Degenerate Mass Operator Perturbation Theory in the Hubbard Model[*]

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The "atomic limit" (kinetic energy zero) of the Hubbard Hamiltonian has extreme degeneracy under very general circumstances. The kinetic energy or hopping term removes this degeneracy. It has been shown by Harris and Lange that there are important first-order manifestations of this fact. For instance, nonlocal correlations exist which invalidate usual Green's function truncation schemes. We present a mass operator perturbation scheme devised on the principle that, first of all, the role of kinetic energy as a breaker of degeneracy must be accounted for. A sort of Taylor's expansion of the mass operator in terms of the kinetic energy is found, the coefficients of which are functionals of the exact Green's functions at zero kinetic energy. The ambiguity due to the degeneracy is removed from these functions self consistently and thereby the degeneracy properly treated. We present a Green's function which accounts for all first-order effects of the kinetic energy.

I. INTRODUCTION

The Hubbard model[1] invites the attention of theorists because of its simplicity and richness. If we could completely understand the physical predictions of this model, we would be helped in the establishment of minimal requirements for metal–nonmetal and magnetic transitions. Once we have decided to analyze a model, however, it is required of us to make no distorting approximations. Little real progress can result from an uncertain treatment of a simplified model. In this brief paper, a method for calculating the true properties of the Hubbard model is outlined.

If one is in the small kinetic energy range of the model, it is natural to begin as Hubbard did and do perturbation theory in the kinetic energy. If there is less than one electron per site there is a degeneracy reflecting the freedom of locating the empty sites in the ground state when the kinetic energy is zero. Even with one electron per site there is a spin degeneracy in the ground state. Therefore, turning on the kinetic energy as a perturbation involves a problem in degenerate perturbation theory.

Harris and Lange[2] have shown that there are physical manifestations of degeneracy which are first order in kinetic energy and are analogous to those associated with choosing wave functions which diagonalize the perturbation in conventional degenerate perturbation theory. The methods they used did not provide, however, a technique for calculation of these effects in detail. We have developed such a technique. It is the first step in a clear sequence of approximations which

tend toward an exact treatment, and within it, a proper degenerate perturbation theory can be constructed.

II. DEFINITIONS

The Hubbard Hamiltonian[1] is

$$H = \sum_{ij\sigma} t_{ij} C_{i\sigma}^{+} C_{j\sigma} + H_0, \tag{1}$$

where

$$H_0 = \tfrac{1}{2} I \sum_{i\sigma} n_{i\sigma} n_{i-\sigma},$$

$$n_{i\sigma} = C_{i\sigma}^{+} C_{i\sigma}, \tag{2}$$

and we choose $t_{ii} = 0$.

The summations are over a lattice of sites and $C_{i\sigma}^{+}$ and $C_{i\sigma}$ create and destroy electrons of spin σ on the ith site. The first term in H describes hopping or kinetic energy and H_0 is a respulsion between two electrons on the same site.

The one-particle Green's function we use is defined by the following equation:

$$G_{ij\sigma}^{U}(tt') = -i \frac{\langle 0 \mid (S(U) C_{i\sigma}(t) C_{j\sigma}^{+}(t'))_{+} \mid 0 \rangle}{\langle 0 \mid (S(U))_{+} \mid 0 \rangle}. \tag{3}$$

The state $\mid 0 \rangle$ is a ground state of H_0. Since H_0 has degenerate ground states, the choice of the state $\mid 0 \rangle$ must be made with care, and this may be considered the key to the problem. The $(\ )_{+}$ symbol signifies usual fermion time ordering[3] and

$$(S(U) C_{i\sigma}(t) C_{j\sigma}^{+}(t'))_{+}$$

$$= \left(\left\{ \exp \left[-i \sum_{\sigma'} \int dt_1 dt'_1 U_{kl}{}^{\sigma'}(t'_1 t_1) \right. \right. \right.$$

$$\left. \left. \left. \times C_{k\sigma'}^{+}(t'_1) C_{l\sigma'}(t_1) \right] \right\} C_{i\sigma}(t) C_{j\sigma}^{+}(t') \right)_{+}. \tag{4}$$

The time dependence in the C's is generated by H_0.

