma})I]^2-[\omega-(1-n_{\bar\sigma})I]\Omega_\sigma(\omega)}\,. \tag{3.10}$$

Here $\Omega_\sigma(\omega)$ is the sum of the scattering correction $\Omega_\sigma'(\omega)$ and the resonance broadening corrections $\Omega_{\bar\sigma}'(\omega)$ and $\Omega_{\bar\sigma}''(\omega)$,

$$\Omega_\sigma(\omega)=\Omega_\sigma'(\omega)+\Omega_{\bar\sigma}'(\omega)+\Omega_{\bar\sigma}''(\omega)\,, \tag{3.11}$$

where

$$\Omega_\sigma'(\omega)=F_\sigma(\omega)-\left(N_a^{-1}\sum_k(F_\sigma(\omega)-\epsilon_k)^{-1}\right)^{-1}, \tag{3.12}$$

and $\Omega_\sigma''(\omega)=-\Omega_\sigma'(I-\omega)$, while $F_\sigma(\omega)=2\pi G_{k\sigma}^{-1}(\omega)+\epsilon_k$. The last term on the right-hand side of Eq. (3.10) is a new correction added to the Hubbard-I solution given by Eq. (3.1). Since, in the narrow-band region, this additional term yields corrections only of order ϵ_k^2/I to the quasiparticle energy $\omega_{k\sigma}^{(1)}$, the total energy $E_0(N)/N$ and the chemical potential $\mu_\sigma(N)$, respectively, it is not possible to remove the instabilities of the solution found under the Hubbard-I approximation, which enters to order ϵ_k. Therefore the Hubbard-III approximation does not give any improvement over the Hubbard-I solution in the narrow-band limit, although it exhibits a metal-nonmetal transition not found in the Hubbard-I solution. As has been proved by Velický *et al.*,[15] the coherent-potential approximation (CPA) solution obtained by Soven[14] under the frozen-lattice approximation is equivalent to the Hubbard-III solution, and hence it is also unstable.

C. The zeroth-order approximation to the self-energy correction

Let us now consider the result contained in Eq. (4.12) of Paper I (Ref. 3)

$$2\pi G_{k\sigma}^{-1}(\omega)=\omega-\epsilon_k-\frac{n_{\bar\sigma}I\omega}{\omega-(1-n_{\bar\sigma})I}-\frac{I^2g(k\sigma)}{[\omega-(1-n_{\bar\sigma})I]^2}-\xi(k\sigma,\omega)\,, \tag{3.13}$$

where

$$g(k\sigma)=n_{\bar\sigma}(1-n_{\bar\sigma})\epsilon_k+(1-2n_\sigma)N_a^{-1}\sum_q\epsilon_q n_{q\bar\sigma}+2N_a^{-2}\sum_{q_1}\sum_{q_2}\epsilon_{k-q_1+q_2}n_{q_1\bar\sigma}n_{q_2\sigma}\,. \tag{3.14}$$

Since $\xi(k\sigma,\omega)$ involving $\delta\langle N\rangle/\delta\epsilon$ etc., yields a correction of order ϵ^2/I, it will be neglected in the following. The third term on the right-hand side of Eq. (3.13) is similar to and smaller than the second term, and hence it will also be neglected in the following, although we have calculated the contributions explicitly.[17] The above result is obtained by inserting the Hubbard-I solution into the basic equation for the self-energy correction given by Eq. (3.25) of Paper I, and the last two terms in Eq. (3.13) are additional correction terms obtained beyond the Hubbard-I approximation. Similar expressions have been obtained by Esterling and Lange[7] and by Fedro and Wilson.[8]

In the absence of ξ, the quasiparticle energy ω is calculated from the cubic equation $G^{-1}(\omega)=0$ as follows:

$$\omega_{k\sigma}^{(1)}=\epsilon_k+\frac{(1-2n_\sigma)}{1-n_{\bar\sigma}}\,\frac{1}{N_a}\sum_q\epsilon_q n_{q\bar\sigma}+\cdots\,. \tag{3.15}$$

The corresponding spectral weights are given by

$$A_{k\sigma}^{(1)}=1-n_{\bar\sigma}+\cdots;\quad A_{k\sigma}^{(2)}=n_{\bar\sigma}+\cdots;\quad A_{k\sigma}^{(3)}\approx 0\,. \tag{3.16}$$

Inserting Eqs. (3.15) and (3.16) into Eq. (2.1) yields the ground-state energy $E_0(N_\sigma,N_{\bar\sigma})$ and hence the chemical potential $\mu(N)$:

$$\mu(N)=\frac{4-n-n^2}{(2-n)^2}\epsilon_{k_F}-\frac{n(1+2n)}{2(2-n)}\,\bar\epsilon_0+\cdots\,. \tag{3.17}$$

The above results again show that $\mu(N)$ is not equal to the quasiparticle energy $\omega_{k_F\sigma}^{(1)}=\epsilon_{k_F}+\cdots$ at the Fermi level, thus violating Eq. (2.11). In the nonmagnetic case ($n_\sigma=n_{\bar\sigma}=\frac{1}{2}n$), the difference $\Delta E_0(N)$ between $\omega_{k_F\sigma}^{(1)}$ and $\mu(N)$ is calculated to be

$$\Delta E_0(N)=-\frac{(3-2n)n}{(2-n)^2}(\epsilon_{k_F}-\bar\epsilon_0)+\frac{n^2}{(2-n)^2}(\tfrac{1}{2}\bar\epsilon_0+\cdots)\,. \tag{3.18}$$

Since $\epsilon_{k_F}>\bar\epsilon_0$ and $\bar\epsilon_0<0$, the above result appears to suggest that $\Delta E_0(N)$ is negative and that the present solution is dynamically unstable. For $n<\frac{1}{2}$, however, terms which are generated from the third term in Eq. (3.14) and which are denoted by $\cdots$ in Eq. (3.18) are positive, and the sign of $\Delta E_0(N)$ cannot be determined until the values of those omitted terms are evaluated explicitly. We also find that the second derivatives are negative in the limit of the nearly-half-filled case, making the zeroth-order approximation solution thermodynamically unstable.

