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Hubbard Model near the Atomic Limit

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Certain statements concerning the Hubbard model in the atomic limit are clarified and corrected. Certain inconsistencies and difficulties associated with various approximate solutions to the Hubbard model near the atomic limit are pointed out.

The Hubbard model describes electrons in a single band moving with their mutual Coulomb repulsion screened out with the exception of two electrons on the same lattice site. If two electrons hop onto the same site, the potential energy of the system is increased by an amount I. Explicitly, the model Hamiltonian is

$$H=\sum_{ij\sigma} T_{ij}c_{i\sigma}{}^{\dagger}c_{j\sigma}+\tfrac{1}{2}I\sum_{i\sigma} n_{i\sigma}n_{i-\sigma}. \tag{1}$$

The sum is over Wannier states labeled by a lattice-site index i. It will be useful to define an effective bandwidth Δ as

$$\Delta\equiv\left(\frac{1}{N}\sum_{ij}|T_{ij}|^2\right)^{1/2} \tag{2}$$

This model Hamiltonian is, from a conceptual standpoint, the simplest possible many-body Hamiltonian describing electron motion in a crystal. Of particular physical interest is the narrow-energy-band regime $kT\ll\Delta\ll I$. Many approximate solutions have been proposed in this regime, each of which in some sense or another takes advantage of the fact that $\Delta/I\ll 1$. The purpose of this note will be to analyze these approaches. First, we will discuss the difficulties associated with any systematic perturbation theory in Δ/I. Closely associated with these difficulties are certain ambiguities in the atomic limit ($\Delta\to 0$). After discussing the atomic limit, we will be in a position to analyze various Green's-function decoupling approaches. This note will be concerned with arbitrary densities, and the associated comments do not necessarily apply for low densities, nor for the half-filled-band case, where special approaches have been developed.

The problem that any perturbation theory will encounter can be stated quite generally and quite succinctly. For simplicity, let the temperature T be zero. We then have two parameters with dimensions of energy in the problem, Δ and I. For $\Delta\ll I$, we have a dimensionless coupling constant Δ/I and should then be able to find an expression for the quantity of interest in powers of Δ/I. Such an expansion exists. However, the coefficients are not well defined. To be specific, consider the case of infinite I. Then the series is "trivial" in that it only consists of one term. However, in order to evaluate that term we must be able to find an exact solution to a generalized excluded-volume problem! For $kT=0$ and $I\to\infty$, the only energy parameter left is Δ. One can write down pseudoexpansions in explicit powers of Δ [e.g., the mass-operator expansion of Esterling and Lange[1] (EL)], but each term is of the same order. In the case of the EL mass-operator expansion, the higher-order terms essentially behave as $\Delta(\Delta/\omega)^p$, where ω is the frequency associated with the Fourier transform. Since the frequencies of interest are also of order Δ, each term is of the same order.[2] This point will be further clarified when we discuss the (related) difficulties with the atomic limit ($\Delta\to 0$).

Even lacking a finite-Δ solution, one can obtain a great deal of information about the finite-Δ problem from the atomic limit. Harris and Lange[3] have derived certain exact sum rules for the spectral weight function (SWF). These sum rules are couched in terms of certain correlation functions. If somehow we knew certain of these correlation functions for ($\Delta\to 0$), we could find, say, the zeroth, first, and second moments of each peak in the SWF correct to $O(\Delta)$. These could then be directly translated into quasiparticle energy levels (from the first moment) and lifetimes (from the second moment).

Esterling and Lange[4] have analyzed the atomic limit and emphasized the physical manifestations of the degeneracy, originally pointed out by Harris and Lange.

Their statements that the single-particle Green's function G_1 is nonlocal even for zero hopping ($\Delta\to 0$) and that various nonlocal correlation functions (e.g., the density-density correlation function) do not factor for zero hopping remain valid. However, their claim to have expressed all the ambiguity in G_2 arising from the degeneracy in terms of the ambiguity in G_1 contains certain inconsistencies.

