Magnetic order in the Hubbard model in three dimensions and the crossover to two dimensions

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Abstract
Systems of fermions described by the three-dimensional (3D) repulsive Hubbard model on a cubic lattice have recently attracted considerable attention due to their possible experimental realization via cold atoms in an optical lattice. Analytical and numerical results are limited away from half-filling. We study the ground state of the doped system from weak to intermediate interaction strengths within the generalized Hartree–Fock approximation. The exact solution to the self-consistent-field equations in the thermodynamic limit is obtained and the ground state is shown to exhibit antiferromagnetic order and incommensurate spin-density waves (SDW). At low interaction strengths, the SDW has unidirectional character with a leading wavevector along the ⟨100⟩-direction, and the system is metallic. As the interaction increases, the system undergoes a simultaneous structural and metal-to-insulator transition to a unidirectional SDW state along the ⟨111⟩-direction, with a different wavelength. We systematically determine the real and momentum space properties of these states. The crossover from 3D to two dimensions (2D) is then studied by varying the inter-plane hopping amplitude, which can be experimentally realized by tuning the distance between a stack of square-lattice layers. Detailed comparisons are made between the exact numerical results and predictions from the pairing model, a variational ansatz based on the pairing of spins in the vicinity of the Fermi surface. Most of the numerical results can be understood quantitatively from the ansatz, which provides a simple picture for the nature of the SDW states.

(Some figures may appear in colour only in the online journal)

1. Introduction

Over the past several years, optical lattices have become an increasingly powerful tool for emulating many systems in condensed matter physics [1–4]. An optical lattice can provide exceptionally clean access to a variety of model many-body Hamiltonians in which parameters can be systematically tuned and controlled. Thus, they make possible quantitative experimental study of the properties of interacting electron models, which have proven extremely challenging for analytic and numerical approaches alone. The combination of these approaches presents unprecedented opportunities for improving our understanding of interacting electron systems, by testing theoretical concepts and increasing the accuracy and predictive power of numerical approaches via comparison with experiment.

The one-band Hubbard model is one of the most fundamental models in condensed matter physics. It has been widely studied in two dimensions (2D) [5–20] as the simplest model for the Cu–O plane in cuprate superconductors. For the three-dimensional (3D) Hubbard model, however, considerably less is known from both theoretical and experimental sides. Optical lattices play, in this respect, a particularly fundamental role as they allow for a clean experimental realization of the 3D model and offer the interesting possibility of tuning the hopping parameter along one direction, $t_\perp$, thereby allowing a systematic study of the evolution of properties as the system crosses over from 3D to 2D.

Thanks to advances in the ability to directly cool atoms in optical lattices [21], experiments are nearing the realization of phases with magnetic order. It is thus particularly important
and timely to understand such phases in the Hubbard model. Somewhat surprisingly, apart from half-filling (one particle per site), which displays antiferromagnetic (AFM) order, the nature of the magnetic properties in the 3D Hubbard model has not been characterized, even at the mean-field level. Several work have discussed the onset of incommensurate order [22–25], including the pioneering work by Penn [22]. However, the actual symmetry of the order parameter in the symmetry-broken phase has not been addressed.

Despite the simple nature of the mean-field approach, the determination of the correct equilibrium properties in these models is not straightforward [20, 26]. The main challenge lies in finding an unbiased strategy to determine the leading wavevector(s) characterizing the spatial dependence of the order parameter. Calculations are performed in a real space simulation cell and most choices of the cell will return solutions that are biased by finite-size effects. This is often further complicated by shell effects and sensitivity of the solution to the topology of the Fermi surface, which often lead to local minimum solutions.

In this work, we study the magnetic properties in the ground states of the 3D Hubbard model and in the crossover regime, using generalized Hartree–Fock (HF) theory. It is shown that the system has a tendency to form unidirectional spin-density wave (SDW) states with AFM order and a modulating wave along either the (100)- (at low $U/t$) or the (111)-direction (at higher $U/t$). We examine the evolution of the SDW wavelength in the full mean-field solution as $U$, density and $t_{\perp}$ vary and characterize the ground state by its properties in real and momentum space.

To overcome the difficulties in determining the true HF solution, it is necessary to move to larger and larger cells and gain insights from the evolution of the corresponding solutions. This line of attack, not possible in the days of Penn [22], has become increasingly possible because of the dramatic increase in computing power and continuous algorithmic progress. In the present work, we combine such an approach with more targeted searches to obtain the global minimum solution of the self-consistent-field (SCF) equations in the thermodynamic limit. Furthermore, we show how the numerical results can be understood by a variational ansatz based on the pairing of spins in the vicinity of the Fermi surface. Detailed comparisons are made between the direct numerical solutions and the pairing ansatz predictions. The excellent agreement helps to provide a simple, predictive picture for the properties of the SDW states.

The mean-field approach is often the starting point in the study of strongly interacting systems such as the Hubbard model. Although the approximations involved can lead to significant errors, mean-field theory often provides insights into qualitative aspects of the behavior of many-body systems. Moreover, comparisons with quantum Monte Carlo results [19] have shown [20] that, in 2D, the mean-field solution captures the basic physics of SDW states at intermediate interaction strengths, and provides a good qualitative (or even quantitative in some aspects) description of the magnetic correlations in the true ground state. Because it is reasonable to expect a similar level of accuracy for the models presently considered, we expect that our findings will provide guidance to many-body approaches and experimental studies alike.

We have limited our study to $U \lesssim 6t$ (and in fact often below 4$t$, half of the 2D bandwidth), where the mean-field approach can be expected to offer useful insight. Below we will discuss the mean-field predictions and their implications (and the caveats) on the true many-body states drawing from the comparison in 2D [19, 20]. Clearly, the form of generalized mean-field theory considered in this work will not capture exotic instabilities, such as unconventional pairing order. Indeed, as $U$ increases, it will become increasingly inadequate for magnetic properties as well.

The remainder of the paper is organized as follows. In section 2, we introduce the Hamiltonian, and briefly outline some of its basic properties to facilitate the ensuing discussion. In section 3, we summarize the strategies used to solve the mean-field equations. Results for the 3D model are presented in section 4; numerical results for the (100)- and the (111)-SDW are followed by a discussion where the pairing ansatz is first introduced and then used to help understand the numerical findings. The dimensional crossover results are then presented in section 5, followed again by a discussion based on insights from the pairing ansatz. We conclude in section 6.