The solutions obtained by Esterling and Lange[7]

and by Fedro and Wilson[8] are similar to our zeroth-order solution. Unfortunately, the two-particle correlation functions involved in these solutions make them difficult to use for the present calculation. By comparing the results with the expression in Eqs. (3.13) and (3.14), however, we find that terms corresponding to the second and third terms in Eq. (3.14) have minus signs in the Fedro-Wilson result, and therefore their result will correspond to

$$\omega_{k\sigma}^{(1)} = \epsilon_k - \frac{1-2n_\sigma}{1-n_{\bar\sigma}} \frac{1}{N_a} \sum_k \epsilon_k f_{k\sigma} \cdots . \tag{3.19}$$

In the nonmagnetic case ($n_\sigma = n_{\bar\sigma} = \frac{1}{2}n$), the difference between $\omega_{k_F\sigma}^{(1)}$ and $\mu(N)$

$$\Delta E_0(N) = -\frac{n}{(2-n)^2}\epsilon_{k_F} + \frac{n}{2(2-n)}\bar\epsilon_0 \cdots , \tag{3.20}$$

remains negative as long as the lower band is more than half filled. Therefore the solution is dynamically unstable for $n_\sigma = n_{\bar\sigma} \gtrsim \frac{1}{3}$. The same conclusion is also obtained for the Esterling–Lange result.

In summary, the approximate solutions discussed in the present subsection are all equally unsatisfactory.

D. Step-1 solution

Before testing the fully renormalized solution, it is instructive to examine the step-1 solution, the complete solution of the restricted equation for the self-energy Σ obtained in Paper II.[4] As has been discussed in Sec. IV of Paper III,[1] the step-1 solution cannot be applied to the cases where the lower band is nearly or completely filled, since the poles of the Green's function become complex, thus violating the basic requirement that G is analytic in the complex ω plane except for the discontinuity along the real axis. Therefore, we have to omit these cases in the following. The lower-band solution $\omega_{k\sigma}^{(1)}$ can then be expanded unambiguously in powers of ϵ_k/I. The result

$$\omega_{k\sigma}^{(1)} = \frac{(1-n_{\bar\sigma})^2}{1-2n_{\bar\sigma}}\epsilon_k + (1-n_{\bar\sigma})P_{k\sigma} + O(\epsilon^2/I) \tag{3.21}$$

is exact up through terms linear in ϵ, where $P_{k\sigma}$ is obtained from Eq. (2.5a) of Paper III by removing bars over $\bar N$, $\bar C^\dagger$, and $\bar C$. By differentiating the total energy $F_0(N_\sigma, N_{\bar\sigma})$, the chemical potential $\mu(N)$ can be expressed as follows:

$$\begin{aligned}\mu(N) = {} & \left(1 + \frac{n_{\bar\sigma}^2}{2(1-2n_{\bar\sigma})}\right)\epsilon_{k_F\sigma} + \frac{1-n_{\bar\sigma}}{2}P_{k_F\sigma} + \left[\left(1 + \frac{n_\sigma}{2(1-2n_\sigma)}\right)\epsilon_{k_F\bar\sigma} + \frac{1-n_\sigma}{2}P_{k_F\bar\sigma}\right]\frac{n_{\bar\sigma}}{1-n_\sigma} \\ & + \frac{1}{2}\sum_k \left((1-n_{\bar\sigma})^2 \frac{\delta P_{k\sigma}}{\delta N_\sigma} f_{k\sigma} + (1-n_\sigma)^2 \frac{\delta P_{k\bar\sigma}}{\delta N_\sigma} f_{k\bar\sigma}\right) - \frac{1}{N_a}\sum_k (1-n_\sigma)P_{k\bar\sigma}f_{k\bar\sigma} \\ & - \frac{1}{N_a}\sum_k \left(1 - \frac{2n_\sigma - 5n_\sigma^2 + 4n_\sigma^3}{2(1-2n_\sigma)^2}\right)\epsilon_k f_{k\bar\sigma} ,\end{aligned} \tag{3.22}$$

where $P_{k\sigma}$ is reduced to

$$P_{k\sigma} = (1-2n_\sigma)\sum_{R'} \frac{\epsilon_{RR'}}{\langle C_{R\sigma}^\dagger C_{R'\sigma}\rangle} + 2\epsilon_k . \tag{3.23}$$

