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Antiferromagnetic symmetry breaking in the half-filled Hubbard model in infinite dimensions

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Abstract. We study the half-filled Hubbard model on a hypercubic lattice in infinite dimensions in the presence of a staggered magnetic field. Using the analyticity of the Anderson impurity model and assuming that for small enough on-site repulsion U the high-temperature phase is a Fermi liquid, we show that at weak coupling the nesting property of the non-interacting band-structure necessarily leads to antiferromagnetic symmetry breaking at a finite temperature.

1. Introduction

A few years ago Metzner and Vollhardt [1] realized that the Hubbard model has a non-trivial limit of infinite dimensions $d \to \infty$ if the nearest-neighbour hopping energy is scaled proportionally to $1/\sqrt{d}$. Since then, the physics of the Hubbard model in $d = \infty$ has been investigated by many authors [2–11]. Recent works have mainly focused on Fermi liquid and Mott insulating phases [5, 7]. The self-consistency equation for the local Green function in the presence of a staggered magnetic field was written in [9, 10], but a detailed analysis of this equation seems not to exist in the literature. In [12] we have shown that technical problems associated with the halfing of the Brillouin zone due to broken translational invariance can be elegantly avoided by choosing the staggered field in the x direction. Here we shall give a more detailed analysis of antiferromagnetic symmetry breaking and derive several exact expressions for the staggered susceptibility.

The Hamiltonian of the Hubbard models under consideration is given by $\mathcal{H} = \mathcal{H}_0 + \mathcal{U}$, with

$$\mathcal{H}_0 = -\sum_{R,r} t_r c_R^\dagger c_{R+r} - h \cdot \sum_R c_R^\dagger \sigma c_R e^{i\Pi \cdot R} \tag{1.1}$$

$$\mathcal{U} = U \sum_R \left(c_{R\uparrow}^\dagger c_{R\uparrow} - \frac{1}{2} \right) \left(c_{R\downarrow}^\dagger c_{R\downarrow} - \frac{1}{2} \right) \tag{1.2}$$

where the R sum is over N sites of a d-dimensional hypercubic lattice, h is a staggered field and $\Pi = [\pi, \ldots, \pi]$ is the antiferromagnetic ordering vector (we set the lattice spacing equal to unity). We have defined two-component operators $c_R^\dagger = [c_{R\uparrow}, c_{R\downarrow}]$, where $c_{R\sigma}^\dagger$ creates spin-σ fermions at site R, and $\sigma = [\sigma^x, \sigma^y, \sigma^z]$ are the Pauli matrices. We allow only hoppings that connect different sublattices, so that $e^{i\Pi \cdot r} = -1$. This implies that the band structure of the non-interacting model, defined by

$$\epsilon_k = -\sum_r t_r e^{ik \cdot r} \tag{1.3}$$

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satisfies the perfect nesting condition

$$\epsilon_{k+\Pi} = -\epsilon_k. \tag{1.4}$$

We have included terms proportional to the density in the definition of the interaction in (1.2), because then at half filling the spectrum of our model has particle–hole symmetry, so that the chemical potential is exactly zero at any temperature and the Hartree correction to the self-energy vanishes. Metzner and Vollhardt [1] first pointed out that a non-trivial limit $d \to \infty$ is only obtained if the t_r are properly rescaled with inverse powers of d to compensate for the increase in the number of neighbours in high dimensions. The nearest-neighbour hopping energy should be scaled as $t_r = t/\sqrt{2d}$. For general hoppings connecting different sublattices, we require that t_r vanishes for large d in such a way that for $d \to \infty$ the density of states at $U = 0$ has a finite limit $\rho(\epsilon)$:

$$\rho(\epsilon) = \lim_{d\to\infty} \lim_{N\to\infty} \frac{1}{N} \sum_k \delta(\epsilon - \epsilon_k). \tag{1.5}$$

The wavevector sum is over the first Brillouin zone $-\pi \leqslant k_i < \pi$, $i = 1, \ldots, d$. Note also that the hopping energies in (1.1) depend only on the distance between the sites, and do not break the translational invariance of the lattice. This is sufficient to ensure† that $\rho(0) > 0$.

2. Antiferromagnetism in infinite dimensions

In this section we shall derive an exact functional-integral equation for the self-energies in the presence of a staggered field. Although an equivalent equation has been written down in [9], we use here an unconventional basis that greatly simplifies the following analysis.