2. Background

Given our goal to study both the 3D case and the crossover from 3D to 2D, it is most convenient to define the 3D Hubbard Hamiltonian as a stack of square-lattice planes. We will use $r \equiv (x, y)$ to denote in-plane coordinates and $z$ to label the planes. With this convention the Hubbard Hamiltonian reads

$$H = -t \sum_{\langle r \sigma,\sigma' \rangle} \left( c_{r \sigma}^\dagger c_{r' \sigma'} + h.c. \right) - t_{\perp} \sum_{\langle z \sigma,\sigma' \rangle} \left( c_{z \sigma}^\dagger c_{z' \sigma'} + c_{z' \sigma'}^\dagger c_{z \sigma} \right) + U \sum_{\langle z \sigma,\sigma' \rangle} n_{z \sigma} n_{z' \sigma'}$$

(1)

where the operator $c_{r \sigma}^\dagger$ ($c_{r \sigma}$) creates (annihilates) a particle with spin $\sigma$ ($\sigma = \uparrow, \downarrow$) at site $(r, z)$ and $n_{r \sigma}$ is the corresponding number operator. The hopping amplitude $t$ is between nearest neighbor sites within a plane (denoted by $(rr')$ in the summation), $t_{\perp}$ is the inter-plane hopping amplitude between nearest neighbor sites belonging to different planes (denoted by $(zz')$ in the summation), and $U > 0$ is the on-site interacting strength. Throughout this work, energy is quoted in units of $t$ and we set $\hbar = 1$. The Hamiltonian in equation (1) describes the 3D cubic Hubbard model when $t_{\perp} = 0$, the crossover between the square and cubic lattices when $0 < t_{\perp} < 1$ and a stack of decoupled 2D Hubbard planes when $t_{\perp} = 0$. Only unpolarized systems are considered, i.e., the average densities of the two spin species are kept equal: $n_{\uparrow} = n_{\downarrow}$. The nature of the ground state is thus characterized by three parameters: the inter-plane hopping
Figure 1. Non-interacting half-filled Fermi surface from different view angles: 3D (top), along [010] (middle), along [111] (bottom). From left to right, the columns are for \( t_\perp = 0, 0.5 \) and 1, respectively. Note that only the surface in one octant is shown in the bottom row. Perfect nesting via \( Q = (\pm \pi, \pm \pi, \pm \pi) \) holds for any \( t_\perp \) at half-filling.

The derivation is as follows: The particle–hole transformation, \( c^\dagger_{\mathbf{r}\sigma} \rightarrow (-1)^{x+y+z}c^\dagger_{\mathbf{r}\sigma} \), maps the \( h < 0 \) sector into the \( h > 0 \) one, regardless of the value of \( t_\perp \) or \( U \), and we therefore confine our study to \( h > 0 \).

At half-filling, \( h = 0 \), the non-interacting Fermi surface is given by \( -2(\cos k_x + \cos k_y + t_\perp \cos k_z) = 0 \). Despite the lack of symmetry between the z- and the r-directions for any \( t_\perp \neq 1 \), perfect nesting via \( Q = (\pm \pi, \pm \pi, \pm \pi) \) remains throughout the whole surface, and causes an AFM instability for any \( t_\perp \neq 0 \) and arbitrary small \( U \) values. The evolution of the non-interacting half-filled Fermi surface as \( t_\perp \) varies is shown in figure 1. In the first column, representing the 2D limit, the Fermi surface has no dependence on \( k_z \) and any wavevector of the form \( (\pm \pi, \pm \pi, q) \) is perfectly nested on it. The arbitrariness of \( q \) is reflected in the complete lack of correlation between the \( r \)-planes. The large nesting degeneracy is abruptly interrupted as soon as \( t_\perp \neq 0 \), and \( Q \) remains the only nesting vector as the system evolves from the 2D limit toward 3D. The middle and bottom rows illustrate projections of the Fermi surface along the (100)- and (111)-directions; as we shall see in sections 4 and 5, the projected area of the Fermi surface plays a central role in determining the character of the SDW in the proximity of \( h = 0 \).

3. Method

The following mean-field formalism in real space is used in this work. A simulation cell of \( N \) sites is defined by three vectors, \( \mathbf{L}_1, \mathbf{L}_2 \) and \( \mathbf{L}_3 \), whose components are integers. Bloch states are then introduced as

\[
c_{\beta}(\mathbf{k}) \propto \sum_{\mathbf{L}} c_{\beta + \mathbf{L}} \exp[i\mathbf{k} \cdot \mathbf{L}],
\]

where \( \mathbf{L} \) are vectors of the form \( \mathbf{L} = n_1 \mathbf{L}_1 + n_2 \mathbf{L}_2 + n_3 \mathbf{L}_3 \). \( \mathbf{k} \) is a reciprocal lattice vector that is free to vary within the first Brillouin zone (BZ) defined by the \( \mathbf{L}_i \)'s, and \( \beta \) labels sites inside the simulation cell. Using these states, the mean-field approximation
Hamiltonian can be decoupled into a sum of $k$-dependent pieces, $H_0 = \sum_k H_0(k)$, with each piece of the form

$$
H_0(k) = [e_i^\dagger e_i^\dagger] \left[ \begin{array}{c} H_1(k) \\ S^- \\ H_4(k - G) \end{array} \right] [e_i e_j]^T, \tag{4}
$$

where $e_i$ ($e_j$) represents a row of operators $c_{\beta\dagger}(k)$ ($c_{\beta\dagger}(k-G)$) with index $\beta$ running through the $N$ sites of the cell. A non-zero value of $G$ causes the spin densities at $\beta$ and $\beta + 1_i$ to be related via a rotation by $G \cdot 1_i$ around the $z$-axis. Charge and spin densities along $z$-direction obey periodic boundary conditions. $H$ and $S^\pm$ are $N \times N$ matrices with elements

$$
\begin{align*}
[H^\pm(k)]_{\beta\gamma} &= -i t_{\beta\gamma}(k) + \delta_{\beta\gamma}(UD_{\beta\sigma} - \mu), \\
[S^\pm(k)]_{\beta\gamma} &= U \delta_{\beta\gamma} S_\beta^\pm,
\end{align*} \tag{5}
$$

where $t_{\beta\gamma}(k) = \sum_{\lambda} \exp(ik \cdot L)_{\beta\gamma} + L$, and $D_{\beta\sigma}, S_\beta^\pm$ and $\mu$ determined by the requirement that the free energy $F = \langle H \rangle_0 - T S_0$ is a minimum for the targeted average density $n = n_\uparrow + n_\downarrow$. This amounts to the following SCF (gap) equations

$$
\begin{align*}
D_{\beta,-\sigma} &= \frac{1}{(2\pi)^3} \int \text{d}k \langle c_{\beta\sigma}(k)c_{\beta\sigma}(k) \rangle_0, \\
S_\beta^\pm &= \frac{1}{(2\pi)^3} \int \text{d}k \langle c_{\beta\dagger\pm\sigma}(k)c_{\beta\dagger,\mp\sigma}(k) \rangle_0, \\
n_\sigma &= \frac{1}{N(2\pi)^3} \sum_{\beta,\sigma} \int \text{d}k \langle c_{\beta\sigma}(k)c_{\beta\sigma}(k) \rangle.
\end{align*} \tag{6}
$$

A similar approach has been recently used in 2D in the presence of a trapping potential [27].