To estimate the magnitude of $P_{k\sigma}$, we assume that $\epsilon_{RR'}$ is nonzero only for nearest neighbors R and R'. Then $\langle C_{R\sigma}^\dagger C_{R'\sigma}\rangle$ may be evaluated explicitly for the one-dimensional case and the three-dimensional case with a spherical Fermi surface (SP) as follows:

$$\langle C_{R\sigma}^\dagger, C_{R'\sigma}\rangle = (1-\tfrac{1}{2}n)S_\sigma(\sigma') , \tag{3.24}$$

where

$$S_\sigma(\sigma') = \begin{cases} (1/\pi)\sin k_F r_0 , \\ (1/2\pi^2)\xi(\sin k_F r_0 - k_F r_0 \cos k_F r_0) , \end{cases} \tag{3.25}$$

(for the one-dimensional and SP cases, respectively, and $r_0 = |R - R'|$ is the nearest-neighbor separation, and ξ is a lattice-dependent number equal to or less than unity.) If the lower band is nearly empty ($n \approx 0$), $S_\sigma(\sigma')$ being proportional to n nearly vanishes and, as the filling n increases, $S_\sigma(\sigma')$ calculated from Eq. (3.24) remains small compared to unity. (This is true even when the lower band is more than half filled and the Fermi surface no longer resembles a sphere.) Therefore terms involving $P_{k\sigma}$ will dominate over other terms in the expression for $\mu(N)$. In the nonmagnetic case ($n_\sigma = n_{\bar\sigma} = \frac{1}{2}n$), the difference $\Delta E_0(N)$ between $\omega_{k\sigma}^{(1)}$ and $\mu(N)$ can be written as

$$\begin{aligned}\Delta E_0(N) = {} & -\frac{n(4-n)}{4(2-n)}\epsilon_{k_F} - \frac{1}{4}\frac{\Delta}{S(n_\sigma)} + \frac{n(1-n)}{(2-n)^2}\frac{\epsilon_{k_F}}{S(n_\sigma)^2} \\ & + (1-n)\epsilon_{k_F} - (2-n)S(n_\sigma)\Delta \\ & + \left(1 - \frac{4n - 5n^2 + 2n^3}{8(1-n)^2}\right)\Delta S(n_\sigma) .\end{aligned} \tag{3.26}$$

If the lower band is significantly more than half filled ($n > \frac{1}{3}$), ϵ_{k_F} becomes positive and large, making the relaxation energy $\Delta E_0(N)$ positive for three-dimensional cases. If the lower band is less than half filled ($n \lesssim \frac{1}{3}$), however ϵ_{k_F} becomes negative making $\Delta E_0(N)$ negative for all cases. Therefore,

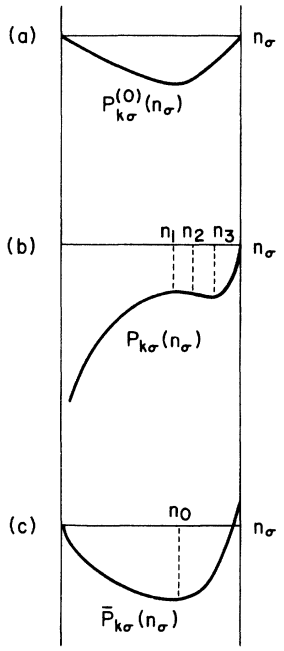

FIG. 1. Plots of $P^{(0)}_{k\sigma}$, $P_{k\sigma}$ and $\bar{P}_{k\sigma}$ as functions of occupation n_σ.

the Hubbard-type solution may be dynamically stable when the lower band is significantly more than half filled ($n > \frac{1}{3}$), but, otherwise, it becomes unstable. Note that the previous results have all exhibited dynamic instability when the lower band is more than half filled.

Unfortunately, the step-1 solution breaks down[5] when the lower band is nearly filled, which is, of course, the most serious defect of that solution. Furthermore, the thermodynamic-stability conditions (2.8) are satisfied in a very narrow region of occupation n. This can be demonstrated by evaluating those stability conditions by using the most dominant terms. These are the ones having the highest derivatives of P with respect to N_σ; that is,

$$\tfrac{1}{2}\sum_k \left((1-n_{\bar\sigma})^2 \frac{\delta^2 P_{k\sigma}}{\delta N_\sigma^2} f_{k\sigma} + (1-n_\sigma)^2 \frac{\delta^2 P_{k\bar\sigma}}{\delta N_\sigma^2} f_{k\bar\sigma} \right) > 0 . \tag{3.27}$$

A plot of $P_{k\sigma}$ defined by Eq. (3.23) and illustrated in Fig. 1(b) shows that $P_{k\sigma}$ is locally maximal at n_1, minimal at n_3, and has a point of inflexion at n_2; $n_1 < n_2 < n_3$. The condition (3.27) is then satisfied only for $n > n_2$. A term which corresponds to $P_{k\sigma}$ does not exist in the Hubbard I nor the Hubbard III. In the zeroth-order approximate solution, the term,

$$P^{(0)}_{k\sigma} \equiv \left((1-2n_\sigma) N_a^{-1} \sum_q \epsilon_q n_{q\bar\sigma} + 2N_a^{-2} \sum_{q_1}\sum_{q_2} \epsilon_{k-q_1+q_2} n_{q_1\bar\sigma} n_{q_2\sigma} \right) \times [\omega - (1-n_{\bar\sigma})I]^{-2} , \tag{3.28}$$

corresponds to $P_{k\sigma}$.

E. The fully renormalized solution

We now want to calculate the ground-state energy $E_0(N_\sigma, N_{\bar\sigma})$ and the chemical potential $\mu(N)$ using the fully renormalized Green's function given by Eq. (2.4) of Paper III and suggest that this solution finally satisfies the dynamic- and thermodynamic-stability conditions for all occupations n.

