Néel order in the Hubbard model within a spin-charge rotating reference frame approach: Crossover from weak to strong coupling

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The antiferromagnetic phase of two-dimensional (2D) and three-dimensional (3D) Hubbard model with nearest neighbor hopping is studied on a bipartite cubic lattice by means of the quantum $SU(2)\times U(1)$ rotor approach that yields a fully self-consistent treatment of the antiferromagnetic state that respects the symmetry properties of the model and satisfy the Mermin-Wagner theorem. The collective variables for charge and spin are isolated in the form of the space-time fluctuating U(1) phase field and rotating spin-quantization axis governed by the SU(2) symmetry, respectively. As a result interacting electrons appear as composite objects consisting of bare fermions with attached U(1) and SU(2) gauge fields. An effective action consisting of a spin-charge rotor and a fermionic field is derived as a function of the Coulomb repulsion U and hopping parameter t. At zero temperature, our theory describes the evolution from a Slater ($U \ll t$) to a Mott-Heisenberg ($U \gg t$) antiferromagnet. The results for zero-temperature sublatice magnetization (2D) and finite temperature (3D) phase diagram of the antiferromagnetic Hubbard model as a function of the crossover parameter U/t are presented and the role of the spin Berry phase in the interaction driven crossover is analyzed.

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I. INTRODUCTION

Effective low-energy theories are frequently employed in essentially all fields of physics. In the realm of strongly correlated electrons, spin only Hamiltonians are examples of effective low-energy theories that apply in the limit of strong interactions. Due to the numerical expense in solving these models for large lattices, it is imperative to look for methods which relay on advanced analytical approaches. A key question in this context concerns the emergence of low-energy scales, much smaller than the bare Coulomb interactions between the electrons, which govern the existence and the competition of different phases. This can be studied by considering prototypical lattice models of strongly correlated electrons. In the strong-coupling limit, the t-J Hamiltonian,[1] derived from the large-U Hubbard model,[2] is often used to describe the low-lying excitations. At half-filling, it directly reduces to the quantum antiferromagnetic Heisenberg model. However, for finite U as in the Hubbard model, the quantum-mechanical objects are not local spins since one has still mobile electrons and one expects that calculation of the ground-state phase diagram as a function of the density and interaction strength is more difficult than for the Heisenberg model. In the weak-coupling limit ($U \ll t$), a Fermi surface instability gives rise to a spin-density-wave ground state as described by Slater,[3] where the antiferromagnetic (AF) long-range order produces a gap in the quasiparticle excitation spectrum. In the strong-coupling regime ($U \gg t$), fermions are effected by the strong Coulomb repulsion causing the Mott-Hubbard localization.[4] The created local magnetic moments subsequently order at low temperature and give rise to a Mott-Heisenberg antiferromagnet. It is well known that even for small but finite interactions the Hartree-Fock (HF) Néel temperature is proportional to U, which is unrealistically high since U is a large energy scale, of the order of eV. This wrong prediction had to be expected since correlations are absent in the HF approach. The requirement of self-consistency by incorporating spin and charge fluctuations, while maintaining the essential spin-rotation symmetry, summarizes the challenging nature of magnetic ordering in strongly correlated systems. A variety of theoretical methods are available for the study of strongly correlated systems. In weak or strong coupling perturbative treatments usually are used.[5] On the other hand numerical—very effective in low-dimensional models—are limited to finite systems, which requires an extrapolation to the thermodynamic limit that is often problematic. As a result the numerical approach does not provide in general a unifying picture, which only analytical approaches can give.

The objective of the present paper is to quantitatively investigate correlation effects in an antiferromagnetic state of the Hubbard model within a spin-rotationally-symmetric scheme that is fully compatible with the Mermin-Wagner theorem.[6] To this end, we describe a theoretical approach which provides a unified view of two- (2D) and three-dimensional model at half-filled Hubbard model for any value of the Coulomb repulsion U, which is able to handle the evolution from the Slater to the Mott-Heisenberg antiferromagnet that captures correctly both the spin and charge degrees of freedom. We address the above questions by implementing the charge-U(1) and spin-SU(2) rotationally invariant handling of the Hubbard model. By recognizing spin and charge symmetries we explicitly factorize the charge and spin contribution to the original electron operator in terms of the corresponding gauge fields that leads to a composite particle, which is the union of an electron with U(1) and SU(2) gauge potentials. In this scheme the charge and spin excitations emerge in terms of a U(1) phase and variable spin-quantization axis: the effective field theory for the strongly correlated problem is thus characterized by the $U(2)=U(1)\times SU(2)$ group, where the gauge potential in U(1) describes the evolution of a particle scalar characteristic, which is naturally associated with an electric charge, while the gauge potential in SU(2) describes the nontrivial

dynamics associated with the evolution of the vector internal characteristic of a particle such as spin.

The outline of the paper is as follows: In Sec. II we introduce the model and, in Secs. III–V, we develop the analytical background needed for the calculations. In Sec. VI we find a closed set of self-consistent equations for the antiferromagnetic gap and order parameter, while the numerical evaluation of self-consistent equations is presented in Sec. VII, where the phase diagrams considering the paramagnetic the antiferromagnetic phase for the Hubbard model and in different dimensionality are calculated.

II. MODEL

Our starting point is the purely fermionic Hubbard Hamiltonian $\mathcal{H}\equiv\mathcal{H}_t+\mathcal{H}_U$ as follows

$$\mathcal{H}=-t\sum_{\langle \mathbf{r}\mathbf{r}'\rangle,\alpha}[c_\alpha^\dagger(\mathbf{r})c_\alpha(\mathbf{r}')+\text{H.c.}]+U\sum_{\mathbf{r}}n_\uparrow(\mathbf{r})n_\downarrow(\mathbf{r}). \quad (1)$$

Here, $\langle \mathbf{r},\mathbf{r}'\rangle$ runs over the different nearest-neighbor (NN) sites, t is the hopping amplitude, U stands for the Coulomb repulsion, while the operator $c_\alpha^\dagger(\mathbf{r})$ creates an electron with spin $\alpha=\uparrow,\downarrow$ at the lattice site $\mathbf{r}$, where $n_\alpha(\mathbf{r})=c_\alpha^\dagger(\mathbf{r})c_\alpha(\mathbf{r})$. Usually, working in the grand canonical ensemble a term is added to $\mathcal{H}$ in Eq. (1) to control the average number of electrons, $\mathcal{H}\to\mathcal{H}-\mu\Sigma_{\mathbf{r}}n(\mathbf{r})$ with μ being the chemical potential and $n(\mathbf{r})=n_\uparrow(\mathbf{r})+n_\downarrow(\mathbf{r})$ the fermionic number operator.

