Single-Particle Excitations in Narrow Energy Bands

A. BROOKS HARRIS*
Theoretical Physics Division, Atomic Energy Research Establishment, Harwell, Didcot, Berkshire, England and Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania
AND
ROBERT V. LANGE†
Theoretical Physics Division, Atomic Energy Research Establishment, Harwell, Didcot, Berkshire, England; Department of Physics, Oxford University, Oxford, England; and Department of Physics, Brandeis University, Waltham, Massachusetts

(Received 15 December 1966)

Hubbard's model for studying correlation effects in systems with narrow energy bands is analyzed by means of a technique which allows the calculation of moments of the individual peaks in the spectral weight function for single-particle excitations. The analysis of the zeroth moments of the peaks shows that the total weight in the bands depends on the strength of the kinetic-energy term in the Hamiltonian even though the bands may be narrow and widely separated. This conclusion is illustrated and verified by an exact calculation for the case when there are only two lattice sites. Analysis of first and higher moments yields results for nonmagnetic or paramagnetic phases which are in qualitative agreement with Hubbard's improved solution. However, we find that (a) there occurs a spin-dependent shift in the band energies which has not been obtained by other treatments of the model and which energetically favors ferromagnetism, and (b) single-particle excitations are more heavily damped in antiferromagnetic than in isomorphic paramagnetic phases.

I. INTRODUCTION

MANY problems in theoretical physics are attacked by considering models with mathematical descriptions which are usefully simpler than those of real systems. So long as the model builder has sufficient insight into the physical mechanisms dominating the real problem and sufficient insight into the model itself, this approach can be very illuminating. Of course, the model is usually not exactly soluble and consequently approximations must be employed. Thus we often find ourselves with approximate solutions to a model problem. When we want to know how to make connection with experiment two levels of question arise. First, how well do the approximate solutions reflect the exact properties of the model, and then second, of course, how well does the model reflect the properties of real systems?

This paper directs itself for the most part at the first type of question. We have devised a method[1] of analyzing the narrow-energy-band model studied by Hubbard[2] and others.[3–6] Our technique illuminates several properties of the spectral weight and density of state functions for the electrons which are unambiguously real within this model and not manifestations of an approximation scheme. Our results therefore shed considerable light on the model and to the extent that the model is sound, give information about the real narrow energy-band systems with which it is associated. Our results can also be used to check particular aspects of approximation schemes to see if the relationships we derive are found to be true for such approximate solutions.

Hubbard's model is essentially a cell model for the electron gas with Coulomb repulsion completely screened out except between electrons in the same cell, or as it is referred to in this context, on the same crystal site. In its simpler form only a single s band is considered, that is, there is just one spatial state per site. Thus this model is essentially the simplest in which the kinetic energy and band shape, the Coulomb repulsion and correlation effects, and of course the exclusion principle can all be seen working together and against one another in a context related to electrical and magnetic properties of the transition metals and transition-metal oxides.

Our approach to the problem is built around moment techniques. We have devised a way to project out of the density of states and spectral weight functions of the theory, those parts referring to individual energy bands. The moments of individual bands can then be expressed in terms of correlation functions in a systematic way. Of course, the correlation functions themselves can only be estimated or approximately calculated, but their relationships to the moments of the bands are rigorous. It is in these relationships that most of our results lie although we do make some further approximations in order to calculate the correlation functions and demonstrate some of the implications of the relationships.

* Supported in part by the Advanced Research Projects Agency.
† Work done in part while on a National Science Foundation Post-Doctoral Fellowship and supported in part by National Science Foundation Grant No. GP5374.

[1] This work was previously described in Bull. Am. Phys. Soc. **11**, 182 (1966).
[2] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963).
[3] J. Kanamori, Progr. Theoret. Phys. (Kyoto) **30**, 275 (1963).
[4] T. Izuyama, D. Kim, and R. Kubo, J. Phys. Soc. Japan **18**, 1025 (1963).
[5] M. Gutzwiller, Phys. Rev. **137**, A1726 (1965).
[6] D. Langreth, Phys. Rev. **148**, 707 (1966).

After defining mathematical quantities in Sec. II, we present in Sec. III an exact solution for the special case in which there are only two sites. Our purpose is to illustrate in a transparent way one of the perhaps most surprising properties of this model and to show in passing that this property is easily expressed as a relationship between band moments and correlation functions. What is shown is that the total number of states in particular energy bands can increase or decrease linearly with the strength of the kinetic energy or "hopping" term in the Hamiltonian, no matter how small this term is compared to the separation between bands.

In Sec. IV we develop the projection technique which gives us the spectral weight associated with each band for the infinite system. We utilize a canonical transformation used by Kohn[7] in a related problem. While our technique is quite general, we can only get explicit expressions for the generator of the transformation and other quantities involved if we make expansions in terms of a parameter proportional to the kinetic divided by the potential energy and thus our explicit results are restricted to the narrow band situations and can not be extended in their present form to cases in which bands broaden to the point of merging. It is in this section that we show how to relate moments of the individual bands to equal time expectation values or particular correlation functions. Our approach is an extension of the well-known moment calculations as applied to nuclear-magnetic- or electron-spin-resonance line shapes.[8–11]

In Sec. V our technique is applied to the question raised in Sec. III, namely to the shift in weight from one band to another due to the hopping or kinetic energy. We find that this shift occurs in the infinite site case as it did in the two site case and contrast this with simple models of alloys and interband mixing for which such a shift does not occur. We also show that the shift does not occur in the one case where it would have a drastic affect on the electrical properties, that is, when there is precisely one electron per site and therefore a precisely filled lower band.

In Sec. VI we illustrate how our relationships can be used to check other forms of calculation by comparing the band narrowing and energy shift predictions in Hubbard's approximate Green's functions calculations[1,12] with our predictions of the same quantities.

Finally we analyze in Secs. VII and VIII the implications of our work in the possible ferromagnetic and antiferromagnetic cases which are embodied in this model. We find that the energy shifts predicted by the moments play a dominant role in ferromagnetic stability. For the one electron per site case in which the ground state is antiferromagnetic we are able to show that the one electron states of precise wave number are broadened to a larger extent than when the system is paramagnetic.

II. FORMALISM AND DEFINITIONS

Using the notation of Hubbard,[2] we write the Hamiltonian for the model as

$$\mathcal{H}=\sum_{ij\sigma} T_{ij}c^{\dagger}_{i\sigma}c_{j\sigma}+I\sum_{i} n_{i\uparrow}n_{i\downarrow}. \tag{2.1}$$

The operator $c^{\dagger}_{i\sigma}$ creates an electron in a Wannier state centered about the atomic core at position R_i with z component of spin $\frac{1}{2}\sigma$, where $\sigma=\pm 1$. We are considering only one Wannier function per atomic site, and those referring to different sites are orthogonal, so that we have the usual Fermion anticommutation relation

$$\{c^{\dagger}_{i\sigma}, c_{j\sigma'}\}_{+}=\delta_{ij}\delta_{\sigma\sigma'}. \tag{2.2}$$

The coefficients T_{ij} in the kinetic energy term are related to the Bloch energies $\epsilon(k)$ corresponding to the single-electron states in the lattice by the relation

$$T_{ij}=N^{-1}\sum_{\mathbf{k}} \epsilon(\mathbf{k})\,\exp[i\mathbf{k}\cdot(\mathbf{R}_i-\mathbf{R}_j)], \tag{2.3}$$

where N is the number of sites. We take $T_{ii}=0$; however our formulas can easily be generalized to the case $T_{ii}\neq 0$. We do not assume a particular form for $\epsilon(\mathbf{k})$ so that the model can be used to discuss bands of different shapes and properties. In Sec. IV we shall find it convenient to write $T_{ij}\equiv\Delta t_{ij}$ where Δ is the root-mean-square band width:

$$\sum_{j}|T_{ij}|^2=\Delta^2; \qquad \sum_{j}|t_{ij}|^2=1. \tag{2.4}$$

Using this convention, one has a single expansion parameter Δ/I, the t_{ij} being regarded as constants which describe the shape of the band but not its size. The constant I is the Coulomb energy due to the repulsion between two electrons of opposite spin at the same site and appears in the Hamiltonian multiplied by the number operator $n_{i\sigma}$ and $n_{i-\sigma}$, where as usual

$$n_{i\sigma}=c^{\dagger}_{i\sigma}c_{i\sigma}. \tag{2.5}$$

By using this model we ignore Coulomb repulsion between electrons unless the electrons are at the same site.

We will use thermodynamic averages defined with respect to the canonical ensemble. For any operator B we define the expectation value of B by

$$\langle B\rangle\equiv Z^{-1}\,\mathrm{Tr}[\exp(-\beta\mathcal{H})B], \tag{2.6}$$

where

$$Z=\mathrm{Tr}\,\exp(-\beta\mathcal{H}). \tag{2.7}$$

[7] W. Kohn, Phys. Rev. **133**, A171 (1964).
[8] J. H. Van Vleck, Phys. Rev. **74**, 1168 (1948).
[9] R. Kubo and K. Tomita, J. Phys. Soc. Japan **9**, 888 (1954).
[10] M. H. L. Pryce and K. W. H. Stevens, Proc. Phys. Soc. (London) **A63**, 36 (1950).
[11] M. McMillan and W. Opechowski, Can. J. Phys. **38**, 1168 (1960).
[12] J. Hubbard, Proc. Roy. Soc. (London) **A281**, 401 (1964).

The trace is the diagonal sum over states having a fixed number N_e of electrons. In Sec. III we will find it useful to indicate explicitly the number of electrons present with subscripts of the form $\{\uparrow\uparrow\downarrow\}$ in which the numbers of up and down arrows specify the number of spin-up and spin-down electrons, respectively.

The one-electron spectral weight function[13,14] (SWF) is defined as follows:

$$A^{\sigma}{}_{ij}(\omega)=2\pi Z^{-1}\sum_{a,b}\delta(\omega-E_b+E_a)\langle a\mid c_{i\sigma}\mid b\rangle\langle b\mid c^{\dagger}{}_{j\sigma}\mid a\rangle\exp(-\beta E_a)$$
$$+2\pi Z^{-1}\sum_{ad}\delta(\omega-E_a+E_d)\langle a\mid c^{\dagger}{}_{j\sigma}\mid d\rangle\langle d\mid c_{i\sigma}\mid a\rangle\exp(-\beta E_a). \quad (2.8)$$

Here $\mid a\rangle$, $\mid b\rangle$, and $\mid d\rangle$ are eigenstates by the full many-body Hamiltonian H with energy eigenvalues E_a, E_b, and E_d. Note that using the canonical ensemble the states $\mid b\rangle$ and $\mid d\rangle$ have, respectively, N_e+1 and N_e-1 particles. If the subscripts i and j are replaced by momentum variables one obtains a definition for the SWF $A^{\sigma}{}_{\lambda\lambda'}(\omega)$ which for a homogeneous system vanishes unless $\lambda=\lambda'$. The electron density of states is defined by

$$\rho^{\sigma}(E)=(2\pi N)^{-1}\sum_{i}A^{\sigma}{}_{ii}(E)=(2\pi N)^{-1}\sum_{\lambda}A^{\sigma}{}_{\lambda\lambda}(E). \quad (2.9)$$

When we confine our attention to homogeneous systems, we have

$$\rho^{\sigma}(E)=(1/2\pi)A^{\sigma}{}_{ii}(E), \quad (2.10)$$

where i refers to an arbitrary site. Multiplying the function $\rho^{\sigma}(E)$ by appropriately chosen Fermi factors gives the density of filled and empty electron states at energy E.

The basis for the moment technique is the relation between the anticommutator and the SWF

$$\langle\{c_{i\sigma}(i),\,c^{\dagger}{}_{j\sigma}(t')\}_{+}\rangle=\int_{-\infty}^{+\infty}A^{\sigma}{}_{ij}(\omega)\,\exp[-i\omega(t-t')](d\omega/2\pi), \quad (2.11)$$

which follows directly from Eq. (2.8).

III. EXACTLY SOLUBLE TWO-SITE MODEL

In this section we will discuss the exact density of states calculated for the version of the model for which there are only two sites. The Hamiltonian is

$$\mathcal{H}=t\sum_{i\neq j,\sigma}c^{\dagger}{}_{i\sigma}c_{j\sigma}+I\sum_{i}n_{i\uparrow}n_{i\downarrow}, \quad (3.1)$$

where i and j range over just two values, 1 and 2. This simple model gives a direct and exact illustration of important points we utilize in our discussion of the infinite crystal in the next section.

The functions we will be studying in this section are $\rho^{\uparrow}{}_{\{\downarrow\}}(E)$ and $\rho^{\uparrow}{}_{\{\uparrow\downarrow\}}(E)$. In accordance with the notation introduced in the previous section these are the density of states for the addition of one up-spin electron to a system already containing, respectively, one down-spin electron, and two electrons of opposite spin.

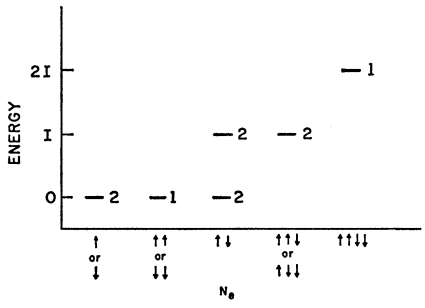

FIG. 1. Energy levels for the two-site model for $t=0$. Each column corresponds to a fixed number of up- and down-spin electrons as indicated by the arrows.

In order to illustrate clearly the changes in $\rho^{\uparrow}{}_{\{\downarrow\}}(E)$ induced by the kinetic energy we first calculate $\rho^{\uparrow}{}_{\{\downarrow\}}(E)_0$, its value for zero t. Thus, we find the density of states for a spin-up electron for the system containing one spin-down electron when no hopping is allowed. For this purpose we have calculated the energy levels and their degeneracies for $t=0$ as shown in Fig. 1. Matrix elements referring to transitions from the first to the third columns in Fig. 1 will be involved. The eigenstates in the case $\{N_e\}=\{\downarrow\}$ are given in Table I. For the four states when $\{N_e\}=\{\uparrow\downarrow\}$, labeled by b in Eq. (2.8) we use those in Table II. Since $Z\{\downarrow\}=2$ we get

$$\rho^{\uparrow}{}_{\{\downarrow\}}(E)_0=\tfrac{1}{2}\sum_{ab}\delta(E-E_b+E_a)\mid\langle b\mid c^{\dagger}{}_{i\uparrow}\mid a\rangle\mid^2 \quad (3.2a)$$

$$=\tfrac{1}{2}\delta(E)+\tfrac{1}{2}\delta(E-I). \quad (3.2b)$$

The density of states is equally distributed between

[13] Had we chosen a grand canonical ensemble, the natural generalization of Eq. (28) would coincide with the usual definition (Ref. 14) of the SWF corresponding to the Green's function

$$G_{ij}{}^{\sigma}(t,t')\equiv-i\langle T(c_{i\sigma}(t)c_{j\sigma}{}^{\dagger}(t'))\rangle.$$

[14] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962).

TABLE I.[a] Eigenstates and eigenvalues for $\{N_e\}=\{\downarrow\}$ and $t=0$.