Imposing the usual periodic boundary conditions, the free part $\mathcal{H}_0$ of our Hamiltonian can be brought into block-diagonal form via Fourier transformation:

$$c_{k\sigma} = N^{-1/2} \sum_R e^{ik\cdot R} c_{R\sigma}. \tag{2.1}$$

Conventionally, one chooses the staggered field in the z direction, $h \cdot \sigma = h\sigma^z$. In this case $\mathcal{H}_0$ can be written as

$$\mathcal{H}_0^z = \sum_{k\in \mathrm{RBZ}} \sum_\sigma \tilde{C}_{k\sigma}^\dagger \begin{pmatrix} \epsilon_k & -\sigma h \\ -\sigma h & \epsilon_{k+\Pi} \end{pmatrix} \tilde{C}_{k\sigma} \tag{2.2}$$

where the momentum sum is over the reduced Brillouin zone of the antiferromagnet, and $\tilde{C}_{k\sigma}^\dagger = [c_{k\sigma}^\dagger, c_{k+\Pi\sigma}^\dagger]$. Note that the sign of the off-diagonal elements in the quadratic form in (2.2) depends on the spin projection. For a derivation of the functional-integral equation for the exact self-energy in $d = \infty$ this introduces unpleasant technical difficulties, because we have to deal with two-component operators that carry in addition a spin index. A

† If we allow for hoppings that break the translational invariance of the lattice, one can construct models with perfect nesting and particle–hole symmetry that have the property $\rho(0) = 0$. I am grateful to P van Dongen for pointing this out to me.

simple trick to avoid this difficulty is to choose the staggered field in the x direction [13], $\boldsymbol{h}\cdot\boldsymbol{\sigma} = h\sigma^x$. In this case (1.1) can be written as

$$\mathcal{H}_0^x = \sum_k C_k^\dagger \begin{pmatrix} \epsilon_k & -h \\ -h & \epsilon_{k+\Pi} \end{pmatrix} C_k \tag{2.3}$$

where the two-component operators are now defined by

$$C_k^\dagger = [c_{k\uparrow}^\dagger, c_{k+\Pi\downarrow}^\dagger]. \tag{2.4}$$

Note that the C_k are composed from operators with a different spin projection, and that the sum in (2.3) is over the full Brillouin zone. Loosely speaking, the antiferromagnetic symmetry breaking is now labeled by a spin flip, so that the extra spin summation in (2.2) can be absorbed in the second component of C_k. Of course, this is only a technical point, but it greatly facilitates the derivation of the functional-integral equation for the exact Green function. In momentum space the interaction part of our Hamiltonian can be written as

$$\mathcal{U} = \frac{U}{N}\sum_{k_1\ldots k_4} \delta^*(k_1 + k_2 - k_3 - k_4)[c_{k_1\uparrow}^\dagger c_{k_3\uparrow} - \tfrac{1}{2}\delta_{k_1,k_3}][c_{k_2+\Pi\downarrow}^\dagger c_{k_4+\Pi\downarrow} - \tfrac{1}{2}\delta_{k_2,k_4}] \tag{2.5}$$

where $\delta_{k,k'}$ is the usual Kronecker δ, and $\delta^*(k) = \frac{1}{N}\sum_R e^{ik\cdot R} = \sum_K \delta_{k,K}$, where $\{K\}$ are the vectors of the reciprocal lattice. In (2.5) we have shifted the momentum of the last two operators by Π. Obviously, this leaves δ^* invariant, so that the interaction term can be expressed entirely in terms of the components of the operator C_k defined in (2.4).

We now introduce the imaginary-time 2×2 matrix Green function

$$\underline{G}(k, \tau - \tau') = -\langle \mathcal{T}[C_k(\tau)C_k^\dagger(\tau')]\rangle \tag{2.6}$$

where $\mathcal{T}$ denotes time ordering in imaginary time, and the time evolution and thermal average are determined by $\mathcal{H}_0^x + \mathcal{U}$. The corresponding non-interacting Matsubara Green function is

$$\underline{G}^{(0)}(k, i\omega_n) = \int_0^{1/T} d\tau\, e^{i\omega_n\tau}\underline{G}^{(0)}(k,\tau) = \begin{pmatrix} i\omega_n - \epsilon_k & h \\ h & i\omega_n - \epsilon_{k+\Pi} \end{pmatrix}^{-1} \tag{2.7}$$

where $\omega_n = \pi T(2n+1)$. The self-energy matrix is defined as usual, $\underline{\Sigma}(k, i\omega_n) = \underline{G}^{(0)-1}(k, i\omega_n) - \underline{G}^{-1}(k, i\omega_n)$. The essential simplification in $d = \infty$ is that momentum conservation can be ignored [2], and we can replace $\delta^*(k) \to 1/N$. The self-energy is then independent of k, and must be of the form

$$\lim_{d\to\infty}\underline{\Sigma}(k, i\omega_n) \equiv \underline{\Sigma}(i\omega_n) = \begin{pmatrix} \Sigma(i\omega_n) & \Gamma(i\omega_n) \\ \Gamma(i\omega_n) & \Sigma(i\omega_n) \end{pmatrix}. \tag{2.8}$$