As we have discussed in Sec. IV of Paper III, the energy $\omega^{(1)}_{k\sigma}$ of an electron added to the system of N electrons in the narrow-band region is given for all occupations n by the completely renormalized solution as

$$\omega^{(1)}_{k\sigma} = [1 - n_{\bar\sigma} - \Phi_\sigma(\bar\sigma)](\epsilon_k + \bar P_{k\sigma}) + \frac{[n_{\bar\sigma}(1-n_{\bar\sigma}) + a]\epsilon_k}{F_\sigma(\bar\sigma)} + \cdots , \tag{3.29}$$

where

$$a = (1-2n_{\bar\sigma})\Phi_\sigma(\bar\sigma) - \Phi_\sigma(\bar\sigma)^2 ,$$

$$F_\sigma(\bar\sigma) = 1 - 2n_{\bar\sigma} - 2\Phi_\sigma(\bar\sigma) - 2[1 - n_{\bar\sigma} - n_{\bar\sigma}(1-2n_{\bar\sigma}) - 2(1-2n_{\bar\sigma})\Phi_\sigma(\bar\sigma) + 2\Phi_\sigma(\bar\sigma)^2]\bar P_{k\sigma}/I + \cdots , \tag{3.30}$$

and $\Phi_\sigma(\bar\sigma) = \Phi_\sigma(R\bar\sigma;\omega)$ is the correction introduced to the equal-time Green's function $\langle N_{R\sigma}(t)\rangle$ by the effect of $\delta\langle N\rangle/\delta\epsilon$ and $\delta\langle C^\dagger C\rangle/\delta\epsilon$. Similarly, contributions from $\delta\langle N\rangle/\delta\epsilon$ and $\delta\langle C^\dagger C\rangle/\delta\epsilon$ modify $P_{k\sigma}$ given by Eq. (3.23) to the form given by Eq. (2.5a) of Paper III, that is,

$$\bar P_{k\sigma} = \sum_{R'} \{ [1 - 2n_\sigma - 2\Phi_\sigma(\sigma)]\epsilon_{RR'} \langle C^\dagger_{R\bar\sigma} C_{R'\bar\sigma}\rangle + \cdots \} D_\sigma^{-1} , \tag{3.31}$$

$$\bar D_\sigma = [\tfrac{1}{2} - n_{\bar\sigma} - \Phi_\sigma(\bar\sigma)]^2 - [\tfrac{1}{2} - n_\sigma - \Phi_\sigma(\sigma)]^2 + \cdots . \tag{3.32}$$

In order to simplify the following illustration, we have neglected terms which correspond to the third term in Eq. (3.14) in the above expressions, although those terms are included in our original calculation.[17]

Since the $\omega^{(\alpha)}_{k\sigma}$ are complex, the ground-state energy should be calculated from Eq. (2.3). In the narrow-

band region where $\mathrm{Im}\omega_{k\sigma}^{(1)}$ and $\mathrm{Im}\Phi_\sigma(\sigma')$ are negligibly small, however, the spectral weight $A_{k\sigma}^{(1)}(\omega)$ defined by Eq. (2.4) may still be replaced by δ function. The ground-state energy is then estimated by inserting

$$A_{k\sigma}^{(1)} = 1 - n_{\bar\sigma} - \Phi_\sigma(\bar\sigma)\cdots , \tag{3.33}$$

and $\omega_{k\sigma}^{(1)}$ given by Eq. (3.29) into Eq. (2.1), yielding

$$\mu(N) = \tfrac{1}{2}(\epsilon_{k_F} + \omega_{k_F\sigma}^{(1)}) + \tfrac{1}{2}\sum_{k,\sigma'}\left(\frac{\delta\omega_{k\sigma'}^{(1)}}{\delta N_\sigma} A_{k\sigma'}^{(1)} f_{k\sigma'} + (\epsilon_k + \omega_{k\sigma'}^{(1)} - \epsilon_{k_F} - \omega_{k_F\sigma'}^{(1)})\frac{\delta A_{k\sigma'}^{(1)}}{\delta N_\sigma} f_{k\sigma'}\right) . \tag{3.34}$$

The Φ's and the P's involved in the expressions (3.29)–(3.34) have been evaluated in Eqs. (3.6), (3.8), (3.15), and (3.16) of Paper III. The results show that, when the lower band is only partly filled, $\Phi_\sigma(\sigma')$ and $\bar P_{k\sigma'}/I$ (or $\omega_{k\sigma'}/I$) are proportional to $\pm[S_\sigma(\bar\sigma)]^{1/2}$ and $\pm(\Delta/I)[S_\sigma(\bar\sigma)]^{1/2}$, respectively, and remain small, but that, when the lower band is nearly filled, their magnitudes increase rapidly and become proportional to $\pm[(I/\Delta)S_\sigma(\bar\sigma)]^{1/3}$ and $\pm[(\Delta/I)^2 S_\sigma(\bar\sigma)]^{1/3}$, respectively. Here $S_\sigma(\bar\sigma)$ defined by Eq. (3.24) is calculated from

$$S_\sigma(\bar\sigma) = N_a^{-1}\sum_k [1 - n_\sigma - \Phi_\sigma(\sigma) - \bar P_{k\sigma}/(2I)\cdots] \times f_{k\sigma} e^{-ik(R-R')} . \tag{3.35}$$