State	Energy
$\|a_1\rangle=c_{1\downarrow}^\dagger\|0\rangle$	0
$\|a_2\rangle=c_{2\downarrow}^\dagger\|0\rangle$	0

[a] The symbol $|0\rangle$ signifies the vacuum state.

two bands,[15] one at zero energy and the other at energy I.

We now let t be nonzero and carry out the same calculation. The degeneracies in the spectrum of Fig. 1 will be split, but we will keep t small so that the energy shifts of the eigenstates are small compared to I. This is the "narrow-band limit" for our simple case. For $N_e=\{\downarrow\}$, the state table is given in Table III. Now,

$$Z_{\{\downarrow\}}=e^{\beta t}+e^{-\beta t}. \tag{3.3}$$

For $\{N_e\}=\{\uparrow\downarrow\}$ the situation is only slightly more complicated. If we take for a basis the four vectors defined by the equations

$$\begin{aligned}
|1\rangle&=(2)^{-1/2}(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}+c^\dagger_{2\uparrow}c^\dagger_{2\downarrow})\,|0\rangle,\\
|2\rangle&=(2)^{-1/2}(c^\dagger_{1\uparrow}c^\dagger_{1\downarrow}-c^\dagger_{2\uparrow}c^\dagger_{2\downarrow})\,|0\rangle,\\
|3\rangle&=(2)^{-1/2}(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}+c^\dagger_{2\uparrow}c^\dagger_{1\downarrow})\,|0\rangle,\\
|4\rangle&=(2)^{-1/2}(c^\dagger_{1\uparrow}c^\dagger_{2\downarrow}-c^\dagger_{2\uparrow}c^\dagger_{1\downarrow})\,|0\rangle,
\end{aligned} \tag{3.4}$$

the Hamiltonian becomes the 4×4 matrix

$$\begin{bmatrix} I & 0 & 2t & 0\\ 0 & I & 0 & 0\\ 2t & 0 & 0 & 0\\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{3.5}$$

Diagonalization of this matrix gives the eigenstates and eigenvalues found in Table IV. In Table IV we use the notation

$$E_\pm=\tfrac{1}{2}I\pm(4t^2+\tfrac{1}{4}I^2)^{1/2}. \tag{3.6}$$

The relevant energy-level diagram is given in Fig. 2. All the degeneracy is removed. The density of states is given by

$$\rho^{\uparrow}_{\{\downarrow\}}(E)=(e^{\beta t}+e^{-\beta t})^{-1}\sum_{ab}\delta(E-E_b+E_a)\exp(-\beta E_a)\,|\langle b\,|\,c^\dagger_{i\sigma}\,|\,a\rangle|^2, \tag{3.7}$$

where the summation is over the a and b states which appear in Tables III and IV, respectively. As expected the density of states is independent of whether operators for site 1 or site 2 are inserted into the above matrix elements, and is given as

$$\begin{aligned}
\rho^{\uparrow}_{\{\downarrow\}}(E)=&[4(1+e^{-2\beta t})]^{-1}\{[(1-\lambda_+)^2/(1+\lambda_+^2)]\delta(E-E_+-t)+\delta(E-I-t)+[(1+\lambda_+)^2/(1+\lambda_+^2)]e^{-2\beta t}\\
&\times\delta(E-E_++t)+e^{-2\beta t}\delta(E-I+t)+\delta(E-t)+[(1-\lambda_-)^2/(1+\lambda_-^2)]\delta(E-E_--t)+e^{-2\beta t}\delta(E+t)\\
&+[(1+\lambda_-)^2/(1+\lambda_-^2)]e^{-2\beta t}\delta(E-E_-+t)\},
\end{aligned} \tag{3.8}$$

where

$$\lambda_\pm=(1/2t)\,E_\pm. \tag{3.9}$$

The function on the right-hand side of Eq. (3.8) has weight at eight distinct energies, four of which are clustered near I forming an upper band and four clustered near zero forming a lower band. The weight in the upper band is given by an integral of $\rho^{\uparrow}_{\{\downarrow\}}(E)$ over a range of energy including the upper band only and is therefore, equal to the sum of coefficients of the first four delta functions in Eq. (3.8). Thus we get

$$\rho_u\equiv\int_{\text{upper band}}\rho^{\uparrow}_{\{\downarrow\}}(E)\,dE, \tag{3.10a}$$

$$\rho_u=\tfrac{1}{2}-\frac{(1-e^{-2\beta t})}{(1+e^{-2\beta t})}\left[\frac{tE_+}{IE_++8t^2}\right], \tag{3.10b}$$

and

$$\rho_l=\int_{\text{lower band}}\rho^{\uparrow}_{\{\downarrow\}}(E)\,dE, \tag{3.11a}$$

$$\rho_l=\tfrac{1}{2}+\frac{(1-e^{-2\beta t})}{(1+e^{-2\beta t})}\left[\frac{tE_+}{IE_++8t^2}\right]. \tag{3.11b}$$

It is obvious that the sum rule

$$\int_{-\infty}^{+\infty}\rho^{\uparrow}_{\{\downarrow\}}(E)\,dE=1 \tag{3.12}$$

[15] Our use of the word "band" may be somewhat unorthodox but we believe quite useful. Band theory is based on the one-electron approximation whereby an effective one-body Hamiltonian is constructed. We prefer to regard this as a particular approximation to the SWF, i.e., the quasiparticle approximation. Whereas finite lifetimes are difficult to reconcile with a band picture, they are naturally incorporated into the SWF which allows one to form a physical picture of approximations more sophisticated than the one-electron models. Accordingly, we refer to an upper and lower band although this type of effect due to correlations cannot be adequately accounted for by the usual band models.

TABLE II. Eigenstates and eigenvalues for $\{N_e\}=\{\uparrow\downarrow\}$ and $t=0$.

State	Energy
$\lvert b_1\rangle=c_{1\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}\lvert 0\rangle$	0
$\lvert b_2\rangle=c_{2\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}\lvert 0\rangle$	0
$\lvert b_3\rangle=c_{1\uparrow}^{\dagger}c_{1\downarrow}^{\dagger}\lvert 0\rangle$	I
$\lvert b_4\rangle=c_{2\uparrow}^{\dagger}c_{2\downarrow}^{\dagger}\lvert 0\rangle$	I

is satisfied for all t. For the narrow band case, $(t/I)\ll 1$, the expressions simplify to

$$\rho_u=\tfrac{1}{2}-(t/I)\,(1-e^{-2\beta t}/1+e^{-2\beta t}), \qquad (3.13a)$$

and

$$\rho_l=\tfrac{1}{2}+(t/I)\,(1-e^{-2\beta t}/1+e^{-2\beta t}). \qquad (3.13b)$$

The atomic-limit value of $\frac{1}{2}$ for ρ_u and ρ_l is obtained only at infinite temperature.

In order to understand this result we must recall the way the degeneracy was removed for the case $\{N_e\}=\{\downarrow\}$ by the nonzero t. In Table III the ground state and excited state are listed and in each there is a definite phase relation between parts referring to different sites. If the previous calculation of ρ_u and ρ_l have been done with these phases randomized rather than kept at their actual values the result would have been $\rho_u=\rho_l=\frac{1}{2}$. At infinite temperature this randomization is effectively carried out since thermodynamic averages become simply expectation values in an equal and incoherent mixture of the ground state and excited state. At any finite temperature the unequal weighting of the two states in thermodynamic average prevents the interference due to these phases from being completely obliterated.

Another quantity which clearly reflects these distinct phases is the expectation value of the interatomic kinetic energy per site $\mathfrak{I}_\sigma$ given by

$$\mathfrak{I}_\sigma=\tfrac{1}{2}t\sum_{i\neq j}\langle c^{\dagger}_{i\sigma}c_{j\sigma}\rangle. \qquad (3.14)$$

We will calculate again for the case $\{N_e\}=\{\downarrow\}$ and use the states from Table III. The necessary matrix elements are

$$\langle a_1\mid c^{\dagger}_{i\downarrow}c_{j\downarrow}\mid a_1\rangle=-\tfrac{1}{2}, \qquad i\neq j \qquad (3.15a)$$

$$\langle a_2\mid c^{\dagger}_{i\downarrow}c_{j\downarrow}\mid a_2\rangle=\tfrac{1}{2}, \qquad i\neq j \qquad (3.15b)$$

so that we get

$$\mathfrak{I}_{\downarrow\{\downarrow\}}=-\tfrac{1}{2}t(1-e^{-2\beta t}/1+e^{-2\beta t}). \qquad (3.16)$$

In this calculation, as in that for ρ_u and ρ_l, the existence

TABLE III. Eigenstates and eigenvalues for $\{N_e\}=\{\downarrow\}$ and nonzero t.

State	Energy
$\lvert a_1\rangle=2^{-1/2}(c_{1\downarrow}^{\dagger}-c_{2\downarrow}^{\dagger})\lvert 0\rangle$	$-t$
$\lvert a_2\rangle=2^{-1/2}(c_{1\downarrow}^{\dagger}+c_{2\downarrow}^{\dagger})\lvert 0\rangle$	t

TABLE IV.[a] Eigenstates[b] and eigenvalues for $\{N_e\}=\{\uparrow\downarrow\}$ and nonzero t.

State	Energy
$\lvert b_1\rangle=(\lambda_-\lvert 1\rangle+\lvert 3\rangle)/(1+\lambda_-^2)^{1/2}$	E_-
$\lvert b_2\rangle=\lvert 4\rangle$	0
$\lvert b_3\rangle=\lvert 2\rangle$	I
$\lvert b_4\rangle=(\lambda_+\lvert 1\rangle+\lvert 3\rangle)/(1+\lambda_+^2)^{1/2}$	E_+

[a] $\lambda_\pm=(1/2t)E_\pm$, see Eq. (3.6).
[b] States $\lvert 1\rangle$, $\lvert 2\rangle$, etc. are defined in Eq. (3.4).

of precise phase relationships in $\lvert a_1\rangle$ and $\lvert a_2\rangle$ is important. In fact, the calculations are closely related and if we wished we could use this result to write for $t\ll I$

$$\rho_u=\tfrac{1}{2}+2\,\mathfrak{I}_{\downarrow\{\downarrow\}}/I, \qquad (3.17a)$$

$$\rho_l=\tfrac{1}{2}-2\,\mathfrak{I}_{\downarrow\{\downarrow\}}/I. \qquad (3.17b)$$

In the next section we will find that the kinetic energy can be related to the redistribution of the density of states among the bands for the infinite crystal as well. The general feature of these calculations which we must carry over to the infinite array is simply the following. There is a great deal of degeneracy in the atomic limit in this model, since the energy of a state is a function only of the number of doubly occupied atoms. When the hopping is turned on there is a zero-order mixing of states of equal unperturbed energy characteristic of degenerate perturbation theory. Ordinarily the detailed nature of this phenomenon can be calculated only for simple situations such as those we discuss in this section. In the general case such a calculation becomes a very difficult excluded volume problem. Although we can not solve such a cooperative problem for the infinite crystal we will assume that matrix elements such as those appearing in Eqs. (3.14) and (3.15) can be nonzero and independent of t/I for t/I small. That is, a quantity like $\mathfrak{I}_\sigma$ is of order t and not of order t^2/I. No approximation scheme based on the notion that quantities such as $\langle c_{i\sigma}^{+}c_{j\sigma}\rangle$ for $i\neq j$ must be at least first order in t/I can possibly treat $\mathfrak{I}_\sigma$ accurately enough to allow a prediction of ρ_u and ρ_l to first order in t/I.

Before going on to the infinite array in the next section, let us see how ρ_u and ρ_l depend on t in the special

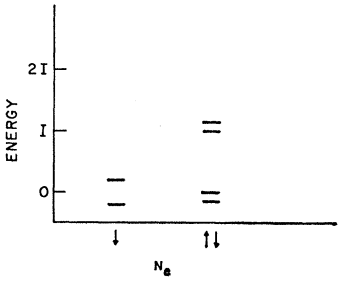

FIG. 2. Energy levels for the two-site model for $t\ll I$. The value $t=0.2I$ was used. Each column corresponds to a fixed number of up- and down-spin electrons as indicated by the arrows.

TABLE V. Eigenstates and eigenvalues needed to evaluate Eq. (3.18).

State	Energy
$\|b\rangle=(\lambda_-\|1\rangle+\|3\rangle)/(1+\lambda_-^2)^{1/2}$	E_-
$\|a_1\rangle=2^{-1/2}(c_{1\downarrow}^\dagger-c_{2\downarrow}^\dagger)c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger\|0\rangle$	$I-t$
$\|a_2\rangle=2^{-1/2}(c_{1\downarrow}^\dagger+c_{2\downarrow}^\dagger)c_{1\uparrow}^\dagger c_{2\uparrow}^\dagger\|0\rangle$	$I+t$
$\|d_1\rangle=2^{-1/2}(c_{1\downarrow}-c_{2\downarrow})\|0\rangle$	$-t$
$\|d_2\rangle=2^{-1/2}(c_{1\downarrow}^\dagger+c_{2\downarrow}^\dagger)\|0\rangle$	t

case of one electron per atom at zero temperature. This is the molecular analogy to substances like NiO or the collection of hydrogenic atoms studied by Kohn.[7] In the atomic limit there are two bands of which the lower one is completely full. There is an energy gap between the empty and filled bands which leads to a prediction of insulating properties. The work of Mott[16] and Hubbard[12] on the transition from insulator to conductor which must occur when the hopping has increased sufficiently depends critically on the lower band being precisely full and the upper band precisely empty as long as the bands are distinct. This guarantees that the gap between the bands acts as an energy gap for single-particle excitations. Our discovery that the density of states in each band can change with the hopping parameters may seem to contradict this picture. If single-particle excitations move from one band to the other, either the lower band will be partially empty or the upper band partially full and the energy gap will lose its significance. However, we now show that when there is one electron per atom the zero temperature values of ρ_u and ρ_l are in fact independent of t. At finite temperature there will of course be thermally excited electrons in the upper band. This effect, which is characteristic of semiconductors is not of interest to us here, however.

At zero temperature $\rho^{\uparrow}{}_{\{\uparrow\downarrow\}}(E)$ is given by

$$\rho^{\uparrow}{}_{\{\uparrow\downarrow\}}(E)=\sum_a \delta(E-E_a+E_b)\,|\langle a\,|\,c_{1\uparrow}^\dagger\,|\,b\rangle|^2+\sum_d \delta(E-E_b+E_d)\,|\langle d\,|\,c_{1\uparrow}\,|\,b\rangle|^2, \tag{3.18}$$

where the states needed are given in Table V.

Performing the summation we get

$$\rho^{\uparrow}{}_{\{\uparrow\downarrow\}}(E)=\frac{(1-\lambda_-)^2}{4(1+\lambda_-^2)}\,\delta(E-I+t+E_-)+\frac{(1+\lambda_-)^2}{4(1+\lambda_-^2)}\,\delta(E-I-t+E_-)$$
$$+\frac{(1+\lambda_-)^2}{4(1+\lambda_-^2)}\,\delta(E-E_-+t)+\frac{(1-\lambda_-)^2}{4(1+\lambda_-^2)}\,\delta(E-E_--t). \tag{3.19}$$

Here we again find weight at energies clustered near I and near zero defining two bands. Integrating $\rho^{\uparrow}{}_{\{\uparrow\downarrow\}}(E)$ over the bands separately we find

$$\rho_u=\frac{(1+\lambda_-)^2}{4(1+\lambda_-^2)}+\frac{(1-\lambda_-)^2}{4(1+\lambda_-^2)}=\tfrac{1}{2}, \tag{3.20a}$$

and likewise

$$\rho_l=\tfrac{1}{2}. \tag{3.20b}$$

Both ρ_u and ρ_l are independent of t and are equal to their values in the atomic limit. Thus as t increases, the lower band remains full and available states for an electron are found only above an energy gap equalling the gap between the bands.

