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NEW METHOD FOR LINEARIZING MANY-BODY EQUATIONS OF MOTION IN STATISTICAL MECHANICS

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A new criterion is proposed for linearizing many-body equations of motion which is well defined and is related to a stationary principle. The method is applied to the problem of correlation in a narrow s band and the results differ considerably from Hubbard's treatment of this problem.

One of the advantages of Green's function[1,2] and equation-of-motion methods[3,4] in statistical mechanics has been the fact that operators can be used which are not strictly fermion or boson operators. For example, the Green's-function method has been used for spins by Tyablikov[5] and others, and for atomic states in narrow energy bands, by Hubbard.[6] The above freedom brings with it disadvantages, however, because the truncation procedures are somewhat arbitrary. We propose here a prescription for truncating equations of motion which is well defined and which is related to a stationary principle.

We discuss the truncation scheme for a general many-body problem and in terms of the equation-of-motion method. We shall later apply it to the narrow s band considered in Hubbard I,[6] whose Hamiltonian is[7]

$$H = U\sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{ij\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma}, \tag{1}$$

where c's are creation and annihilation operators for Wannier sites, and the notation is as in Ref. 7. In the equation-of-motion method, we attempt to construct a creation or annihilation operator A for a quasiparticle, which satisfies in some approximation

$$[A, H] = \omega A. \tag{2}$$

Here, if we think of A as an annihilation operator, then ω is the quasiparticle energy. More generally, we might attempt to find a basis set of operators $\{A_i\}$ such that

$$[A_i, H] = \sum_j K_{ij} A_j. \tag{3}$$

If we obtain Eq. (3), we can then diagonalize K to give Eq. (2). Of course, for systems with interactions, Eqs. (2) and (3) are not in general satisfied by simple operators, so that one must make approximations. What is usually done is to replace some operators on the right-hand side by their expectation values. The simplest example is the Hartree-Fock approximation, for which we use only one-fermion operators and for which in our example we have, using $c_{i\sigma}$ as the basis set,

$$K_{ij}^{\sigma} = t_{ij} + U\langle n_{-\sigma}\rangle. \tag{4}$$

Higher approximations have been worked out by many authors, and we mention especially Suhl and Werthamer's[4] work in which they show how to include all three-fermion operators in the set $\{A_i\}$ and to truncate expressions with five-fermion operators. However, in Hubbard's[6] work it was shown that the most important correlations in a narrow energy band are those on a single atomic site, so that he proposed decoupling according to particular states of occupancy of atomic sites rather than according to the number of fermion operators involved. In particular, for the case of the narrow s band he singled out one type of three-fermion operator, $n_{-\sigma}c_{i\sigma}$. The result of Hubbard's first calculation was criticized by Harris and Lange,[8] who showed that certain moments of the spectral function[8,2] were not reproduced correctly. This seems to be a result of the ambiguities in truncating equations of motion with one but not all three-fermion operators.

Our proposal is to use the following prescription for determining the K_{ij} self-consistently: Let us commute or anticommute, according to the statistics, both sides of Eq. (3) with another member of the set and then take either the expec-

tation value in the ground state, or the thermal average, of both sides. This gives

$$\langle[[A_i,H],A_l^+]_\mp\rangle \equiv E_{il} = \sum K_{ij}\langle[A_j,A_l^+]_\mp\rangle, \qquad (5)$$

where the upper sign is for bosons or an even number of fermions, and the lower sign is for an odd number of fermions. Then, to the extent that the various averages can be calculated, this gives a well-defined method for determining the K_{ij} of Eq. (3), provided that the matrix $N_{ij} = \langle A_i, A_j^+]_\mp\rangle$ is nonsingular. The matrices E_{ij} and N_{ij} are Hermitian, though K_{ij} need not be.

It should take only a little thought to convince oneself that Eq. (5) reduces to the Hartree-Fock approximation if we keep only single-particle operators. Also, for any problem for which a Hartree-like approximation can be used, Eq. (5) will reproduce the standard result. An example is the equation-of-motion approach to superconductivity.[9] Furthermore, if we let the set A_i consist of one-particle and three-particle operators, and further approximate all of the brackets by the corresponding quantity obtained by requiring momenta to match in pairs, the "second random phase approximation" of Suhl and Werthamer[4] is reproduced.

The relation to the variational principle is as follows: Suppose that an operator A exists which obeys Eq. (2) with ω real. Then we can readily prove that if we vary A and A^+,

$$\delta\{\langle[[A,H],A^+]_\mp\rangle - \omega\langle[A,A^+]_\mp\rangle\} = 0. \qquad (6)$$

That is, if an exact A exists, then the frequency obeys a stationary condition. The expectation value involved can be in the exact ground state, or in any eigenstate of H for which $\langle[A,A^+]_\mp\rangle$ is finite. Then if we assume that A is given by a linear combination of the members of our set A_i, with constant coefficients, variation of Eq. (7) with respect to the coefficients yields an eigenvalue equation whose solutions are just the eigenvalues of K_{ij}.