As long as the lower band is only partly filled, terms involving the $\bar P$'s are the most dominant terms in the expression (2.1) for the ground-state energy. Hence the ground-state energy is minimal when both $\bar P_{k\sigma}$ and $\bar P_{k\bar\sigma}$ are negative. This can be achieved if the condition (3.2a) of Paper III

$$\Phi_{\bar\sigma}(\bar\sigma) = \Phi_\sigma(\sigma);\quad \Phi_{\bar\sigma}(\sigma) = \Phi_\sigma(\bar\sigma) \tag{3.36}$$

is assumed and if the upper signs are taken in Eqs. (3.6) and (3.8) of III. If, instead, the condition (3.2b) of III is assumed, we find a state having a total energy higher than the ground-state energy. For the partly-filled-lower-band case with $\delta = \frac{1}{2} - n_0 > |\Phi_\sigma(\sigma)|$ and $|\omega/I|$, the quantity $S_\sigma(\bar\sigma)$ calculated from Eq. (3.35) is roughly equal to $\sin x$ with $x = \pi - k_F(R - R')$ and hence

$$\Phi_\sigma(\sigma) \approx -\Phi_\sigma(\bar\sigma) \approx \tfrac{1}{8}(\pi K \sin x/x)^{1/2} , \tag{3.37a}$$

$$\bar P_{k\sigma} \approx -2\Delta[x\sin x/(\pi K)]^{1/2} , \tag{3.37b}$$

which yield

$$\frac{\delta\Phi_\sigma(\sigma)}{\delta N_\sigma} = -\frac{\delta\Phi_\sigma(\bar\sigma)}{\delta N_\sigma} > 0 , \tag{3.38a}$$

$$\frac{\delta A_{k\sigma}}{\delta N_\sigma} > 0 \tag{3.38b}$$

for $n_\sigma = n_{\bar\sigma} < \frac{1}{2} - |\Phi_\sigma(\sigma)|$. Although $\bar P_{k\sigma}$ is minimal when the lower band is nearly half filled ($n_\sigma = n_{\bar\sigma} \approx \frac{1}{3}$) and

$$\frac{\delta\bar P_{k\sigma}}{\delta N_\sigma} \lesssim 0 ,\quad n_\sigma = n_{\bar\sigma} \lesssim \sim\tfrac{1}{3} . \tag{3.39}$$

We find

$$\frac{\delta\omega_{k\sigma}^{(1)}}{\delta N_\sigma} = \frac{[1 - n_{\bar\sigma} - \Phi_\sigma(\bar\sigma)]\delta\bar P_{k\sigma}}{\delta N_\sigma} - \frac{(\epsilon_k + \bar P_{k\sigma})\delta\Phi_\sigma(\bar\sigma)}{\delta N_\sigma} < 0 , \tag{3.40}$$

for $n_\sigma = n_{\bar\sigma} < \frac{1}{2} - |\Phi_\sigma(\sigma)|$, because when the lower band is more than half filled, the second term involving $\delta\Phi_\sigma(\bar\sigma)/\delta N_\sigma$ becomes dominant over $\delta\bar P/\delta N$. Inserting Eqs. (3.38b) and (3.40) into Eq. (3.34) yields

$$\mu(N) < 0 , \tag{3.41}$$

$$\Delta E_0(N) = \omega_{k_F\sigma}^{(1)} - \mu(N) > 0 , \tag{3.42}$$

in the partly-filled-lower-band case. We also find that the magnitude of $\Delta E_0(N)$ is of order Δ.

Exactly the same analysis can be extended to the evaluation of second derivatives, finding the thermodynamic-stability conditions (2.8) satisfied.[17]

If the number N of electrons increases further and $\delta = \frac{1}{2} - n_\sigma$ becomes comparable to $|\omega/I|$ and $|\Phi_\sigma(\sigma)|$, the solution satisfying the condition (3.36) no longer yields the ground state because, for $\delta < \Phi_\sigma(\sigma)$, $\bar P_{k\sigma}$ given by Eq. (3.37b) becomes positive. In this region, $\Phi_{\bar\sigma}(\bar\sigma)$ and $\Phi_{\bar\sigma}(\sigma)$ will deviate from $\Phi_\sigma(\sigma)$ and $\Phi_\sigma(\bar\sigma)$, respectively, and, in the nearly-half-filled limit, a solution satisfying the condition (3.2b) of Paper III,

$$\Phi_{\bar\sigma}(\sigma) = \Phi_\sigma(\sigma);\quad \Phi_{\bar\sigma}(\bar\sigma) = \Phi_\sigma(\bar\sigma) , \tag{3.43}$$

yields the ground state having the lowest energy.