Another way we can see that this has to be the case is to look at the energy level diagram, Fig. 1. For $t=0$, the lowest state for the three-electron system lies at an energy I above the lowest state for the two-electron system. This is because there is precisely one electron on each atom in the ground state and another electron cannot be added without some atom being doubly occupied. For nonzero but small $t(t\ll I)$ these ground-state energies change only slightly and there is still an energy of the order of I which must be supplied to add an electron. This must be reflected in the band picture as a full band separated by a gap from an empty band. Only in the one electron per atom case is there such a simple relationship between the band picture and the energy levels for the entire system. In the next section we will see that the relationship between kinetic energy and the band weights ρ_u and ρ_l is more complicated than is suggested by Eq. (3.17) but that it is modified in a way which yields the special result for this half-filled band case.

To summarize the results of this section: We have shown that for a two-site model the total weights in the lower and upper bands are not maintained at their atomic-limit values as the hopping is turned on. It might be argued that these effects are of order $(1/N)$ and hence become unimportant for large systems. As we shall see in the next section this is not the case; that is, the shift in weight from one band to the other is of order 1 and not of order $(1/N)$ and hence persists even for large systems.

IV. THE MOMENT TECHNIQUE

We now turn our attention toward approximate calculations for the many-body system. We aim to obtain

[16] N. F. Mott, Proc. Phys. Soc. (London) **A62**, 416 (1949); Phil. Mag. **6**, 287 (1961).

information about the spectral weight function (SWF) by calculating some of the lowest-order moments associated with the peaks in the SWF. This approach is most useful when the SWF consists of isolated peaks whose breadth is much less than the separation between successive peaks. For $\Delta \ll I$ this condition is probably well fulfilled, so that a moment calculation is expected to be fruitful.

The moments of the SWF are defined as

$$M^n{}_{uv\sigma}=\int_{-\infty}^{+\infty} A^\sigma{}_{uv}(\omega)\omega^n(d\omega/2\pi), \tag{4.1}$$

where u and v are either position or momentum labels. For convenience we introduce the characteristic function $f^\sigma{}_{uv}(t)$:

$$f^\sigma{}_{uv}(t)=\sum_n M^n{}_{uv\sigma}(-it)^n(n!)^{-1}$$

$$=\int_{-\infty}^{+\infty} A^\sigma{}_{uv}(\omega)e^{-i\omega t}(d\omega/2\pi). \tag{4.2}$$

According to (2.11) the characteristic function has a simple interpretation:

$$f^\sigma{}_{uv}(t-t')=\langle\{c_{u\sigma}(t), c^\dagger{}_{v\sigma}(t')\}_+\rangle. \tag{4.3}$$

Note that according to (4.2)

$$M^n{}_{uv\sigma}=(i\partial/\partial t)^n f^\sigma{}_{uv}(t)\mid_{t=u} \tag{4.4a}$$

$$=(i\partial/\partial t)^r(-i\partial/\partial t')^{n-r}f^\sigma{}_{uv}(t-t')\mid_{t=t'}, \tag{4.4b}$$

irrespective of the choice of r. Explicitly Eq. (4.4b) is

$$M^n{}_{uv\sigma}=\langle\{[\cdots[[c_{u\sigma},\underbrace{\mathcal{H}],\mathcal{H}],\cdots,\mathcal{H}}_{r\text{ factors}}],$$
$$[\underbrace{\mathcal{H},\cdots,[\mathcal{H},[\mathcal{H},c^\dagger{}_{v\sigma}]]\cdots]}_{n-r\text{ factors}}\}_+\rangle. \tag{4.5}$$

In general the lowest few moments of the full SWF give little insight into the detailed shape of the SWF. On the other hand, from the lowest few moments of the individual peaks in the SWF we can obtain a great deal of useful information.

We decompose the Hamiltonian as follows:

$$\mathcal{H}=\mathcal{H}_0+V, \tag{4.6}$$

where

$$\mathcal{H}_0=I\sum_i n_{i\uparrow}n_{i\downarrow}, \tag{4.7a}$$

$$V=\Delta\sum_{ij\sigma} t_{ij}c^\dagger{}_{i\sigma}c_{j\sigma}. \tag{4.7b}$$

If $\Delta=0$ it is easy to see that the SWF will be nonzero only at the precise energies 0 and I. This result obtains because the Hamiltonian $\mathcal{H}_0$ has eigenstates which can be labeled by the number d of doubly occupied sites and the energy of such a state is then just equal to dI. If the system is initially in an eigenstate and an electron is added (removed), the resulting eigenstate will have either one more (less) or the same number of doubly occupied sites and therefore the energy increase (decrease) of the system will be precisely 0 or I. Thus, as one sees from Eq. (2.8), the SWF will be a sum of weighted delta functions centered at these two energies.

For small but nonzero Δ one expects the degeneracy of the energy levels to be at least partially lifted. The wave functions with energy near pI consist mainly of zero-order wave functions of that energy, but zero-order wave functions of energy $(p+1)I$ are admixed in first order in Δ/I and those of energy $(p+r)I$ are admixed in rth order in Δ/I. Due to the lifting of the degeneracy the delta functions in the SWF are broadened and due to the admixing the coefficients of the delta functions can be modified [c.f. Eq. (3.8)]. Also new "satellite" peaks whose intensity is at most of order $(\Delta/I)^r$ will appear near energies $(r+1)I$ and $-rI$. One expects the width of the peaks to be proportional to Δ, so that the nth moment of each peak is of order $A\Delta^n$ where A is the intensity of the peak. Thus, one sees that generally the nth moment of the peak in the SWF near energy pI is at most of order

$$\Delta^n(\Delta/I)^{|p-1/2|-1/2}. \tag{4.8}$$

This situation is similar to the problem of nuclear magnetic resonance line shapes, which has been treated by Kubo and Tomita,[9] and others.[10,11]

We can see from Eq. (2.8) that the problem of considering individual peaks in the SWF separately is equivalent to the problem of achieving a spectral decomposition of the field operators as follows:

$$c_{i\sigma}=\sum_p c_{i\sigma;pI}, \tag{4.9a}$$

$$c^\dagger{}_{i\sigma}=\sum_p c^\dagger{}_{i\sigma;pI}, \tag{4.9b}$$

where the sums are over all positive and negative integers. The operators $c_{i\sigma;pI}$ and $c^\dagger{}_{i\sigma;pI}$ are to be constructed so that they only connect states which differ in unperturbed energy by pI. That is,

$$\langle b\mid c_{i\sigma;pI}\mid a\rangle=0, \tag{4.10a}$$

$$\langle b\mid c^\dagger{}_{i\sigma;pI}\mid a\rangle=0, \tag{4.10b}$$

unless

$$E_b-E_a=pI+O(\Delta). \tag{4.11}$$

We adhere to the convention that the energy subscript on an operator gives the allowed change in unperturbed energy so that

$$O^\dagger{}_E=(O_{-E})^\dagger. \tag{4.12}$$

According to this convention the product of such operators O_{E_1}, $O_{E_2}\cdots O_{E_n}$ only connects states which differ in unperturbed energy by $E_1+E_2+\cdots E_n$:

$$\langle b\mid O_{E_1}O_{E_2}\cdots O_{E_n}\mid a\rangle=0$$

unless

$$E_b-E_a=E_1+E_2+\cdots E_n+O(\Delta). \tag{4.13}$$

Such a spectral decomposition of $c_{i\sigma}$ and $c^\dagger{}_{i\sigma}$ would allow us to write

$$A^\sigma{}_{ij}(\omega)=\sum_p A^\sigma{}_{ij;pI}(\omega), \tag{4.14}$$

where

$$A^{\sigma}_{ij;pI}(\omega)=2\pi Z^{-1}\sum_{ab}\exp(-\beta E_a)\{\delta(\omega-E_b+E_a)\langle a\mid c_{i\sigma;-pI}\mid b\rangle \times\langle b\mid c^{\dagger}_{j\sigma;pI}\mid a\rangle+\delta(\omega-E_a+E_b)\langle a\mid c^{\dagger}_{j\sigma;pI}\mid b\rangle\langle b\mid c_{i\sigma;-pI}\mid a\rangle\}. \quad (4.15)$$

In other words, $A^{\sigma}_{ij;pI}(\omega)$ would be nonzero only for ω near pI. In analogy with Eqs. (4.2) and (4.3) we would also have

$$f^{\sigma}_{ij;pI}(t-t')=\int_{-\infty}^{+\infty}A^{\sigma}_{ij;pI}(\omega)\exp[-i\omega(t-t')](d\omega/2\pi), \quad (4.16)$$

where

$$f^{\sigma}_{ij;pI}(t-t')=\langle\{c_{i\sigma;-pI}(t),c^{\dagger}_{j\sigma;pI}(t')\}\rangle, \quad (4.17)$$

and therefore, as for the full SWF, we would have a characteristic function for each peak which is just an expectation value of an anticommutator.[17] The moments of each peak could then be studied in terms of time derivatives of these anticommutators as outlined in Eqs. (4.4) and (4.5).

For $\Delta=0$ the spectral decomposition of Eq. (4.9) is trivial. Consider the equation

$$c_{i\sigma}=n_{i-\sigma}c_{i\sigma}+(1-n_{i-\sigma})c_{i\sigma}. \quad (4.18)$$

The operator $n_{i-\sigma}c_{i\sigma}$ destroys an electron on a site already occupied by an electron of opposite spin thus decreasing the number of doubly occupied sites and hence decreasing the energy of the system by I. On the other hand the operator $(1-n_{i-\sigma})c_{i\sigma}$ destroys an electron on an otherwise empty site with no resulting energy change. Hence, for $\Delta=0$,

$$c_{i\sigma;0}=(1-n_{i-\sigma})c_{i\sigma}, \quad (4.19a)$$

$$c_{i\sigma;-I}=n_{i-\sigma}c_{i\sigma}, \quad (4.19b)$$

$$c_{i\sigma;pI}=0, \qquad p\neq 0,-1. \quad (4.19c)$$

Treating these operators as fundamental is the motivation for Hubbard's "atomic representation" for this problem.[18]

However, for $\Delta\neq 0$ this spectral decomposition is nontrivial. While $n_{i-\sigma}c_{i\sigma}$ for instance, creates an electron on an occupied site, the other electron can quickly hop away and such a process does not necessarily increase the energy of the system by I. However by means of a canonical transformation[7] we can achieve the desired decomposition for $\Delta\neq 0$. We define a unitary transformation $U\equiv e^{-S}$ such that

$$c^{\dagger}_{i\sigma}=\exp[S(\bar{c})]\,\bar{c}^{\dagger}_{i\sigma}\exp[-S(\bar{c})], \quad (4.20)$$

where the operator S is expressed in terms of $\bar{c}_{i\sigma}$ and $\bar{c}^{\dagger}_{i\sigma}$. The operator $\bar{c}^{\dagger}_{i\sigma}$ creates a new kind of particle which may be thought of as a dressed electron. S is chosen so that these new particles have the property that although they do hop around, their hopping does not change the effective number of doubly occupied sites. In this context effective occupation numbers refer to the new particles. Stated in more formal language the procedure is as follows. We write

$$\mathcal{H}=\mathcal{H}_0(\bar{c})+\bar{V}(\bar{c}), \quad (4.21)$$

where

$$\mathcal{H}_0(\bar{c})=I\sum_i\bar{n}_{i\uparrow}\bar{n}_{i\downarrow}, \quad (4.22)$$

$$\bar{n}_{i\sigma}=\bar{c}^{\dagger}_{i\sigma}\bar{c}_{i\sigma}, \quad (4.23)$$

and S is chosen in such a way that

$$[\mathcal{H},\mathcal{H}_0(\bar{c})]=[\mathcal{H}_0(\bar{c}),\bar{V}(\bar{c})]=0. \quad (4.24)$$

In order to make explicit use of this canonical transformation, we restrict ourselves to the case $(\Delta/I)\ll 1$ and assume that S and $\bar{V}$ can be expanded in power series in the parameter (Δ/I). According to the condition (4.24) the eigenvalue of $\mathcal{H}_0(\bar{c})$ (i.e., the effective number of doubly occupied sites) is a good quantum number and is also an approximation to the energy good to order Δ. Therefore $c_{i\sigma;pI}$ is that part of $c_{i\sigma}$ which changes the eigenvalue of $\mathcal{H}_0(\bar{c})$ by pI:

$$[\mathcal{H}_0(\bar{c}),c_{i\sigma;pI}]=pIc_{i\sigma;pI}. \quad (4.25)$$

The usefulness of the canonical transformation lies in the simplicity of the criterion (4.25) for the construction of the spectral decomposition of $c_{i\sigma}$.

Before continuing this program let us determine explicitly the lowest terms in the power series expansions

[17] This decomposition is widely accepted to be reasonable for a nuclear spin system (Refs. 8–11), for which case the degenerate unperturbed levels are split by an amount $g\beta H_0\gg g\beta H_d$, where H_d is a field measuring the strength of the dipolar interactions which are treated perturbatively. However, a mathematically rigorous treatment of the decomposition of the SWF has not, to our knowledge, been given. The crucial step is to show that a perturbation expansion of the canonical transformation [see Eq. (4.27)] for the many-body system is valid. In fact, for long-range interactions such a dipolar interaction is a difficult mathematical problem. It is this same step in the argument which is lacking here. Hence we feel that our calculations, while not rigorous, have the same status as their analogs for the nuclear spin system.