[1] J. Hubbard, Proc. Roy. Soc. (London) **A276**, 238 (1963); **A281**, 401 (1964).

[2] A. B. Harris and R. V. Lange, Phys. Rev. **157**, 295 (1967).

[3] P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1243 (1959).

The function $U_{kl}{}^{\sigma'}(t'_1 t_1)$ is an arbitrary external field but note that if

$$U_{kl}{}^{\sigma}(t'_1 t_1) = t_{kl}\,\delta(t'_1 - t_1),\qquad(5)$$

the $S(U)$ is the S matrix which makes G the correct Green's function for the full Hubbard Hamiltonian so long as the ground state $|\,0\rangle$ is the one such that

$$\left(\exp\left[-i\int dt'\sum_{klo'} t_{kl}C_{k\sigma'}{}^+(t')C_{l\sigma'}(t')\right]\right)_+ |\,0\rangle \propto |\,0\rangle.\qquad(6)$$

The two-particle Green's function is given by

$$G_{iljk}{}^{\sigma\sigma'U}(t_1 t_2 t_1' t_2') = -\left[\delta G_{ij\sigma}{}^U(t_1 t_1')/\delta U_{kl}{}^{\sigma}(t_2' t_2)\right]$$

$$= \;+G_{ij\sigma}{}^U(t_1 t_1')G_{lk\sigma'}{}^U(t_2 t_2').\qquad(7)$$

The mass operator Σ is defined by

$$G_{ij}{}^{U-1}(t_1 t_1') = G_{ij}{}^{0-1}(t_1 t_1') - U_{ij}{}^{\sigma}(t_1 t_1') - \Sigma_{ij}{}^{\sigma U}(t_1 t_1'),\qquad(8)$$

where

$$G^0{}_{ij}{}^{-1}(t_1 t_1') = \delta_{ij}\delta(t_1 - t_1')i(\partial/\partial t_1).\qquad(9)$$

III. THE MASS OPERATOR EXPANSION

The first-order term in a functional Taylor's expansion for the mass operator in which we sum over repeated space and spin indices and integrate over repeated times is as follows:

$$\Sigma_{ij\sigma}{}^U(t_1 t_1') - \Sigma_{ij\sigma}{}^{U_0}(t_1 t_1') \approx (\delta\Sigma_{ij\sigma}(t_1 t_1')/\delta U_{lm}{}^{\sigma'}(t_2' t_2))_{U_0}$$

$$\times (U_{lm}{}^{\sigma'}(t_2' t_2) - U_{0,lm}{}^{\sigma'}(t_2' t_2)).\qquad(10)$$

Functionally differentiating Eq. (8) and using Eq. (7) we can express $(\delta\Sigma/\delta U)_{U_0}$ in terms of the one- and two-particle Green's function for the field U_0. Putting this into Eq. (10) and then plugging the resulting form for Σ into Eq. (8) we get the form for the inverse of the one-particle Green's function correct to first order in the change in external field, $(U - U^0)$:

$$G_{ij\sigma}{}^{-1U}(t_1 t_1') = G_{ij}{}^{0-1}(t_1 t_1') - U_{ij}{}^{\sigma}(t_1 t_1') - \Sigma_{ij\sigma}{}^{U_0}(t_1 t_1')$$

$$-\,[-G_{ip\sigma}{}^{-1U_0}(t_1 t_3')G_{plqk}{}^{\sigma\sigma'U_0}(t_3 t_2 t_3' t_2')G_{qj\sigma}{}^{-1U_0}(t_3 t_1')$$

$$+\,G_{ij\sigma}{}^{-1U_0}(t_1 t_1')G_{lk\sigma'}{}^{U_0}(t_2 t_2')$$

$$-\,\delta_{\sigma\sigma'}\delta_{il}\delta_{kj}\delta(t_1 - t_2')\delta(t_2 - t_1')]$$

$$\times[U_{kl}{}^{\sigma'}(t_2' t_2) - U_{0kl}{}^{\sigma'}(t_2' t_2)].\qquad(11)$$

IV. PERTURBATION THEORY IN THE KINETIC ENERGY

In order for our change in external field to represent turning on the kinetic energy in the Hubbard Hamiltonian, we must choose $U_0 = 0$ and U must be given by

Eq. (5). To evaluate the terms appearing in Eq. (11) we then need Σ and the one- and two-particle Green's function at zero kinetic energy, that is at U_0 where $U_0 = 0$.