This expression for G_2 in terms of G_1 is given in Eq. (70) of I. In order to see explicitly what causes the inconsistency, it is necessary to include in the expression for G_2 all the terms of explicit order Δ that were dropped. Rather than rederiving such an equation using the somewhat laborious techniques of I, it will be easier to derive here a suitable expression for G_2 using the technique of functional derivatives.

The following definitions will be employed:

$$G(11'\sigma)\equiv -i\langle(c_{1\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle, \tag{3}$$

$$\Gamma(11'\sigma)\equiv -i\langle(n_{1-\sigma}c_{1\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle, \tag{4}$$

$$G(121'2';\sigma\sigma')\equiv -\langle(c_{1\sigma}c_{2\sigma'}c_{2'\sigma'}^{\dagger}c_{1'\sigma}^{\dagger})_{+}\rangle. \tag{5}$$

Here the usual expectation values have been redefined by introducing a fictitious external field. Specifically,

$$\langle(\ )_{+}\rangle\to\langle(S\ )_{+}\rangle/\langle(S)_{+}\rangle, \tag{6}$$

where

$$S=\exp\Big[-i\sum_{R_2R_2'\sigma}\int dt_2\int dt_{2'}\,U(2'2\sigma)c_{2'\sigma}^{\dagger}c_{2\sigma}\Big] \tag{7}$$

is the S matrix and all the operators are to be considered in the interaction representation. Hence, the equations of motion for the *operators* are not modified [they involve the original Hamiltonian in Eq. (1)], but the equations of motion for the Green's functions pick up additional terms because of the implicit time dependence in S.[5]

The functional derivatives will yield relationships among the various Green's functions. Essentially, taking a functional derivative yields a higher-order Green's function. In particular,

$$\frac{\delta G(11'\sigma)}{\delta U(2'2\sigma')}=-[G(121'2';\sigma\sigma')-G(11'\sigma)G(22'\sigma')]. \tag{8}$$

If we make the definition

$$G^{0}(12)^{-1}=i(\partial/\partial t_1)\delta(12), \tag{9}$$

then the equation of motion for G becomes

$$[G^{0}(12)^{-1}-T(12)-U(12\sigma)]G(21'\sigma)=\delta(11')+I\Gamma(11'\sigma). \tag{10}$$

In a similar fashion, an equation of motion for Γ may be derived. Next, an equation for the two-particle Green's function may be derived by taking the functional derivative of Eq. (10). This involves $\delta\Gamma/\delta U$, which may be obtained from differentiating the equation for Γ. After some straightforward matrix manipulation, we obtain the following equation for $\delta G/\delta U$, evaluated at $U=0$:

$$\begin{aligned}
&[\delta(13)+I\Gamma(13\sigma)]\frac{\delta G(31'\sigma)}{\delta U(2'2\sigma')}\\
&\quad=G(12'\sigma)G(21'\sigma)\delta_{\sigma\sigma'}+\frac{\delta\Gamma(11'\sigma)}{\delta U(2'2\sigma')}\\
&\qquad+G(13\sigma)T(33')\frac{\delta\Gamma(3'1'\sigma)}{\delta U(2'2\sigma')}+IG(13\sigma)\Gamma(33'\sigma)\\
&\qquad\times\frac{\delta\Gamma(3'1'\sigma)}{\delta U(2'2\sigma')}-G(11'\sigma)(i)\frac{\delta G(1'4-\sigma)}{\delta U(2'2\sigma')}\Big|_{4=1'+}\\
&\qquad-\delta_{\sigma\sigma'}G(12'\sigma)(-i)\langle(n_{2'-\sigma}c_{2\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle\\
&\qquad-\delta_{\sigma,-\sigma'}G(12'\sigma)(-i)\langle(c_{2'\sigma}c_{2'-\sigma}^{\dagger}c_{2-\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle\\
&\qquad+\delta_{\sigma,-\sigma'}G(12\sigma)(-i)\langle(c_{2'-\sigma}^{\dagger}c_{2-\sigma}c_{2\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle\\
&\qquad-G(13\sigma)T(33')(-i)\frac{\delta\langle(n_{3-\sigma}c_{3'\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle}{\delta U(2'2\sigma')}\\
&\qquad-G(13\sigma)T(33')(-i)\frac{\delta\langle(c_{3\sigma}c_{3-\sigma}^{\dagger}c_{3'-\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle}{\delta U(2'2\sigma')}\\
&\qquad+G(13\sigma)T(33')(-i)\frac{\delta\langle(c_{3'-\sigma}^{\dagger}c_{3-\sigma}c_{3\sigma}c_{1'\sigma}^{\dagger})_{+}\rangle}{\delta U(2'2\sigma')}.
\end{aligned} \tag{11}$$

