Finite-Temperature Magnetism in the Hubbard Model

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A novel and physically transparent approach to the finite-temperature Hubbard model at half filling is proposed. It recovers not only the correct dimensionality dependence of antiferromagnetism but, in $d = 3$, interpolates properly between weak and strong coupling interaction strengths for the Néel temperature, and enables extraction of related thermodynamic properties.

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The canonical model of interacting fermions on a lattice is the Hubbard model, specified by the Hamiltonian

$$\hat{H} = -t \sum_{\langle ij\rangle,\sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \qquad (1)$$

with the $\langle ij\rangle$ sum here over nearest neighbor (NN) sites on a d-dimensional hypercubic lattice. It bridges itinerant and localized descriptions of quantum magnetism, reducing at half filling in the strong coupling limit $\tilde{U} = U/t \to \infty$ to the spin-$\frac{1}{2}$ antiferromagnetic (AF) Heisenberg model of localized spins,

$$\hat{H}_{\mathrm{Heis}} = \tfrac{1}{2} \sum_{i,j(\neq i)} J_{ij} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j, \qquad (2)$$

with solely NN exchange couplings $J_{ij} \equiv J_\infty = 4t^2/U$. It thus provides a vital testbed for theories of finite-temperature band magnetism, where considerable progress has occurred for nearly two decades; see, e.g., [1–6], and references therein. These theories employ functional integral methods, most within the static approximation; their aim is to determine the $\hat{U}$-T phase diagram (and associated thermodynamic properties), i.e., the Néel temperature $T_N(\tilde{U})$ for loss of AF long-ranged order (AFLRO). While interpolating with some success between weak and strong coupling $\tilde{U}$, the theories share common limitations; for example, all yield the molecular field result for the Heisenberg model as $\tilde{U} \to \infty$, $T_N^{\mathrm{MF}} = zt^2/U$, with $z = 2d$ the lattice coordination number. This is skewed for $d = 3$, where the accepted [3,4,7,8] $T_N \simeq 3.83t^2/U$ from high-temperature series expansions, and for $d = 2$, clearly cannot predict the well known absence of AFLRO at any $T > 0$.

We describe here a new, simple, and physically transparent theory for the half-filled Hubbard model at finite T, consisting of two essential steps as sketched below. (i) An approximate mapping of the low-energy excitations of the Hubbard model (1) on to those of a Heisenberg model (2) is made for *finite* $\tilde{U} > 0$, and with no constraint to NN exchange couplings, the $\{J_{ij}(\tilde{U})\}$ being determined directly. (ii) Thermodynamic properties of the effective $\hat{H}_{\mathrm{Heis}}$ are then examined. We focus here mainly on $T_N(\tilde{U})$, as found by a standard molecular field treatment [9] of the $\tilde{U}$-dependent $\hat{H}_{\mathrm{Heis}}$ to give $T_N^{\mathrm{MF}}(\tilde{U})$, followed by a self-consistent Onsager reaction field correction [9,10], leading to a much improved description of short-ranged magnetic ordering and a strong (and d-dependent) renormalization of $T_N(\tilde{U})$ below $T_N^{\mathrm{MF}}(\tilde{U})$. The resultant theory recovers the correct d dependence of AFLRO, as is mentioned above. In $d = 3$ it interpolates properly between weak and strong coupling $\tilde{U}$. For example, we find $T_N(\tilde{U}) = 3.96t^2/U$ as $\tilde{U} \to \infty$, and that second and third NN exchange couplings play an important role for weak to moderate $\tilde{U}$. With a caveat later discussed, Monte Carlo (MC) results [7,8] for the $d = 3$ half-filled Hubbard model are also well reproduced. Moreover, the theory, in addition, naturally permits extraction of the full range of thermodynamic and/or magnetic properties (and hence more extensive comparison with MC results).