A. Grassmann action

The functional integral representation of models for correlated electrons allows us to implement efficiently the method of treatment. It is customary to introduce Grassmann fields, $c_\alpha(\mathbf{r}\tau)$ depending on the "imaginary time" $0\leqslant\tau\leqslant\beta\equiv 1/k_BT$ (with T being the temperature) that satisfy the antiperiodic condition $c_\alpha(\mathbf{r}\tau)=-c_\alpha(\mathbf{r}\tau+\beta)$, to write the path integral for the statistical sum $\mathcal{Z}=\int[\mathcal{D}\bar{c}\mathcal{D}c]e^{-\mathcal{S}[\bar{c},c]}$ with the fermionic action

$$\mathcal{S}[\bar{c},c]=\mathcal{S}_B[\bar{c},c]+\int_0^\beta d\tau\mathcal{H}[\bar{c},c] \quad (2)$$

that contains the fermionic Berry term[7]

$$\mathcal{S}_B[\bar{c},c]=\sum_{\mathbf{r}\alpha}\int_0^\beta d\tau\bar{c}_\alpha(\mathbf{r}\tau)\partial_\tau c_\alpha(\mathbf{r}\tau), \quad (3)$$

which will play an important role in our considerations.

III. SU(2)×U(1) ACTION

It is customary to introduce auxiliary fields for the spin and charge fluctuations via a Hubbard-Stratonovich (HS) transformation to decouple the interaction term in the Hubbard Hamiltonian. However, such a procedure usually leads to a loss of the spin-rotational invariance. For strongly correlated system in order to properly account for the nature of elementary excitation it is crucial to construct a formulation of the theory which naturally preserves the existing symmetry present in the Hubbard Hamiltonian. For this purpose the density-density product in Eq. (1) we write, following Ref. 8, in a spin-rotational invariant way,

$$\mathcal{H}_U=U\sum_{\mathbf{r}}\left\{\frac{1}{4}n^2(\mathbf{r}\tau)-[\mathbf{\Omega}(\mathbf{r}\tau)\cdot\mathbf{S}(\mathbf{r}\tau)]^2\right\}, \quad (4)$$

where $S^a(\mathbf{r}\tau)=\frac{1}{2}\Sigma_{\alpha\alpha'}c_\alpha^\dagger(\mathbf{r}\tau)\hat{\sigma}^a_{\alpha\alpha'}c_{\alpha'}(\mathbf{r}\tau)$ denotes the vector spin operator $(a=x,y,z)$ with $\hat{\sigma}^a$ being the Pauli matrices. The unit vector

$$\mathbf{\Omega}(\mathbf{r}\tau)=[\sin\vartheta(\mathbf{r}\tau)\cos\varphi(\mathbf{r}\tau),\sin\vartheta(\mathbf{r}\tau)\sin\varphi(\mathbf{r}\tau),\cos\vartheta(\mathbf{r}\tau)] \quad (5)$$

written in terms of polar angles, labels varying in space-time spin-quantization axis. In order to maintain spin-rotational invariance, one should consider the spin-quantization axis to be *a priori* arbitrary and integrate over all possible directions of $\mathbf{\Omega}(\mathbf{r}\tau)$ in the partition function. The reason for choosing the decomposition in Eq. (4) is that it allows us to recover the Hartree-Fock solution at the saddle-point level within the functional integral formalism. By decoupling spin and charge density terms in Eq. (4) using auxiliary fields $\varrho(\mathbf{r}\tau)$ and $iV(\mathbf{r}\tau)$, respectively, we write down the partition function in the form

$$\mathcal{Z}=\int[\mathcal{D}\mathbf{\Omega}]\int[\mathcal{D}V\mathcal{D}\varrho]\int[\mathcal{D}\bar{c}\mathcal{D}c]e^{-\mathcal{S}[\mathbf{\Omega},V,\varrho,\bar{c},c]}, \quad (6)$$

where $[\mathcal{D}\mathbf{\Omega}]\equiv\Pi_{\mathbf{r}\tau_k}\frac{\sin\vartheta(\mathbf{r}\tau_k)d\vartheta(\mathbf{r}\tau_k)d\varphi(\mathbf{r}\tau_k)}{4\pi}$ is the spin-angular integration measure. The effective action reads

$$\mathcal{S}[\mathbf{\Omega},V,\varrho,\bar{c},c]=\sum_{\mathbf{r}}\int_0^\beta d\tau\left[\frac{\varrho^2(\mathbf{r}\tau)}{U}+\frac{V^2(\mathbf{r}\tau)}{U}+iV(\mathbf{r}\tau)n(\mathbf{r}\tau)+2\varrho(\mathbf{r}\tau)\mathbf{\Omega}(\mathbf{r}\tau)\cdot\mathbf{S}(\mathbf{r}\tau)\right]+\mathcal{S}_B[\bar{c},c]+\int_0^\beta d\tau\mathcal{H}_t[\bar{c},c]. \quad (7)$$

We devise a systematic way of decomposing the fluctuating fields contained in the action in Eq. (7) that enables us to obtain a low-energy effective theory. In the following we introduce bosonic fields describing charge and spin fluctuations, and the fluctuating spin-quantization axis.