[18] J. Hubbard, Proc. Roy. Soc. (London) **A285**, 542 (1965).

of S and $\bar{V}(\bar{c})$. Substituting Eq. (4.20) into Eq. (4.6) we obtain

$$\mathcal{H}=\exp[S(\bar{c})]\{\sum_i I\bar{n}_{i\uparrow}\bar{n}_{i\downarrow}+\Delta\sum_{ij\sigma}t_{ij}\bar{c}^\dagger_{i\sigma}\bar{c}_{j\sigma}\}\exp[-S(\bar{c})]. \tag{4.26}$$

We define the expansions we need as follows:

$$S(\bar{c})=\sum_{n=1}^{\infty}S_n(\bar{c})\,(\Delta/I)^n, \tag{4.27}$$

$$\bar{V}(\bar{c})=\Delta\sum_{n=0}^{\infty}V_n(\bar{c})\,(\Delta/I)^n. \tag{4.28}$$

Substituting these expansions into Eq. (4.26) we obtain to second order in Δ/I the following:

$$\mathcal{H}=\mathcal{H}_0(\bar{c})+\{(\Delta/I)[S_1(\bar{c}),\mathcal{H}_0(\bar{c})]+V(\bar{c})\}+\{(\Delta/I)^2[S_2(\bar{c}),\mathcal{H}_0(\bar{c})]$$
$$+\tfrac{1}{2}(\Delta/I)^2[S_1(\bar{c}),[S_1(\bar{c}),\mathcal{H}_0(\bar{c})]]+(\Delta/I)[S_1(\bar{c}),V(\bar{c})]\}, \tag{4.29}$$

where $\mathcal{H}_0(\bar{c})$ was given in Eq. (4.22) and $V(\bar{c})$ is given by

$$V(\bar{c})=\Delta\sum_{ij\sigma}t_{ij}\bar{c}^\dagger_{i\sigma}\bar{c}_{j\sigma}. \tag{4.30}$$

In order to simplify the algebra we introduce the notation [in conformity with Eq. (4.9)]

$$V(\bar{c})=\Delta[V_I+V_0+V_{-I}], \tag{4.31}$$

where

$$V_I=\sum_{ij\sigma}t_{ij}\bar{n}_{i-\sigma}(1-\bar{n}_{j-\sigma})\,\bar{c}^\dagger_{i\sigma}\bar{c}_{j\sigma}, \tag{4.32a}$$

$$V_0=\sum_{ij\sigma}t_{ij}(1-\bar{n}_{i-\sigma}-\bar{n}_{j-\sigma}+2\bar{n}_{i-\sigma}\bar{n}_{j-\sigma})\,\bar{c}^\dagger_{i\sigma}\bar{c}_{j\sigma}, \tag{4.32b}$$

$$V_{-I}=\sum_{ij\sigma}t_{ij}\bar{n}_{j-\sigma}(1-\bar{n}_{i-\sigma})\,\bar{c}^\dagger_{i\sigma}\bar{c}_{j\sigma}, \tag{4.32c}$$

so that

$$[\mathcal{H}_0(\bar{c}),V_{pI}]=pIV_{pI}. \tag{4.33}$$

The requirement $[\mathcal{H}_0(\bar{c}),\bar{V}(\bar{c})]=0$ will be fulfilled to first order in Δ/I providing

$$[\mathcal{H}_0(\bar{c}),(\Delta/I)[S_1(\bar{c}),\mathcal{H}_0(\bar{c})]+\Delta[V_I+V_0+V_{-I}]]=0, \tag{4.34}$$

which may be satisfied by the choice

$$S_1(\bar{c})=V_I-V_{-I}. \tag{4.35}$$

In second order the condition $[\mathcal{H}_0(\bar{c}),\bar{V}(\bar{c})]=0$ yields

$$[\mathcal{H}_0(\bar{c}),(\Delta/I)[S_2(\bar{c}),\mathcal{H}_0(\bar{c})]+(\Delta/2I)[S_1(\bar{c}),[S_1(\bar{c}),\mathcal{H}_0(\bar{c})]]+[S_1(\bar{c}),V(\bar{c})]]=0. \tag{4.36}$$

Using Eqs. (4.35), (4.33), and (4.31) we can write this as

$$[\mathcal{H}_0(\bar{c}),I^{-1}[S_2(\bar{c}),\mathcal{H}_0(\bar{c})]+[V_I,V_{-I}]+[V_I-V_{-I},V_0]]=0. \tag{4.37}$$

Using the cyclic properties of commutators we see that

$$[\mathcal{H}_0(\bar{c}),[V_I,V_{-I}]]=I[V_{-I},V_I]+I[V_I,V_{-I}]=0, \tag{4.38}$$

so that Eq. (4.37) will be satisfied if we choose $S_2(\bar{c})$ to satisfy

$$[S_2(\bar{c}),\mathcal{H}_0(\bar{c})]=I[V_{-I}-V_I,V_0]. \tag{4.39}$$

Using (4.33) one can verify that

$$I[V_{-I}-V_I,V_0]=[[V_I+V_{-I},V_0],\mathcal{H}_0(\bar{c})]. \tag{4.40}$$

Thus, Eq. (4.39) can be satisfied by the choice

$$S_2(\bar{c})=[V_I+V_{-I},V_0]. \tag{4.41}$$

At this point we can write out explicitly expressions[19,20] for S to order $(\Delta/I)^2$ and for $\mathcal{H}$ to order Δ^2/I:

$$S=(\Delta/I)\sum_{ij\sigma} t_{ij}(\bar{n}_{i,-\sigma}-\bar{n}_{j,-\sigma})\,\bar{c}^{\dagger}_{i\sigma}\bar{c}_{j\sigma}+(\Delta/I)^2\sum_{ijl\sigma}\{t_{ij}t_{jl}(\bar{n}_{i,-\sigma}-\bar{n}_{l,-\sigma})(1-2\bar{n}_{j,-\sigma})\,\bar{c}^{\dagger}_{i\sigma}\bar{c}_{l\sigma}$$
$$+2t_{ij}t_{jl}(1-\delta_{il})(\bar{n}_{l\sigma}-\bar{n}_{i,-\sigma})\,\bar{c}^{\dagger}_{j,-\sigma}\bar{c}_{l,-\sigma}\bar{c}^{\dagger}_{i\sigma}\bar{c}_{j\sigma}+t_{ij}t_{il}(1-\bar{n}_{j,-\sigma}-\bar{n}_{l\sigma})(1-\delta_{jl})\,\bar{c}^{\dagger}_{i,-\sigma}\bar{c}_{l,-\sigma}\bar{c}^{\dagger}_{i\sigma}\bar{c}_{j\sigma}$$
$$-t_{ji}t_{li}(1-\bar{n}_{j,-\sigma}-\bar{n}_{l\sigma})(1-\delta_{jl})\,\bar{c}^{\dagger}_{l,-\sigma}\bar{c}_{i,-\sigma}\bar{c}^{\dagger}_{j\sigma}\bar{c}_{i\sigma},\quad(4.42)$$

$$\mathcal{H}=I\sum_{i}\bar{n}_{i\uparrow}n_{i\downarrow}+\Delta\sum_{ij\sigma}t_{ij}(1-\bar{n}_{i,-\sigma}-\bar{n}_{j,-\sigma}+2\bar{n}_{i,-\sigma}\bar{n}_{j,-\sigma})\,\bar{c}^{\dagger}_{i\sigma}\bar{c}_{j\sigma}+(\Delta^2/I)\sum_{ijl\sigma}[t_{ij}t_{li}(1-\bar{n}_{i,-\sigma})\bar{n}_{j,-\sigma}\bar{n}_{l,-\sigma}\bar{c}^{\dagger}_{l\sigma}\bar{c}_{j\sigma}$$
$$-t_{ij}t_{jl}(1-\bar{n}_{i,-\sigma})\bar{n}_{j,-\sigma}(1-\bar{n}_{l,-\sigma})\,\bar{c}^{\dagger}_{i\sigma}\bar{c}_{l\sigma}+t_{ij}t_{il}(1-\bar{n}_{l,-\sigma})\bar{n}_{j\sigma}\bar{c}^{\dagger}_{i\sigma}\bar{c}_{l\sigma}\bar{c}^{\dagger}_{i,-\sigma}\bar{c}_{j,-\sigma}+t_{ij}t_{lj}\bar{n}_{l,-\sigma}\bar{c}^{\dagger}_{l\sigma}\bar{c}_{j\sigma}(1-\bar{n}_{i\sigma})\,\bar{c}^{\dagger}_{i,-\sigma}\bar{c}_{j,-\sigma}$$
$$-t_{ij}t_{li}\bar{n}_{j\sigma}\bar{n}_{l,-\sigma}\bar{c}^{\dagger}_{i,-\sigma}\bar{c}_{j,-\sigma}\bar{c}^{\dagger}_{l\sigma}\bar{c}_{i\sigma}-t_{ij}t_{jl}(1-\bar{n}_{i\sigma})\,\bar{c}^{\dagger}_{i,-\sigma}\bar{c}_{j,-\sigma}(1-\bar{n}_{l,-\sigma})\,\bar{c}^{\dagger}_{j\sigma}\bar{c}_{l\sigma}].\quad(4.43)$$

Having obtained explicit formulas for S and $\mathcal{H}$ up to second order in Δ/I, we return to the problem of obtaining the spectral decomposition of $c_{i\sigma}$. We will first obtain the analogous decomposition of $\bar{c}_{i\sigma}$. One can easily verify that

$$[\mathcal{H}_0(\bar{c}),\,\bar{n}_{i,-\sigma}\bar{c}_{i\sigma}]=-I\bar{n}_{i,-\sigma}\bar{c}_{i\sigma},\quad(4.44)$$

$$[\mathcal{H}_0(\bar{c}),\,(1-\bar{n}_{i,-\sigma})\,\bar{c}_{i\sigma}]=0.\quad(4.45)$$

Thus, the spectral decomposition of $\bar{c}_{i\sigma}$ is trivial:

$$\bar{c}_{i\sigma}=\bar{c}_{i\sigma;0}+\bar{c}_{i\sigma;-I},\quad(4.46)$$

$$\bar{c}_{i\sigma;0}=(1-\bar{n}_{i,-\sigma})\,\bar{c}_{i\sigma},\quad(4.47)$$

$$\bar{c}_{i\sigma;-I}=\bar{n}_{i,-\sigma}\bar{c}_{i\sigma}.\quad(4.48)$$

Hence, by expressing $c_{i\sigma}$ in terms of $\bar{c}_{i\sigma}$, decomposing $\bar{c}_{i\sigma}$ according to Eq. (4.46), and using the property (4.13), we can obtain the desired decomposition of $c_{i\sigma}$. Thus, the operators $\bar{c}_{i\sigma;0}$ and $\bar{c}_{i\sigma;-I}$ play a fundamental role even when $\Delta\neq 0$. Accordingly it is convenient to rewrite Eq. (4.32) in terms of these operators:

$$V_I=\sum_{ij\sigma}t_{ij}\bar{c}^{\dagger}_{i\sigma;I}\bar{c}_{j\sigma;0},\quad(4.49a)$$

$$V_0=\sum_{ij\sigma}t_{ij}[\bar{c}^{\dagger}_{i\sigma;I}\bar{c}_{j\sigma;-I}+\bar{c}^{\dagger}_{i\sigma;0}\bar{c}_{j\sigma;0}],\quad(4.49b)$$

$$V_{-I}=\sum_{ij\sigma}t_{ij}\bar{c}^{\dagger}_{i\sigma;0}\bar{c}_{j\sigma;-I}.\quad(4.49c)$$

According to Eq. (4.20) and using Eqs. (4.35), (4.41), and (4.46) we can express $c_{i\sigma}$ in terms of the $\bar{c}_{i\sigma;pI}$ correct to order $(\Delta/I)^2$ as

$$c_{i\sigma}=\sum_{p=0,-1}\bar{c}_{i\sigma;pI}+(\Delta/I)\sum_{p=-1,0}[V_I-V_{-I},\,\bar{c}_{i\sigma;pI}]+(\Delta/I)^2\sum_{p=-1,0}\{[[V_I+V_{-I},\,V_0],\,\bar{c}_{i\sigma;pI}]$$
$$+\tfrac{1}{2}[V_I-V_{-I},\,[V_I-V_{-I},\,\bar{c}_{i\sigma;pI}]]\}.\quad(4.50)$$

From this expression using the property (4.13) we can read off the operators $c_{i\sigma;pI}$ correct to order $(\Delta/I)^2$:

$$c_{i\sigma;2I}=\tfrac{1}{2}(\Delta/I)^2[V_I,\,[V_I,\,\bar{c}_{i\sigma;0}]],\quad(4.51a)$$

$$c_{i\sigma;I}=(\Delta/I)[V_I,\,\bar{c}_{i\sigma;0}]+(\Delta/I)^2\{[[V_I,\,V_0],\,\bar{c}_{i\sigma;0}]+\tfrac{1}{2}[V_I,\,[V_I,\,\bar{c}_{i\sigma;-I}]]\},\quad(4.51b)$$

$$c_{i\sigma;0}=\bar{c}_{i\sigma;0}+(\Delta/I)[V_I,\,\bar{c}_{i\sigma;-I}]+(\Delta/I)^2\{[[V_I,\,V_0],\,\bar{c}_{i\sigma;-I}]-\tfrac{1}{2}[V_I,\,[V_{-I},\,\bar{c}_{i\sigma;0}]]-\tfrac{1}{2}[V_{-I},\,[V_I,\,\bar{c}_{i\sigma;0}]]\},\quad(4.51c)$$

$$c_{i\sigma;-I}=\bar{c}_{i\sigma;-I}-(\Delta/I)[V_{-I},\,\bar{c}_{i\sigma;0}]+(\Delta/I)^2\{[[V_{-I},\,V_0],\,\bar{c}_{i\sigma;0}]-\tfrac{1}{2}[V_I,\,[V_{-I},\,\bar{c}_{i\sigma;-I}]]-\tfrac{1}{2}[V_{-I},\,[V_I,\,\bar{c}_{i\sigma;-I}]]\},\quad(4.51d)$$

$$c_{i\sigma;-2I}=-(\Delta/I)[V_{-I},\,\bar{c}_{i\sigma;-I}]+(\Delta/I)^2\{[[V_{-I},\,V_0],\,\bar{c}_{i\sigma;-I}]+\tfrac{1}{2}[V_{-I},\,[V_{-I},\,\bar{c}_{i\sigma;0}]]\},\quad(4.51e)$$

$$c_{i\sigma;-3I}=\tfrac{1}{2}(\Delta/I)^2[V_{-I},\,[V_{-I},\,\bar{c}_{i\sigma;-I}]].\quad(4.51f)$$

Since

$$[V_{-I},\,\bar{c}_{i\sigma;-I}]=0=[V_I,\,\bar{c}_{i\sigma;0}],\quad(4.52)$$

[19] It is well known that to obtain energies correct to second order in the perturbation one need only calculate the unitary transformation correct to first order. Our interest lies in obtaining $c_{i\sigma}$ correct to second order to verify explicitly the existence of satellite peaks in the SWF. One notes that Eq. (4.43) reproduces the well-known (Ref. 20) result that for one electron per atom the effective Hamiltonian is that of a Heisenberg antiferromagnet.

[20] P. W. Anderson, in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1963), Vol. 14, p. 99.

we see that $c_{i\sigma;2I}$ and $c_{i\sigma;-3I}$ vanish in order $(\Delta/I)^2$ and that $c_{i\sigma;I}$ and $c_{i\sigma;-2I}$ are actually of order $(\Delta/I)^2$ and not of order (Δ/I) as the arguments leading to Eq. (4.8) would suggest. The adjoints of Eq. (4.51) give the corresponding decomposition of $c^\dagger{}_{i\sigma}$ as follows from Eq. (4.12).