We first recall the simplest approach to a half-filled Hubbard model at $T = 0$. This begins with an unrestricted Hartree-Fock (UHF) mean-field approximation: The lattice is bipartite, so the UHF ground state is a two-sublattice Néel AF for all $U > 0$, with the UHF local moment $\mu_i \equiv 2\langle \hat{s}_{iz}\rangle_{\mathrm{HF}}$ found from the usual self-consistent gap equation [11]. Linearized excitations about the broken symmetry UHF state follow via a familiar random phase approximation (RPA), transverse spin excitations being of lowest energy as there is always a gap for charge excitations. The effect of zero-point transverse spin excitations in, e.g., reducing the sublattice magnetization from its UHF value, $|\mu_i| \equiv |\mu|$, may then be found by a one-loop calculation [11]. For $d = 2$ in particular, this approach is remarkably successful at $T = 0$ for strong coupling: It gives exactly the results of linear spin wave (LSW) theory [12] for the $\tilde{U} \to \infty$ $\hat{H}_{\mathrm{Heis}}$, and agrees very well with MC results [13], e.g., the sublattice magnetization reduction and ground state energy. Qualitatively similar results are expected for $d \geq 3$ (for $d = 1$, one-loop quantum spin fluctuations destroy AFLRO at $T = 0$ [11], as is correct).

Since there is a gap to charge and longitudinal spin excitations for all $\tilde{U} > 0$, we expect the lowest energy transverse spin excitations to be largely spin-wave-like (save possibly for very small $\tilde{U}$). Our essential step (i) above is thus, for any $\tilde{U} > 0$, (a) to construct a site representation of the RPA equations of motion about the finite-T UHF Néel state for the Hubbard model,

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and then (b) under the assumption (whose accuracy may be verified) that the lowest N (= number of sites) of the resultant transverse excitations are spin waves, to decouple that N-dimensional subset of the RPA equations which pertains to on-site spin deviations from the Néel local moment axes. These are then compared to the LSW equations of an arbitrary Heisenberg model as obtained readily by a linearized Holstein-Primakoff transformation. This yields directly an effective $\hat{H}_{\rm Heis}$ (2), with $\tilde{U}$-dependent exchange couplings $\{J_{ij}(\tilde{U})\}$ (whose accuracy we do not expect to be sensitive to their extraction by comparison of linearized theories, RPA and LSW). Full details will be given elsewhere. We find

$$J_{ij}(\tilde{U}) = 2|\mu_i \mu_j|[{}^0\boldsymbol{\chi}^{-1}]_{ij}\,, \tag{3}$$

with $|\mu_i| \equiv |\mu(T)|$ the UHF Néel local moment magnitude found from the usual finite-T gap equation at the chosen $\tilde{U}$, and $[{}^0\boldsymbol{\chi}^{-1}]_{ij}$ the inverse of the UHF static ($\omega = 0$) transverse susceptibility matrix in a site representation; from this the Fourier transform $J(\mathbf{q})$ may be found in closed analytical form. To check the accuracy of the approach, the full $T = 0$ RPA transverse spin spectrum of the Hubbard model $N_T^{\rm RPA}(\omega)$ may be calculated at any $\tilde{U}$ (via the RPA transverse susceptibility matrix $\boldsymbol{\chi}(\omega) = {}^0\boldsymbol{\chi}(\omega)[\mathbf{1} - U\,{}^0\boldsymbol{\chi}(\omega)]^{-1}$), and compared to $N_T^{\rm LSW}(\omega)$ found by LSW on the effective $\hat{H}_{\rm Heis}(\tilde{U})$. $N_T^{\rm RPA}$ consists of a gapless low-ω spin-wave-like band containing N excitations, separated by a gap from a band of $(N/2)(N-2)$ weakly renormalized Stoner-like excitations centered on $\omega \sim U$. As $\tilde{U} \to \infty$ the Stoner band is effectively eliminated, and $N_T^{\rm RPA}(\omega)$ reduces to the exact LSW spectrum $N_T^{\rm LSW}$ of the $\tilde{U} \to \infty$ NN $\hat{H}_{\rm Heis}$. But the underlying success of the effective mapping for a very wide $\tilde{U}$ range arises because the spectral gap in $N_T^{\rm RPA}$ persists down to weak coupling $\tilde{U} = U/t$, of around 2 for $d = 3$, the spin wave component of $N_T^{\rm RPA}$ being well reproduced by $N_T^{\rm LSW}(\omega)$ for the effective $\hat{H}_{\rm Heis}(\tilde{U})$.