To locate the ground state we proceed with two complementary approaches. In the first approach we select the $L_i$s so that they span a large supercell containing $O(5000)$ sites. A twisted boundary condition [28, 29] is applied, namely, using a single randomly selected $k$-point in place of the integrals in equation (6). The iterative process is started with various initial states, including random ones, and multiple annealing cycles are performed. In each cycle a random perturbation (whose strength can be controlled) is applied to a converged solution and the self-consistent process is repeated. Separate calculations for different $k$-points are done to check for consistency. (More details are in reference [20].)

Once an understanding of the character of the ground state is gained, we use a second approach to target the specific family of states compatible with the results of the random search. For instance, suppose the random search finds a unidirectional SDW at small $U$ values with wavevector along the $\langle 100\rangle$-direction. We then choose a cluster of $L_1 = (L, 0, 0)$, $L_2 = (0, 1, 0)$ and $L_3 = (0, 0, 1)$ with $G = \pi((-1)^{k+2L}, 1, 1)$, where $L$ is the number of oscillations of the order parameter, chosen to be an integer or half an integer. For a given set of the three parameters ($t_\perp, U, h$), $L$ is finely scanned (with $L$ on the order of 50 and step size of 1) until the energy minimum is found. A large number of $k$-points is used (on the order of 100 in the two short directions and a few in the other) so that the character and properties of the targeted states can be accurately determined. This approach allows us to study different forms of SDW and long wavelength modes without increasing the computational cost.

In our study, we mix the two numerical approaches as needed and use them in complementary ways. For example, comparison of energies among several families of SDW is made with the second approach. To confirm the correctness of the ground state, the solutions are then checked against different initial states and annealing procedures using the first approach on a supercell commensurate with the optimal wavelength.

Various observables are computed to characterize the converged solutions. The local charge density $\rho$ and the local order parameter, identified as the local staggered magnetization $m$, are defined as

$$
\rho(r) \equiv \langle n_{\uparrow r} \rangle + \langle n_{\downarrow r} \rangle, \tag{7}
$$

$$
m(r) \equiv (-1)^{\dagger + \dagger + \dagger} \left( \langle n_{\uparrow r} \rangle - \langle n_{\downarrow r} \rangle \right), \tag{8}
$$

and used to characterize the state in real space (here $\rho \equiv (r, z)$). Since all the minimum energy solutions we find are unidirectional spin/charge density waves (SDW/CDW), it is natural to characterize them by their modulation wavelength around a relevant Cartesian axis, $\lambda_{\text{SDW/CDW}}$, defined by the leading component of the Fourier transform of $\rho$ and $m$, respectively. The minima in the CDW are found to coincide with nodes in the SDW, thus $2\lambda_{\text{CDW}} = \lambda_{\text{SDW}}$. Below we will sometimes discuss our results in terms of a single wavelength $\lambda = \lambda_{\text{CDW}}$, which can also be identified as the distance between two consecutive nodes of the order parameter. When we refer to the direction of the modulation, we will use ($100$) to denote symmetry-equivalent $[100]$-directions, and similarly for $[110]$ and $[111]$.

To characterize the system in momentum space, we use the momentum distribution $n_k$ and the momentum-resolved single-particle spectral function $A_k(\omega)$, defined as

$$
n_{k\sigma} \equiv \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle, \tag{9}
$$

$$
A_{k\sigma}(\omega) \equiv \frac{1}{\pi} \text{Im}(c_{k\sigma}(\omega - H_0 - i\eta)^{-1} c_{k\sigma}^\dagger), \tag{10}
$$

with $c_{k\sigma} \propto \sum_R \exp(-i k \cdot R)c_{R\sigma}$. We use $n_k$ to compare the converged mean-field solution with the pairing ansatz prediction and $A_k$ to characterize the Fermi surface of the ordered phase.

4. 3D results

4.1. SDW correlation in the $\langle 100\rangle$-direction

At half-filling, the existence of perfect nesting allows an AFM solution for any $U > 0$. Away from half-filling, perfect nesting ceases to exist and a finite critical value of the interaction is needed to cause the onset of order. The critical value $U_c$ depends on $h$. Using the first approach described in section 3, we have determined that, just above $U_c$, the ground state of the system is an SDW with modulation along the $\langle 100\rangle$-direction. Figure 2 illustrates the spatial dependence of $\rho$ and $m$ in a $16 \times 16 \times 16$ supercell at $h = 13/128 \approx 0.10$ and $U = 2.5$. The SDW is characterized by a single wavevector and $\lambda_{\langle 100 \rangle} = 8$. 


Figure 2. Charge density $\rho$ (left) and order parameter $m$ (right) of the solution for the 3D Hubbard model. Shown is a $16 \times 16 \times 16$ supercell, with $\delta = 13/128$ at $U = 2.5$. A linear wave is seen along the $z$-direction, with uniform AFM order in the $xy$-plane. The bottom panel shows a line cut along $z$-direction, with dots the actual data and the line a sinusoidal fit.

Figure 3. Spatial dependence of the order parameter $m$ for $\delta = 13/128$, same as in figure 2, but with $U = 2.9$, on a $16 \times 16 \times 16$ supercell (left) and a $16 \times 16 \times 14$ supercell (right). Uniform AFM order in the $xy$-plane disappears for $L_z = 16$, but linear SDW along $z$-direction is seen again on the right with $L_z = 14$.

The amplitude of the SDW is $\simeq 0.1$, roughly thirty times larger than that of the CDW. The simple form of the order found for $m(R)$ is indicative of the proximity of $U$ to $U_c$. All of the observations above are consistent with the pairing model, as discussed below in section 4.3.