But, there are no unique Green's functions at zero kinetic energy because of the degeneracy in H_0. Thus, we essentially need the Green's function for $U_0 \to 0$ rather than $U_0 = 0$.

Hubbard wrote as his solution for $t_{ij} = 0$ the Green's function

$$G_{ij\sigma}(\omega) = \delta_{ij}\left[\frac{\langle n_{i-\sigma}\rangle}{\omega - I} + \frac{1 - \langle n_{i-\sigma}\rangle}{\omega}\right].\qquad(12)$$

This solution is not unique and the most general solution for the one-particle Green's function for $t_{ij} = 0$ is, in fact,

$$G_{ij\sigma}(\omega) = \delta_{ij}\left[\frac{\langle n_{i-\sigma}\rangle}{\omega - I + i\epsilon} + \frac{1 - \langle n_{i-\sigma}\rangle}{\omega + i\epsilon}\right] + 2\pi i\delta(\omega)g_{ij\sigma},\qquad(13)$$

where

$$g_{ii\sigma} = \langle n_{i\sigma}\rangle,\qquad(14)$$

and, otherwise, $g_{ij\sigma}$ is an arbitrary real symmetric function of i and j. Thus, in the atomic limit there can be spatially and spin-dependent static correlations which are arbitrary and the specification of which is equivalent to fixing the ground state $|\,0\rangle$ in the Green's function definition.

By a careful analysis of the equations of motion at zero kinetic energy, we were able to show that all ambiguity in the two-particle Green's function can be completely expressed in terms of the same function, $g_{ij\sigma}$ [or its Fourier transform, $g_{\sigma}(k)$]. Thus, all the functions needed to specify the right-hand side of Eq. (11) can be expressed in terms of the function $g_{ij\sigma}$. To choose this function prematurely would be to prejudice the possible manifestations of the degeneracy of H_0.

V. RESULTING GREEN'S FUNCTION

When all the steps introduced up to now are carried out, we arrive at the following form for the space and time Fourier transform of the inverse Green's function from Eq. (11) for the case $\langle n_{i\sigma}\rangle = \langle n_{i-\sigma}\rangle = n$:

$$G_{\sigma}{}^{-1}(k\omega) = \omega - \mathcal{E}(k) - \frac{nI\omega}{\omega - I(1-n)} + \frac{I^2(T - L(k))}{[\omega - I(1-n)]^2}.\qquad(15)$$

In this expression,

$$\mathcal{E}(k) = N^{-1}\sum_j \exp\left[-ik\cdot(R_i - R_j)\right]t_{ij},\qquad(16)$$

$$T = N^{-1}\sum_j t_{ij}\langle C_{i-\sigma}{}^+ C_{j-\sigma}\rangle,\qquad(17)$$

$$L(k) = N^{-1}\sum_j \exp\left[-ik\cdot(R_i - R_j)\right]t_{ij}[D_{ij}{}^{-\sigma} + S_{ij}{}^{-\sigma}],$$

where

$$D_{ij}^{-\sigma} = \langle (n_{i-\sigma} - \langle n_{i-\sigma}\rangle)(n_{j-\sigma} - \langle n_{j-\sigma}\rangle)\rangle, \quad (19)$$

$$S_{ij}^{-\sigma} = \langle C_{i\sigma}C_{i-\sigma}^{+}C_{j-\sigma}C_{j\sigma}^{+}\rangle. \quad (20)$$

T can be simply expressed in terms of $g_{ij-\sigma}$.

D and S are particular projections of the two-particle Green's function which can also be expressed in terms of $g_{ij\sigma}$. Since the expressions for D and S are complicated and will not be explicitly analyzed further in this paper, we will not write them out here. What is most important to notice is that a momentum-dependent term proportional to particular density and spin correlations does come into the inverse Green's function to first order in kinetic energy. $L(k)$ is nonzero precisely because of the degeneracy in H_0.