The resultant NN, 2NN, and 3NN exchange couplings for $d = 3$ are shown in Fig. 1 as a function of $\tilde{U}$ (at $T = 0$). The bipartite lattice is composed of two disjoint sublattices, and we find $J_{ij} > 0$ (< 0) for all sites j on the opposite (same) sublattice to i, whence magnetic ordering is always AF. $J_{\rm NN}$ itself reaches a maximum for $\tilde{U} \sim 9$, after which it steadily approaches from below the exact strong coupling asymptote for the half-filled Hubbard model $J_\infty = 4t^2/U$. $|J_{2;\rm NN}|$ and $J_{3;\rm NN}$ are always an order of magnitude less than $J_{\rm NN}$, and correctly vanish as $\tilde{U} \to \infty$, but as we will see they play a significant role for $\tilde{U} \lesssim 15$. Couplings beyond third NN play only a minor role in practice.

To calculate the Néel temperature, step (ii) above, we use first a standard [9] molecular field (MF) approximation to the effective $\hat{H}_{\rm Heis}(\tilde{U})$, approaching the AF phase from the high-T paramagnet. This gives $T_N^{\rm MF}(\tilde{U}) = \frac{1}{4}|J(\mathbf{Q})|$, with $\mathbf{Q} = \boldsymbol{\pi}$ the AF ordering vector [$|J(\mathbf{q})|$ is a maximum at $\mathbf{q} = \boldsymbol{\pi}$ for all $\tilde{U}$]. By itself, this suffers from the limitations previously described, reflecting an inadequate treatment of short-ranged magnetic ordering (SMO). To alleviate this, a self-consistent Onsager reaction field (ORF) correction [9,10] is employed: The reaction field of a spin cannot contribute to its own alignment, and must thus be removed from the MF. This improves greatly the treatment of SMO. For an arbitrary AF $\hat{H}_{\rm Heis}$ it yields [9]

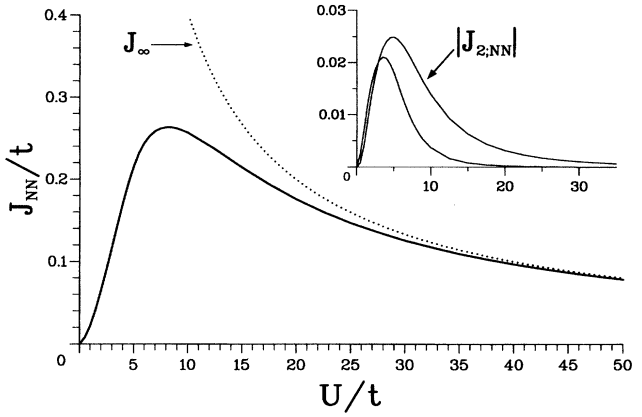

FIG. 1. Nearest neighbor $J_{\rm NN}/t$ vs $\tilde{U} = U/t$; the strong coupling limit $J_\infty = 4t^2/U$ is also shown. Inset: $|J_{2;\rm NN}|$ and $J_{3;\rm NN}$ vs $\tilde{U}$.