We next examine the evolution of $\lambda_{(100)}$ as the interaction strength changes. Keeping $\delta$ and the simulation cell unchanged and increasing $U$ from 2.5 to 2.9, the random search returns the state displayed on the left panel of figure 3, which suggests that a more complicated type of order is seemingly settling in. We apply our second approach, using a dense $k$-point grid and a $1 \times 1 \times L$ simulation cell, to search for the optimal wavelength. We use large $L$ (containing about 8 nodes in the cell) and vary its value until an energy minimum
the 16 × λ those of by the 1 × obtained in the 16 supercell calculations of figure 3, to verify that the energy α with wavelengths. Our results are summarized in figure 5, are done on large supercells whose sizes are commensurate k value using a dense state, computed by fixing the density and converging the energy of this state, computed by fixing the density and converging the imposed constraint. The energy of this self-consistent solution in a large supercell then finds a different pattern that corresponds to the true ground state of the characteristics of the two types of approaches. The supercell being incommensurate prevents the solution from an incommensurate supercell size. We next find the predicted state with the wavelength of the minimum energy SDW state and that the pattern in the left panel of figure 3 is a result of frustration from an incommensurate supercell size. We next find the predicted state with the wavelength of the minimum energy SDW state and that the pattern in the left panel of figure 3 is a result of frustration from an incommensurate supercell size.

In figure 4, we report the energies of the two large supercell calculations of figure 3, to verify that the energy obtained in the 16 × 16 × 16 supercell is correctly reproduced by the 1 × 1 × L cluster search with λ(100) = 7. The energy of the 16 × 16 × 16 calculation, on the other hand, falls between those of λ(100) = 7 and 8. This gives a clear illustration of the characteristics of the two types of approaches. The supercell being incommensurate prevents the solution from collapsing onto the lowest energy SDW state of λ(100) = 7.

We proceed to determine the exact dependence of the wavelengths on h and U by explicit solutions of the SCF equations in 1 × 1 × L clusters. Verifications of the results are done on large supercells whose sizes are commensurate with the wavelengths. Our results are summarized in figure 5, with α(100) defined as

\[ \alpha_{(100)} = h \lambda_{(100)}. \]  

(11)

is found. Figure 4 shows the result of such minimization in terms of λ(100); the minimum occurs when λ(100) = 7, indicating that the 16 × 16 × 16 supercell is not commensurate with the wavelength of the minimum energy SDW state and that the pattern in the left panel of figure 3 is a result of frustration from an incommensurate supercell size. We next return to our first approach, and perform a new mean-field calculation, with random initial guess and annealing, on a 16 × 16 × 14 supercell, a size which is commensurate with the wavelength of the minimum energy solution. And indeed we find the predicted state with λ(100) = 7 correctly reproduced (right panel in figure 3).

When the doping is small, the wavelength of the modulation is proportional to 1/h, with α(100) almost independent of U and roughly equal to 2/3. For larger h, α(100) converges to a slightly larger value. There is a general trend of an increase of 100/α as U approaches 100. The figure illustrates the existence of Uc, the (100)-SDW/CDW amplitudes increase with U and the solution evolves from a sinusoidal wave to domain walls. The CDW amplitude is much weaker than that of the SDW.

The evolution of the properties of the 3D SDW state with interaction U is similar to what is observed in 2D. Figure 6 shows 1D cuts of m and ρ in the z-direction, the direction of the modulation. Beyond Uc, the (100)-SDW/CDW amplitudes increase with U and the solution evolves from a sinusoidal wave to domain walls. The CDW amplitude is much weaker than that of the SDW.

Figure 4. Energy of (100)-SDW (blue) versus λ(100) for a system of h = 13/128 and U = 2.9. Horizontal lines are the energies of the calculations shown in figure 3. The minimum of (100)-SDW is reached when λ(100) = 7. The state in the left panel of figure 3 leads to an energy higher than the minimum but lower than the energy with λ(100) = 8.

Figure 5. Characteristic wavelength as a function of U at various doping. α(100) gives the modulation wavelength, λ(100), in units of 1/h. As U is increased, the value of α(100) converges to approximately 2/3 at small h (slightly larger at larger h).

Figure 6. Charge density ρ (top) and order parameter m (bottom) versus U. The system has doping h = 0.05. Each curve is a 1D cut along z-direction, the direction of the modulation. Beyond Uc, the (100)-SDW/CDW amplitudes increase with U and the solution evolves from a sinusoidal wave to domain walls. The CDW amplitude is much weaker than that of the SDW.

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characterized by domain walls or stripes, with holes localized in the nodal regions.

There exists an important difference in the physics of the mean-field ground state of the 3D system and its 2D counterpart. While, in the latter, the system remains insulating when lightly doped, the 3D model immediately turns metallic. The difference is a consequence of the different behaviors of the modulating wavelength. In 2D, $\alpha$ is unity, independent of $h$ and $U$, while in 3D it varies with parameters and has a non-integer value. To illustrate this in a simple case, consider a value of doping $h$ such that $\lambda \equiv \alpha/h$ is an integer. For such a system to be an insulator, the number of particles in a $1 \times 1 \times \lambda$ cell, $(1 - h)\lambda = \lambda - \alpha$, will have to be an integer. However, because $\alpha \sim 2/3$ in the limit of small doping, the condition cannot be satisfied, and the system is necessarily metallic. A related way to see this is to consider the case of domain wall states, for example $U = 3.5$ in figure 6. Inside each domain wall (nodal region) are localized holes whose integrated (along the direction of the modulation) density is $\alpha$. Thus the domain wall as a whole will act as a quasi-2D liquid of holes with non-integer density. We will discuss the corresponding momentum space signature in section 4.2.

4.2. SDW modulation along the $\langle 111 \rangle$-direction

As shown above and further discussed in section 4.3, an orientation of the SDW other than $\langle 100 \rangle$ is not the solution in the proximity of $U_c$. However, when the interaction grows larger, other Fermi liquid instabilities become possible. This fact is clearly displayed when calculations on supercells commensurate with the optimal $\langle 100 \rangle$-wavelength for a given $U$ do not yield a state with $\langle 100 \rangle$-SDW order. Figure 7 shows the occurrence of such a case in a calculation with $h = 1/8$ and $U = 5.0$, for which $\lambda_{\langle 100 \rangle} = 5.5$. The $16 \times 16 \times 22$ supercell should have precisely accommodated four nodal planes of the order parameter, but rather than doing so, the random search produces the lower energy solution shown in the left panel of the figure.

To search for the solution at higher $U$, we investigate unidirectional SDW’s with modulation lying along either the $\langle 110 \rangle$- or $\langle 111 \rangle$-direction. An example is given in figure 8. The energies from constrained searches using the second approach are shown as a function of $\lambda$ for a scan of $U$ values. It is seen that, at and above $U = 4.5$, the lowest energy state is given by a $\langle 111 \rangle$-SDW, instead of the $\langle 100 \rangle$-order at lower $U$. For $U = 5$, the minimum energy solution is correctly reproduced by a random search in a $16 \times 16 \times 16$ supercell as shown in the right panel of figure 7. In our searches, $\langle 110 \rangle$-direction SDW’s are never found to be the global ground state.