Particle–hole symmetry implies that

$$\Sigma(i\omega_n) = -\Sigma(-i\omega_n) \tag{2.9}$$

$$\Gamma(i\omega_n) = \Gamma(-i\omega_n). \tag{2.10}$$

The exact on-site Green function is then given by

$$\underline{G}_n = \frac{1}{N}\sum_k \left[\underline{G}^{(0)-1}(k, i\omega_n) - \underline{\Sigma}_n\right]^{-1} \tag{2.11}$$

where we use the abbreviation $\underline{G}_n = \underline{G}(i\omega_n)$ and $\underline{\Sigma}_n = \underline{\Sigma}(i\omega_n)$. From (2.7) it is clear that in general the summand on the left-hand side of (2.11) depends on ϵ_k and $\epsilon_{k+\Pi}$, and that therefore the summation cannot be reduced to an integration over the density of states. However, if we require that the non-interacting band structure satisfies the perfect nesting condition (1.4), the summand in (2.11) depends on ϵ_k only, so that

$$\underline{G}_n = \int_{-\infty}^{\infty} d\epsilon\, \rho(\epsilon) \begin{pmatrix} i\omega_n - \epsilon - \Sigma_n & h - \Gamma_n \\ h - \Gamma_n & i\omega_n + \epsilon - \Sigma_n \end{pmatrix}^{-1}. \tag{2.12}$$

The unique signature of perfect nesting is that the energy ϵ enters in the upper and lower diagonal elements with opposite sign.

The functional-integral equation for the exact Green function is now derived in the standard way [2]. One defines a variational Green function

$$\underline{\tilde{G}}_n^{-1} = \underline{G}_n^{-1} + \underline{\Sigma}_n \tag{2.13}$$

and a single-site impurity action

$$S_{\rm imp} = -\frac{1}{T}\sum_n C_n^\dagger \underline{\tilde{G}}_n^{-1} C_n + U\int_0^{1/T} d\tau \left[n_\uparrow(\tau) - \tfrac{1}{2}\right]\left[n_\downarrow(\tau) - \tfrac{1}{2}\right] \tag{2.14}$$

where $C^\dagger(\tau) = [C_\uparrow^\dagger(\tau), C_\downarrow^\dagger(\tau)]$ are imaginary-time two-component Grassmann fields, with Matsubara components

$$C_n = T\int_0^{1/T} d\tau\, e^{i\omega_n\tau} C(\tau)$$

and $n_\sigma(\tau) = C_\sigma^\dagger(\tau)C_\sigma(\tau)$. The functional-integral equation for the self-energies $\{\underline{\Sigma}_n\}$ is then a 2×2 matrix equation

$$\underline{G}_n = -\frac{1}{T}\frac{\int \mathcal{D}\{C, C^\dagger\}\exp(-S_{\rm imp})C_n C_n^\dagger}{\int \mathcal{D}\{C, C^\dagger\}\exp(-S_{\rm imp})} \equiv -\frac{1}{T}\langle C_n C_n^\dagger\rangle_{S_{\rm imp}}. \tag{2.15}$$

Because $S_{\rm imp}$ depends on all $\{\underline{\Sigma}_n\}$, the right-hand side of (2.15) is in general a non-linear functional of the self-energies, while the left-hand side is a non-linear function of $\underline{\Sigma}_n$. Hence, (2.15) is a very complicated non-linear functional-integral equation. To calculate Σ_n, one should first calculate the exact Green function of the impurity model in (2.14) for general choice of the $\{\Sigma_n\}$, and obtain an explicit expression for the right-hand side of (2.15). After that, one should solve the resulting non-linear integral equation. Of course, such a calculation can only be performed numerically. However, to examine the possibility of symmetry breaking, it is not necessary to explicitly solve these equations.

3. Staggered susceptibility and vertex function

Suppose that $\underline{G}_n$ is a solution of (2.15). In the presence of a symmetry breaking field, the exact Green function is of the form

$$\underline{G}_n = \begin{pmatrix} G_n & F_n \\ F_n & G_n \end{pmatrix} \tag{3.1}$$

where the anomalous Green function F_n is related to the staggered magnetization $M(h, T)$ of the underlying Hubbard Hamiltonian via

$$M(h, T) = T \sum_n F_n = \sum_n \langle C_n^\dagger \sigma^x C_n \rangle_{S_{\text{imp}}}. \tag{3.2}$$

Note that *antiferromagnetic* symmetry breaking in the original Hubbard model translates into *ferromagnetic* symmetry breaking in the impurity model. Because the impurity model is essentially zero-dimensional, no spontaneous symmetry breaking can occur in this model. Thus, the spin-susceptibility $\tilde{\chi}$ of the impurity model, defined via

$$\tilde{\chi}(T) = T \int_0^{1/T} d\tau \int_0^{1/T} d\tau' \langle C^\dagger(\tau)\sigma^x C(\tau) C^\dagger(\tau')\sigma^x C(\tau') \rangle_{S_{\text{imp}}} \tag{3.3}$$

remains finite for all values of T and U [14]. However, $\tilde{\chi}$ is not identical with the staggered susceptibility χ of the Hubbard model, which is defined by

$$\chi(T) = \lim_{h \to 0} \frac{\partial M(h, T)}{\partial h}. \tag{3.4}$$

Because the self-energies are complicated functions of the external field, the derivative in (3.4) does not simply produce the correlation function in (3.3). Below we shall make the relation between χ and $\tilde{\chi}$ precise, and show that the self-consistency condition (2.15) assures that χ can diverge at a finite temperature, while $\tilde{\chi}$ remains finite.

