Narrow-Band Expansions in the Hubbard Model: A Comment*

Robert A. Bari
Lincoln Laboratory, Massachusetts Institute of Technology, Lexington, Massachusetts 02173
(Received 2 March 1970)

The connection between a solution of the Hubbard Hamiltonian obtained by Esterling and Lange and the low-density solution is discussed. It is shown that their solution agrees to first order in the bandwidth with the exact solution for the two-electron N-site case. However, even this correct first-order expansion fails to adequately account for the low-frequency behavior of the Green's function and related quantities.

I. INTRODUCTION

In a recent paper, Roth[1] has obtained an approximate solution to the single-band Hubbard Hamiltonian and has discussed its failures in the low-density limit and also related these failures to a paper by Esterling and Lange.[2] It is the purpose of this comment to clarify the connection between the work by the authors in Ref. 2 (EL) and results obtained in the low-density limit.

The procedure used by EL was to make a Taylor expansion of the mass operator in powers of the bandwidth about the zero-bandwidth limit. It will be shown here that the results of EL agree to first order in the bandwidth with the exact solution for the two-electron N-site Hubbard model. Further comments will be made concerning the nature of this expansion.

II. EXACT SOLUTION

For two electrons in an N-site Hubbard model, it is convenient to write the Hamiltonian[3] in the Bloch representation:

$$H=\sum_k \epsilon(k)(C_{k\uparrow}^\dagger C_{k\uparrow}+C_{k\downarrow}^\dagger C_{k\downarrow}) + (I/N)\sum_{p,q,q'} C_{q\uparrow}^\dagger C_{q-p\uparrow} C_{q'\downarrow}^\dagger C_{q'+p\downarrow} \quad . \tag{1}$$

Here $\epsilon(k)$, I, and $C_{k\sigma}^\dagger$ specify the Bloch (bandwidth parameter) energy, interaction parameter, and creation operator for Bloch state k and spin up ($\uparrow$), respectively. The summation is over the N k vectors in the first Brillouin zone. The following Green's function is defined:

$$G^q(k,t-t')\equiv -i\,{}_t\langle K+q\,|\,(C_{k-q\uparrow}(t)C_{k\uparrow}^\dagger(t'))_+\,|K\rangle_t \quad . \tag{2}$$

The symbol $(\,)_+$ denotes the usual fermion time ordering and the state $|K\rangle_t$ denotes $C_{K\downarrow}^\dagger(t)|\mathrm{vac}\rangle$. Thus, Eq. (2) describes the propagation of a spin-up electron in a system otherwise containing a single spin-down electron. For the Hubbard Hamiltonian, $|K\rangle_t$ is trivially an exact eigenstate. From the equation of motion for $C_{k-q\uparrow}(t)$, it follows that

$$\left\{ i\frac{\partial}{\partial t}-\epsilon(k-q)-\epsilon(K+q)+\epsilon(K)\right\} G^q(k,t-t') = \delta_{q,0}\,\delta(t-t')-i(I/N)\sum_{p,q'}{}_t\langle K+q\,|\,(C_{q'\downarrow}^\dagger(t) \times C_{q'+p\downarrow}(t)\,C_{k-q-p\uparrow}(t)\,C_{k\uparrow}^\dagger(t'))_+\,|K\rangle_t \quad . \tag{3}$$

It is easily seen that

$$-i\,{}_t\langle K+q\,|\,(C_{q'\downarrow}^\dagger(t)C_{q'+p\downarrow}(t)C_{k-q-p\uparrow}(t)\,C_{k\uparrow}^\dagger(t'))_+\,|K\rangle_t = \delta_{q+K,q'}\,G^{q+p}(k,t-t') \quad . \tag{4}$$

After transforming to frequency space, Eq. (3) becomes

$$\{\omega-\epsilon(k-q)-\epsilon(K+q)+\epsilon(K)\}\,G^q(k,\omega) = \delta_{q,0}+(I/N)\textstyle\sum_p G^{q+p}(k,\omega) \quad . \tag{5}$$

The summation over p is independent of q (since $q+p$ can always be reduced to a vector in the first Brillouin zone) and, from Eq. (5),

$$\sum_q G^q(k,\omega)=[\omega-\epsilon(k)]^{-1}\left(1-\frac{I}{N}\sum_q\frac{1}{\omega-\epsilon(k-q)-\epsilon(K+q)+\epsilon(K)}\right)^{-1} \quad . \tag{6}$$

Therefore, $G^q(k,\omega)$ is written explicitly as

$$G^q(k,\omega)=\left[\delta_{q,0}+\frac{I/N}{\omega-\epsilon(k)}\left(I-\frac{I}{N}\sum_q\frac{1}{\omega-\epsilon(k-q)-\epsilon(K+q)+\epsilon(K)}\right)^{-1}\right]\Big/\,[\omega-\epsilon(k-q)-\epsilon(K+q)+\epsilon(K)] \quad . \tag{7}$$

The mass operator is defined by $\Sigma(k,\omega)\equiv\omega-\epsilon(k)-[G(k,\omega)]^{-1}$, where $G(k,\omega)$ is given by Eq. (2) with $q=0$. Thus,

$$\Sigma(k,\omega)=\left(\frac{I}{N}\right)\Big/\left(1-\frac{I}{N}\sum_{q\neq 0}\frac{1}{\omega-\epsilon(k-q)-\epsilon(K+q)+\epsilon(K)}\right) \tag{8}$$

is the exact mass operator for two electrons in the N-site Hubbard model. The mass-operator expansion of EL is compared with this result in Sec. III.