By repeating the same procedure, we construct the equation of states for $U = 3$ and 4 contained in figure 9. At $U = 3$, there is no density regime where the $\langle 111 \rangle$-SDW is the global ground state. In contrast, for $U = 4$, a discontinuous transition from $\langle 100 \rangle$ to $\langle 111 \rangle$ occurs around $n = 0.9$ with a small coexistence region. In both cases the low-doping ground state is characterized by a linear energy-density dispersion. This bears two important consequences. First, contrary to what is observed using variational states with a uniform spiral order parameter [30], there is no sign of phase separation into a half-filled, AFM region and a hole-rich region. Second, the effective interaction between domain walls is short-ranged and their precise location in the hole-diluted limit is therefore irrelevant as long as they stay sufficiently far apart.

We find $\alpha_{\langle 111 \rangle} = 1$ at any density for which the $\langle 111 \rangle$-SDW is the ground state. The $\langle 111 \rangle$-SDW states are fully gapped, owing to the integer value of $\alpha_{\langle 111 \rangle}$, in contrast to the metallic behavior of the $\langle 100 \rangle$ states. Upon increase of $U$ at a constant $h$, the structural transition is therefore always accompanied by a metal-to-insulator transition. We have verified, for selected cases, that random searches on larger supercells with sizes commensurate to the optimal wavevector always return unidirectional SDW’s with the same

Figure 7. Order parameter $m$ at $h = 1/8$ and $U = 5.0$ in a $16 \times 16 \times 22$ supercell (left) and a $16 \times 16 \times 16$ supercell (right). Though the supercell of $16 \times 16 \times 22$ is commensurate with the optimal $\langle 100 \rangle$-wavelength, the random search produces a lower energy solution. The minimum energy solution is an SDW along the $\langle 111 \rangle$-direction, which is correctly reproduced by a random search in a $16 \times 16 \times 16$ supercell as shown on the right.
Figure 8. Energies per site of SDW in ⟨100⟩-, ⟨110⟩- and ⟨111⟩-directions versus λ for h = 1/8. At and above U = 4.5, the lowest energy state is modulated along the ⟨111⟩- instead of ⟨100⟩-direction.

Figure 9. Ground state energy per site from constrained search of ⟨100⟩-, ⟨110⟩- and ⟨111⟩-SDW at U = 3 (left) and U = 4 (right). A linear common shift has been applied to the energies to highlight the convexity and the different trends. At U = 3, ⟨111⟩-SDW is not the global ground state. (The inset shows a zoom of the energy difference between ⟨111⟩- and ⟨100⟩-SDW states as n → 1.) At U = 4, the ground state is ⟨111⟩-SDW for n ≳ 0.92.

predicted wavelength and orientation. This provides a strong indication that the character of intermediate U instabilities remains that of a unidirectional SDW. Thus, as we increase U at constant density, the system is always expected to undergo a discontinuous transition from a ⟨100⟩- to a ⟨111⟩-SDW ground state.

4.3. A variational pairing ansatz

The so-called pairing model is a variational ansatz that has proved extremely helpful in rationalizing the properties of SDW’s in the mean-field treatment of the electron gas [31, 26] and the 2D Hubbard model [20]. Similarly here, the model helps to explain the numerical results and provides a simple conceptual framework that captures the essential physics of the SDW states in 3D and in the crossover regime discussed in the next section. We first summarize the formalism, and then apply it to the case of ⟨100⟩-SDW at modest U, followed by the ⟨111⟩-SDW.

At low U and small h, the pairing model is defined by spin–orbitals of the form

$$\phi_{k\sigma}^{\dagger} \equiv u_{k}c_{k\sigma}^{\dagger} + \sigma v_{k}c_{k+q\sigma}^{\dagger}.$$

(12)
The construction requires excitations to outside the Fermi sea. It is reminiscent of the ansatz used to construct the BCS pairing states for attractive interactions, except that here the tendency for small excitations is perhaps more ‘natural’, because of the repulsive interaction. A collection of spin pairs in orbitals given by equation (12) leads to a uniform charge density, $\rho (R) = n$, and a spin density of the form

$$s(R) = \frac{4}{N} \sum_{k \in R} a_k \cos (q_k \cdot R)$$

(13)

with $a_k = a_{k^\prime}v_k$. The region $R$ over which $k$ is summed will be closely related to the non-interacting Fermi sea, and preserving the volume of $4\pi^3 n$, but will in general be slightly modified from the variational optimization, as we further discuss below. To ensure orthogonality amongst the spin–orbitals, $q_k$ must be such that $k + q_k \notin R$ and $k + q_k \neq k^\prime + q_k$. The corresponding potential energy per site is then given by

$$V = Un^2 - \frac{U}{4N} \sum_R \chi^2 (R).$$

(14)

The potential energy lowering relative to the paramagnetic (PM) solution is thus:

$$\Delta V = -\frac{U}{N^2} \sum_{k, k^\prime \in R} a_k a_{k^\prime} [\delta(q_k + q_{k^\prime}) + \delta(q_k - q_{k^\prime})].$$

(15)

where the Kronecker $\delta$ is intended as periodic on the reciprocal lattice, i.e., modulo $2\pi$ in any direction.

Equation (15) makes it clear that the maximum reduction in $V$ is achieved by having as many pairs as possible with $q_k$ parallel or anti-parallel to each other. Noting that the vector $Q$ is perfectly nested when $h = 0$, let us consider the following explicit construction for $R$: displace the half-filled Fermi surface in each octant of the first BZ by $\pm \Delta q/2$, choosing the direction that shrinks the Fermi sea, and with a length $\Delta q$ such that the enclosed volume is reduced to $4\pi^3 n$. This construction is illustrated in the top panel in figure 10 for the case of the (100)-SDW (discussed next in section 4.3.1). The surface of $R$ can now anchor spin pairs with one common pairing vector, by making $a_k$ less than 1 in a small layer immediately inside the surface of $R$, and correspondingly $v_k = \sqrt{1 - |a_k|^2} > 0$.

For small $h$, we can determine $\Delta q$ directly from the construction:

$$\Delta q \int_S \hat{e}_{\Delta q} \cdot dS = h \frac{\Omega_{\text{BZ}}}{2},$$

(16)

where $S$ is the half-filled surface, $\hat{e}_{\Delta q}$ is the direction of $\Delta q$, and $\Omega_{\text{BZ}} = (2\pi)^3$ is the volume of the first BZ. Equation (16) implies a linear relationship between $h$ and $\Delta q$, and, using $\lambda = \pi/(\Delta q \cdot \hat{e})$, provides the following estimate of $\alpha$ (equation (11))

$$\alpha_{\Delta q} = \frac{1}{4\pi^3} \hat{e}_{\Delta q} \cdot \hat{e} \int_S \hat{e}_{\Delta q} \cdot dS.$$ 

(17)

where $\hat{e}$ is a relevant Cartesian unit vector.