To derive an expression for the staggered susceptibility, let us first assume that the hopping energies t_r in (1.1) are only non-vanishing for nearest-neighbour sites. In the weak coupling regime, the generalization to arbitrary hoppings, subject to the restrictions mentioned earlier, is trivial and will be given shortly. Setting $t_r = t/\sqrt{2d}$ for r connecting neighbouring sites, the density of states in $d = \infty$ is [2]

$$\rho(\epsilon) = \rho_0 \exp(-\pi \rho_0^2 \epsilon^2) \tag{3.5}$$

with $\rho_0 \equiv \rho(0) = \left(t\sqrt{2\pi}\right)^{-1}$. The integration in (2.12) can then be done analytically, and we find that the diagonal and off-diagonal elements of $\underline{G}_n$ are given by

$$G_n = -\pi \rho_0 R_n \frac{i\omega_n - \Sigma_n}{\Omega_n} \tag{3.6}$$

$$F_n = \pi \rho_0 R_n \frac{h - \Gamma_n}{\Omega_n} \tag{3.7}$$

where

$$\Omega_n = [-(i\omega_n - \Sigma_n)^2 + (h - \Gamma_n)^2]^{1/2} \tag{3.8}$$

$$R_n = \operatorname{erfc}\left(\sqrt{\pi}\rho_0 \Omega_n\right) \exp(\pi \rho_0^2 \Omega_n^2). \tag{3.9}$$

Here erfc (x) is the complimentary error function, and the root in (3.8) should be taken such that $\mathrm{Re}\,\Omega_n \geqslant 0$. The leading terms of R_n for small and large $\rho_0|\Omega_n|$ is

$$R_n \sim \begin{cases} 1 & \text{for } \rho_0|\Omega_n| \ll 1 \\ (\pi\rho_0\Omega_n)^{-1} & \text{for } \rho_0|\Omega_n| \gg 1 \end{cases}. \tag{3.10}$$

Thus, R_n acts as a high-energy cutoff for frequency summations. As long as the Matsubara sums are dominated by the infrared regime $\rho_0|\omega_n| \ll 1$, the precise form of the cutoff is irrelevant. Inclusion of hoppings between the sublattices beyond the nearest neighbours will lead to a different value of the cutoff ρ_0, and a different functional form of the function R_n at high frequencies. However, the low-frequency behaviour of (3.6)–(3.8) will be unchanged, because the form of these equations carries the unique signature of perfect nesting. Hence, for $\rho_0 U \ll 1$ all calculations presented below also hold for arbitrary hoppings, provided we substitute the value of ρ_0 and the cutoff function R_n corresponding to the particular choice of hoppings.

To examine the stability of the paramagnetic phase, we now calculate the staggered susceptibility χ. Substituting (3.7) into (3.2), differentiating with respect to h and letting $h \to 0$, we obtain an exact relation between the staggered susceptibility and the self-energy of the Hubbard model

$$\chi = T\sum_n \chi_n \tag{3.11}$$

$$\chi_n = \lim_{h\to 0}\frac{\partial F_n}{\partial h} = \pi\rho_0 R_n \frac{\Lambda_n}{\Omega_n} \tag{3.12}$$

where we have used the fact that, in a parameter regime where the symmetry is not spontaneously broken, $\lim_{h\to 0}\Gamma_n = 0$. It is understood that Ω_n and R_n are now defined by setting $h = \Gamma_n = 0$ in (3.8) and (3.9). The vertex function Λ_n is defined via the Ward identity

$$\Lambda_n = 1 - \lim_{h\to 0}\frac{\partial\Gamma_n}{\partial h}. \tag{3.13}$$

To obtain an exact equation relating the vertices Λ_n and the self-energies Σ_n, we differentiate the off-diagonal components of both sides of (2.15) with respect to h and then take the limit $h \to 0$. This yields the following infinite system of linear equations for Λ_n:

$$\pi\rho_0 R_n \frac{\Lambda_n}{\Omega_n} = \sum_m \frac{\tilde{\chi}_{nm}}{2}\left[1 + \Lambda_m\left(\frac{1}{\pi\rho_0 R_m \Omega_m} - 1\right)\right] \tag{3.14}$$

where the kernel $\tilde{\chi}_{nm}$ is the dynamic spin-susceptibility of the impurity model

$$\tilde{\chi}_{nm} = \frac{1}{T^2}\langle C_n^\dagger \sigma^x C_n C_m^\dagger \sigma^x C_m\rangle_{S_{\mathrm{imp}}}. \tag{3.15}$$