In the nearly-half-filled limit, the magnitude of $S_\sigma(\bar\sigma)$ is mostly determined by $-\Phi_\sigma(\bar\sigma) - \bar P_{k\sigma}/I$ involved on the right-hand side of Eq. (3.35), making $S_\sigma(\bar\sigma)$ of order Δ/I. Under the condition (3.36), furthermore,

$$S_\sigma(\bar\sigma) = -S_\sigma(\sigma) , \tag{3.44}$$

and, as $n_\sigma = n_{\bar\sigma}$ increases, the magnitudes of $S_\sigma(\sigma)$ and $S_\sigma(\bar\sigma)$ increase as illustrated in Fig. 2. $\Phi_\sigma(\sigma)$ calculated from Eq. (3.15) of III is then negative and of order unity, while $\bar P_{k\bar\sigma}$ and $\omega_{k\bar\sigma}^{(1)}$ evaluated from Eq. (3.16) of III are negative and $\bar P_{k\bar\sigma} \ll \bar P_{k\sigma}$ and $\bar\omega_{k\bar\sigma}^{(1)} \ll \bar\omega_{k\sigma}^{(1)}$. The spectral weight for an added electron $k\sigma$,

$$A_{k\sigma}^{(1)} \approx 1 - n_{\bar\sigma} - \Phi_\sigma(\bar\sigma) + \cdots \approx \tfrac{1}{2} - |\Phi_\sigma(\bar\sigma)| , \tag{3.45}$$

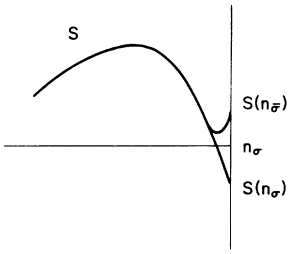

FIG. 2. Plots of $S_\sigma(\sigma)$ and $S_\sigma(\bar{\sigma})$ as functions of occupations n_σ.

is appreciably smaller than $\frac{1}{2}$, while the spectral weight for the corresponding electron k with opposite spin $\bar{\sigma}$

$$A_{k\bar{\sigma}}^{(1)} \approx 1 - n_\sigma - \Phi_\sigma(\sigma) + \cdots \approx \tfrac{1}{2} + |\Phi_\sigma(\bar{\sigma})| \qquad (3.46)$$

is nearly equal to one. This leads to the conclusion that, in the nearly-half-filled limit ($n_\sigma = n_{\bar{\sigma}} \approx \frac{1}{2}$), all states are occupied by single electrons with optimum energy $\omega_{k\bar{\sigma}}^{(1)}$ with $A_{k\bar{\sigma}}^{(1)} \approx 1$, and whenever an electron k with spin $\sigma = \uparrow$ or $\downarrow$ is added, the electron feels as if the state k is occupied by another electron with opposite spin $\bar{\sigma}$ and the added electron with $A_{k\sigma}^{(1)} \ll 1$ has difficulty finding an unoccupied state in the lower band, making its energy $\omega_{k\sigma}^{(1)}$ appreciably higher than that of the corresponding electron k with opposite spin $\bar{\sigma}$. Because the derivative of $S_\sigma(\bar{\sigma})$ introduces the factor,

$$[S_\sigma(\bar{\sigma})]^{-1}[\delta S_\sigma(\bar{\sigma})/\delta N_\sigma], \qquad (3.47)$$

of order I/Δ, derivatives of the Φ's and the P's can be accurately estimated giving

$$\begin{aligned} &\delta A_{k\bar{\sigma}}^{(1)}/\delta N_\sigma > 0, \\ &\delta \omega_{k\bar{\sigma}}^{(1)}/\delta N_\sigma < 0. \end{aligned} \qquad (3.48)$$

Since $A_{k\bar{\sigma}}^{(1)} \gg A_{k\sigma}^{(1)}$ for all k,[18] the chemical potential $\mu(N)$ evaluated from Eq. (3.34) is determined by the two quantities in Eq. (3.48), yielding

$$\mu(N) < 0, \qquad (3.49)$$

$$\Delta E_0(N) = \omega_{k_F\sigma}^{(1)} - \mu(N) > 0. \qquad (3.50)$$

We further find from Eq. (3.47) that $\Delta E_0(N)$ is of order I.

By increasing the filling $n_\sigma = n_{\bar{\sigma}}$ from zero to $\frac{1}{2}$, the state satisfying the condition (3.36) will gradually change to the state satisfying the condition (3.43), but an explicit calculation of such a gradual transition is difficult. In Ref. 17, instead, we have assumed Eq. (3.36) for $0 < n_\sigma < n_0$ and Eq. (3.43) for $n_0 < n_\sigma < \frac{1}{2}$ and show the dynamic stability for all n_σ, where n_0 is a number smaller than but nearly equal to $\frac{1}{2}$. Second derivatives can also be estimated in exactly the same manner, leading to the result that thermodynamic-stability conditions (2.8) are again satisfied.

In conclusion, the fully renormalized solution satisfies the dynamic- and thermodynamic-stability conditions for all occupations in the narrow-band limit.

IV. DISCUSSION

The results obtained in Sec. III may be summarized as follows. The Green's functions used have been obtained under various approximations. For each approximate Green's function the poles are, in principle, calculated correctly through terms linear in ϵ_k and hence are exact in the narrow-band limit ($\Delta/I \to 0$) within the approximation used to obtain each Green's function. The ground-state energy, the chemical potential, and the stability conditions, calculated by using a rigorous formalism, are therefore "exact" consequences of the approximate Green's function and reflect the nature of the approximate Green's function precisely in this limit. The power series expansions in Δ/I used in evaluating these quantities will not modify the conclusions of Sec. III.