$$T_N(\tilde{U}) = T_N^{\rm MF}(\tilde{U})/G(s = 1+)\,. \tag{4}$$

Here $G(s) \equiv {\rm Re}G(E)$ with $E = s + i0+$, and $G(E) = N^{-1}\sum_{\mathbf{q}}[E - J(\mathbf{q})/J(\mathbf{Q})]^{-1}$. Mathematically, $G(E)$ is equivalent to the site-diagonal Green's function for an arbitrary one-band tight-binding Hamiltonian in d dimensions. Thus, crucially, $G(s \to 1+)$ diverges logarithmically for $d = 2$ [14] (a result not confined to NN J_{ij}). From (4) the simple ORF treatment thus predicts, for all $\tilde{U} > 0$, the absence of AFLRO for any $T > 0$ in $d = 2$. Further, the $G(s \to 1+)$ divergence leads to an exponentially divergent spin correlation length as $T \to T_N(\tilde{U}) = 0$. For $\tilde{U} \to \infty$, this is given by $\xi(T) = C\exp(\pi T_N^{\rm MF}/2T) = C\exp(2\pi\rho_s/T)$, with C a T-independent constant and $\rho_s = J_\infty/4$ the LSW spin stiffness constant, in good agreement with the $d = 2$ pure NN Heisenberg model [15].

Now consider the $d = 3$ simple cubic lattice where $G(s = 1)$ is finite. We calculated its $\tilde{U}$ dependence numerically; as $\tilde{U} \to \infty$, we recover the known limit [9] $G(s = 1) = 1.5164$. Figure 2 shows the resultant $T_N^{\rm MF}(\tilde{U})$ and the ORF $T_N(\tilde{U})$ vs $\tilde{U}$. The effects of SMO inherent in the ORF reduce markedly T_N below $T_N^{\rm MF}$ for all but the smallest interaction strengths. In the strong coupling limit $\tilde{U} \to \infty$, $T_N^{\rm MF}(\tilde{U}) \to 6t^2/U$ as expected. In contrast, $T_N(\tilde{U}) \to 3.96t^2/U$, which is within ~3% of the accepted strong coupling limit $T_N \simeq 3.83t^2/U$ mentioned above: The simple ORF again captures well

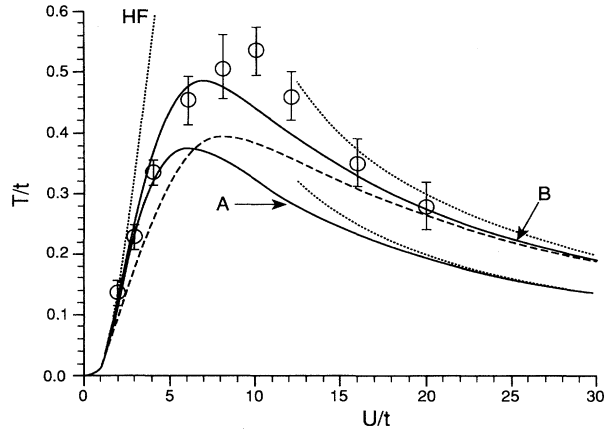

FIG. 2. Néel temperature in $d = 3$. Curve A: Onsager reaction field $T_N(\tilde{U})$. Curve B: molecular field $T_N^{\mathrm{MF}}(\tilde{U})$ vs $\tilde{U}$. Also shown are MC results [8] (circles), T_N^{MF} with solely NN J_{ij} (dashed line), T_{HF} (dotted), and the $\tilde{U} \to \infty$ asymptotes $T_N^{\mathrm{MF}} = 6t^2/U$, and $T_N = 3.96t^2/U$ from the present theory.