Equation (3.14) is valid for all values of U and temperatures larger than the Néel temperature $T_N(U)$. The solution of (3.14) can be written in the form

$$\Lambda_n = \psi_n^{-1}\sum_m (1 - \hat{H})^{-1}_{nm}\psi_m \tag{3.16}$$

with

$$\psi_n = \left(\frac{\pi T R_n}{L\Omega_n}\right)^{1/2} \tag{3.17}$$

$$\hat{H}_{nm} = \frac{L}{\tilde{T}}\frac{\psi_n}{\pi R_n}[\delta_{nm} - (\hat{\chi}^{-1})_{nm}]\frac{\psi_m}{\pi R_m} \tag{3.18}$$

$$\hat{\chi}_{nm} = \frac{\tilde{\chi}_{nm}}{2\pi\rho_0 R_n \pi\rho_0 R_m} \qquad \tilde{T} = \rho_0 T. \tag{3.19}$$

The numerical constant L is defined via the requirement that the vector $|\psi\rangle$ with components $\langle n|\psi\rangle = \psi_n$ is a normalized vector in the Hilbert space ℓ^2, i.e. $\langle\psi|\psi\rangle = \sum_n \psi_n^2 = 1$. This yields

$$L = \sum_n \frac{\pi T R_n}{\Omega_n}. \tag{3.20}$$

It is extremely important that the solution of (3.14) can be written in terms of a pseudo-Hamiltonian $\hat{H}$, which is a Hermitian operator in the Hilbert space ℓ^2. This enables us to apply standard quantum mechanical perturbation theory to study the spectrum of $\hat{H}$.

If at a certain temperature T_0 one of the eigenvalues of $\hat{H}$ reaches unity, there exists some divergent linear combination of the vertex functions Λ_n. However, the physical susceptibility χ defined in (3.11) is a weighted sum over all vertex functions, and *a priori* one cannot exclude the following possibilities. (i) χ diverges at a temperature T_N where all eigenvalues of $\hat{H}$ are still smaller than unity. In this case $T_N > T_0$. (ii) The linear combination of the Λ_n that diverges does not contribute to χ, so that $T_N < T_0$. To illustrate these possibilities, let us directly look at the expression for χ. From (3.11), (3.12) and (3.16) we obtain

$$\chi = \rho_0 L\langle\psi|(1 - \hat{H})^{-1}|\psi\rangle. \tag{3.21}$$

The above possibility (i) means that L diverges at a temperature where the matrix element $\langle\psi|(1 - \hat{H})^{-1}|\psi\rangle$ is still finite, while (ii) means that the eigenspace associated with the eigenvalue of $\hat{H}$ that first reaches unity is orthogonal to $|\psi\rangle$. Within the Hartree–Fock approximation $|\psi\rangle$ is an eigenvector of $\hat{H}$. We therefore isolate in $\hat{H}$ the Hartree–Fock part by setting

$$\hat{H} = L\tilde{U}\hat{P}_\psi + \hat{V} \qquad \tilde{U} = \rho_0 U \tag{3.22}$$

where $\hat{P}_\psi = |\psi\rangle\langle\psi|$. At weak coupling we expect that $L\tilde{U} = O(1)$ close to T_N, while the matrix elements of $\hat{V}$ are of higher order in $\tilde{U}$. Suppose now we choose an orthonormal basis $\{|\psi\rangle, |\phi_\alpha\rangle, \alpha = 1, 2, \ldots\}$ of the Hilbert space ℓ^2 which diagonalizes $\hat{V}$ in the subspace orthogonal to $|\psi\rangle$:

$$\langle\phi_\alpha|\hat{V}|\phi_\beta\rangle = \delta_{\alpha\beta}\epsilon_\alpha \qquad \langle\psi|\phi_\alpha\rangle = 0. \tag{3.23}$$

In this case at least one of the matrix elements

$$V_{0\alpha} = \langle\psi|\hat{V}|\phi_\alpha\rangle \tag{3.24}$$

must be non-zero, because $\hat{V}$ and $\hat{P}_\psi$ do not commute. Using

$$\det\begin{pmatrix} E_0 & V_{01} & V_{02} & \cdots \\ V_{01} & E_1 & 0 & \cdots \\ V_{02} & 0 & E_2 & 0 \\ \vdots & \vdots & 0 & \ddots \end{pmatrix} = \left(\prod_{\alpha=0}^{\infty} E_\alpha\right)\left(1 - \sum_{\alpha=1}^{\infty} \frac{V_{0\alpha}^2}{E_0 E_\alpha}\right) \tag{3.25}$$

it is straightforward to show that χ can be written as

$$\chi = \frac{\rho_0 L}{1 - L\tilde{U} - V^{(1)} - V^{(2)}} \tag{3.26}$$

$$V^{(1)} = \langle\psi|\hat{V}|\psi\rangle \tag{3.27}$$

$$V^{(2)} = \sum_{\alpha=1}^{\infty} \frac{V_{0\alpha}^2}{1 - \epsilon_\alpha}. \tag{3.28}$$