A. U(1) rotor charge frame

We observe now that the Hubbard Hamiltonian has a local U(1) gauge symmetry, when expressed in terms of the underlying electron variables. This points out a possibility of an emergent U(1) dynamical gauge field as a fluctuating complex field attached to fermionic variables, which is dynamically generated, by interacting fermions. In the modern language it is called a fermion-flux composite. Technically, the appearance of the U(1) field is based on the Hubbard-Stratonovich decoupling of the four-fermion interaction—a typical way to "bosonize" a fermionic system in higher-dimensional problems. The essence of the method is to elimi-

nate a mixed fermion-boson term in the resulting action by a gauge transformation.[9] The U(1) formulation begins by rewriting the electron as the product of a charge-neutral fermionic spinon and a charge-carrying U(1) rotor, which is constrained to lie on the unit circle in the complex plane. To this end, we write the fluctuating "imaginary chemical potential" $iV(\mathbf{r}\tau)$ as a sum of a static $V_0(\mathbf{r})$ and periodic function $V(\mathbf{r}\tau)=V_0(\mathbf{r})+\tilde{V}(\mathbf{r}\tau)$ using Fourier series

$$\tilde{V}(\mathbf{r}\tau)=\frac{1}{\beta}\sum_{n=1}^{\infty}[\tilde{V}(\mathbf{r}\omega_n)e^{i\omega_n\tau}+\text{c.c.}] \tag{8}$$

with $\omega_n=2\pi n/\beta$ $(n=0,\pm1,\pm2)$ being the (Bose) Matsubara frequencies. Now, we introduce the U(1) *phase* field $\phi(\mathbf{r}\tau)$ via the Faraday-type relation

$$\dot{\phi}(\mathbf{r}\tau)\equiv\frac{\partial\phi(\mathbf{r}\tau)}{\partial\tau}=e^{-i\phi(\mathbf{r}\tau)}\frac{1}{i}\frac{\partial}{\partial\tau}e^{i\phi(\mathbf{r}\tau)}=\tilde{V}(\mathbf{r}\tau). \tag{9}$$

Furthermore, by performing the local gauge transformation to the *new* fermionic variables $f_\alpha(\mathbf{r}\tau)$,

$$\begin{bmatrix}c_\alpha(\mathbf{r}\tau)\\ \bar{c}_\alpha(\mathbf{r}\tau)\end{bmatrix}=\begin{bmatrix}z(\mathbf{r}\tau) & 0\\ 0 & \bar{z}(\mathbf{r}\tau)\end{bmatrix}\begin{bmatrix}f_\alpha(\mathbf{r}\tau)\\ \bar{f}_\alpha(\mathbf{r}\tau)\end{bmatrix}, \tag{10}$$

where the unimodular parameter $|z(\mathbf{r}\tau)|^2=1$ satisfies $z(\mathbf{r}\tau)=e^{i\phi(\mathbf{r}\tau)}$, we remove the imaginary term $i\int_0^\beta d\tau\tilde{V}(\mathbf{r}\tau)n(\mathbf{r}\tau)$ for all the Fourier modes of the $V(\mathbf{r}\tau)$ field, except for the zero frequency. Accordingly, the integration measure over the group manifold becomes

$$\int[\mathcal{D}\phi]\equiv\sum_{\{m(\mathbf{r})\}}\prod_{\mathbf{r}}\int_0^{2\pi}d\phi_0(\mathbf{r})\int_{\phi(\mathbf{r}0)=\phi_0(\mathbf{r})}^{\phi(\mathbf{r}\beta)=\phi_0(\mathbf{r})+2\pi m(\mathbf{r})}\mathcal{D}\phi(\mathbf{r}\tau). \tag{11}$$

Since the homotopy group $\pi_1[\mathrm{U}(1)]$ forms a set of integers, discrete configurations of $\phi(\mathbf{r}\tau)$ matter, for which $\phi(\mathbf{r}\beta)-\phi(\mathbf{r}0)=2\pi m(\mathbf{r})$, where $m(\mathbf{r})=0,\pm1,\pm2,\ldots$. Here, $m\in Z$ labels equivalence classes of homotopically connected paths. Thus the paths can be divided into topologically distinct classes, characterized by a winding number defined as the net number of times the world line wraps around the system in the "imaginary time" direction.[10]

B. Rotating SU(2) spin reference frame

Subsequent SU(2) transformation from $f_\alpha(\mathbf{r}\tau)$ to $h_\alpha(\mathbf{r}\tau)$ operators,

$$\begin{bmatrix}f_1(\mathbf{r}\tau)\\ f_2(\mathbf{r}\tau)\end{bmatrix}=\mathbf{R}(\mathbf{r}\tau)\begin{bmatrix}h_1(\mathbf{r}\tau)\\ h_2(\mathbf{r}\tau)\end{bmatrix} \tag{12}$$

takes away the rotational dependence on $\mathbf{\Omega}(\mathbf{r}\tau)$ in the spin sector. This parametrization makes clear that the SU(2) matrix rotor is identical to the more familiar O(4) rotor, a quantum particle constrained to the three-sphere

$$\mathbf{R}(\mathbf{r}\tau)=\begin{bmatrix}e^{-i/2(\varphi+\chi)}\cos\left(\frac{\vartheta}{2}\right) & -e^{-i/2(\varphi-\chi)}\sin\left(\frac{\vartheta}{2}\right)\\ e^{i/2(\varphi-\chi)}\sin\left(\frac{\vartheta}{2}\right) & e^{i/2(\varphi+\chi)}\cos\left(\frac{\vartheta}{2}\right)\end{bmatrix} \tag{13}$$

with the Euler angular variables $\varphi(\mathbf{r}\tau)$, $\vartheta(\mathbf{r}\tau)$, and $\chi(\mathbf{r}\tau)$, respectively. The link between SO(3) and SU(2) rotations is established by means of the Hopf map[11]

$$\mathbf{R}(\mathbf{r}\tau)\hat{\sigma}^z\mathbf{R}^\dagger(\mathbf{r}\tau)=\hat{\boldsymbol{\sigma}}\cdot\mathbf{\Omega}(\mathbf{r}\tau) \tag{14}$$

that is based on the enlargement from two-sphere S_2 to the three-sphere $S_3\sim\mathrm{SU}(2)$. Here, the extra variable $\chi(\mathbf{r}\tau)$ represents the U(1) gauge freedom of the theory as a consequence of $S_2\to S_3$ mapping. One can summarize Eqs. (10) and (12) by the single joint gauge transformation exhibiting electron operator factorization

$$c_\alpha(\mathbf{r}\tau)=\sum_{\alpha'}\mathcal{U}_{\alpha\alpha'}(\mathbf{r}\tau)h_{\alpha'}(\mathbf{r}\tau), \tag{15}$$

where

$$\mathcal{U}(\mathbf{r}\tau)=z(\mathbf{r}\tau)\mathbf{R}(\mathbf{r}\tau) \tag{16}$$