the known limit, reached in practice for $\tilde{U} \gtrsim 15-20$. Moreover, in weak coupling the ORF (as well as MF) T_N is also physically sound, as seen (Fig. 2) from the temperature $T_{\mathrm{HF}}(\tilde{U})$ at which the UHF local moment $|\mu(T)|$ vanishes (obtained simply from the finite-T UHF gap equation). It is clear physically [see, e.g., (3)] that AFLRO can potentially occur only if local moments persist, so $T_N(\tilde{U})$ must asymptotically approach $T_{\mathrm{HF}}(\tilde{U})$ as $\tilde{U} \to 0$, as indeed is found. $T_{\mathrm{HF}}(\tilde{U})$ itself naturally sets an upper limit for applicability of our theory, but, save for the lowest $\tilde{U} \lesssim 2$, it is far in excess of T_N or T_N^{MF}, as $T_{\mathrm{HF}}(\tilde{U}) \sim \frac{1}{4}U$ for large $\tilde{U}$, an asymptote reached in practice for $\tilde{U} \gtrsim 4$. The importance of second and third NN exchange couplings is also clear in Fig. 2, where we show $T_N^{\mathrm{MF}}(\tilde{U})$ obtained by constraint solely to the NN J_{ij}. The effect of couplings beyond purely NN clearly increases $T_N^{\mathrm{MF}}(\tilde{U})$ significantly for both weak and moderate coupling strengths up to $\tilde{U} \sim 15$ or so, commensurate with Fig. 1 for the J_{ij}. [Similar behavior occurs for $T_N(\tilde{U})$; it is omitted for clarity.]

Figure 2 also shows the Néel temperature of the Hubbard model on a simple cubic lattice, inferred from MC by Scalettar *et al.* [8]; for $\tilde{U} \gtrsim 6-8$, these results are reduced significantly from the earlier pioneering MC work by Hirsch [7] on smaller (4^3) lattices. Our *molecular field* $T_N^{\mathrm{MF}}(\tilde{U})$ clearly agrees very well with $T_N^{\mathrm{MC}}(\tilde{U})$, lying within MC error bars for all but two points ($\tilde{U} = 10, 12$, and even here it is close). This is interesting, for Hasegawa [4] has since argued that the method used to extract T_N^{MC} produces the Weiss temperature (rather than the true T_N)—which is what is obtained from a MF theory—and thus still overestimates T_N. While not wishing to enter the controversy [3,4,8], our T_N^{MF} does reproduce well the MC results, and it is curious that, even for $\tilde{U}$ as large as 20, the MC result is still apparently far from the large coupling asymptote $T_N \simeq 3.83t^2/U$ (cf. also Fig. 1 for the J_{ij}).

To compare our results for the $d = 3$ Hubbard model with the functional integral theories mentioned earlier, Fig. 3 shows $T_N(\tilde{U})$ for the single-site spin-fluctuation (SSF) theory of Hubbard and Hasegawa [1]; the Gutzwiller-type variational approaches of Kakehashi, Fulde, and Samson [2] (VA) and, more recently, Hasegawa [4] (HA); the SSF and VA results are taken from [3]. For $\tilde{U} \gtrsim 10$, SSF and VA essentially coincide with our molecular field $T_N^{\mathrm{MF}}(\tilde{U})$ (Fig. 2). But clearly none do as well as T_N^{MF} in reproducing the MC results, especially for weak to moderate coupling, $\tilde{U} \lesssim 10$. It is also worth noting that T_N^{MF} with J_{ij} confined solely to NN's, also shown in Fig. 3, bridges smoothly between SSF for $\tilde{U} \lesssim 6$ and HA for $\tilde{U} \gtrsim 10$. Note again, however, that none of these theories behaves correctly in the strong coupling $\tilde{U}$ limit, all reducing to the MF asymptote.

We have focused mainly on the Néel temperature, one of the hardest quantities to obtain from MC calculations. But our approximate mapping of the low-energy excitations of the half-filled Hubbard model onto an effective $\hat{H}_{\mathrm{Heis}}(\tilde{U})$ naturally enables extraction of the full gamut of thermodynamic and/or magnetic properties, including where appropriate $\tilde{U}$-dependent one-loop contributions from transverse spin fluctuations (e.g., energy, specific heat, and staggered magnetization). These will be detailed in an expanded paper. Here, for illustration, we consider the T dependence of the important spin correlation functions (SCF) $\langle \hat{s}_{iz}\hat{s}_{jz}\rangle$ in the paramagnetic regime. Figure 4 shows the NN, 2NN, and 3NN $|\langle \hat{s}_{iz}\hat{s}_{jz}\rangle|$ vs T/t for fixed $\tilde{U} = 12$, compared to Hirsch's [7] MC results on a 4^3 lattice (the NN and 3NN SCF's are always negative). Spin correlations beyond NN buildup