All results following from all approximate Green's functions, including Hubbard I and the fully renormalized solution, clearly suggest that as long as I is finite, electrons in the Hubbard model do not behave like quasielectrons in the Landau theory of Fermi liquids, and the "quasielectron" energy $\omega_{k\sigma}$ calculated from the poles of the Green's function cannot be reproduced from the derivative of the ground-state energy with respect to the occupation of that electron, $\delta E_0(N)/\delta n_{k\sigma}$. This failure of the Landau theory is due to the fact that, when an electron is added to the system of N electrons, the whole system relaxes and the ground-state energy $E_0(N+1)$ of $N+1$ electrons is not given by the sum of the ground-state energy $E_0(N)$ of N electrons and the quasiparticle energy ω of the added electron in the split-band limit. Instead, a relaxation energy $\Delta E_0(N)$ appears between the two, yielding Eq. (1.1);

$$E_0(N+1) = E_0(N) + \omega_{k_F\sigma} - \Delta E_0(N). \qquad (4.1)$$

Consequently, the lowest energy of an electron added to the system of N electrons is not equal to the chemical potential $\mu(N)$

$$\begin{aligned} \mu(N) &= E_0(N+1) - E_0(N) \\ &= \omega_{k_F\sigma} - \Delta E_0(N) \neq \omega_{k_F\sigma}, \end{aligned} \qquad (4.2)$$

and, instead, a gap equal to $\Delta E_0(N)$ (>0) appears.

According to our estimate, the value of the gap $\Delta E_0(N)$ calculated from the fully renormalized solution is indeed positive for all occupations, (and of order Δ for the partly-filled-lower-band case and of order I for the nearly-filled-band case provided I is finite), illustrating that the system of $N+1$

electrons obtained by adding an electron is stable. Although this calculation involves approximations beyond simple expansions in powers of Δ/I and hence the result is no longer exact, the conclusions will remain valid, demonstrating the existence of a solution with the Hubbard-type two-peak structure. Our calculations also show that only the fully renormalized solution satisfies dynamic stability. All other solutions yield negative values for $\Delta E_0(N)$ for some occupations n, demonstrating their dynamic instability. Those previous solutions also yield thermodynamic instability for some occupations n, while the fully renormalized solution satisfies the thermodynamic-stability conditions for all occupations n. The reason for the appearances of those instabilities is obvious. Electron correlations are included insufficiently in all previous solutions, while sufficient correlations are included in our fully renormalized solution. This also suggests that thermodynamic properties of the Hubbard model cannot be calculated correctly unless the fully renormalized solution is used, at least in the narrow-band limit. We further note that, since the fully renormalized solution (and also the step-1 solution in Sec. III D) is exact up through terms in ϵ_k, our conclusions may be regarded as "rigorous" consequences of the Hubbard model when the lower band is half filled ($n_\sigma = n_{\bar\sigma} \approx \frac{1}{3}$) and the renormalization factors Φ involved in $\bar P_{k\sigma}$ are not dominant.

In Sec. III E, we have demonstrated that the nature of the solution in the region where the lower band is nearly or completely filled is quite different from that in the low-density region where the lower band is only partly filled. Here we shall show that these two types of solutions are already apparent among the previous solutions and allow us to classify them into two groups. The Hubbard-I and -III solutions belong to group I, where the leading term in the quasielectron energy $\omega^{(1)}_{k\sigma}$ has the form

$$\omega^{(1)}_{k\sigma} = (1 - n_{\bar\sigma})\epsilon_k + \cdots , \tag{4.3}$$

explicitly suggesting that the space occupied by electrons with opposite spin $\bar\sigma$ is not available for the motion of electrons with spin σ. This interpretation is supported by the fact that the Hubbard-III solution is equivalent to the CPA solution under the frozen-lattice approximation.[15] The solutions given by Eqs. (3.13), (3.19), and (3.21) belong to group II. The first one is the zeroth-order approximate solution discussed in Sec. II C, the second one is obtained by Esterling and Lange, and also by Fedro and Wilson, and the third one (step-1 solution) is the complete solution of the restricted equation discussed in Sec. III D, in which renormalization factors Φ are not included. The first two are expanded as

$$\omega^{(1)}_{k\sigma} = \epsilon_k + \cdots , \tag{4.4}$$

while the last one as

$$\omega^{(1)}_{k\sigma} = \frac{(1 - n_\sigma)^2}{1 - 2n_\sigma}\epsilon_k + \cdots . \tag{4.5}$$

Here electrons appear to hop through the lattice without the volume exclusion observed in the group-I solutions. The magnitude of the "kinetic" energy in Eq. (4.5) is, in fact, greater than that of the free-particle energy ϵ_k to compensate for restriction that, because of the small spectral weight $A^{(1)}_{k\sigma} \approx 1 - n_{\bar\sigma} < 1$, only a portion of each state is available for occupation by electrons in the lower band, thus increasing the total energy.

The fully renormalized solution exhibits the above two distinct properties. When the lower band is only partly filled, the volume exclusion will not appear since, just before an electron with spin σ tries to hop into an occupied site, the second electron $\bar\sigma$ can easily find an unoccupied site to move in and to avoid the large repulsive interaction I. Consequently, the probability for an electron σ to hop into a site may not be determined solely by the fact that, until a moment before the intended move, the site was occupied by another electron $\bar\sigma$, and hence the spectral weight $A^{(1)}_{k\sigma}$ for the first electron σ is by no means a "conjugate" of $A^{(1)}_{k\bar\sigma}$ for the second electron $\bar\sigma$. Instead, the motion of electron $k\sigma$ cannot be distinguished from that of electron $k\bar\sigma$, thus yielding $A^{(1)}_{k\sigma} = A^{(1)}_{k\bar\sigma}$, that is, $\Phi_{\bar\sigma}(\sigma) = \Phi_\sigma(\sigma)$ and $\Phi_{\bar\sigma}(\sigma) = \Phi_\sigma(\bar\sigma)$ and satisfying the condition (3.36). Our solution given by Eq. (3.29) can indeed be reduced to the form of the step-1 solution given by Eq. (3.21) except that $P_{k\sigma}$ is replaced by $\bar P_{k\sigma}$ given by Eq. (3.31). Hence, it can be expanded as shown in Eq. (4.5) but not in the form given by Eq. (4.3).