is a U(2) matrix which rotates the spin-charge quantization axis at site $\mathbf{r}$ and time τ. Equation (15) reflects the composite nature of the interacting electron formed from bosonic spinorial and charge degrees of freedom given by $R_{\alpha\alpha'}(\mathbf{r}\tau)$ and $z(\mathbf{r}\tau)$, respectively as well as remaining fermionic part $h_\alpha(\mathbf{r}\tau)$. In the new variables the action in Eq. (7) assumes the form

$$\mathcal{S}[\mathbf{\Omega},\phi,\varrho,\bar{h},h]=\mathcal{S}_B[\bar{h},h]+\int_0^\beta d\tau\mathcal{H}_{\mathbf{\Omega},\phi}[\rho,\bar{h},h]+\mathcal{S}_0[\phi]$$
$$+2\sum_{\mathbf{r}}\int_0^\beta d\tau\mathbf{A}(\mathbf{r}\tau)\cdot\mathbf{S}_h(\mathbf{r}\tau), \tag{17}$$

where $\mathbf{S}_h(\mathbf{r}\tau)=\frac{1}{2}\Sigma_{\alpha\gamma}\bar{h}_\alpha(\mathbf{r}\tau)\hat{\boldsymbol{\sigma}}_{\alpha\gamma}h_\gamma(\mathbf{r}\tau)$. Furthermore,

$$S_0[\phi]=\sum_{\mathbf{r}}\int_0^\beta d\tau\left[\frac{\dot{\phi}^2(\mathbf{r}\tau)}{U}+\frac{1}{i}\frac{2\mu}{U}\dot{\phi}(\mathbf{r}\tau)\right] \tag{18}$$

stands for the kinetic and Berry term of the U(1) phase field in the charge sector. The SU(2) gauge transformation in Eq. (12) and the fermionic Berry term in Eq. (2) generate SU(2) potentials given by

$$\mathbf{R}^\dagger(\mathbf{r}\tau)\partial_\tau\mathbf{R}(\mathbf{r}\tau)=\mathbf{R}^\dagger\left(\dot{\varphi}\frac{\partial}{\partial\varphi}+\dot{\vartheta}\frac{\partial}{\partial\vartheta}+\dot{\chi}\frac{\partial}{\partial\chi}\right)\mathbf{R}=-\hat{\boldsymbol{\sigma}}\cdot\mathbf{A}(\mathbf{r}\tau), \tag{19}$$

where

$$A^x(\mathbf{r}\tau)=\frac{i}{2}\dot{\vartheta}(\mathbf{r}\tau)\sin\chi(\mathbf{r}\tau)-\frac{i}{2}\dot{\varphi}(\mathbf{r}\tau)\sin\theta(\mathbf{r}\tau)\cos\chi(\mathbf{r}\tau),$$

$$A^y(\mathbf{r}\tau)=\frac{i}{2}\dot{\vartheta}(\mathbf{r}\tau)\cos\chi(\mathbf{r}\tau)+\frac{i}{2}\dot{\varphi}(\mathbf{r}\tau)\sin\theta(\mathbf{r}\tau)\sin\chi(\mathbf{r}\tau),$$

$$A^z(\mathbf{r}\tau) = \frac{i}{2}\dot{\varphi}(\mathbf{r}\tau)\cos\,\vartheta(\mathbf{r}\tau) + \frac{i}{2}\dot{\chi}(\mathbf{r}\tau) \tag{20}$$

are the explicit expression for the vector potential in terms of the Euler angles.

C. Integration over V_0 and ϱ

We observe that the spatial and temporal fluctuations of the fields $V_0(\mathbf{r})$ and $\varrho(\mathbf{r}\tau)$ will be energetically penalized, since they are gapped and decouple from the angular and phase variables. Therefore, in order to make further progress we subject the functional to a saddle-point HF analysis: the expectation value of the static (zero frequency) part of the fluctuating electrochemical potential $V_0(r)$ we calculate by the saddle-point method to give

$$V_0(r) = i\left(\mu - \frac{U}{2}n\right) \equiv i\bar{\mu} \tag{21}$$

where $n = \Sigma_\alpha \langle \bar{h}_\alpha(\mathbf{r}\tau)h_\alpha(\mathbf{r}\tau)\rangle$ and the saddle point with respect to ρ gives

$$\rho(\mathbf{r}\tau) = (-1)^{\mathbf{r}}\Delta_c,$$

$$\Delta_c = U\langle S^z(\mathbf{r}\tau)\rangle, \tag{22}$$

with Δ_c setting the magnitude for the Mott-charge gap. The choice delineated in Eq. (22) corresponds to the saddle point of the antiferromagnetic (with staggering Δ_c) type. Note that the notion "antiferromagnetic" here does not mean an actual long-range ordering—for this the angular spin-quantization variables have to be ordered as well. The fermionic sector, in turn, is governed by the effective Hamiltonian

$$\begin{aligned}\mathcal{H}_{\mathbf{\Omega},\phi} = &\sum_{\mathbf{r}} \varrho(\mathbf{r}\tau)[\bar{h}_\uparrow(\mathbf{r}\tau)h_\uparrow(\mathbf{r}\tau) - \bar{h}_\downarrow(\mathbf{r}\tau)h_\downarrow(\mathbf{r}\tau)] \\ &- t\sum_{\langle \mathbf{r},\mathbf{r}'\rangle}\sum_{\alpha\gamma}[\mathcal{U}^\dagger(\mathbf{r}\tau)\mathcal{U}(\mathbf{r}'\tau)]_{\alpha\gamma}\bar{h}_\alpha(\mathbf{r}\tau)h_\gamma(\mathbf{r}'\tau) \\ &- \bar{\mu}\sum_{\mathbf{r}\alpha}\bar{h}_\alpha(\mathbf{r}\tau)h_\alpha(\mathbf{r}\tau),\end{aligned} \tag{23}$$

where $\bar{\mu} = \mu - nU/2$ is the chemical potential with a Hartree shift originating from the saddle-point value of the static variable V_0.