Suppose we were to drop the last three terms, all of explicit order Δ. Now in the $\Delta\to 0$, $I\to\infty$ limit, the remaining terms simplify somewhat since in that limit $\Gamma\to 0$, $\delta\Gamma/\delta U\to 0$, and

$$I\Gamma(11'\sigma)\to n_{-\sigma}\delta(11'). \tag{12}$$

Further, evaluate Eq. (11) for $2'=2^{+}$, $2=1$, and $\sigma'=-\sigma$. In that case, Eq. (11) becomes

$$(i)(1-n_{-\sigma})[\Gamma(11'\sigma)-n_{-\sigma}G(11'\sigma)]=iG(11'\sigma)[\langle(n_{1-\sigma}n_{1'-\sigma})_{+}\rangle-n_{-\sigma}^{2}] \tag{12'}$$

or

$$(1-n_{-\sigma})\Gamma(11'\sigma)=-G(11'\sigma)[\langle(n_{1-\sigma}n_{1'-\sigma})_{+}\rangle-n_{-\sigma}]. \tag{12''}$$

For $I\to\infty$, the left-hand side is zero and the right-hand side is nonzero. Hence, we have a contradiction. Hence, we were not justified in neglecting the terms of explicit order Δ even for $\Delta\to 0$.

These terms of order Δ are of the form $G\times T\times$(correlation function). In order to see explicitly how these terms remain nonzero as $\Delta\to 0$, it will be useful to analyze the simple free-electron-gas (FEG) problem. Indeed, it was just such an analysis of the FEG problem which led EL to recognize the importance of the nonlocality of G_1 in the Hubbard atomic limit.

The equation of motion for G_1 in the FEG case is

$$G^0(12)^{-1}G(21')=\delta(11')+T(12)G(21'), \tag{13}$$

$$G(11')=G^0(11')+G^0(12)T(23)G(31'). \tag{14}$$

By definition, G^0 is local. If we dropped the second term, we would obtain a local G_1. However, the explicit solution to Eq. (14) is

$$G_{11'}=\frac{-i}{N}\sum_k \exp[i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_{1'})] \times[\theta(t_1-t_{1'})n_k-\theta(t_{1'}-t_1)(1-n_k)] \times\exp[-i\epsilon_k(t_1-t_{1'})] \tag{15a}$$

$$\underset{\Delta\to 0}{\longrightarrow}\frac{-i}{N}\sum_k \exp[i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_{1'})] \times[\theta(t_1-t_{1'})n_k-\theta(t_{1'}-t_1)(1-n_k)], \tag{15b}$$

so that, for example,

$$\langle c_1 c_{1'}{}^{\dagger}\rangle|_{t_1=t_{1'}}=\frac{1}{N}\sum_{k<k_F}\exp[i\mathbf{k}\cdot(\mathbf{R}_1-\mathbf{R}_{1'})] =3n\left(\frac{\sin k_F R-k_F R\cos k_F R}{(k_F R)^3}\right), \tag{16}$$

where $n=(k_F^3/6\pi^2)^{1/3}$ is the density and $R\equiv|\mathbf{R}_1-\mathbf{R}_{1'}|$.