If the correction terms $V^{(1)}$ and $V^{(2)}$ are small, then χ is almost of the form predicted by the random-phase approximation. $V^{(1)}$ is the usual first-order perturbative shift in the ground-state energy of $\hat{H}$, while $V^{(2)}$ contains all higher orders. Using $1 = |\psi\rangle\langle\psi| + \sum_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$ and writing $(1 - \epsilon_\alpha)^{-1} = 1 + \epsilon_\alpha(1 - \epsilon_\alpha)^{-1}$, it is easy to show that $V^{(2)}$ can also be written as

$$V^{(2)} = \left(\langle\psi|\hat{V}^2|\psi\rangle - \langle\psi|\hat{V}|\psi\rangle^2\right) + \sum_{\alpha=1}^{\infty} \frac{\epsilon_\alpha V_{0\alpha}^2}{1 - \epsilon_\alpha}. \tag{3.29}$$

The term in brackets on the right-hand side is the variance of the operator $\hat{V} = \hat{H} - L\tilde{U}\hat{P}_\psi$ in the Hartree–Fock eigenstate. Equations (3.26)–(3.29) are the main result of this section. These equations are exact and could be the starting point of a systematic numerical calculation of the Néel temperature.

4. Calculation of T_N at weak coupling

So far no approximation has been made. To make further progress, we need to know the properties of the operator $\hat{V}$ defined in (3.22), which is determined by the spin-susceptibility of the impurity model. For impurity models with a non-interacting Green function of the form $\tilde{G}_n = (i\omega_n + i\Delta\text{sign}\omega_n)^{-1}$, Zlatić and Horvatić [15] have rigorously proven that the perturbation series for the spin susceptibility is absolutely convergent for any $|U|<\infty$, and that in the weak coupling regime the first few terms of the series yield an extremely accurate approximation of the exact result. Although the self-consistent Green function $\tilde{G}_n$ in (2.14) will not be of the form assumed in [15], it is plausible that the validity of perturbation theory does not depend on the precise form of the non-interacting Green function. The fact that the Anderson impurity model is analytic in U has also been used by Zhang and co-workers [6] in their recent study of the Mott transition. Hence the matrix $\hat{\chi}$, which determines $\hat{V}$ via (3.18) and (3.22), can be calculated perturbatively in the weak-coupling limit. A simple calculation gives

$$\hat{\chi}_{nm} = \delta_{nm} + \tilde{T}\tilde{U}\pi^2 R_n R_m - \tilde{T}\tilde{U}^2\pi^2 R_n R_m (K_{n+m} - K_0) + O(\tilde{T}\tilde{U}^3) \tag{4.1}$$

where

$$K_n = \frac{T}{\rho_0}\sum_{\nu} G_{\nu}^{(0)} G_{n-\nu}^{(0)} \qquad G_n^{(0)} = -i\pi\rho_0 R_n \operatorname{sign}\omega_n. \tag{4.2}$$

Inverting (4.1), and using the definitions (3.18) and (3.22), we find

$$\langle n|\hat{V}|m\rangle = -L\tilde{U}\big[\tilde{U}\psi_n\psi_m K_{n+m} + O(\tilde{U}^2)\big] \tag{4.3}$$

so that

$$V^{(1)} = -L\tilde{U}\left(\tilde{U}\sum_{n,m}\psi_n^2\psi_m^2 K_{n+m} + O(\tilde{U}^2)\right) = -L\tilde{U}\big[\tilde{U}K_0 + O(\tilde{U}^2)\big]. \tag{4.4}$$

Because K_n is, for $\rho_0\Omega_n \ll 1$, independent of n, the leading term in (4.4) is determined by K_0. For $\tilde{T} \ll 1$ we obtain $K_0 = \sqrt{2}\ln(1+\sqrt{2})$. Using the fact that by construction ϵ_α and the matrix elements $V_{0\alpha}$ are of order $\tilde{U}$, we see that the last term in (3.29) is of order $\tilde{U}^3$. Moreover, although $\langle\psi|\hat{V}^2|\psi\rangle$ and $\langle\psi|\hat{V}|\psi\rangle^2$ are both of order $\tilde{U}^2$, the difference of these terms is of order $\tilde{U}^3$, so that $V^{(2)} = O(\tilde{U}^3)$. The Néel temperature is therefore determined by