IV. SPIN-ANGULAR ACTION

Since we are interested in the magnetic properties of the system a natural step is to obtain the effective action that involves the spin-directional degrees of freedom $\mathbf{\Omega}$, which important fluctuations correspond to rotations. This can be done by integrating out fermions as follows:

$$\mathcal{Z} = \int [\mathcal{D}\phi\mathcal{D}\mathbf{\Omega}]\int [\mathcal{D}\bar{h}\mathcal{D}h]e^{-\mathcal{S}[\varphi,\phi,\vartheta,\bar{h},h]} \equiv \int [\mathcal{D}\mathbf{\Omega}]e^{-\mathcal{S}[\mathbf{\Omega}]}, \tag{24}$$

where

$$\mathcal{S}[\mathbf{\Omega}] = -\ln\int [\mathcal{D}\phi\mathcal{D}\bar{h}\mathcal{D}h]e^{-\mathcal{S}[\varphi,\phi,\vartheta,\bar{h},h]} \tag{25}$$

generates the cumulant expansions for the low-energy action in the form $\mathcal{S}[\mathbf{\Omega}] = \mathcal{S}_B[\mathbf{\Omega}] + \mathcal{S}_J[\mathbf{\Omega}]$.

A. Topological theta term

In general, in addition to the usual exchange term, the action describing antiferromagnetic spin systems is expected to have a topological Berry-phase term

$$\mathcal{S}_B[\mathbf{\Omega}] = -2\sum_{\mathbf{r}\mathbf{r}'}\int_0^\beta d\tau\mathbf{A}(\mathbf{r}\tau)\cdot\langle\mathbf{S}_h(\mathbf{r}'\tau')\rangle, \tag{26}$$

where

$$\langle S_h^z(\mathbf{r}\tau)\rangle = \frac{1}{2}(n_\uparrow - n_\downarrow) = \frac{\Delta_c}{U}, \tag{27}$$

which results from the saddle-point value in Eq. (22). In terms of angular variables, the Berry term becomes

$$\mathcal{S}_B[\mathbf{\Omega}] = \frac{\theta}{i}\sum_{\mathbf{r}}\int_0^\beta d\tau[\dot{\varphi}(\mathbf{r}\tau)\cos\,\vartheta(\mathbf{r}\tau) + \dot{\chi}(\mathbf{r}\tau)]. \tag{28}$$

If we work in Dirac "north pole gauge $\chi(\mathbf{r}\tau) = -\varphi(\mathbf{r}\tau)$ one recovers the familiar form $\mathcal{S}_B[\mathbf{\Omega}] = \frac{\theta}{i}\Sigma_{\mathbf{r}}\int_0^\beta d\tau\dot{\varphi}(\mathbf{r}\tau)[1 - \cos\,\vartheta(\mathbf{r}\tau)]$. Here, the integral of the first term in Eq. (28) has a simple geometrical interpretation as it is equal to a solid angle swept by a unit vector $\mathbf{\Omega}(\vartheta,\varphi)$ during its motion. The extra phase factor coming from the Berry phase requires some little extra care, since it will induce quantum-mechanical phase interference between configurations. In regard to the nonperturbative effects, we realized the presence of an additional parameter with the topological angle or so-called theta term

$$\theta = \frac{\Delta_c}{U}, \tag{29}$$

which is related to the Mott gap. In the large-U limit one has $\Delta_c \to U/2$, so that $\theta \to \frac{1}{2}$ is relevant for the half-integer spin. However, for arbitrary U the theta term will be different from that value, which, as we show will be instrumental for destruction of the antiferromagnetic order away from the spin-localized $U \to \infty$ limit.

B. Antiferromagnetic exchange

Now we proceed with the calculation of the exchange term in the spin-angular action. We concentrate on the second order cumulant term in the hopping element t containing four fermion operators as follows:

$$\begin{aligned}\mathcal{S}^{(2)}[\bar{h},h] &= -\frac{t^2}{2}\int_0^\beta d\tau d\tau'\Bigg\langle\sum_{|\mathbf{r}_1-\mathbf{r}_1'|=\mathrm{NN}}\bar{z}(\mathbf{r}_1\tau)z(\mathbf{r}_1'\tau) \\ &\times\sum_{\alpha\alpha'}[\mathbf{R}^\dagger(\mathbf{r}_1\tau)\mathbf{R}(\mathbf{r}_1'\tau)]_{\alpha\alpha'}\bar{h}_\alpha(\mathbf{r}_1\tau)h_{\alpha'}(\mathbf{r}_1'\tau)\end{aligned}$$

$$\times \sum_{|\mathbf{r}_2-\mathbf{r}_2'|=\mathrm{NN}} \bar{z}(\mathbf{r}_2\tau')z(\mathbf{r}_2'\tau') \times \sum_{\gamma\gamma'} [\mathbf{R}^\dagger(\mathbf{r}_2\tau')\mathbf{R}(\mathbf{r}_2'\tau')]_{\gamma\gamma'}\bar{h}_\gamma(\mathbf{r}_2\tau')h_{\gamma'}(\mathbf{r}_2'\tau') \Big\rangle, \tag{30}$$

where $\langle\cdots\rangle$ denotes averaging over U(1) phase fields and fermions. The averaging in the charge sector is performed with the use of the U(1) phase action in Eq. (18) to give

$$\langle \bar{z}(\mathbf{r}_1\tau)z(\mathbf{r}_1'\tau)\bar{z}(\mathbf{r}_2\tau')z(\mathbf{r}_2'\tau')\rangle \simeq (\delta_{\mathbf{r}_1,\mathbf{r}_1'}\delta_{\mathbf{r}_2,\mathbf{r}_2'} + \delta_{\mathbf{r}_1,\mathbf{r}_2'}\delta_{\mathbf{r}_1',\mathbf{r}_2}) \times \exp\left\{-\frac{U}{2}\left[|\tau-\tau'| - \frac{(\tau-\tau')^2}{\beta}\right]\right\}. \tag{31}$$