Now exact solutions of Eq. (2) do in fact exist, of the form $|n\rangle\langle m|$, where n and m are two different eigenstates of the total Hamiltonian, with ω given by $\epsilon_m - \epsilon_n$. To be definite, let us assume that the expectation value in Eq. (7) is in the ground state. Then we must have either n or m, say n, be the ground state, and the energy involved is then the difference in energy between states $A^+|0\rangle$ and $|0\rangle$. The eigenvalues of H are well known to be stationary. The difference from the usual variational result is that we are varying the operators rather than the wave functions.

While the stationary principle gives some weight to our arguments, what we would really like to prove is that our prescription leads to an upper bound for the total energy. This we have not succeeded in doing as yet. However, we feel that if the variational method gives one a hunting license for choosing trial wave functions, our prescription at least gives us poaching rights, and Eq. (5) gives us in some sense the best equation-of-motion results for a given choice of quasiparticle operators.

Our result is particularly useful when applied to the calculation of Green's functions. If we use the notation of Zubarev,[2] then from the equation of motion for the Green's function,[2,6] along with Eq. (5), we can construct a whole "brace" of retarded Green's functions:

$$\langle\langle A_i, B^+\rangle\rangle_\omega = \frac{1}{2\pi}\sum_j [(\omega + i\epsilon - K)^{-1}]_{ij}\langle[A_j,B^+]_\mp\rangle. \qquad (7)$$

We can then use standard Green's-function methods for evaluating the various expectation values that occur.

As an illustration of the method, let us consider the narrow-band problem of Eq. (1). We take as a basis set the operators

$$c_{\vec{k}\sigma} = \sum \exp(i\vec{k}\cdot\vec{R}_i)c_{i\sigma}, \qquad d_{\vec{k}\sigma} = \sum \exp(i\vec{k}\cdot\vec{R}_i)n_{i-\sigma}c_{i\sigma}. \qquad (8)$$

This is the same basis set used in Hubbard I. We can then evaluate the 2×2 matrices E_{ij} and N_{ij} for each spin:

$$E_\sigma = \begin{pmatrix} \epsilon_{\vec{k}} + Un_{-\sigma} & (U+\epsilon_{\vec{k}})n_{-\sigma} \\ (U+\epsilon_{\vec{k}})n_{-\sigma} & Un_{-\sigma} + \epsilon_{\vec{k}}n_{-\sigma}{}^2 + n_{-\sigma}(1-n_{-\sigma})W_{\vec{k}-\sigma} \end{pmatrix}, \qquad (9)$$

$$N_\sigma = \begin{pmatrix} 1 & n_{-\sigma} \\ n_{-\sigma} & n_{-\sigma} \end{pmatrix}, \qquad (10)$$

where $\epsilon_{\vec{k}} = \Sigma_j t_{0j} \exp(i\vec{k}\cdot\vec{R}_j)$, and where

$$n_\sigma(1-n_\sigma)W_{\vec{k}\sigma} = \sum_{j\neq 0} t_{0j}\langle c_{0\sigma}{}^{+}c_{j\sigma}(1-n_{0-\sigma}-n_{j-\sigma})\rangle$$

$$-\sum t_{0j}\exp(i\vec{k}\cdot\vec{R}_j)(n_\sigma{}^2-\langle n_{i\sigma}n_{j\sigma}\rangle+\langle c_{j-\sigma}{}^{+}c_{0\sigma}{}^{+}c_{j\sigma}c_{0-\sigma}\rangle+\langle c_{j-\sigma}{}^{+}c_{j\sigma}{}^{+}c_{0\sigma}c_{0-\sigma}\rangle). \quad (11)$$

Then from Eqs. (5) and (7) we can construct Green's functions, in particular, the one-particle Green's function

$$\langle\langle c_{\vec{k}}; c_k{}^{+}\rangle\rangle = \frac{\omega - U(1-n_{-\sigma}) - W_{\vec{k}-\sigma}}{(\omega-\epsilon_{\vec{k}}-U)(\omega-W_{\vec{k}-\sigma})+U(\epsilon_{\vec{k}}-W_{\vec{k}-\sigma})(1-n_{-\sigma})}. \quad (12)$$

This result is the same as the result of Hubbard I except for the appearance of the term $W_{\vec{k}\sigma}$. To interpret this term, let us look at the poles of the Green's function (or the eigenvalues of K_{ij}) in the limit of very large U:

$$E_{\vec{k}\sigma}{}^{a} \sim (1-n_{-\sigma})\epsilon_{\vec{k}} + n_{-\sigma}W_{\vec{k}-\sigma}, \quad (13)$$

$$E_{\vec{k}\sigma}{}^{b} \sim U + n_{-\sigma}\epsilon_{\vec{k}} + (1-n_{-\sigma})W_{\vec{k}-\sigma}. \quad (14)$$