$$1 = L\tilde{U}\big[1 - K_0\tilde{U} + O(\tilde{U}^2)\big]. \tag{4.5}$$

Note that the derivation of this equation is based on the analyticity of the Anderson impurity model. Let us now consider the factor L defined in (3.20). Introducing the finite-temperature approximation to the wavefunction renormalization factor [16]

$$Z^{-1} = 1 - \frac{\operatorname{Im}\Sigma_0}{\omega_0} \tag{4.6}$$

we have for small frequencies $\Omega_n = Z^{-1}|\omega_n|$, so that

$$L = Z\ln\tilde{T}^{-1} + L_0 + O(\tilde{U}) \tag{4.7}$$

where L_0 is a numerical constant of order unity. Combining (4.5) and (4.7) we conclude that the Néel temperature in the weak-coupling limit is given by

$$\begin{aligned}\rho_0 T_N &= \exp\left[-Z^{-1}\left(\frac{1}{\tilde{U}(1-K_0\tilde{U})} - L_0 + O(\tilde{U})\right)\right] \\ &= \exp\big[-Z^{-1}\big(\tilde{U}^{-1} + K_0 - L_0 + O(\tilde{U})\big)\big].\end{aligned} \tag{4.8}$$

Obviously the vanishing of the wavefunction renormalization factor Z at the phase transition implies that symmetry breaking does not occur at finite temperatures. We now assume that the spin rotationally invariant high-temperature phase is a Fermi liquid, and argue that Z can be calculated perturbatively. Within second-order perturbation theory one finds in arbitrary dimension d

$$Z_k^{-1} = 1 + \frac{U^2}{N^2}\sum_{k_1k_2k_3}\delta^*\big(k-(k_1+k_2-k_3)\big)\frac{f(\epsilon_{k_1})f(\epsilon_{k_2})f(-\epsilon_{k_3}) + f(-\epsilon_{k_1})f(-\epsilon_{k_2})f(\epsilon_{k_3})}{(\epsilon_{k_1}+\epsilon_{k_2}-\epsilon_{k_3})^2 + (\pi T)^2} \tag{4.9}$$

where $f(\epsilon)$ is the Fermi function. In $d = \infty$ we may replace $\delta^* \to 1/N$. Then it is easy to see that the integral in (4.9) is finite even at $T = 0$, so that

$$Z^{-1} = 1 + z_1 \tilde{U}^2 + O(\tilde{U}^3) \tag{4.10}$$

where z_1 is a numerical constant of order unity. It is important to stress that (4.9) can be continued below T_N by replacing $|\epsilon_k| \to \sqrt{\epsilon_k^2 + (mU/2)^2}$, where m is the mean-field staggered magnetization. Hence perturbation theory suggests that, in $d = \infty$, the symmetry breaking has no effect on the wavefunction renormalization factor Z. Physically, this means that the low-lying excited states above the relevant vacuum are in one-to-one correspondence with the low-lying non-interacting eigenstates. The wavefunction renormalization factor Z should not be confused with the overlap $\langle FL|SDW\rangle$ between the non-interacting ground state $|FL\rangle$ and spin-density wave ground state $|SDW\rangle$. Within mean-field theory one finds for finite but large N

$$|\langle FL|SDW\rangle|^2 = \exp(-Nm\tilde{U}). \tag{4.11}$$

For $m\tilde{U} > 0$ this overlap vanishes in the thermodynamic limit $N \to \infty$. Because there is no sign of a breakdown of perturbation theory, it is at least very reasonable to assume that for sufficiently small $\tilde{U}$ the perturbative result $Z^{-1} = 1 + z_1 \tilde{U}^2$ is accurate. Inserting (4.10) into (4.8), we see that the Hartree–Fock result T_N^{HF} for the Néel temperature is renormalized by a finite factor even in the limit $\tilde{U} \to 0$:

$$\lim_{\tilde{U}\to 0} \frac{T_N}{T_N^{HF}} = \exp(-K_0) = \frac{1}{(1+\sqrt{2})^{\sqrt{2}}} \approx 0.29. \tag{4.12}$$

Equation (4.12) was first derived by van Dongen from the Onsager reaction field correction to Hartree–Fock theory [3]. In our derivation we have used the well known analyticity of the Anderson impurity model to show that at weak coupling the only approximation necessary to derive (4.12) that is not completely controlled is the perturbative form of the wavefunction renormalization factor Z given in (4.10). *A priori* one cannot exclude the possibility that the perturbation series for Z^{-1} contains at nth order a term proportional to $\tilde{U}(L\tilde{U})^{n-1}$. Because $L\tilde{U} \approx 1$ close to the phase transition, this term would renormalize the coefficient in (4.12). However, even if such a term exists, a finite Z in the low-temperature regime is sufficient to imply spontaneous symmetry breaking at a finite temperature.