Manifestly this G_1 is nonlocal and the second term in Eq. (14) is nonzero even for $\Delta\to 0$. Crudely speaking, we can say that the implied integration over the time variable for G_1 in Eq. (14) introduces a factor of $1/\epsilon_k$ arising from the last exponential in Eq. (15a). This combines with the explicit ϵ_k, so that the second term is zeroth order in explicit powers of Δ. However, the momentum dependence in n_k remains even as $\Delta\to 0$. Through its dependence on n_k, the second term is momentum dependent, or equivalently its Fourier transform is nonlocal.

This term in Eq. (14) for G_1 has a structure similar to the terms we neglected in Eq. (11). Lacking a complete solution, we can only conjecture that these terms conspire to give a nonlocal contribution in an analogous fashion.

Finally, we consider the various Green's-function factoring schemes. The straightforward factoring schemes of Hubbard[6] and others[7] suffer from the defect that the assumed factoring is incorrect to zeroth order in Δ. This point has already been emphasized in I, and follows from the nontrivial nature of the problem even as $\Delta\to 0$ which we have just discussed.

More sophisticated decoupling schemes have been proposed.[8–10] In particular, these approaches preserve the Harris-Lange moments just as the EL mass-operator expansion does. However, they suffer from a similar difficulty in that the results are couched in terms of certain correlation functions. The moment-preserving scheme of Tahir-Kheli and Jarrett does not in its present form provide any procedure for evaluating the correlation functions. Roth uses an RPA-like factoring in Ref. 9. This suffers from the flaws associated with any factoring in that zeroth-order terms are neglected. In Ref. 10, she provides a procedure for evaluating the correlation function. However, even given that the variational principle is valid, her prescription [Eq. (32) of Ref. 10] has only been shown valid for operators in her original basis set (in her notation, the set $\{A_n\}$). For the new operators given in Eq. (33)–(36) of Ref. 10, a more complicated prescription is required involving yet more complicated correlation functions.[11]

Recently, Appelbaum and Penn[12] have proposed an approximate solution to a similar model in which the Coulomb interaction was confined to a single site, interactions being neglected on other sites. The inconsistencies associated with factoring in the Hubbard model carry over to their model. Indeed, they obtain a contradiction in their paper which is similar to the one we have obtained in Eq. (12″). Although they feel that a better factoring scheme will remove this difficulty, this author is of the opinion that contradictions will always remain for any factoring.

In conclusion, although several approximation schemes have been proposed for the model Hamiltonian, none of the approaches discussed in this note yields meaningful or consistent results. Further, even the atomic limit of the model remains an extremely nontrivial problem.

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[1] D. M. Esterling and R. V. Lange, Rev. Mod. Phys. **40**, 796 (1968).
[2] This behavior has been shown explicitly in a paper by R. Bari (unpublished) for the exactly soluble two-electron N-site case. The EL expansion does, however, preserve the exact sum rules as they claim. The reason is that sum rules on the spectral weight function can be related to the high-frequency behavior of the Green's function. For $\omega\gg\Delta$, the EL series converges.
[3] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).
[4] D. M. Esterling and R. V. Lange, Phys. Rev. B **1**, 2231 (1970) (hereafter referred to as I).
[5] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962), Chap. 5.
[6] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963); **A281**, 401 (1964).
[7] R. Kishore and S. K. Joshi, Phys. Rev. **186**, 484 (1969).
[8] R. Tahir-Kheli and H. S. Jarrett, Phys. Rev. **180**, 544 (1968).
[9] L. Roth, Phys. Rev. Letters **20**, 1431 (1968).
[10] L. Roth, Phys. Rev. **184**, 451 (1969).
[11] H. S. Jarrett (private communication).
[12] J. Appelbaum and D. Penn, Phys. Rev. **188**, 874 (1969).