Furthermore, with the help of the gradient expansion

$$\mathbf{R}(\mathbf{r}\tau') = \mathbf{R}(\mathbf{r}\tau) + (\tau'-\tau)\partial_\tau\mathbf{R}(\mathbf{r}\tau) + O[(\tau'-\tau)^2],$$

$$\mathbf{h}(\mathbf{r}\tau') = \mathbf{h}(\mathbf{r}\tau) + (\tau'-\tau)\partial_\tau\mathbf{h}(\mathbf{r}\tau) + O[(\tau'-\tau)^2], \tag{32}$$

we write the relevant part of the action in the form

$$\mathcal{S}_J[\mathbf{\Omega}] = -\frac{t^2}{2}\int_0^\beta d\tau d\tau' \exp\left[-\frac{U}{2}|\tau-\tau'|\right] \times \sum_{|\mathbf{r}-\mathbf{r}'|=a}\sum_{\substack{\alpha\alpha'\\ \gamma\gamma'}} [\mathbf{R}^\dagger(\mathbf{r}\tau)\mathbf{R}(\mathbf{r}'\tau)]_{\alpha\alpha'}[\mathbf{R}^\dagger(\mathbf{r}'\tau)\mathbf{R}(\mathbf{r}\tau)]_{\gamma\gamma'} \times \langle\bar{h}_\alpha(\mathbf{r}\tau)h_{\gamma'}(\mathbf{r}\tau)\rangle\langle h_{\alpha'}(\mathbf{r}'\tau)\bar{h}_\gamma(\mathbf{r}'\tau)\rangle. \tag{33}$$

In the low temperature limit (on the energy scale given by U), by making use of the formula

$$\lim_{\tau\to 0}\int_0^\beta d\tau' e^{-|\tau-\tau'|U/2} = \frac{2}{U} - \frac{2e^{-\beta U/2}}{U} \tag{34}$$

and with the aid of the fermionic occupation numbers

$$\langle h_{\alpha'}(\mathbf{r}'\tau)\bar{h}_\gamma(\mathbf{r}'\tau)\rangle = (1-n_\gamma)\delta_{\alpha'\gamma},$$

$$\langle \bar{h}_\alpha(\mathbf{r}\tau)h_{\gamma'}(\mathbf{r}\tau')\rangle = n_\alpha\delta_{\alpha\gamma'}, \tag{35}$$

we arrive at

$$\mathcal{S}_J[\mathbf{\Omega}] = \frac{t^2}{U}\int_0^\beta d\tau \sum_{|\mathbf{r}-\mathbf{r}'|=a}\sum_{\alpha\gamma} \times [\mathbf{R}^\dagger(\mathbf{r}\tau)\mathbf{R}(\mathbf{r}'\tau)]_{\alpha\gamma}[\mathbf{R}^\dagger(\mathbf{r}'\tau)\mathbf{R}(\mathbf{r}\tau)]_{\gamma\alpha}(n_\gamma-1)n_\alpha. \tag{36}$$

Finally, making use of the following composition formula for the SU(2) matrices:

$$[\mathbf{R}^\dagger(\mathbf{r}\tau)\mathbf{R}(\mathbf{r}'\tau)]_{\alpha\gamma}[\mathbf{R}^\dagger(\mathbf{r}'\tau)\mathbf{R}(\mathbf{r}\tau)]_{\gamma\alpha} = \tfrac{1}{2}[1-\mathbf{\Omega}(\mathbf{r}\tau)\cdot\mathbf{\Omega}(\mathbf{r}'\tau)](1-\delta_{\alpha\gamma}) + \tfrac{1}{2}[1+\mathbf{\Omega}(\mathbf{r}\tau)\cdot\mathbf{\Omega}(\mathbf{r}'\tau)]\delta_{\alpha\gamma}, \tag{37}$$

we obtain the desired part of the spin action

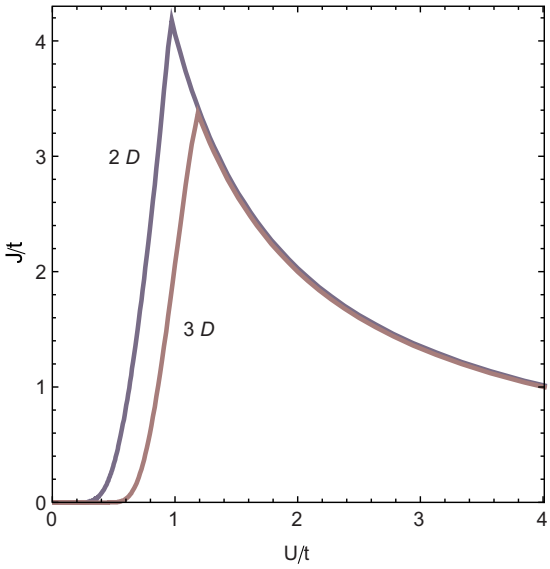

FIG. 1. (Color online) The antiferromagnetic exchange parameter J as a function of the Coulomb interaction U in two and three dimensions. The fermionic occupation number is fixed by $n=1$.

$$\mathcal{S}_J[\mathbf{\Omega}] = \frac{J}{4}\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\int_0^\beta d\tau[\mathbf{\Omega}(\mathbf{r}\tau)\cdot\mathbf{\Omega}(\mathbf{r}'\tau) + n(n-2)] \tag{38}$$

with the AF-exchange coefficient

$$J(\Delta_c) = \frac{4t^2}{U}(n_\uparrow - n_\downarrow)^2 \equiv \frac{4t^2}{U}\left(\frac{2\Delta_c}{U}\right)^2. \tag{39}$$

The factor $\sim t^2/U$ comes from integration over U(1) charge degrees of freedom [see Eqs. (31) and (34)], whereas the occupation numbers result from integration over fermionic variables [see Eq. (27)]. From Eq. (39) it is evident that for $U\to\infty$ one has $J(\Delta_c)\sim\frac{4t^2}{U}$ since $\frac{2\Delta_c}{U}\to 1$ in this limit. In general the AF-exchange parameter persists as long as the charge gap Δ_c exists. However, $J(\Delta_c)$ diminishes rapidly in the $U/t\to 0$ weak-coupling limit, see Fig. 1.