III. COMPARISON WITH ESTERLING AND LANGE

In order to compare Eq. (8) with the results of EL, the former is expanded to first order in the Bloch energy parameter. This gives, with $n = 1/N$,

$$\Sigma(k,\omega)=\frac{In\omega}{\omega-I(1-n)}-\frac{I^2[n\epsilon(K)+n^2\epsilon(k)]}{[\omega-I(1-n)]^2}+(\text{higher order terms}); \tag{9}$$

here, $\sum_q \epsilon(q)=0$, without loss of generality. It is to be noted that the expansion requires $|\epsilon(k)/I|<1$ and $|\epsilon(k)/\omega|<1$ for all k.

It is interesting to compare Eq. (9) with Eqs. (15)–(20) of Ref. 2. In order to see that the mass-operator expansion of EL does reduce to Eq. (9) for the case of two electrons in N sites, their mass operator is written as

$$\Sigma(k,\omega)=\frac{In\omega}{\omega-I(1-n)}-I^2\left(\frac{1}{N}\sum_k \epsilon(k)\langle C_{k\uparrow}^\dagger C_{k\uparrow}\rangle-\frac{1}{N}\sum_q \epsilon(k+q)(D_q+S_q)\right)\Big/[\omega-I(1-n)]^2 , \tag{10}$$

where

$$D_q=\sum_j e^{-iq\cdot(R_i-R_j)}(\langle n_{i\uparrow}n_{j\downarrow}\rangle-n^2) \tag{11}$$

and

$$S_q=\sum_j e^{-iq\cdot(R_i-R_j)}\langle C_{i\uparrow}C_{i\uparrow}^\dagger C_{j\downarrow}C_{j\downarrow}^\dagger\rangle . \tag{12}$$

(The indices i and j refer to Wannier sites.) Since the expectation value refers to the state $|K\rangle_t$, it follows that $\langle C_{k\uparrow}^\dagger C_{k\uparrow}\rangle=\delta_{k,K}$, $D_q=n-n\delta_{q,0}$, and $S_q=n$. With these connections, it is readily seen that the mass operator given by EL agrees with the exact expression to first order as given by Eq. (9). Thus the claim made by EL, that they have presented a Green's function that accounts for all first-order effects in the kinetic (Bloch) energy, has been verified by the exact solution for two electrons in an arbitrary number of sites.

IV. DISCUSSION

Roth has argued that EL have unjustly claimed to have an exact result in the "strongly correlated limit." EL have, in fact, claimed to account for all first-order effects in the kinetic energy. This latter claim is correct, as has been verified above. Roth's argument is based on the fact that the EL mass operator does not agree in the low-density limit with the T approximation to the mass operator. However, the T approximation, which for two electrons is the first order in the density expansion of Eq. (8), contains terms of all orders in the kinetic energy parameter $\epsilon(k)$. Therefore, in comparing the results of EL with the T-approximation mass operator, one must expand the latter to first order in the Bloch energy and see if the EL mass operator agrees with it or not. That it does agree has been demonstrated above.

A different, but more subtle, question concerns the nature of the Bloch energy power expansion of the mass operator. From Eq. (8), two serious conclusions can be drawn: (1) Near zero frequency the mth power term in the expansion of the mass operator behaves as ω^{1-m}; (2) the expansion does not yield finite lifetimes in any finite order. This implies that, if lifetime effects are important at a frequency ω_0, the expansion of Eq. (8) is being carried out beyond its radius of convergence in ω^{-1}. The singular behavior of terms with $m \geq 2$ and the lack of finite lifetimes points out the inadequacies of an expansion in powers of the Bloch energy. An approximation (to the mass operator) which contains terms of all orders in the Bloch energy is necessary for obtaining finite lifetimes.

ACKNOWLEDGMENTS

It is a pleasure to thank D. M. Esterling and R. V. Lange for several conversations and Laura M. Roth for helpful remarks.

*Work sponsored by the Department of the Air Force.

[1]L. M. Roth, Phys. Rev. 184, 451 (1969).
[2]D. M. Esterling and R. V. Lange, Rev. Mod. Phys. 40, 796 (1968).
[3]J. Hubbard, Proc. Roy. Soc. (London) A276, 238 (1963).