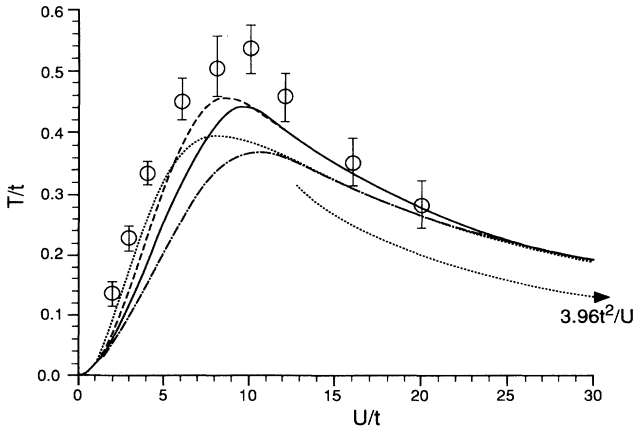

FIG. 3. Previous approximations for T_N in $d = 3$: SSF [1] (dashed line), VA [2] (solid), and HA (point-dash). As $\tilde{U} \to \infty$ all yield the MF limit. Also shown are MC results [8] (circles) and our $T_N^{\mathrm{MF}}(\tilde{U})$ for solely NN J_{ij} (dotted).

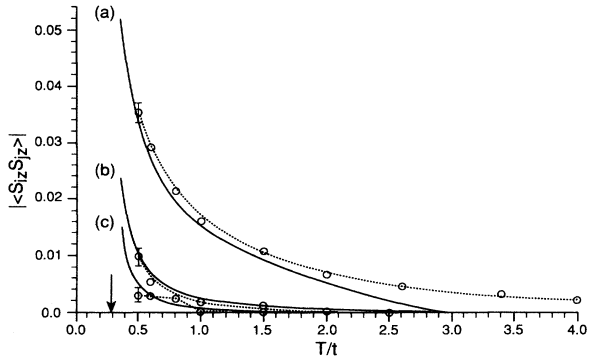

FIG. 4. Spin correlation functions $|\langle \hat{s}_{iz}\hat{s}_{jz}\rangle|$ vs T/t in the paramagnet, for $\tilde{U} = 12$; $T_N(\tilde{U})$ is marked by an arrow. (a) Nearest neighbor, (b) 2NN, and (c) 3NN. Circles show Hirsch's [7] 4^3 MC results.

only below $T/t \simeq 1$. And the theory clearly agrees remarkably well with MC results over a very wide T range above the ORF $T_N(\tilde{U}) \simeq 0.3t$ (despite the extant disparity between T_N and T_N^{MC}), agreement being noticeably poorer if the ORF contribution is omitted. As expected from the discussion above, the good agreement weakens (for the NN SCF) only for temperatures approaching $T_{\mathrm{HF}}(\tilde{U}) \simeq 3t$ ($\simeq 10T_N$) at which the UHF local moments are thermally destroyed.

In summary, by the simple and physically transparent expedient of mapping approximately the low-energy excitations of a half-filled Hubbard model onto those of an effective, $\tilde{U}$-dependent Heisenberg model, combined with a thermal mean-field approximation which includes an Onsager reaction field treatment of short-ranged magnetic ordering, we have proposed a theory which recovers the correct d dependence of AFLRO, interpolates properly for $d = 3$ between weak and strong coupling strengths in describing the magnetic phase boundary of the Hubbard model, and yields associated thermodynamic properties. We add further that the underlying theory can also be adapted more generally to the AF phase of a disordered Hubbard model, as we will discuss in a later paper.

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