The spectral weight function corresponding to the Green's function in Eq. (15) and correct to first order, is

$$A(k\omega)/2\pi = Z_1(k)\delta(\omega - E_1(k)) + Z_2(k)\delta(\omega - E_2(k)), \quad (21)$$

where

$$E_1(k) = (1-n)\mathcal{E}(k) - [T - L(k)][1-n]^{-1},$$

$$Z_1(k) = 1 - n - 2n(1-n)\mathcal{E}(k)I^{-1} - 2[T - L(k)]I^{-1},$$

$$E_2(k) = I + n\mathcal{E}(k) - [T - L(k)]n^{-1},$$

$$Z_2(k) = n + 2n(1-n)\mathcal{E}(k)I^{-1} + 2[T - L(k)]I^{-1}. \quad (22)$$

The energies $E_1(k)$ and $E_2(k)$ are the wave-number-dependent energies in the lower and upper parts of the band split by I. The numbers $Z_1(k)$ and $Z_2(k)$ give their respective weights. We find no broadening of the peaks in the spectral weight function to first order. Pursuing the next order in the functional Taylor's expansion of Eq. (10) will introduce this effect. We emphasize that even to first order there are important renormalizations to both the energies, E, and the weight, Z, due to the degeneracy.

VI. CALCULATION OF $g_\sigma(k)$

The final task in this program is to determine $g_\sigma(k)$. From Eq. (13), one can show that

$$g_\sigma(k) = \langle n_\sigma(k)\rangle \quad (23)$$

at zero kinetic energy. But we can calculate from our $G_\sigma(k\omega)$ the quantity $\langle n_\sigma(k)\rangle$ for finite t_{ij} and then take the limit $\Delta \to 0$ where

$$t_{ij} = \Delta\tau_{ij}. \quad (24)$$

This properly breaks the degeneracy and gives us an equation for $g_\sigma(k)$ since all the quantities appearing in $G_\sigma(k\omega)$ are known functionals of $g_\sigma(k)$.

For finite t_{ij} and less than one electron per site,

$$\langle n_0(k)\rangle = Z_1(k), \qquad E_1(k) < \mu$$

$$= 0, \qquad E_1(k) > \mu, \quad (25)$$

As $\Delta \to 0$, μ must tend to zero so that

$$\sum_k \langle n_\sigma(k)\rangle = n. \quad (26)$$

Since at $\Delta = 0$, $Z_1(k) = 1-n$, μ must tend to zero in such a way that those k for which $E_1(k) < \mu$ must fill a volume in momentum space equal to $(2\pi)^3 n(1-n)^{-1}$.

To simplify the present analysis, assume $E_1(k)$ is monotonic in $|k|$ and spherically symmetric. Then we will have $E_1(k) < \mu$ for $|k| < k_0$, where

$$\tfrac{4}{3}\pi k_0^3 = n(1-n)^{-1}(2\pi)^3,$$

and therefore

$$g_\sigma(k) = 1 - n, \qquad |k| < [6\pi n/(1-n)]^{1/3}$$

$$= 0, \qquad |k| > [6\pi n/(1-n)]^{1/3}. \quad (27)$$

If a calculation of T, $L(k)$ and therefore $E_1(k)$ using this simple $g_\sigma(k)$ should yield an $E_1(k)$ which is not monotonic, then the determination of $g_\sigma(k)$ would have to be done self consistently. Also, of course, lack of spherical symmetry in the lattice must also complicate the calculation. In general, one must solve the equations,

$$g_\sigma(k) = (1-n)\theta(\mu - E_1(k)) \quad (28)$$

and

$$n(1-n)^{-1}(2\pi)^3 = \int d^3k\,\theta(\mu - E_1(k)), \quad (29)$$

where, of course, $E_1(k)$ is the functional of $g_0(k)$ determined by Eqs. (17)–(20) and Eq. (22).

VII. CONCLUSION

We have not completely analyzed in this brief paper, the full implications of the Green's functions we have found. They do contain the subtle effects which we knew must appear in a good solution of the Hubbard model.[2] What is established here, is a method which gives an accurate statement of the content of the model to the order it has been applied, and which when analyzed in detail and carried out to higher orders will tell us how a Hubbard metal would really behave.