5. Conclusions

The existence of an antiferromagnetic instability in the weak-coupling regime of the half-filled Hubbard models with perfect nesting is not surprising. Such an instability is predicted by Hartree–Fock theory in all dimensions. While in one dimension this instability is known to be an artifact of mean-field theory, conventional wisdom is that at least in high enough dimensions Hartree–Fock theory becomes very accurate. In the present work we have shown that in finite dimensions spontaneous symmetry does indeed occur at a finite temperature if $Z > 0$, i.e. if the spin rotationally invariant high-temperature phase is a Fermi liquid. In this case perfect nesting and particle–hole symmetry are sufficient to lead at weak coupling to a spontaneous magnetization at a finite temperature.

What is the relevance of our result to finite dimensions? For $d < \infty$ the density of states $\rho(\epsilon)$ vanishes outside a fixed interval. However, we have seen that in the weak-coupling regime the only parameter that determines the infrared behaviour of Matsubara sums is $\rho(0)$. Therefore, we believe that in all dimensions $d \geqslant 3$ the half-filled repulsive Hubbard model has indeed antiferromagnetic long-range order below a finite temperature $T_N(U)$. Obviously this result does not extrapolate to $d = 1$, where we know that there is no spontaneous magnetization for all U, even at $T = 0$ [17]. In $d = 2$ Hartree–Fock theory is completely incorrect at $T > 0$, because it predicts spontaneous symmetry breaking at low temperatures, although the rigorous Mermin–Wagner theorem [18] tells us that this can happen only at $T = 0$. Note also that in two dimensions $\rho(0) = \infty$ due to Van Hove singularities. Thus, at weak coupling the extrapolation of the physics in $d = \infty$ to $d = 2$ is not possible. For nearest-neighbour hopping and large U, the half-filled square-lattice Hubbard model is equivalent to a two-dimensional quantum Heisenberg antiferromagnet, which seems to be ordered at $T = 0$. There remains the possibility that the order in the ground state is destroyed in the weak-coupling regime [19,20]. It can be shown [21] that, even for arbitrarily small U, the perturbation expansion is not governed by a small parameter, and that, in contrast to $d \geqslant 3$, corrections to Hartree–Fock theory in $d = 2$ lead to a Néel temperature that is for $U \to 0$ exponentially small compared with the Hartree–Fock result. Furthermore, it is not difficult to see that the lowest-order correction to the inverse wavefunction renormalization Z_k^{-1} given in (4.9) diverges in $d = 2$ for $T \to T_N = 0$ if k is located at the corners of the Brillouin zone. Thus, $d = 2$ seems to be closer to $d = 1$, and a simple Hartree–Fock description of antiferromagnetism at weak coupling seems not to be justified.

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References

[1] Metzner W and Vollhardt D 1989 *Phys. Rev. Lett.* **62** 324
[2] Müller-Hartmann E 1989 *Int. J. Mod. Phys.* B **3** 2169
Vollhardt D 1991 *Physica* B **169** 277
van Dongen P G J 1991 *Mod. Phys. Lett.* **5** 861
[3] van Dongen P G J 1991 *Phys. Rev. Lett.* **67** 757
[4] Jarrell M 1992 *Phys. Rev. Lett.* **69** 168
Pruschke Th, Cox D L and Jarrell M 1993 *Europhys. Lett.* **21** 593
[5] Rozenberg M J, Zhang X Y and Kotliar G 1992 *Phys. Rev. Lett.* **69** 1236
[6] Zhang X Y, Rozenberg M J and Kotliar G 1993 *Phys. Rev. Lett.* **70** 1666
[7] Georges A and Krauth W 1992 *Phys. Rev. Lett.* **69** 1240
[8] Georges A and Kotliar G 1992 *Phys. Rev.* B **45** 6479
[9] Georges A, Kotliar, G and Si Q 1992 *Int. J. Mod. Phys.* B **6** 257
[10] Janis V and Vollhardt D 1992 *Int. J. Mod. Phys.* B **6** 283
[11] Bartkowiak M and Chao K A 1993 *Phys. Rev.* B **47** 4193
[12] Kopietz P 1994 *Physica* B **194–196** 271
[13] Georges A and Yedidia J S 1991 *Phys. Rev.* B **43** 3475
[14] Schrieffer J R and Mattis D C 1965 *Phys. Rev.* **140** A1412
[15] Zlatić V and Horvatić B 1983 *Phys. Rev.* B **28** 6904
Horvatić B and Zlatić V 1985 *J. Physique* **46** 1459

[16] Serene J W and Hess D W 1991 *Phys. Rev.* B **44** 3391
[17] Lieb E H and Wu F Y 1968 *Phys. Rev. Lett.* **20** 1455
[18] Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
[19] Kopietz P 1992 *Physica* A **188** 644; 1992 *Z. Phys.* B **89** 351
[20] Oitmaa J and Henderson J A 1991 *Phys. Rev.* B **44** 7433
[21] Kopietz P 1993 *Phys. Rev.* B **48** 13789