Figure 10. Illustration of the pairing model for the (100)-SDW state in 3D. The schematic diagram is drawn on the actual momentum distribution from the exact numerical solution for $h = 1/8$ and $U = 4.0$. The top panel shows the pairing construction on the contour plot of the (110) cut. The white dashed lines represent the half-filled surface, across which is the nesting vector $Q$. The reconstructed surface, shown as magenta solid lines, is obtained by displacing the half-filled one along the $z$-direction by a distance $\Delta q_{100}/2$, as given by equation (16). The nesting vector across the shifted surface, $q_{100}$, is shown by the long solid line with arrow. The bottom panel shows $n(k)$ of the $k_z = \pi$ plane. This is in a region where the Fermi surface survives the onset of order and where it differs more severely from the pairing construction. The actual Fermi surface, seen distinctly inside the reconstructed surface, differs little from the non-interacting Fermi surface (black solid line). $\phi_k$ drops sharply, and no pairing is present in this region.

Different directions of $\Delta q$ lead to different reconstructions of the non-interacting doped Fermi surface. The kinetic energy cost of the pairing ansatz can therefore be thought of as the combination of two contributions: the reconstruction energy due to using $R$ rather than the true non-interacting Fermi sea, and the kinetic energy change due to moving particles from $k$ (inside $R$) to $k + q_k$ (outside), i.e., the non-zero values of $v_k$. It is easy to see that, similar to 2D [20], at sufficiently large $U$ the potential energy lowering will overtake the kinetic energy increase for the constructions discussed here. The correct state is determined by maximizing the gain in the potential energy from pairing (larger areas near the Fermi surface participating with parallel $\Delta q$) while minimizing the kinetic energy cost.
The ansatz gives a clear picture for the onset of the instability. First, by its form, the model captures how the energetically costly CDW can be suppressed compared to the SDW. Second, it indicates that amongst different possible choices of $\mathbf{q}_k$, the one involving only parallel and anti-parallel vectors are optimal. Third, the direction of $\pm \Delta \mathbf{q}$ must be such as to lead to the minimal possible reconstruction of the doped Fermi surface. These findings are in qualitative agreement with the numerical results obtained by the solution of the SCF equations: (1) the SDW is much stronger than the accompanying CDW, (2) the Fermi surface reconstructs in a way to enhance pairing and the SDW order tends to be unidirectional as a result, (3) more drastic reconstructions are only possible with larger $U$. Much quantitative information can be obtained with straightforward calculations using this model, as we discuss next for the (100)- and (111)-SDW states, respectively.

4.3.1. Analysis of the (100)-SDW. Among all directions, only a $\Delta \mathbf{q}$ along the (100)-direction causes the Fermi surface in each octant to shrink equally and this, it can be shown, leads to the minimum kinetic energy increase at small $h$. An SDW with (100) modulation is thus the lowest energy solution at low $h$ and just above $U_c$, consistent with the results from explicit solutions of the SCF equations in section 4.1. We numerically calculate the projected area along the (100)-direction (shown in the right middle panel in figure 1) and obtain $\alpha_{(100)} \simeq 0.63$, in very good agreement with the exact results from direct solutions shown in figure 5, where $\alpha_{(100)} \simeq 0.66$. That the estimated value is slightly smaller is consistent with the presence of surviving Fermi surface inside the reconstructed doped Fermi surface as seen in figure 10.

A direct comparison between the pairing model and the exact SCF solution can also be made in momentum space. We will identify the Fermi surface in the numerical solution from mean-field theory as the locus of points where $n_{k_\sigma} = 0.5$. Depending on the system and the value of $U$, the momentum distribution of the exact mean-field ground state can maintain a true Fermi surface, characterized by a discontinuity in $n_{k_\sigma}$, or have it smeared out by large pairing amplitudes (i.e., $u_k$ close to $1/\sqrt{2}$ near the boundary of $\mathcal{R}$). The two scenarios can occur in the same system at different $k$ values. The identification using $n_{k_\sigma} = 0.5$ is consistent with both.

Figure 10 shows, in particular, that the portion of the Fermi surface where pairing takes place is in very good agreement with the construction based on the pairing model, which indicates that the ansatz captures the dominant ingredient of the physics of the SDW state. The figure also provides a direct explanation for the survival of the Fermi surface around $k_z = \pi$ as it is there that the pairing construction shows large discrepancy with the true Fermi surface. This, in turn, implies that pairing in that region would be associated with too large a kinetic energy cost to be favorable. The absence of any gap from pairing at the Fermi surface in the $k_z = \pi$ plane is consistent with the picture discussed earlier of a quasi-2D liquid within each domain wall. These effects are amplified at smaller values of $U$ as shown in figure 11, where a larger part of the Fermi surface survives the onset of order; the parts that do not survive are in areas around the ‘hot spots’ $k \simeq (\pm \pi/2, \pm \pi/2, \pm \pi/2)$, where the pairing construction and the doped Fermi surface are most similar, and the change in $\frac{\partial \alpha}{\partial k}$ is at a minimum implying a closer proximity to a perfect common pairing vector.

These understandings allow quantitative explanations of all the features of the data on $\alpha_{(100)}$ shown in figure 5. For example, figure 12 shows that the distance along $z$-direction between the doped and half-filled Fermi surfaces is at a minimum around the hot spots. Given that such distance equals $\Delta q/2$ in the pairing construction, one finds that the local $\Delta q$ value is smaller at the hot spots than when computed as the average distance over the entire surface. Hence, when only the hot spots are involved in pairing, a larger $\alpha_{(100)}$ results, as seen at lower values of $U$ just above $U_c$. Obviously, the pairing reconstruction becomes increasingly accurate as $h$ approaches 0. In this limit, one therefore finds the increasingly smaller $U_c$ and the faster convergence (in $U$) to the saturated value of $\alpha_{(100)} \sim 2/3$ shown in figure 5.