The technique for generating the moments of the individual peaks in the SWF is as follows. We define

$$m^n{}_{ij\sigma;pI}\equiv\int_{-\infty}^{+\infty}(\omega-pI)^n A^\sigma{}_{ij;pI}(\omega)\,(d\omega/2\pi). \tag{4.53}$$

The moments of the peak near energy pI are taken about that energy which is to lowest order in Δ/I the energy of this peak. Therefore,

$$m^n{}_{ij\sigma;pI}=\int_{-\infty}^{+\infty}(d\omega/2\pi)\,([i(\partial/\partial t)-pI]^n\exp[-i\omega(t-t')]A^\sigma{}_{ij;pI}(\omega))_{t=t'} \tag{4.54a}$$

$$=([i(\partial/\partial t)-pI]^n f^\sigma{}_{ij;pI}(t-t'))_{t=t'} \tag{4.54b}$$

$$=\langle\{[i(\partial/\partial t)-pI]^n c_{i\sigma;-pI}(t),\,c^\dagger{}_{j\sigma;pI}(t)\}_+\rangle, \tag{4.54c}$$

where we have used Eqs. (4.16) and (4.17). However, since

$$[c_{i\sigma;-pI}(t),\,\mathcal{H}-\mathcal{H}_0(\bar{c})]=[i(\partial/\partial t)-pI]c_{i\sigma;pI}(t), \tag{4.55}$$

we obtain the expression

$$m^n{}_{ij\sigma;pI}=\langle\{\underbrace{[\cdots[[c_{i\sigma;-pI},\,\bar{V}(\bar{c})],\,\bar{V}(\bar{c})]\cdots\bar{V}(\bar{c})]}_{n\text{ factors}},\,c^\dagger{}_{j\sigma;pI}\}_+\rangle \tag{4.56}$$

involving the n-fold repeating commutator with the operator $\bar{V}(\bar{c})\equiv\mathcal{H}-\mathcal{H}_0(\bar{c})$. Just as in the case of Eq. (4.5) we can also write

$$m^n{}_{ij\sigma;pI}=\langle\{\underbrace{[\cdots[[c_{i\sigma;-pI},\,\bar{V}(\bar{c})],\,\bar{V}(\bar{c})]\cdots\bar{V}(\bar{c})]}_{n-r\text{ factors}},\,\underbrace{[\bar{V}(\bar{c})\cdots[\bar{V}(\bar{c}),\,[V(\bar{c})}_{r\text{ factors}},\,c^\dagger{}_{j\sigma;pI}]]\cdots]\}_+\rangle \tag{4.57}$$

irrespective of the choice of r.

While these expressions have not been difficult to derive, they are quite cumbersome and we therefore utilize an additional simplification wherever possible in what follows. Since the expectation value appearing in our expressions is a thermodynamic average in a canonical ensemble, energy eigenstates are weighted by the usual Boltzmann factors and therefore any eigenstate of $\mathcal{H}_0(\bar{c})$ with eigenvalue pI is weighted by the factor $\exp[-(pI+O(\Delta))/kT]$. Since I is of the order of 1–10 eV,[21] $I/k\approx10^4-10^5$ °K, and therefore at normal temperatures we need keep only states of the lowest possible eigenvalue of $\mathcal{H}_0(\bar{c})$ in our thermodynamic ensemble. Without loss of generality we restrict ourselves to a number of electrons less than or equal to the number of sites, so that the lowest possible eigenvalue of $\mathcal{H}_0(\bar{c})$ is zero. The simplification therefore comes from the fact that any product of operators which would lower the eigenvalue of $\mathcal{H}_0(\bar{c})$ gives zero when acting on a state from our restricted ensemble. For example,

$$\bar{c}_{i\sigma;-I}\,|\,\rangle=0, \tag{4.58a}$$

$$\bar{c}_{i\sigma;0}\,|\,\rangle\neq0. \tag{4.58b}$$

Also

$$V_{-I}V_{-I}\bar{c}^\dagger{}_{i\sigma;I}\,|\,\rangle=0, \tag{4.58c}$$

$$V_0\bar{c}_{i\sigma;-I}V_0\,|\,\rangle=0. \tag{4.58d}$$

But

$$V_0V_{-I}\bar{c}^\dagger{}_{i\sigma;I}\,|\,\rangle\neq0. \tag{4.58e}$$

These are examples of the type of simplification we will repeatedly use without explicit mention each time. In the same vein, to lowest order one can obviously equate expectation values of barred and unbarred operators. Further, one has

$$\langle\bar{n}_{i\sigma}\rangle=\langle n_{i\sigma}\rangle+O((\Delta/I)^2).$$

Consequently, in the results of our moment calculations we will simply replace barred operators by unbarred ones with no error to the order in Δ/I to which we work.

In summary the procedure for finding the moments of the peaks in the SWF is as follows. We substitute Eq. (4.51) into (4.57), affect any simplifications exemplified by Eq. (4.58), and finally express the barred operators in terms of the unbarred operators by inverting Eq. (4.20). As we have mentioned, to the order in Δ/I we consider, this last step is trivial. Thus, we will obtain expressions for the peaks in the SWF in terms of equal time commutators. Specific examples will be discussed in the following sections.

V. THE SHIFT IN WEIGHT FROM BAND TO BAND

In this section we will discuss a property whose general features are inadequately represented by one-electron approximations, namely the shift of weight in the density-of-states function from one band to the other. As a preliminary let us discuss two simplified one-electron models: first, the problem of electrons in an alloy, and second, the problem of interband mixing.

[21] A. P. Klein and A. J. Heeger, Phys. Rev. Letters **15**, 786 (1965); Phys. Rev. **144**, 458 (1966).

The unifying features of these two models is that when the widths of the bands are small in comparison to the gap between bands, the number of states in each band is conserved as the interband interaction is turned on.

The model for the alloy problem we treat is

$$\mathcal{H}=\sum_{i\sigma} E_i c^\dagger_{i\sigma} c_{i\sigma} - \Delta \sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma}, \tag{5.1}$$

where

$$E_i=0, \quad \text{if } i \text{ is an } A \text{ site} \tag{5.2a}$$

$$E_i=I, \quad \text{if } i \text{ is a } B \text{ site.} \tag{5.2b}$$

From Eq. (2.8) one sees that the SWF for $\Delta=0$ is

$$A^\sigma_{ii}(\omega)=2\pi\delta(\omega-E_i), \tag{5.3}$$

so that the density of states as defined by Eq. (2.9) is

$$\rho^\sigma(E)=x_A\delta(E)+(1-x_A)\delta(E-I), \tag{5.4}$$

where x_A is the fractional amount of A sites. The similarity between this density of states function and that for our narrow-band model is apparent. The total weight in the upper band is clearly $(1-x_A)$ and that in the lower band x_A.

Let us study the change in the SWF as the hopping is turned on, i.e., for $\Delta \ll I$. The Hamiltonian of Eq. (5.1) is diagonalized by the canonical transformation

$$q^\dagger_{n\sigma}=\sum_i \Gamma_{ni} c^\dagger_{i\sigma}, \qquad \Gamma^\dagger\Gamma=\mathbf{1}. \tag{5.5}$$

The new one-electron orbitals have energies λ_n, which may be found by diagonalizing the matrix $\mathbf{E}-\Delta\mathbf{t}$ or equivalently are given by the singularities in the function $f(\lambda)$ where

$$f(\lambda)=\mathrm{Tr}\{\mathbf{E}-\Delta\mathbf{t}-\lambda\mathbf{1}\}^{-1}, \tag{5.6}$$

where $E_{ij}=E_i\delta_{ij}$ and $\mathbf{1}$ is the unit matrix. Assume t_{ij} to be of short range:

$$\Delta\sum_j |t_{ij}| < T. \tag{5.7}$$

Then for $T<|\lambda|$ and $T<|I-\lambda|$ the power-series expansion of the matrix appearing in Eq. (5.6) converges, since

$$\left|\mathrm{Tr}(\mathbf{E}-\lambda\mathbf{1})\sum_n\{\Delta\mathbf{t}(\mathbf{E}-\lambda\mathbf{1})^{-1}\}^n\right| \leq \sum_n |\mathrm{Tr}(\mathbf{E}-\lambda\mathbf{1})| \max\{|T/\lambda|^n, |T/(I-\lambda)|^n\}. \tag{5.8}$$

Accordingly, the singularities of $f(\lambda)$ lie on the real axis in the intervals $-T\leq\lambda\leq T$ and $I-T\leq\lambda\leq I+T$. By considering the contour integral which gives the number of roots near zero energy,

$$(2\pi i)^{-1}\oint_{|z|=I/2} f(z)\,dz, \tag{5.9}$$

one can easily show that roots cannot jump from one interval to the other. The density-of-states function for $\Delta\neq 0$ is easily found since

$$\rho^\sigma(E)=(2\pi N)^{-1}\sum_i A_{ii}(E) \tag{5.10a}$$

$$=(2\pi N)^{-1}\sum_{inm}\Gamma^*_{in}\Gamma_{im}A_{nm}(E)$$

$$=(2\pi N)^{-1}\sum_n A_{nn}(E) \tag{5.10b}$$

$$=N^{-1}\sum_n \delta(E-\lambda_n), \tag{5.10c}$$

where A_{nm} is the SWF corresponding to the operators q_n and $q^\dagger_m$, the sums over n and m are over all orbitals. The total weight in the lower band is just the fraction of orbitals in the lower band which, for small Δ according to our argument, does not vary from its value for $\Delta=0$.

The second and equally trivial model is a one-electron Hamiltonian which describes interband mixing;

$$\mathcal{H}=\sum_{\mathbf{k},\sigma,\alpha=1,2}\epsilon_{\mathbf{k}\alpha}c^\dagger_{\mathbf{k}\alpha\sigma}c_{\mathbf{k}\alpha\sigma}+\sum_{\mathbf{k}\sigma}V_{12}(\mathbf{k})c^\dagger_{\mathbf{k}1\sigma}c_{\mathbf{k}2\sigma} +\sum_{\mathbf{k}\sigma}V_{12}^*(\mathbf{k})c^\dagger_{\mathbf{k}2\sigma}c_{\mathbf{k}1\sigma}, \tag{5.11}$$

where $\alpha=1, 2$ labels the two bands. We suppose that the bands are well separated and that the interband mixing is small so that

$$\max\{\epsilon_{\mathbf{k}1}\}<\min\{\epsilon_{\mathbf{k}2}\}, \tag{5.12a}$$

$$|V_{12}(\mathbf{k})|\ll\min\{\epsilon_{\mathbf{k}2}\}-\max\{\epsilon_{\mathbf{k}1}\}. \tag{5.12b}$$

With the obvious generalization of the labeling of the electron operators in Eq. (2.8) we have, for $V_{12}(\mathbf{k})=0$

$$A^\sigma_{\alpha\beta}(\mathbf{k},\omega)=2\pi\delta_{\alpha\beta}\delta(\omega-\epsilon_{\mathbf{k}\alpha}). \tag{5.13}$$

In this case the appropriate definition of the density-of-states function is

$$\rho^\sigma(E)=(2\pi N)^{-1}\sum_{\mathbf{k}\alpha}A^\sigma_{\alpha\alpha}(\mathbf{k},E), \tag{5.14}$$

so that for $\Delta=0$

$$\rho^\sigma(E)=N^{-1}\sum_{\mathbf{k}\alpha}\delta(E-\epsilon_{\mathbf{k}\alpha}) \tag{5.15}$$

which has unit weight in each band.

For nonzero $V_{12}(\mathbf{k})$ we introduce new operators $\bar{c}^\dagger_{\mathbf{k}\alpha\sigma}$ according to

$$c^\dagger_{\mathbf{k}\alpha\sigma}=\sum_\beta\Gamma_{\alpha\beta}(\mathbf{k})\bar{c}^\dagger_{\mathbf{k}\beta\sigma}, \qquad \mathbf{\Gamma}^\dagger(\mathbf{k})\mathbf{\Gamma}(\mathbf{k})=\mathbf{1} \tag{5.16}$$

such that the Hamiltonian of Eq. (5.11) is diagonalized. The new band energies $\bar{\epsilon}_{\mathbf{k}\alpha}$ are the roots of

$$\det\begin{vmatrix}\epsilon_{\mathbf{k}1}-\bar{\epsilon}_{\mathbf{k}\alpha} & V_{12}(\mathbf{k})\\ V_{12}^*(\mathbf{k}) & \epsilon_{\mathbf{k}2}-\bar{\epsilon}_{\mathbf{k}\alpha}\end{vmatrix}=0. \tag{5.17}$$

The SWF is then

$$A^\sigma_{\alpha\beta}(\mathbf{k},\omega)=2\pi\sum_\gamma\Gamma_{\alpha\gamma}^*(\mathbf{k})\Gamma_{\beta\gamma}(\mathbf{k})\delta(\omega-\bar{\epsilon}_{\mathbf{k}\gamma}), \tag{5.18}$$

so that $A^\sigma_{11}(\mathbf{k},\omega)$, for instance, has weight not only in

band 1, but also some in band 2, since for $V_{12}(\mathbf{k})\neq 0$, $\Gamma_{12}(\mathbf{k})\neq 0$. However, because of the unitarity of the transformation of Eq. (5.16), one sees that the density-of-states function is

$$\rho^{\sigma}(E)=N^{-1}\sum_{\mathbf{k}\alpha}\delta(\omega-\bar{\epsilon}_{\mathbf{k}\alpha}), \tag{5.19}$$

so that, as in the alloy problem, for a small perturbation there is no shift in weight in the density of states from one band to the other.

In view of these simple examples one is naturally led to ask if this is a general result, applicable, for instance, to the narrow-band Hamiltonian we have considered in the previous sections. Recalling the results of Sec. III it is not surprising that the answer to this question should be in the negative. This is easily seen by calculating the zeroth moment (weight) of each peak in the SWF. Using the methods of Sec. IV we find, correct to order Δ/I,

$$m^{\sigma}{}_{ii\sigma;0}=1-\langle n_{i-\sigma}\rangle-(2\Delta/I)\sum_{j}t_{ij}\langle c^{\dagger}{}_{i-\sigma}c_{j-\sigma}\rangle, \tag{5.20a}$$

$$m^{\sigma}{}_{ii\sigma;I}=\langle n_{i-\sigma}\rangle+(2\Delta/I)\sum_{j}t_{ij}\langle c^{\dagger}{}_{i-\sigma}c_{j-\sigma}\rangle. \tag{5.20b}$$

These formulas when applied to the two-site model of Sec. III agree with the results found there. For a homogeneous system these expressions give the total weight in the lower and upper bands of the density of states. For less than one electron per site $\langle c^{\dagger}{}_{i-\sigma}c_{j-\sigma}\rangle$ is negative, so that the weight in the lower band is increased at the expense of the upper band. This phenomenon can be easily understood by considering the correlation between an electron added to the system and an electron of opposite spin on the site to which it is added. In the case when no hopping is allowed, the result

$$m^{0}{}_{ii\sigma;0}=1-\langle n_{i,-\sigma}\rangle \tag{5.21}$$

is obvious, since then $1-\langle n_{i,-\sigma}\rangle$ is just the probability that an added electron will land on an unoccupied site. For $\Delta\neq 0$, however, we need only ask which of the following two-multiple processes is more likely: first, that an electron occupying a site will leave when another electron is added to it, or second, that an electron will hop to a site to which we have just added an electron. Due to the repulsion between electrons the first process is the dominant one. Therefore, there are effectively fewer occupied sites when hopping is allowed. The additional electron, through its interaction with those already present, in effect, clears a space for itself and thereby increases the probability of being added with lower energy.