Looking at the lower set of levels, (13), we see that in addition to the band-narrowing term which Hubbard obtained, there is a shift of the center of gravity of the band given by the first term of Eq. (11). The second term of Eq. (11) represents an additional band narrowing, and is smaller than the first. This result is exactly the same as that obtained by Harris and Lange[8] from their moment calculation, when we omit terms which vanish for $U \to \infty$. In this connection let us remark that the one-particle Green's function for finite U is exactly what results if we assume two poles on the real axis and fit the relative weights and positions to the first three moments of the spectral function, i.e., the imaginary part of $\langle\langle c_{\vec{k}\sigma}; c_{\vec{k}\sigma}{}^{+}\rangle\rangle$. This would indeed seem to be the best we could do within the limitations of Hubbard's two-peak approximation.

The result also reduces (for finite or infinite U) to energies obtained in the author's variational calculation for the case in which the ground state was ferromagnetic.[7] That work was primarily concerned with spin waves, but single-particle states were also obtained and the present calculation generalizes these results to the case of partial- or no-spin alignment.

As Harris and Lange point out, the band shift makes it more likely that the ground state of the system is ferromagnetic. To investigate the predictions of our method as to the occurrence of ferromagnetism in this model, we have self-consistently evaluated n_σ and $W_{\vec{k}\sigma}$ by Green's-function methods.[2,4] The results for $U \to \infty$ give, assuming only the lower set to be occupied,

$$n_\sigma = (1-n_{-\sigma})\sum_{\vec{k}} f(E_{\vec{k}\sigma}{}^{a}), \quad (15)$$

$$n_\sigma(1-n_\sigma)W_{\vec{k}\sigma} = -\sum_j t_{0j}n_{j\sigma} - \sum_j t_{0j}\exp(i\vec{k}\cdot\vec{R}_j)[n_{j\sigma}{}^2(1-n_\sigma)+n_{j\sigma}n_{j-\sigma}]/(1-n_\sigma-n_{-\sigma}), \quad (16)$$

where f is the Fermi function and where

$$n_{j\sigma} = \sum_k \exp(ik\cdot\vec{R}_j) f(E_{\vec{k}\sigma}{}^{a}).$$

Eqs. (13), (15), and (16) must be solved self-consistently. For the case of nearest-neighbor interactions, this is not difficult once we know the density of states for the noninteracting case, because the shape of the bands is not altered by the interactions. What we do is to vary the unperturbed Fermi energies of the two spin bands, which determines the Fermi surfaces and the various parameters, until the perturbed Fermi energies match up. We have carried out the calculation for a simple cubic lattice using Wolfram and Calloway's[10] density of states; and we find regions of n, the number of electrons per site, for which solutions exist for $n_\uparrow \neq n_\downarrow$. The magnetization is plotted in Fig. 1 versus n. We also include a plot of the total energy of the system versus n, as calculated from the one-particle Green's function.[1,2]

The existence of magnetic solutions for this

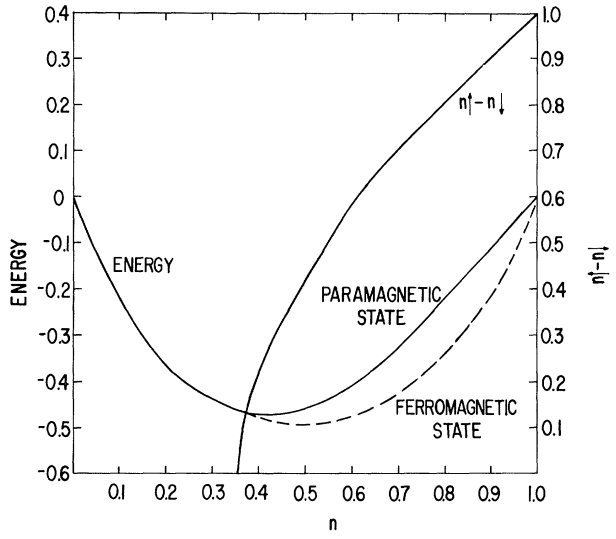

FIG. 1. Magnetization ($2\langle S_z \rangle$) and total energy per site plotted against the number of electrons per site. Units of energy are such that the bandwidth is 6.

model in the infinite-U limit brings this theory in line with the work of Nagaoka,[11] who showed that for the almost-half-filled case the ground state is ferromagnetic, and with the author's previous work on the model.[7] In this sense we have rescued the "Hubbard I" theory. Outside of the truncation procedure we are, of course, making all of the other approximations of that theory, including neglect of spin waves and of level broadening. We hope to apply the method to Hubbard's improved versions (II and III) of the theory. The approach should be particularly helpful in the orbitally degenerate case (II), where we can put in projection operators for states of occupancy of the ions. We believe that the method should have further applications in statistical mechanics.

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