V. FERMIONIC SECTOR

Now we evaluate the effective interaction between fermions by integrating out by means of cumulant expansion the gauge degrees of freedom. To this end we write the partition function as

$$\mathcal{Z} = \int[\mathcal{D}\phi\mathcal{D}\mathbf{\Omega}]\int[\mathcal{D}\bar{h}\mathcal{D}h]e^{-\mathcal{S}[\varphi,\phi,\vartheta,\bar{h},h]} \equiv \int[\mathcal{D}\bar{h}\mathcal{D}h]e^{-\mathcal{S}[\bar{h},h]}, \tag{40}$$

where

$$\mathcal{S}[\bar{h},h] = -\ln\int[\mathcal{D}\phi\mathcal{D}\mathbf{\Omega}]e^{-\mathcal{S}[\varphi,\phi,\vartheta,\bar{h},h]} \tag{41}$$

generates cumulant expansion for the effective fermionic action. Since, both U(1) and SU(2) gauge fields couple to the

hopping element t, in the lowest order of cumulant expansion we reveal the hopping renormalization $t \to tg$,

$$g = g_c g_s,$$

$$g_c = \langle \bar{z}(\mathbf{r}\tau) z(\mathbf{r}'\tau) \rangle,$$

$$g_s = \langle [\mathbf{R}^\dagger(\mathbf{r}\tau)\mathbf{R}(\mathbf{r}'\tau)]_{\uparrow\uparrow} \rangle = \langle [\mathbf{R}^\dagger(\mathbf{r}\tau)\mathbf{R}(\mathbf{r}'\tau)]_{\downarrow\downarrow} \rangle, \quad (42)$$

where the coefficients g_c and g_s contribute to the band renormalization in a way, which is similar to the action of the Gutzwiller factors,[12] and have to be calculated self-consistently, according to the Eq. (42) that involve charge and spin-angular correlation functions. However as long as there is no ordering in the charge sector, $\langle \bar{z}(\mathbf{r}\tau) z(\mathbf{r}'\tau) \rangle = 0$ and $g=0$ resulting in renormalized hopping $t=0$. Thus, we have to rest on the second order of the cumulant expansion, in which one obtains a contribution to the effective action in the form

$$\mathcal{S}^{(2)}[\bar{h},h] = -\frac{2t^2}{U} \int_0^\beta d\tau \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \mathcal{F}^\dagger(\mathbf{r}\tau\mathbf{r}'\tau) \mathcal{F}(\mathbf{r}\tau\mathbf{r}'\tau), \quad (43)$$

with the bond operators

$$\mathcal{F}(\mathbf{r}\tau\mathbf{r}'\tau) = \frac{\bar{h}_\uparrow(\mathbf{r}\tau) h_\uparrow(\mathbf{r}'\tau) + \bar{h}_\downarrow(\mathbf{r}\tau) h_\downarrow(\mathbf{r}'\tau)}{\sqrt{2}}. \quad (44)$$

Since the $\mathcal{S}^{(2)}[\bar{h},h]$ is quartic in the fermionic variables, we resort to the Hubbard-Stratonovich decoupling with the help of the complex variables defined on the links of the lattice

$$e^{-\mathcal{S}^{(2)}[\bar{h},h]} = \int [\mathcal{D}^2\xi] e^{-\Sigma_{\langle \mathbf{r}\mathbf{r}' \rangle} \int_0^\beta d\tau (2/J)|\xi|^2 + \xi\bar{\mathcal{F}} + \bar{\xi}\mathcal{F})}, \quad (45)$$

where $\mathcal{D}^2\xi = \Pi_{\langle \mathbf{r}\mathbf{r}' \rangle, \tau} d^2\xi(\mathbf{r}\tau\mathbf{r}'\tau)$ and $d^2\xi = d\,\mathrm{Re}\,\xi\, d\,\mathrm{Im}\,\xi$. Saddle point with respect to ξ gives

$$\xi = \frac{J}{2} \langle \mathcal{F}(\mathbf{r}\tau\mathbf{r}'\tau) \rangle = \frac{J}{2\sqrt{2}} \sum_\alpha \langle \bar{h}_\alpha(\mathbf{r}\tau) h_\alpha(\mathbf{r}'\tau) \rangle. \quad (46)$$

Denoting

$$v = \sum_\alpha \langle \bar{h}_\alpha(\mathbf{r}\tau) h_\alpha(\mathbf{r}'\tau) \rangle, \quad (47)$$

which plays the role of the kinetic energy parameter for fermions, we obtain

$$\mathcal{S}^{(2)}[\bar{h},h] = -\frac{Jv^2}{4} + t_J \sum_{\langle \mathbf{r}\mathbf{r}' \rangle \alpha} [\bar{h}_\alpha(\mathbf{r}\tau) h_\alpha(\mathbf{r}'\tau) + \mathrm{H.c.}], \quad (48)$$

where

$$t_J = \tfrac{1}{4} J v \quad (49)$$

is the effective hopping parameter that involves the antiferromagnetic exchange parameter J. The interaction dependence of this quantity is depicted in Fig. 2. Summarizing the results we obtain for the fermionic action

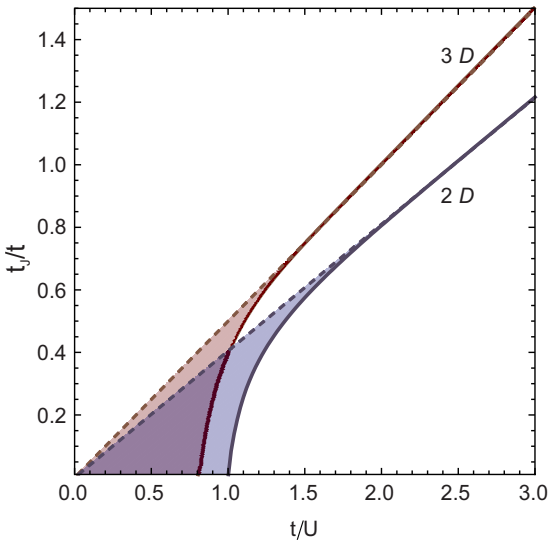

FIG. 2. (Color online) The effective hopping parameter t_J/t [see Eq. (49)] related to the AF exchange as a function of t/U at $n=1$ for two- and three-dimensional Hubbard model at $n=1$.