These results are not in disagreement with Luttinger's theorem[22] that for normal fermion systems the volume of the Fermi sea is unaffected by perturbations. This theorem was only proposed for a perturbative calculation about a single-particle Hamiltonian, whereas for the narrow-band model we treat, we consider perturbations about the Hamiltonian, $\sum_{i}In_{i\uparrow}n_{i\downarrow}$, which is not a single-particle Hamiltonian. Furthermore, the concept of a Fermi surface seems to be meaningless since all the single-particle states have a finite lifetime, i.e., a finite width to their SWF. Thus, there is nothing anomalous in the result that there is a shift of weight in the density-of-states function from one band to the other as the hopping is turned on.

Let us now study the case of one electron per site more carefully. In this case $\langle c^{\dagger}{}_{i,-\sigma}c_{j,-\sigma}\rangle$ is of order Δ/I, so that to first order in Δ/I the weights of the two peaks remain at their values for $\Delta=0$:

$$m^{0}{}_{ii\sigma;0}=1-\langle n_{i,-\sigma}\rangle, \tag{5.22a}$$

$$m^{0}{}_{ii\sigma;I}=\langle n_{i,-\sigma}\rangle. \tag{5.22b}$$

Although we have only shown this result to be valid to order Δ/I, it actually holds to order $(\Delta/I)^3$ but not to order $(\Delta/I)^4$ due to the emergence of the satellite peaks. The weights of these satellite peaks at energies $-I$ and $2I$, $\rho^{\sigma}(-I)$ and $\rho^{-\sigma}(2I)$ are readily calculated using the formalism of the preceding section, especially Eq. (4.51a) and (4.51d): We find

$$m^{0}{}_{jj-\sigma;2I}=m^{0}{}_{jj\sigma;-I}$$
$$=(\Delta/I)^4\sum_{i\neq k}|t_{ij}t_{jk}|^2\{\langle n_{i\sigma}(2n_{k,-\sigma}n_{j\sigma}+n_{k\sigma}n_{j,-\sigma})\rangle\}. \tag{5.23}$$

To estimate the size of this effect let us assume a simple cubic lattice with

$$t_{ij}=t, \qquad i,j \text{ nearest-neighboring sites} \tag{5.24a}$$

$$=0, \qquad \text{otherwise.} \tag{5.24b}$$

Also we approximate the expectation value in Eq. (5.23) as

$$\langle n_{i\sigma}(2n_{k,-\sigma}n_{j\sigma}+n_{k\sigma}n_{j,-\sigma})\rangle$$
$$\approx\langle n_{i\sigma}\rangle\{2\langle n_{k,-\sigma}\rangle\langle n_{j\sigma}\rangle+\langle n_{k\sigma}\rangle\langle n_{j,-\sigma}\rangle\}. \tag{5.25}$$

For a paramagnetic state $\langle n_{i\sigma}\rangle=\frac{1}{2}$, so that

$$\rho^{-\sigma}(2I)=\rho^{\sigma}(-I)=m^{0}{}_{j\gamma\sigma;-I} \tag{5.26a}$$

$$\approx(\Delta/I)^4t^4z(z-1)\tfrac{3}{8}=\tfrac{5}{16}(\Delta/I)^4, \tag{5.26b}$$

where $z=6$ is the number of nearest-neighboring sites and we have used the definition of Eq. (2.4) which here is

$$zt^2=1. \tag{5.27}$$

For "complete" ferromagnetism

$$n_{i\uparrow}=1, \tag{5.28a}$$

$$n_{i\downarrow}=0, \tag{5.28b}$$

so that

$$\rho^{-\sigma}(2I)=\rho^{\sigma}(-I)=m^{0}{}_{jj\sigma;-I}\approx 0. \tag{5.29}$$

[22] J. M. Luttinger, Phys. Rev. **119**, 1153 (1960).

For "complete" antiferromagnetism with NaCl-type ordering,

$$\langle n_{i\sigma}\rangle\langle n_{k,-\sigma}\rangle\langle n_{j\sigma}\rangle=0, \tag{5.30a}$$

$$\langle n_{i\sigma}\rangle\langle n_{k\sigma}\rangle\langle n_{j,-\sigma}\rangle=\langle n_{j,-\sigma}\rangle, \tag{5.30b}$$

when sites i and k are nearest neighbors of site j, so that

$$m^0{}_{jj\sigma;-I}\approx\tfrac{5}{6}(\Delta/I)^4\langle n_{j,-\sigma}\rangle, \tag{5.31a}$$

$$\rho^{-\sigma}(2I)=\rho^{\sigma}(-I)=N^{-1}\sum_j m^0{}_{jj\sigma;-I}\approx\tfrac{5}{12}(\Delta/I)^4, \tag{5.31b}$$

in this case. Of course, the sum rule

$$\int_{-\infty}^{+\infty} A^{\sigma}{}_{ii}(\omega)\,(d\omega/2\pi)=1 \tag{5.32}$$

must be satisfied by a concomitant loss of weight in the main peaks of the SWF at energies 0 and I.

This readjustment of weight is such that the insulator property for this case as embodied in the existence of an energy gap between filled bands and empty bands is not changed as Δ is increased. That is, although there is a realignment of weight among the peaks in the SWF as Δ is changed, no partially filled bands are created either by holes appearing in filled bands or by electrons moving into empty ones, just as we saw in Sec. III. To see this we note that so long as $\Delta\ll I$ all the intermediate states $|\,b\rangle$ in the product

$$\langle a\,|\,c_{i\sigma}\,|\,b\rangle\langle b\,|\,c^{\dagger}{}_{i\sigma}\,|\,a\rangle \tag{5.33a}$$

have energies nearly equal to or greater than I, while those in the product

$$\langle a\,|\,c^{\dagger}{}_{i\sigma}\,|\,b\rangle\langle b\,|\,c_{i\sigma}\,|\,a\rangle \tag{5.33b}$$

have energies nearly equal to or greater than zero, if $\langle a\,|$ is the ground state or a member of our restricted ensemble having no effectively doubly occupied sites. Taking E' to lie in the band gap (e.g., $E'\sim I/2$) we calculate the total weight, W, of all peaks of the SWF, near pI with $p\leq 0$ as

$$W=\int_{-\infty}^{E'}\rho^{\sigma}(E)\,dE=Z^{-1}\sum_{ab}\int_{-\infty}^{E'}\exp(-\beta E_a)\,dE[\delta(E-E_b+E_a)\times\langle a\,|\,c_{i\sigma}\,|\,b\rangle\langle b\,|\,c^{\dagger}{}_{i\sigma}\,|\,a\rangle+\delta(E+E_b-E_a)\langle a\,|\,c^{\dagger}{}_{i\sigma}\,|\,b\rangle\langle b\,|\,c_{i\sigma}\,|\,a\rangle] \tag{5.34a}$$

$$=Z^{-1}\sum_{ab}\{\theta(E'-E_b+E_a)\langle a\,|\,c_{i\sigma}\,|\,b\rangle\langle b\,|\,c^{\dagger}{}_{i\sigma}\,|\,a\rangle+\theta(E'+E_b-E_a)\langle a\,|\,c^{\dagger}{}_{i\sigma}\,|\,b\rangle\langle b\,|\,c_{i\sigma}\,|\,a\rangle\}\exp(-\beta E_a). \tag{5.34b}$$

However, according to our arguments, the first theta function vanishes and the second one is always unity so that

$$W=n_{i\sigma}, \tag{5.35}$$

i.e., the total weight in the SWF below the band gap is equal to the number of σ-spin electrons. Thus adding an electron involves adding the gap energy when there is one electron per site already present. We see even in this case, however, that the filled band one visualizes in the band theory has a complicated behavior for nonzero Δ, since the existence of satellite peaks in the SWF at negative energies tells us that removing an electron can require the addition of energy to the system of various multiples of I.

A physical picture of this phenomenon as it might in principle be observed via positron annihilation is the following. The main peaks in the SWF at energies 0 and I correspond to processes in which an electron is removed from a singly or doubly occupied site respectively. The satellite peaks at energies $-I$ and $2I$ correspond to multiple processes in which one electron is removed and the state of the crystal is changed by an electron hopping so as to increase by one the number of doubly occupied sites or vice versa, as is shown schematically in Fig. 3. Since these are higher-order processes their probability is reduced [by a factor $(\Delta/I)^4$] from the zero-order processes corresponding to the main peaks in the SWF.

VI. COMPARISON WITH HUBBARD'S THEORIES

In this section we wish to examine Hubbard's calculations[2,12] for the narrow-band model to see how well his approximate Green's functions satisfy the sum rules we have derived. Hubbard's solutions were obtained by a decoupling of the hierarchy of equations of motion for the Green's functions based on the idea that correlations were of relatively short range in space. The chief virtue of his calculations is that they provide an approximate interpolation scheme between the atomic ($\Delta\to 0$) and band ($I\to 0$) limits. His work has provided insight into and emphasized the role of electron correlations and therefore it is not surprising that other aspects such as the shift in weight in the density-of-states function may not be given correctly. Our moment calculations are useful as a means of

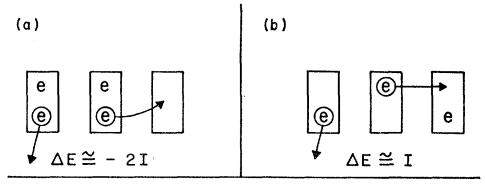

FIG. 3. Processes corresponding to the satellite peaks in the SWF. A box represents a site and "e" an electron. Process (a) contributes to the peak at energy $2I$ and process (b) contributes to the peak at energy $-I$.

studying such properties which are not easily accessible via decoupling approximations.

From the moments associated with the SWF $A^{\sigma}{}_{\lambda\lambda}(\omega)$ we can calculate the average energy $\langle\epsilon_{\lambda\sigma;pI}\rangle$ of the peak near energy pI as

$$\langle\epsilon_{\lambda\sigma;pI}\rangle = m^{1}{}_{\lambda\sigma;pI}/m^{0}{}_{\lambda\sigma;pI}, \tag{6.1}$$

and the root-mean-square width $\langle\delta\epsilon_{\lambda\sigma;pI}\rangle$ of this peak as

$$\langle\delta\epsilon_{\lambda\sigma;pI}\rangle = [(m^{2}{}_{\lambda\sigma;pI}/m^{0}{}_{\lambda\sigma;pI}) - \langle\epsilon_{\lambda\sigma;pI}\rangle^{2}]^{1/2}. \tag{6.2}$$

A particularly simple and physically revealing treatment of correlations in narrow bands has been given by Hubbard in Ref. 2. Expanding the SWF derivable from his approximate Green's functions one obtains to first order in Δ/I (in our notation)

$$A^{\sigma}{}_{\lambda\lambda}(\omega) = 2\pi[1-n_{-\sigma}-n_{-\sigma}(\epsilon_{\lambda}/I)]\delta(\omega-(1-n-\sigma)\epsilon_{\lambda}) + 2\pi[n_{-\sigma}+n_{-\sigma}(\epsilon_{\lambda}/I)]\delta(\omega-I-n_{-\sigma}\epsilon_{\lambda}), \tag{6.3}$$

where throughout this section $n_{-\sigma}=\langle n_{i,-\sigma}\rangle$ and is assumed to be independent of i and thus describes a paramagnetic or ferromagnetic state. For a SWF of this form $\langle\delta\epsilon_{\lambda\sigma;pI}\rangle=0$, so that such an approximate treatment is incapable of describing the damping of electron excitations.

Let us check the weight (zeroth moment) and average energy of the low-energy peak in the SWF given by Eq. (6.3) against the moments calculated according to Sec. IV. The discussion of the high-energy peaks in the SWF is analogous and will be omitted. From Hubbard's SWF of Eq. (6.3) it is trivial to calculate the zeroth moment of the low-energy peak in the SWF as

$$m^{0}{}_{\lambda\lambda\sigma;0} = 1-n_{-\sigma}-n_{-\sigma}(\epsilon_{\lambda}/I). \tag{6.4}$$

Correspondingly, the total number of states in the two bands is

$$\rho_{l}{}^{\sigma} = \int_{\text{lower band}} \rho^{\sigma}(\omega)d\omega = N^{-1}\sum_{\lambda} m^{0}{}_{\lambda\lambda\sigma;0} = 1-n_{-\sigma}, \tag{6.5a}$$

$$\rho_{u}{}^{\sigma} = \int_{\text{upper band}} \rho^{\sigma}(\omega)d\omega = N^{-1}\sum_{\lambda} m^{0}{}_{\lambda\lambda\sigma;I} = n_{-\sigma}. \tag{6.5b}$$

The average energy of the low-energy peak in Hubbard's SWF is given as

$$\langle\epsilon_{\lambda\sigma;0}\rangle = (1-n_{-\sigma})\epsilon_{\lambda}. \tag{6.6}$$

These results should be compared with the results exact to order Δ/I which can be obtained by the methods of Sec. IV:

$$m^{0}{}_{\lambda\lambda\sigma;0} = 1-n_{-\sigma}-2(\mathfrak{I}_{-\sigma}/I+n_{-\sigma}\epsilon_{\lambda}/I)+2(\Delta/I)\sum_{j}\exp(i\boldsymbol{\lambda}\cdot\mathbf{r}_{ij})t_{ij}\{\langle n_{i,-\sigma}n_{j,-\sigma}+c^{\dagger}{}_{j\sigma}c_{j,-\sigma}c^{\dagger}{}_{i,-\sigma}c_{i\sigma}\rangle\}, \tag{6.7}$$

$$\rho_{l}{}^{\sigma} = 1-n_{-\sigma}-(2/I)\mathfrak{I}_{-\sigma}, \tag{6.8a}$$

$$\rho_{u}{}^{\sigma} = n_{-\sigma}+(2/I)\mathfrak{I}_{-\sigma}, \tag{6.8b}$$

and

$$\langle\epsilon_{\lambda\sigma;0}\rangle = \epsilon_{\lambda}(1-n_{-\sigma})-\mathfrak{I}_{-\sigma}/(1-n_{-\sigma})+\Delta/(1-n_{-\sigma})\sum_{j}\exp(i\boldsymbol{\lambda}\cdot\mathbf{r}_{ij})t_{ij}\{\langle n_{i-\sigma}n_{j-\sigma}\rangle-n_{-\sigma}{}^{2}+\langle c^{\dagger}{}_{j\sigma}c_{j,-\sigma}c^{\dagger}{}_{i,-\sigma}c_{i\sigma}\rangle\}. \tag{6.9}$$

We note that although Eq. (6.4) shows a shift in weight from one band to the other for an excitation of wave number $\boldsymbol{\lambda}$, it differs from the exact expression, Eq. (6.7). Also we see that according to Hubbard's theory, Eq. (6.5), there is no change in the total number of states in the two bands in order Δ/I in contrast to the exact result, Eq. (6.8), which we discussed more fully in the previous section. In order to compare the expressions for the average energy let us analyze Eq. (6.9) further. The bracketed expression in this equation is a sum of terms, the first of which is proportional to density fluctuations which are energetically unfavorable and therefore small, and the second of which is proportional to the magnetic energy. Since magnetic ordering critical temperatures are usually negligible compared to the band width, we can say that the term $\mathfrak{I}_{-\sigma}/(1-n_{-\sigma})$ is probably the most important one since it is in fact of the order of the band width. Thus, we have approximately,

$$\langle\epsilon_{\lambda\sigma;0}\rangle \approx \epsilon_{\lambda}(1-n_{-\sigma})-\mathfrak{I}_{-\sigma}/(1-n_{-\sigma}), \tag{6.10}$$

which differs from Hubbard's result, Eq. (6.6), by the addition of the correction term $-\mathfrak{I}_{-\sigma}/(1-n_{-\sigma})$ which is independent of $\boldsymbol{\lambda}$. For the nonmagnetic case this correction term is the same for both up and down spins and hence leads to a trivial shift in the Fermi energy. For magnetic states, as we shall see in the next section, this term becomes important for studying the relative stability of magnetic versus nonmagnetic states.