When the lower band is nearly filled, however, almost all sites are occupied and it is difficult for a second electron $\bar\sigma$ to find an unoccupied neighboring site to hop in, thus introducing a volume exclusion in this region. For example, if a site is occupied by a second electron $\bar\sigma$, the first electron σ cannot hop into the site, because the probability of finding the second electron $\bar\sigma$,

$$\sum_k A^{(1)}_{k\bar\sigma} f_{k\bar\sigma} e^{-ikR}/N_{\bar\sigma} \approx 1 - \langle N_\sigma \rangle \approx 1 - n_\sigma - \Phi_{\bar\sigma}(\sigma) , \tag{4.6}$$

at the site R at this time is nearly equal to unity, while the probability for the first electron σ to hop into the site R

$$\sum_k A^{(1)}_{k\sigma} f_{k\sigma} e^{-ikR}/N_\sigma \approx 1 - \langle N_{\bar\sigma} \rangle \approx 1 - n_{\bar\sigma} - \Phi_\sigma(\bar\sigma) \tag{4.7}$$

is nearly zero. This suggests that, in the nearly-

filled-lower-band case, condition (3.43) is satisfied and $\Phi_{\bar{\sigma}}(\sigma)=\Phi_{\sigma}(\sigma)$ and $\Phi_{\bar{\sigma}}(\bar{\sigma})=\Phi_{\sigma}(\bar{\sigma})$. In this region, our solution given by Eq. (3.29) can indeed be expanded in the form given by Eq. (4.3) but not in the form shown in Eq. (4.5) because of $F_{\sigma}(\bar{\sigma})$ given by Eq. (3.30). The foregoing discussion demonstrates the ability of the fully renormalized solution to exhibit the two types of properties. The above results, Eqs. (4.6) and (4.7), also show that, even though the lower band is not completely filled, an electron σ with a fixed momentum k will have difficulty finding vacant sites to hop through in the lower band in the atomic limit.

None of the previous solutions includes the fluctuations described by the Φ's explicitly, thus failing to satisfy the stability conditions in the nearly-filled-lower-band limit. In the partly filled case, we have shown that the most important quantity is $\bar{P}_{k\sigma}$. This quantity is not included in Hubbard I nor III, thus making those solutions unstable for all occupations n. In the zeroth-order approximate solution discussed in Sec. III C, the corresponding quantity $P_{k\sigma}^{(0)}$ has the form given by Eq. (3.28) and illustrated in Fig. 1(a), making this solution unstable when the lower band is more than half filled. In the absence of a renormalization, furthermore, the magnitude of $P_{k\sigma}^{(0)}$ is too small to maintain the stability even in the lower-density region. In the solutions obtained by Esterling and Lange and by Fedro and Wilson, the sign of $P_{k\sigma}^{(0)}$ is reversed, introducing more confusions but yielding equally unsatisfactory results. In the step-1 solution, renormalizations are overestimated in $P_{k\sigma}$ introducing the divergence in the perturbation expansion and instability of the solution in a large region of the occupations n.

It is also possible to explain why previous solutions exhibit either the properties in the partly filled case or the properties in the nearly filled case but none of them exhibits both of these properties. In Hubbard I and III, collisions between two electrons with opposite spins σ and $\bar{\sigma}$ are replaced by an average field by decoupling them. Hence sites occupied by electrons with opposite spin $\bar{\sigma}$ are permanently excluded, yielding the group-I solutions. In the group-II solutions, on the other hand, the collision terms, $\langle\langle C_{R\sigma}C_{R\bar{\sigma}}^{\dagger}C_{R''\bar{\sigma}};\ C_{R'\sigma}^{\dagger}\rangle\rangle$ etc., are calculated without including the strong repulsive interaction I, thus the volume exclusion involved in the nearly-filled-lower-band limit is completely neglected.

In the pathological limit $I=\infty$, the inequality $|\omega/I|>\frac{1}{2}-n_{\sigma}=\delta$ can never be satisfied and the solution given by Eqs. (3.14)–(3.16) of Paper III never appear. Instead, we find that the self-consistent solution satisfying Eqs. (2.15)–(2.22) of III is $\Phi_{\sigma}(\sigma)\simeq-\Phi_{\sigma}(\bar{\sigma})\simeq\frac{1}{2}$, yielding $\bar{P}_{k\sigma}(\omega)\simeq 0$ and $A_{k\sigma}^{(1)}\simeq 1$ or 0. The gap $\Delta E_0(N)$ then vanishes in agreement with Brinkman and Rice's calculation.[12,19] We shall discuss the relaxation mechanism yielding the energy gap and consequences of the energy gap in the following paper (Ref. 11).

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terial also appears in Current Physics Microfilm, the monthly microfilm edition of the complete set of journals published by AIP, on the frames immediately following this journal article.

[18]The ground state of N electrons is constructed by adding spin-up and spin-down electrons one by one. σ denotes the spin of an added electron and can be up or down.

[19]This pathological limit has been calculated in Ref. 17. See Eqs. (3.67)–(3.70) of Ref. 17.