4.3.2. Application to the (111)-SDW. By taking a displacement $\Delta \mathbf{q}$ along the (111)-direction, we can apply the pairing construction straightforwardly to the diagonal-modulated SDW. Analogously to the (100) case, figure 13 shows a remarkable agreement between the shifted half-filled surface and the calculated Fermi surface of the SDW. The two cuts in the figure clearly show broken cubic symmetry, where the Fermi surface in one pair of the octants is further away from the half-filled one so as to share the common modulation wavevector $\mathbf{q}_{(111)}$ with the other three pairs. The (111)-SDW state offers, in this respect, a particularly clear example where Fermi surface reconstruction can be observed. It also shows how an accurate experimental characterization of the momentum distribution in optical lattices can be used to characterize the band structure and pairing at the Fermi surface which, in turn, provides momentum space evidence on the real space character of the SDW.

Using equation (17) we have estimated the wavelength of the (111)-SDW, and found $\alpha_{(111)} = 0.93$. The exact SCF calculations in section 4.2 showed, instead, that $\alpha_{(111)}$ is precisely pinned at 1 in a fairly large regime of $U$. This somewhat large discrepancy is a consequence of the natural tendency of the system to ‘lock’ the integrated density of states over the entire Fermi surface and further lower the ground state energy.

5. Dimensional crossover results

5.1. Results from full numerical HF solutions

The mean-field ground state of the doped 2D Hubbard model shares many similarities with its 3D counterpart. Just above $U_c$, the 2D system develops a sinusoidal SDW with a
modulating wave along the $\langle 10 \rangle$-direction and a much weaker accompanying CDW. As $U$ is increased, the SDW increases its amplitude before the SDW state eventually changes into a collection of weakly interacting domain walls. Above a certain $U$, there is a discontinuous transition to a phase where the modulation is along the $\langle 11 \rangle$-direction. The crossover from SDW to domain walls occurs before the $\langle 10 \rangle$ to $\langle 11 \rangle$ transition at small $h$, but after at larger $h$ [20]. A peculiarity of the 2D case, due to the special topology of the 2D half-filled surface, is that $\alpha = 1$ and the system is an insulator regardless of
doping. $U$ or direction of the modulation wavevector apart from a region close to $U_c$.

By controlling the distance between square-lattice layers, optical lattice experiments allow the study of the evolution of the system as it crosses over from 2D to 3D. This situation is theoretically described by an increase of $t_L$ in Hamiltonian (1) and the question, within mean-field theory, concerns the ensuing evolution of the ground state properties. The pairing model and the arguments described in section 4.3 remain valid in the crossover regime. We thus restrict our investigation to unidirectional SDW ground states, although we did use the first approach to carry out some searches, finding no additional structures. As in 3D, we verify that the SDW solution with minimum energy, identified using the second approach, can be obtained by the first approach in a large supercell that is commensurate with the optimal wavelengths, even when starting from random initial guesses. SDW in directions different from (100) or (111) are not found to be the global ground state for any value of $t_L$.

Results are summarized in the $t_L$–$U$ mean-field phase diagram of figure 14. An overall increase in the critical $U$ values is seen as doping increases, as a result of a greater deformation from the perfectly nested half-filled Fermi surface and the need for more excitations to achieve reconstruction of the Fermi surface for pairing. As before, numerical calculations focus on small doping ($h \leq 0.2$) and low to intermediate interactions ($U \leq 5.5$), where mean-field theory can be expected to be more accurate. Upon increase of $U$, and similarly to 3D, the system undergoes a first transition to a (100)-SDW state followed by a second, discontinuous transition to a (111)-SDW state. The absence of cubic symmetry away from $t_L = 1$ causes the modulation wavevector for (100)-SDW to lie in the $xy$-plane. This is because the elongation of the Fermi surface along $z$-direction (as illustrated in figure 1), meaning that $\Delta q$ along $z$-direction leads to less surface area for pairing than along $x$- or $y$-directions. Wavevectors along the (111)-direction continue, on the other hand, to remain equivalent under the symmetry operation of the tetragonal group.

The critical value of the interaction strength for the transition from the paramagnetic (PM) phase to (100)-SDW, $U_{\text{PM}}\rightarrow(100)$, monotonically increases from 2D to 3D, due to the wider band width and smaller density of states at the Fermi energy for larger $t_L$. The transition values decrease to 0 when $h$ approaches 0 as $U_c = 0$ for the half-filled system at any $t_L$. The critical $U$ value for the transition from (100)-to (111)-SDW, $U_{\text{PM}}\rightarrow(111)$, has a lower bound lying close to the $h = 1/32$ line in the figure, so that no (111)-SDW exists below $U \simeq 3$ regardless of the smallness of $h$ and the value of $t_L$. In contrast with $U_{\text{PM}}\rightarrow(100)$, $U_{\text{PM}}\rightarrow(111)$ displays a non-monotonic behavior with $t_L$, whose origin we will address in section 5.2.

The evolution of the modulation wavelength is summarized in figure 15 in terms of $\alpha$ as a function of $t_L$. Numerical results are obtained at $U$ values around the transition line

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**Figure 13.** Schematic illustration of the pairing model for the (111)-SDW state, shown on the contour plots of the (110) (top) and the (110) (bottom) cuts of $n_k$ for a system of $h = 1/8$ and $U = 5.0$. The white dashed lines are the half-filled surface, across which is the nesting vector $Q$. The magenta solid lines show the pairing construction, obtained by shifting the half-filled surface along [111]-direction by a distance of $\Delta q_{(111)}/2$. In the upper panel, $q_{(111)}$ and $\bar{q}_{(111)}$ give two equivalent representations (differing by a reciprocal lattice vector) of the pairing vector across the reconstructed Fermi surface. Note the asymmetry between the two diagonal directions in the upper panel.

**Figure 14.** Mean-field phase diagram of the ground state in the crossover regime. Phase boundaries for several values of doping are indicated by symbols. The lines are to guide the eye. Solid lines separate the PM phase from the AFM phase, and dashed lines show transitions from (100)- to (111)-SDW. The inset plots the value of $U_{(100)\rightarrow(111)}/U_{\text{PM}\rightarrow(100)}$.
display a correct trend but a consistent underestimation of wavelengths. The quantitative disagreement is not surprising. The most significant reason behind it is the tendency of \( \alpha \) to be locked at 1, on which we have already commented and which apparently involves more global considerations than contained in the pairing model. The smaller discrepancy for the \((100)\)-SDW outside the immediate vicinity of 2D, which increases for higher \( h \), is due to the surviving FS that remains inside the reconstructed doped FS, as we have already remarked in the 3D results.