We now discuss an improved solution, also given by Hubbard,[12] designed to describe the conductor to insulator transition for the case of one electron per atom and which of necessity involves peaks in the SWF of nonzero width. This improved solution is sufficiently complicated that analytic evaluation of the SWF is difficult. However, for the special case of one electron per atom the details were worked out analytically for the nonmagnetic system with $n_{i\sigma}=\frac{1}{2}$. The SWF is determined by the roots of a cubic polynomial. Hubbard treated the case of a parabolic density of states

$$\rho_{0}(\omega) = (2\pi\Delta^{2})^{-1}(4\Delta^{2}-\omega^{2})^{1/2}, \quad |\omega| \leq 2\Delta, \tag{6.11a}$$

$$= 0, \quad \text{otherwise}, \tag{6.11b}$$

where $\rho_0(\omega)$, which we shall henceforth refer to as the unperturbed density of states, is defined as

$$\rho_0(\omega)=N^{-1}\sum_{\lambda}\delta(\omega-\epsilon_\lambda). \tag{6.12}$$

Note that our definition of Δ differs from that of Hubbard since we require

$$\int_{-\infty}^{+\infty}\rho_0(\omega)\,d\omega=1, \tag{6.13a}$$

$$\int_{-\infty}^{+\infty}\rho_0(\omega)\omega^2 d\omega=\Delta^2. \tag{6.13b}$$

The results are most conveniently displayed in terms of the new variables

$$\sin\theta=\omega/2\Delta, \tag{6.14a}$$

$$\sin\theta_k=\epsilon_k/2\Delta, \tag{6.14b}$$

so that Eq. (6.11a) takes the form

$$\rho_0(\omega)=(\pi\Delta)^{-1}\cos\theta. \tag{6.15}$$

In the limit $I\gg\Delta$ we have obtained explicit expressions for the SWF using Hubbard's theory and find the following results:

$$A^\sigma_{jj}(\omega)=\Delta^{-1}\cos\theta, \qquad |\omega|\leq 2\Delta \tag{6.16a}$$

$$=A^\sigma_{jj}(\omega-I), \qquad |\omega-I|\leq 2\Delta \tag{6.16b}$$

$$=0, \qquad \text{otherwise}, \tag{6.16c}$$

$$A^\sigma_{\lambda\lambda}(\omega)=\frac{12\Delta^{-1}\cos\theta}{(5\sin\theta-4\sin\theta_\lambda)^2+9\cos^2\theta}, \qquad |\omega|\leq 2\Delta \tag{6.17a}$$

$$=A^\sigma_{\lambda\lambda}(\omega-I), \qquad |\omega-I|\leq 2\Delta \tag{6.17b}$$

$$=0, \qquad \text{otherwise}. \tag{6.17c}$$

The SWF for $I\to\infty$ calculated from Eq. (6.17a) is shown in Fig. 4 for various values of λ. Using the results of Eqs. (6.16) and (6.17) we can calculate the associated moments of the peaks in the SWF at energies 0 and I:

$$\int_{\text{l.b.}}A^\sigma_{\lambda\lambda}(\omega)\,(d\omega/2\pi)=\int_{\text{u.b.}}A^\sigma_{\lambda\lambda}(\omega)\,(d\omega/2\pi)=\tfrac{1}{2}, \tag{6.18a}$$

$$\int_{\text{l.b.}}A^\sigma_{jj}(\omega)\,(d\omega/2\pi)=\int_{\text{u.b.}}A^\sigma_{jj}(\omega)\,(d\omega/2\pi)=\tfrac{1}{2}, \tag{6.18b}$$

$$\int_{\text{l.b.}}A^\sigma_{\lambda\lambda}(\omega)\,(\omega d\omega/2\pi)=\int_{\text{u.b.}}A^\sigma_{\lambda\lambda}(\omega)[(\omega-I)\,d\omega/2\pi]=\tfrac{1}{4}\epsilon_\lambda, \tag{6.18c}$$

$$\int_{\text{l.b.}}A^\sigma_{jj}(\omega)\,(\omega d\omega/2\pi)=\int_{\text{u.b.}}A^\sigma_{jj}(\omega)[(\omega-I)\,d\omega/2\pi]=0, \tag{6.18d}$$

$$\int_{\text{l.b.}}A^\sigma_{\lambda\lambda}(\omega)\,(\omega^2 d\omega/2\pi)=\int_{\text{u.b.}}A^\sigma_{\lambda\lambda}(\omega)[(\omega-I)^2 d\omega/2\pi]=\tfrac{1}{8}(3\Delta^2+\epsilon_\lambda^2), \tag{6.18e}$$

$$\int_{\text{l.b.}}A^\sigma_{jj}(\omega)\,(\omega^2 d\omega/2\pi)=\int_{\text{u.b.}}A^\sigma_{jj}(\omega)[(\omega-I)^2 d\omega/2\pi]=\tfrac{1}{2}\Delta^2. \tag{6.18f}$$

One must recognize that these results are only correct to lowest order in Δ/T. In the limit $I\to\infty$ Eqs. (6.18a) through (6.18d) are the same as the corresponding results of Eqs. (6.4)–(6.6) obtained using Hubbard's simpler theory. The lowest moments which are different in the improved treatment are the second moments given by Eqs. (6.18e) and (6.18f). For the moment given in Eq. (6.18f), Hubbard's simpler theory gives the value $\Delta^2/8$ rather than $\Delta^2/2$. It is a simple matter to evaluate this same moment using our techniques and indeed we find the value $\Delta^2/2$ in agreement with Eq. (6.18f). [Unfortunately, a comparison with the moment in Eq. (6.18e) would involve a lengthy discussion of many approximations of correlation functions beyond the purposes of this section.] We therefore confirm that the simpler theory overestimates the band narrowing due to correlation. This excessive narrowing can be linked to a neglect of the damping giving rise to width of one-electron excitations comprising a band. Hubbard's more complex theory includes

these effects, as can be seen from the fact that this theory gives

$$\langle \delta\epsilon_{\lambda\sigma;0}\rangle = \langle \delta\epsilon_{\lambda\sigma;I}\rangle = (3/4)^{1/2}\Delta, \tag{6.19}$$

where the simpler theory gives zero.

In the above discussion we have referred to the narrowing of the bands but have only calculated second moments. As we see from Fig. 4 the SWF has a Gaussian-looking shape only for states near the center of the band if anywhere. In general it would take more than a single moment to specify the effective width of a band with respect to some physical property. Second moments yield bandwidths only in the crudest sense. One might give physical arguments as to why Gaussian or Lorentzian or intermediate approximations might be applicable for various regions and under various circumstances, but it is sufficient for our present purpose to accept the limitation on the direct physical relevance of such moments and accept that strictly speaking such quantities should only be compared with like quantities, i.e., second moments in one theory with second moments in another. The comparisons made in this section have a validity as comparisons regardless of band shape or complexity since they are of this direct nature.

VII. APPLICATIONS TO FERROMAGNETIC STATES

In the previous sections we have discussed the applications of the sum rules to the study of the SWF of paramagnetic states. In this section and the next we shall discuss the effect of ferromagnetic and antiferromagnetic ordering respectively on the SWF. In the case of ferromagnetic ordering we have already remarked that there is a wave-vector-independent shift in the average excitation energy which is important for any discussion of the stability of magnetic phases. Thus, in contrast to Hubbard's expression for the excitation energy Eq. (6.6) we take

$$\langle \epsilon_{\lambda\sigma;0}\rangle \approx \epsilon_\lambda(1-n_{-\sigma}) - \mathfrak{I}_{-\sigma}/(1-n_{-\sigma}). \tag{7.1}$$

In order to see the effect of this correction term, let us study the condition for ferromagnetism neglecting the damping of the excitations.

First we consider a special case for which precise calculations can be done and which shows explicitly the importance and correctness of the wave-number-independent shift in energies embodied in the approximate Eq. (7.1). This is the case of N sites, $N-1$ electrons and infinite I studied by Nagaoka[23] and shown by him to have a ground state which is completely ferromagnetic. We can show that in this circumstance Eq. (7.1) is almost exact and the term $\mathfrak{I}_{-\sigma}/(1-n_{-\sigma})$ is necessary to make the ground state ferromagnetic. At zero temperature we can express

[23] Y. Nagaoka, Solid State Commun. **3**, 409 (1965).

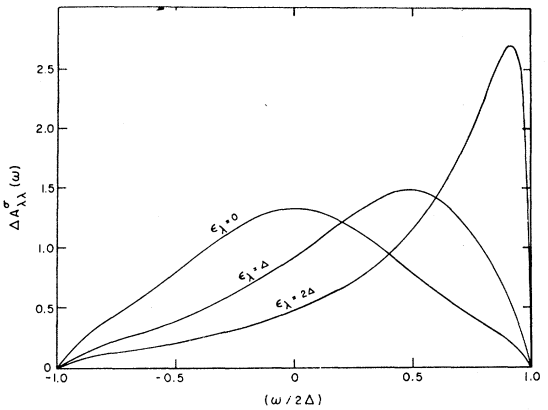

FIG. 4. The SWF $A^{\sigma}_{\lambda\lambda}(\omega)$ as given by Hubbard's improved theory for $\omega \lessgtr 0$ according to Eq. (6.17a) for various values of ϵ_λ. Note that similar peaks (not shown) also appear near energy I.

the SWF entirely in terms of matrix elements between the ferromagnetic ground state of the $N-1$ particle system Φ_0 and the states of the $N-2$ and N particle systems where Φ_0 is simply given by

$$\Phi_0 = \prod_{\lambda}{}' c^\dagger_{\lambda\uparrow} \mid 0\rangle. \tag{7.2}$$

In the product all λ appear except the λ referring to that momentum state with the largest single-particle energy $\epsilon_{\max}$. That is, since all electrons have the same spin, they do not interact through the potential term in the Hamiltonian and we can just fill up the $N-1$ single-particle states of lowest kinetic energy. It is a trivial result then that, since we are dealing with essentially free up-spin particles,

$$A_{\lambda\lambda}{}^{\uparrow}(\omega) = 2\pi\delta(\omega-\epsilon_\lambda), \tag{7.3}$$

and

$$\langle \epsilon_{\lambda\uparrow;0}\rangle = \epsilon_\lambda, \tag{7.4}$$

a result consistent with Eq. (7.1) since $n_\downarrow$ and $\mathfrak{I}_\downarrow$ are both zero, there being no down-spin electrons present.

We now calculate $A_{\lambda\lambda}{}^{\downarrow}(\omega)$. This of course is given by

$$A_{\lambda\lambda}{}^{\downarrow}(\omega) = 2\pi \sum_b \delta(\omega - E_b + E_0)\,\langle \Phi_0 \mid c_{\downarrow\lambda} \mid b\rangle \times \langle b \mid c^\dagger_{\downarrow\lambda} \mid \Phi_0\rangle. \tag{7.5}$$

Here E_0 is the energy of the ground state Φ_0 and is just

$$E_0 = \sum_{\lambda\ \mathrm{occ}} \epsilon_\lambda = -\epsilon_{\max}, \tag{7.6}$$

where we sum over the λ referring to occupied states in Φ_0 and use the fact that

$$\sum_\lambda \epsilon_\lambda = N\Delta t_{ii} = 0. \tag{7.7}$$

It is now a simple task to observe that the states $\mid b\rangle$ in Eq. (7.5) must all have precisely zero energy for infinite I, since when I tends to infinity the N electrons

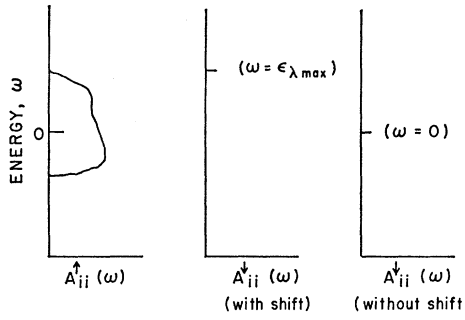

FIG. 5. The SWF at zero temperature for a state with $N-1$ up-spin electrons. $A\uparrow_{ii}(\omega)$ is the same as the unperturbed density of states; i.e., it displays no energy shift. $A\downarrow_{ii}(\omega)$ has an important energy shift. Hubbard's simple theory would predict no shift.

present in state $|b\rangle$ are prevented from hopping regardless of their spin. Thus, we have

$$A^{\downarrow}_{\lambda\lambda}(\omega) = (2\pi/N)\,\delta(\omega-\epsilon_{\max}), \tag{7.8}$$

where the multiplicative constant $(2\pi/N)$ has been determined through the relation

$$\int_{-\infty}^{+\infty} (d\omega/2\pi)\,A^{\downarrow}_{\lambda\lambda}(\omega) = \langle\Phi_0 \mid c_{\downarrow\lambda}c^{\dagger}_{\downarrow\lambda} \mid \Phi_0\rangle \tag{7.9a}$$

$$= 1/N. \tag{7.9b}$$

From this SWF we can calculate $\langle\epsilon_{\lambda\downarrow;0}\rangle$ and find

$$\langle\epsilon_{\lambda\downarrow;0}\rangle = \epsilon_{\max}, \tag{7.10}$$

which we must compare with Eq. (7.1). The virtue of this special case is that in addition to these results it is trivial to calculate $\mathfrak{I}_{\uparrow}/(1-n_{\uparrow})$ as well. $\mathfrak{I}_{\uparrow}$ is defined to be kinetic energy per site, which in this case is to be calculated in the ground state Φ_0. It is therefore just $-\epsilon_{\max}/N$. Furthermore $(1-n_{\uparrow})$ in the ground state is just $1/N$ so that

$$-\mathfrak{I}_{\uparrow}/(1-n_{\uparrow}) = \epsilon_{\max}, \tag{7.11}$$

and Eq. (7.1) becomes

$$\langle\epsilon_{\lambda\downarrow;0}\rangle \approx \epsilon_{\max} + \epsilon_{\lambda}/N. \tag{7.12}$$

For a large system we then see that the result of Eq. (7.10) is accounted for, by the energy shift $\mathfrak{I}_{\uparrow}/(1-n_{\uparrow})$, the term in Eq. (7.12) proportional to $1/N$ being negligible.[24] The density-of-states functions are plotted in Fig. 5. Note that without inclusion of the energy-shift term one would have

$$\langle\epsilon_{\lambda\downarrow;0}\rangle \approx \epsilon_{\lambda}/N \approx 0, \tag{7.13}$$

which is the result obtained from Hubbard's simple theory, Eq. (6.6). If the weight in $A\downarrow_{ii}(\omega)$ were not shifted up to $\epsilon_{\max}$, away from the mean energy at 0, the ferromagnetic state with which we started would not be the ground state, since one could clearly decrease the energy by shifting spins from the up states to the down states. Thus, in this case we see not only the importance of the shift but its necessity in the light of Nagaoka's independent proof of the ferromagnetic ground state. The zero-energy transition which can occur by shifting a spin into the down state at $\epsilon_{\max}$ can be shown from further arguments to correspond to a trivial rotation of the magnetization direction.