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Discussion of Esterling and Lange's Paper

G. W. PRATT (MIT): I'd like to say I agree with your approach of looking at this thing as a quantum mechanics problem. I'd

like to make a suggestion. Mattheiss has carried out the solution of six hydrogen atoms on a ring, where he has taken all possible states into account at all interatomic distances and so forth and he gets the sort of thing you are talking about, a very highly degenerate ground state when you pull these hydrogen atoms apart. He seems to get this spectral weight function which develops as you suggested it would. I think it would be a very interesting thing to take Mattheiss' solution, where all the eigenstates and energies are known, and translate it into Green's function language and just see how it turns out. I think it would be a rather instructive thing to do.

R. V. Lange: Brooks Harris and I published a paper which I understand is unreadable, but we tried. Anyway, we published a paper in which we derived a moment technique which gives these same things phenomenologically. It shows that the weights and the bands must be related to correlation functions but it was not microscopic in the sense that we could not also calculate the correlation functions. In this new work we have the function g and everything is in terms of it; g can be determined at the end of the calculation without much difficulty because all you have to do is take your answer for the one-particle Green's function, take the atomic limit of it and you get an equation for g and hence for all those correlation functions and the Green's functions which are then determined. We have checked this against the rigorous moment results that Harris and I got and it does check those out exactly. So this is a microscopic Green's function now which reproduces all of that complicated phenomenology that we had previously produced.

D. Adler (Massachusetts Institute of Technology): I'd like to point out that for the case of an initially half-filled band the average kinetic energy term vanishes, and there is neither a shift in weight between the bands nor a shift of the band centers oi gravity. Consequently, when there is exactly one electron per atom present, the material will be a Mott insulator, at least near the atomic limit. In this respect the solution presented here is better than the one originally suggested by Hubbard.

R. V. Lange: Just let me take one minute to illustrate just what that band-shift effect does. If you have an exactly half-filled band, you do get an energy gap. If you have one half an electron per site of each spin and you analyze those moments which I threw on that slide, you will find you have a separation between the full and empty parts of the spectral weight function. However, if you have anything but a half-filled band, one can see just how band theory doesn't work. Imagine we remove one electron from a lower subband. We can see that band theory is a

dangerous point of view because in the first place, Hubbard showed that one state drops down so that where your holes are depends very much on where your electrons are. Not only that, the rigorous results show that more than one state dribbles down. It isn't just one. How much more comes down is just a function of the kinetic energy of the opposite spin electron. That has a very simple physical interpretation. The weight in the lower subband is related to "what's the chance I can stick in an electron and land on an empty site." Then I don't have to add much energy. The weight in the upper subband is related to the chance I can stick in an electron and force a double occupancy. Then I'll have to add energy I. But if there is hopping, then what can happen? If I toss an electron on an empty site, an electron could hop over real quickly and force me to add energy I. As long as it hops over within a time less than $1/I$ so to speak, I might have to add energy I even though I put the electron on an empty site. Likewise, if I put the electron on a full site, then the other one could hop away and I don't have to add energy I after all. Now which of those two effects is more likely? Obviously the second one is, because these are repulsive particles and it is more likely that adding an electron to an occupied site will drive the other one away than adding an electron to an empty site will suck one over to form a double occupancy. So that means that it is a little bit easier to put electrons into this system with low energy than you would expect due to the correlation effects. Now that's a very physical process. At this stage is where I want to start using physical intuition. Now we have got the problem where we can maybe think about the true properties of the model and start using physical intuition at this point and ask whether these processes carry over into more realistic models. One shouldn't guess too early in the game.

T. A. Kaplan (MIT Lincoln Lab): Buried in your results should be an antiferromagnetic order and a spin wave spectrum, at least for the case of one electron per site. Have you looked into this?

R. V. Lange: If we have one electron per site, then you have to choose a properly generalized spin-dependent function g. You see the degeneracy is removed in a different way. In other words, you can put it in this same ambiguous function and determine it at the end of the calculation, but now the degeneracy refers to spin arrangement. But I haven't pushed it as far for the one electron per site as I have for the fewer than one electron site. The hopping breaks the degeneracy to second order here. But if you have fewer than one electron per site it breaks the degeneracy to first order and you get all sorts of wild things to first order.