We next address the origin of the non-monotonic behavior of \( U_{(100)\rightarrow(111)} \). This is the result of two competing factors. On the one hand, the increasing band width with dimensionality leads to an increase of \( U_c \), as demonstrated in the monotonicity of \( U_{PM\rightarrow(100)} \). On the other hand, the geometrical properties of the Fermi surface are such that the angle between \( \Delta q_{(111)} \) and the Fermi surface in some of the octants is small when \( t_\perp \) is small. This means that the displaced Fermi surfaces in those octants will remain close to the half-filling counterparts in the construction of \( \mathcal{R} \) (section 4.3). As a result, the other components of the Fermi surface must be displaced further to preserve total volume, causing a more uneven reconstruction which requires more excitations from the non-interacting Fermi sea, hence larger \( U_c \). The 2D case offers an extreme example of this as it is characterized by a large fraction of the reconstructed doped surface remaining exactly pinned on the half-filled one [20]. To separate this factor from that of the band width, we examine \( U_{(100)\rightarrow(111)}/U_{PM\rightarrow(100)} \), which is plotted in the inset of figure 14. A monotonic decrease is seen with \( t_\perp \). Therefore, \( U_{(100)\rightarrow(111)} \) first decreases and then increases as \( t_\perp \) goes from 0 to 1.

6. Summary and discussion

This work addressed quantitative aspects of possible inhomogeneous magnetic phases of the 3D Hubbard model that emerge as the average density deviates from one particle per site. Because of the ease with which experiments are expected to be able to transition between the 2D and 3D regimes, we also studied the evolution of the inhomogeneous ground state as a function of the hybridization between parallel layers of square lattices. Within mean-field theory, we have shown that the leading instability of the PM ground state is an SDW with long wavelength modulation along the \((100)\)-direction. No tendency toward phase separation was seen, even at small values of doping. The system remains metallic, regardless of the proximity to half-filling, because of a non-integer density of holes per wavelength of modulation. This density is largely determined by an entirely geometric property of the Fermi surface: its projected area along the direction of modulation. At larger \( U \) values, the ground state continues to be a unidirectional SDW, but with \((111)\)-orientation. This phase is insulating and characterized by a significant distortion of the momentum distribution. Such distortion leads, quite naturally, to the identification of a reconstructed Fermi surface whose observation in optical lattice experiments should be feasible.
We showed that much of these results can be understood by a simple variational ansatz with pairing orbitals formed by a linear combination of two plane waves. By placing a pair of up- and down-spin particles into a pair of such orbitals, an SDW is formed with constant charge density. Straightforward analysis of the energetics from this ansatz leads to quantitative predictions of the wavelength and nature of the SDW modulation which are verified by our direct numerical solutions of the SCF equations.

The true many-body ground state will modify the mean-field solutions in several ways. For example, quantum Monte Carlo calculations in periodic simulation cells will restore translational invariance, and the inhomogeneities seen here will be manifested in spin–spin correlations and such. A deeper issue is the possible existence of additional competing instabilities once a fuller treatment of quantum fluctuations is included. Certainly, the tendency for magnetic inhomogeneous order is exaggerated in mean-field theory, and a more accurate description of the many-body correlation at a certain $U$ value tends to be given by the mean-field results at a significantly weaker $U$. However, as we have shown in 2D, mean-field theory appears to capture the correct basic picture of the magnetic correlations when compared to quantum Monte Carlo results [20, 19]. This indicates that the results in the present paper can provide a useful framework for understanding the magnetic correlations in 3D and in the crossover regime for weak to intermediate interaction strengths.

Apart from the obvious omissions inherent in the mean-field approximation, this study has not addressed the fact that experiments are performed in the presence of a confining potential. Nor have we addressed how the situation is modified by a finite magnetization. Generalization of the present approach to address such issues will be valuable, and technically straightforward.

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References

[1] Morsch O and Oberthaler M 2006 Rev. Mod. Phys. 78 179
[2] Lewenstein M, Sanpera A, Ahufinger V, Damski B, Sen A and Sen U 2007 Adv. Phys. 56 243
[3] Bloch I, Dalibard J and Zwerger W 2008 Rev. Mod. Phys. 80 885
[4] Esslinger T 2010 Annu. Rev. Condens. Matter Phys. 1 129
[5] Su W P 1988 Phys. Rev. B 37 9904
[6] Zaanen J and Gunnarsson O 1989 Phys. Rev. B 40 7391
[7] Schulz H J 1989 J. Physique 50 2833
[8] Schulz H J 1990 Phys. Rev. Lett. 64 1445
[9] Kato M, Machida K, Nakanishi H and Fujita M 1990 J. Phys. Soc. Japan 59 1047
[10] Singh A and Tešanović Z 1990 Phys. Rev. B 41 614
[11] Inui M and Littlewood P B 1991 Phys. Rev. B 44 4415
[12] Yang J and Su W P 1991 Phys. Rev. B 44 6838
[13] Ichimura M, Fujita M and Nakao K 1992 J. Phys. Soc. Japan 61 2027
[14] Zitzler R, Pruschke Th and Bulla R 2002 Eur. Phys. J. B 27 473
[15] Aimi T and Imada M 2007 J. Phys. Soc. Japan 76 113708
[16] Capone M and Kotliar G 2006 Phys. Rev. B 74 054513
[17] Capone M and Kotliar G 2006 Phys. Rev. B 74 054513
[18] Takimoto T and Moriya T 2002 Phys. Rev. B 44 614
[19] Washburn B, Fritz L, Zinner N T, Manousakis E and Demler E 2010 Phys. Rev. A 81 032616
[20] Poilblanc D 1994 J. Low Temp. Phys. 95 169
[21] Zhang S, Carlson J and Gubernatis J E 1997 Phys. Rev. Lett. 78 4486
[22] Takimoto T and Moriya T 2002 Phys. Rev. B 44 614
[23] Lonan M and Littlewood P B 1991 Phys. Rev. B 44 4415
[24] Penn D R 1966 Phys. Rev. 142 350
[25] Tahvildar-Zadeh A N, Freericks J K and Jarrell M 1997 Phys. Rev. B 55 942
[26] Morsch O and Oberthaler M 2006 Rev. Mod. Phys. 78 179
[27] Takimoto T and Moriya T 2002 Phys. Rev. B 66 134516
[28] Zhang S and Ceperley D M 2008 Phys. Rev. Lett. 100 236404
[29] Singh A and Tešanović Z 1990 Phys. Rev. B 41 614
[30] Inui M and Littlewood P B 1991 Phys. Rev. B 44 4415
[31] Ichimura M, Fujita M and Nakao K 1992 J. Phys. Soc. Japan 61 2027
[32] Zitzler R, Pruschke Th and Bulla R 2002 Eur. Phys. J. B 27 473
[33] Aimi T and Imada M 2007 J. Phys. Soc. Japan 76 113708
[34] Capone M and Kotliar G 2006 Phys. Rev. B 74 054513
[35] Ichimura M, Fujita M and Nakao K 1992 J. Phys. Soc. Japan 61 2027