We will proceed to analyze other cases, taking Eq. (7.1) seriously, and finding the effect of the shift, neglecting the further effects due to damping of the one-particle excitations. As Hubbard has discussed,[2] complete ferromagnetism is favored when there is a high density of states away from the center of the band. Following Hubbard, we consider the following unperturbed density of states

$$\rho_0(E) = \delta^{-1}, \quad -\tfrac{1}{2}\Delta' \le E \le -\tfrac{1}{2}\Delta' + \tfrac{1}{2}\delta \tag{7.14a}$$

$$= \delta^{-1}, \quad \tfrac{1}{2}\Delta' \leftarrow \tfrac{1}{2}\delta \le E \le \tfrac{1}{2}\Delta' \tag{7.14b}$$

$$= 0, \quad \text{otherwise.} \tag{7.14c}$$

For concreteness consider the case of $\frac{1}{2}$ electron per atom in a supposedly stable ferromagnetic state. In Fig. 6 the results for the SWF according to Hubbard's theory are contrasted to these from Eq. (7.1). If $\delta < \Delta'$

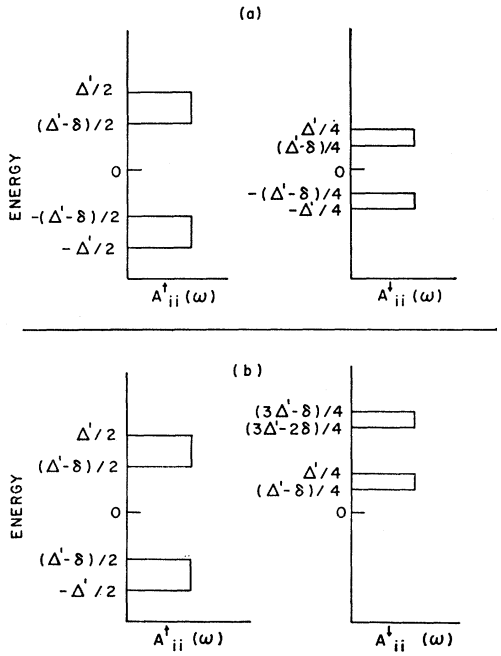

FIG. 6. The SWF for the unperturbed density of states given by Eq. (7.14) and for $\frac{1}{2}$ electron per site using (a) Hubbard's simple theory, Eq. (6.6) and (b) Eq. (7.1), i.e., including the energy shift. The analogous peaks in the SWF near energy I are not shown. The height of the peaks in the SWF is $1/\delta$ and the Fermi energy is at $-(\Delta'-\delta)/2$.

[24] The fact that Eq. (7.1) is not exact is to be expected since it was obtained by neglecting some of the terms in the exact result, Eq. (6.9). These neglected terms can be shown to give a contribution to $\langle\epsilon_{\lambda\sigma;0}\rangle$ of $-(1/N)\epsilon_{\lambda}$ thus explaining the discrepancy between Eqs. (7.10) and (7.12). In general, these neglected terms will be of order 1 and not of order $(1/N)$, but hopefully, as we have argued, they will be small.

this configuration is indeed stable as Hubbard has discussed, and ferromagnetism can occur. However, consider the effect on the band energies of the shift term. Noting that $\mathfrak{I}_\uparrow<0$ we see that the inclusion of this term moves the unoccupied down-spin band towards higher energies as we have shown in the figures. Using Eq. (7.1) the magnitude of this shift is easily found to be

$$-\mathfrak{I}_{-\sigma}/(1-n_{-\sigma})=(2\Delta'-8\delta)/4. \qquad (7.15)$$

Clearly, this energy shift has the effect of increasing the stability of the ferromagnetic array. Hence, we conclude that in this case Hubbard's simple theory gives too restrictive a condition for ferromagnetism.

The generality of this conclusion is apparent. Consider the stability of a saturated ferromagnetic state, where we assume without loss of generality less than one electron per site so that $n_\downarrow=0$. The up-spin band has no energy shift, since there are no down spins present. The down-spin band is shifted towards higher energy since $-\mathfrak{I}_{-\sigma}/(1-n_{-\sigma})$ is always positive. Thus, we conclude that Hubbard's theory, since it neglects this energy shift, always underestimates the stability of the ferromagnetic state. In other words, although correlations make ferromagnetism less stable than the Stoner theory would predict, this effect of correlation is somewhat overemphasized in Hubbard's treatment.

VIII. APPLICATION TO THE ANTIFERROMAGNETIC STATE WITH ONE ELECTRON PER SITE

In this section we shall give a treatment of antiferromagnetic ordering which avoids the complications inherent in the use of the equations-of-motion technique occasioned by the presence of two magnetically inequivalent sublattices. As we shall see, this situation creates no algebraic difficulties for the moment method. We discuss the effect of magnetic ordering on the SWF for the case of one electron per atom. For simplicity we treat the case of zero temperature and assume t_{ij} to be nonzero only if i and j are nearest-neighboring lattice sites and the lattice to be simple cubic or body-centered cubic. For such lattices it is accepted that the ground state is antiferromagnetic, one sublattice having spins aligned predominantly along the z direction (i.e., $n_\uparrow\approx1$, $n_\downarrow\approx0$) and vice versa for the other sublattice. To a good approximation we can neglect spin fluctuations in the ground state,[25] that is we can take

$$\langle n_{i\sigma}+n_{j\sigma}\rangle\cong0, \qquad (8.1a)$$

$$\sum_\sigma\langle n_{i\sigma}n_{j-\sigma}\rangle\cong-\langle n_{i\sigma}n_{j\sigma}\rangle\cong1, \qquad (8.1b)$$

$$\langle S_i^+S_j^-\rangle=\langle S_i^-S_j^+\rangle\cong0, \qquad (8.1c)$$

where i and j here refer to different sublattices. We now insert these approximations into the expressions for the first and second moments which we can obtain using the methods of Sec. IV. Explicitly we use the formula

$$m'_{ij\sigma;0}=\Delta t_{ij}\langle(1-n_{i-\sigma})(1-n_{j-\sigma})+c^\dagger_{j\sigma}c_{j,-\sigma}c^\dagger_{i,-\sigma}c_{i\sigma}\rangle-\delta_{ij}\mathfrak{I}_{-\sigma}. \qquad (8.2)$$

However, for the present case $\mathfrak{I}_\sigma=0$ and using the approximations of Eq. (8.1) one sees that the other terms also vanish, so that

$$m'_{ij\sigma;0}\cong0. \qquad (8.3a)$$

Similar analysis yields the following results

$$m'_{ij\sigma;I}\cong0, \qquad (8.3b)$$

$$m^2_{ij\sigma;0}=m^2_{ij,-\sigma;I}\cong\delta_{ij}\Delta^2(1-n_{i-\sigma}), \qquad (8.3c)$$

and to lowest order we have

$$m^0_{ij\sigma;0}=m^0_{ij,-\sigma;I}=(1-n_{i-\sigma})\,\delta_{ij}. \qquad (8.3d)$$

For an antiferromagnet the unit cell contains two magnetically inequivalent sites and hence the first Brillouin zone is half as large as for the same sample in its paramagnetic phase, but each wave vector has two single-particle excitations associated with it. The approximate excitation operators are $q^\dagger_{\lambda\sigma\rho}$ where $\rho=1,2$ distinguishes between the excitations for a given wave vector where

$$q^\dagger_{\lambda\sigma\rho}=\alpha_{\rho0}(\lambda\sigma)c^\dagger_0(\lambda\sigma)+\alpha_{\rho\tau}(\lambda\sigma)c^\dagger_\tau(\lambda\sigma). \qquad (8.4)$$

Here,

$$c^\dagger_0(\lambda\sigma)=N_{\rm uc}^{-1/2}\sum_{\mathbf R}c^\dagger_{\mathbf R\sigma}\exp(i\lambda\cdot\mathbf R), \qquad (8.5a)$$

$$c_\tau^\dagger(\lambda\sigma)=N_{\rm uc}^{-1/2}\sum_{\mathbf R}c^\dagger_{\mathbf R+\tau,\sigma}\exp[i\lambda\cdot(\mathbf R+\boldsymbol\tau)], \qquad (8.5b)$$

$N_{\rm uc}=N/2$ is the number of unit cells, $\mathbf R$ is summed over unit cells, and the vectors 0 and $\boldsymbol\tau$ give the positions of the two sites within the unit cell. The coefficients $\alpha_{\rho0}(\lambda\sigma)$ and $\alpha_{\rho\tau}(\lambda\sigma)$ cannot be determined from symmetry considerations.

It is natural to introduce the SWF

$$A_{\lambda\sigma\rho}(\omega)=\text{F.T.}\langle\{q_{\lambda\sigma\rho}(t),q^\dagger_{\lambda\sigma\rho}(t')\}_+\rangle, \qquad (8.6)$$

[25] D. L. Bullock, Phys. Rev. **137**, A1877 (1965).

where F.T. means Fourier transform, cf. Eq. (2.11). This SWF can be decomposed into its components $\alpha_{\lambda\sigma\rho;pI}(\omega)$ which have moments $m^n{}_{\lambda\sigma\rho;pI}$ taken relative to $\omega=pI$. These quantities can be readily calculated using the results of Eq. (8.3) since $A_{\lambda\sigma\rho}(\omega)$ can be expressed in terms of $A^\sigma{}_{ij}(\omega)$ using Eqs. (8.4) and (8.5). Thus we find

$$m^0{}_{\lambda\sigma\rho;0}=|\alpha_{\rho0}(\lambda\sigma)|^2(1-\langle n_{0-\sigma}\rangle)+|\alpha_{\rho\tau}(\lambda\sigma)|^2(1-\langle n_{\tau-\sigma}\rangle), \tag{8.7a}$$

$$m^0{}_{\lambda\sigma\rho;I}=1-m^0{}_{\lambda\sigma\rho;0}, \tag{8.7b}$$

$$m^1{}_{\lambda\sigma\rho;0}=m^1{}_{\lambda\sigma\rho;I}=0, \tag{8.7c}$$

$$m^2{}_{\lambda\sigma\rho;0}=|\alpha_{\rho0}(\lambda\sigma)|^2\Delta^2(1-\langle n_{0-\sigma}\rangle)+|\alpha_{\rho\tau}(\lambda\sigma)|^2\Delta^2(1-\langle n_{\tau-\sigma}\rangle), \tag{8.7d}$$

$$m^2{}_{\lambda\sigma\rho;I}=|\alpha_{\rho0}(\lambda\sigma)|^2\Delta^2\langle n_{0-\sigma}\rangle+|\alpha_{\rho\tau}(\lambda\sigma)|^2\Delta^2\langle n_{\tau-\sigma}\rangle, \tag{8.7e}$$

so that the root-mean-square width of the peaks in the SWF is given as

$$\langle\delta\epsilon_{\lambda\sigma\rho;0}\rangle=\left\{\frac{m^2{}_{\lambda\sigma\rho;0}}{m^0{}_{\lambda\sigma\rho;0}}-\left(\frac{m^1{}_{\lambda\sigma\rho;0}}{m^0{}_{\lambda\sigma\rho;0}}\right)^2\right\}^{1/2}=\Delta, \tag{8.8a}$$

$$\langle\delta\epsilon_{\lambda\sigma\rho;I}\rangle=\left\{\frac{m^2{}_{\lambda\sigma\rho;I}}{m^0{}_{\lambda\sigma\rho;I}}-\left(\frac{m^1{}_{\lambda\sigma\rho;I}}{m^0{}_{\lambda\sigma\rho;I}}\right)^2\right\}^{1/2}=\Delta. \tag{8.8b}$$

It would be very interesting to compare these calculations with the corresponding calculations made assuming (incorrectly) paramagnetic ordering, but the expressions for the second moments are too complex. However, it is possible to calculate $\{\langle\langle\delta\epsilon_{\lambda\sigma\rho;0}\rangle^2\rangle_\lambda\}^{1/2}$, where the $\langle\ \rangle_\lambda$ indicates an average over λ. This should give us a qualitative estimate of the linewidth for the paramagnetic case. In fact Hubbard's improved solution indicates, see Eq. (6.20), that this quantity is independent of λ in which case taking the average would introduce no error at all. Thus, we obtain

$$\{\langle\langle\delta\epsilon_{\lambda\sigma\rho;0}\rangle^2\rangle_\lambda\}^{1/2}=\left\{\frac{m^2{}_{ii\sigma;0}}{m^0{}_{ii\sigma;0}}-N^{-1}\sum_\lambda\left(\frac{m^1{}_{\lambda\lambda\sigma;0}}{m^0{}_{\lambda\lambda\sigma;0}}\right)^2\right\}^{1/2}=(\tfrac{3}{4})^{1/2}\Delta, \tag{8.9a}$$

$$\{\langle\langle\delta\epsilon_{\lambda\sigma\rho;I}\rangle^2\rangle_\lambda\}^{1/2}=\left\{\frac{m^2{}_{ii\sigma;I}}{m^0{}_{ii\sigma;0}}-N^{-1}\sum_\lambda\left(\frac{m^1{}_{\lambda\lambda\sigma;0}}{m^0{}_{\lambda\lambda\sigma;I}}\right)^2\right\}^{1/2}=(\tfrac{3}{4})^{1/2}\Delta. \tag{8.9b}$$

Comparing Eqs. (8.8) and (8.9) we see that the peaks in the SWF are broader for antiferromagnetic ordering than for the paramagnetic phase. In other words the electron excitations have a longer lifetime in the paramagnetic phase than in the antiferromagnetic plase. This phenomenon would be quite interesting to observe experimentally.

IX. CONCLUSION

We have shown how the moment method may be used to discuss effects which are difficult to treat using the usual decoupling schemes for the equations of motion of the Green's functions. In particular we have been able to estimate quantitatively the shift in weight among the main peaks in the SWF and also the intensity of the first satellite peaks in the SWF. We have verified that Hubbard's improved treatment of his model is indeed improved in the sense that the moments obtained from the SWF agree more closely with the exact results than would be the case using his simpler theory. We have pointed out that in addition to band narrowing one should also include the spin-dependent shifts in the band energy which favor ferromagnetism when discussing questions of magnetic stability. We have also shown that the effect of antiferromagnetic ordering is to broaden the peaks corresponding to single-particle excitations in comparison to the disordered or ferromagnetic state.

ACKNOWLEDGMENTS

The authors would like to thank Dr. W. Marshall for the hospitality of the Atomic Energy Research Establishment at Harwell. It is a pleasure to acknowledge many stimulating discussions with Dr. J. Hubbard. We would also like to thank Professor J. R. Schrieffer for some instructive comments on band theory. One of us (R.V.L.) would like to thank Professor R. Peierls for hospitality at Oxford University.