$$\mathcal{S}[\bar{h},h] = \mathcal{S}_B[\bar{h},h] + \int_0^\beta d\tau \mathcal{H}[\bar{h},h], \quad (50)$$

with the effective Hamiltonian

$$\mathcal{H}[\bar{h},h] = \sum_{\mathbf{r}} (-1)^{\mathbf{r}} \Delta_c [\bar{h}_\uparrow(\mathbf{r}\tau) h_\uparrow(\mathbf{r}\tau) - \bar{h}_\downarrow(\mathbf{r}\tau) h_\downarrow(\mathbf{r}\tau)] - (tg - t_J) \sum_{\langle \mathbf{r},\mathbf{r}',\alpha \rangle} \bar{h}_\alpha(\mathbf{r}\tau) h_\alpha(\mathbf{r}'\tau) - \bar{\mu} \sum_{\mathbf{r}\alpha} \bar{h}_\alpha(\mathbf{r}\tau) h_\alpha(\mathbf{r}\tau). \quad (51)$$

The result of the gauge transformations is that we have managed to cast the strongly correlated problem into a system of mutually noninteracting fermions, submerged in the bath of strongly fluctuating U(1) and SU(2) fields, whose dynamics is governed by the energy scale set by the Coulomb interaction U coupled to fermions via hopping term and with the Zeeman-type contribution with the massive field $\varrho(\mathbf{r}\tau)$ related to the Mott gap Δ_c. To calculate the latter one has to introduce two inequivalent sublattices, let say A and B, and write the Hamiltonian in terms of two sublattice operators in the reduced Brillouin zone (RBZ). The fermionic propagator then reads

$$\mathbf{G}(\mathbf{k}\omega_n) = \frac{\begin{pmatrix} i\nu_n + \epsilon_{\mathbf{k}} - \bar{\mu} & \Delta_c \\ \Delta_c & i\nu_n - \epsilon_{\mathbf{k}} - \bar{\mu} \end{pmatrix}}{(i\nu_n - \epsilon_{\mathbf{k}} - \bar{\mu})(i\nu_n + \epsilon_{\mathbf{k}} - \bar{\mu}) - \Delta_c^2}, \quad (52)$$

where $\nu_n = \pi(2n+1)/\beta$, $n = \pm 1, \pm 2, \ldots$ are the fermionic Matsubara frequencies. The self-consistency equations for the Mott gap, the kinetic energy bond parameter, and fermionic occupation number are given by

$$\Delta_c = \frac{1}{\beta N} \sum_{\mathbf{k}\nu_n,\alpha}{}' G_{\uparrow\downarrow}(\mathbf{k}\nu_n),$$

$$v = \frac{1}{\beta N} \sum_{\mathbf{k}\nu_n,\alpha}{}' \gamma(\mathbf{k}) G_{\alpha\alpha}(\mathbf{k}\nu_n),$$

$$n = 1 - \frac{1}{\beta N} \sum_{\mathbf{k}\nu_n,\alpha}{}' G_{\alpha\alpha}(\mathbf{k}\nu_n), \tag{53}$$

where the sums with prime index denote the summations over wave vectors inside the RBZ and $\gamma(\mathbf{k}) = (\cos k_x + \cos k_y)/2$. By performing the summations over Matsubara frequencies one obtains explicitly with the use of the fermionic distribution $n_F(x) = 1/(e^{\beta x}+1)$ the following:

$$1 = \frac{U}{2N} \sum_{\mathbf{k}} \frac{n_F(-E_{\mathbf{k}} - \bar{\mu}) - n_F(E_{\mathbf{k}} - \bar{\mu})}{E_{\mathbf{k}}} \tag{54}$$

for the gap parameter,

$$1 = \frac{J}{N} \sum_{\mathbf{k}} \gamma^2(\mathbf{k}) \frac{n_F(-E_{\mathbf{k}} - \bar{\mu}) - n_F(E_{\mathbf{k}} - \bar{\mu})}{E_{\mathbf{k}}}, \tag{55}$$

the fermion kinetic energy parameter,

$$n = \frac{1}{N} \sum_{\mathbf{k}} [n_F(-E_{\mathbf{k}} - \bar{\mu}) + n_F(E_{\mathbf{k}} - \bar{\mu})] \tag{56}$$

and the occupation number, respectively. At half-filling, solutions of Eq. (54) for the gap Δ_c are stabilized for any arbitrarily small U; however, by computing of the free energy one can find that no stable antiferromagnetic solutions away from $n=1$ exist.[13] Solutions of the self-consistency equation for the gap Δ_c leading to densities away from half-filling correspond to maxima instead of minima in the free energy. If a certain occupation near the half-filling is enforced, the system will experience a phase separation in a half-filled antiferromagnetic and a non-half-filled paramagnetic region.

VI. CP[1] FORMULATION

Since the fermionic field can be systematically integrated out, the main practical difficulty comes from the dynamics of spin-directional fluctuations. To proceed with the spin-bosonic action we resort to the CP[1] representation (see, e.g., Ref. 14). In the CP[1] representation, the SU(2) rotation matrix is expressed in terms of two Schwinger bosons:

$$\mathbf{R}(\mathbf{r}\tau) = \begin{bmatrix} \zeta_1(\mathbf{r}\tau) & -\bar{\zeta}_2(\mathbf{r}\tau) \\ \zeta_2(\mathbf{r}\tau) & \bar{\zeta}_1(\mathbf{r}\tau) \end{bmatrix} \tag{57}$$

with the constraint $|\zeta_1(\mathbf{r}\tau)|^2 + |\zeta_2(\mathbf{r}\tau)|^2 = 1$. The unimodular constraint can be resolved by using the Euler angle parametrization

$$\zeta_1(\mathbf{r}\tau) = e^{-i/2[\varphi(\mathbf{r}\tau)+\chi(\mathbf{r}\tau)]} \cos\left[\frac{\vartheta(\mathbf{r}\tau)}{2}\right],$$

$$\zeta_2(\mathbf{r}\tau) = e^{i/2[\varphi(\mathbf{r}\tau)-\chi(\mathbf{r}\tau)]} \sin\left[\frac{\vartheta(\mathbf{r}\tau)}{2}\right], \tag{58}$$

which make link between the $\zeta_1(\mathbf{r}\tau)$, $\zeta_2(\mathbf{r}\tau)$ fields and $\mathbf{\Omega}(\mathbf{r}\tau)$ variables. By definition

$$\mathbf{S}_\zeta(\mathbf{r}\tau) = \frac{1}{2} \sum_{\alpha\gamma} \bar{\zeta}_\alpha(\mathbf{r}\tau) \hat{\boldsymbol{\sigma}}_{\alpha\gamma} \zeta_\gamma(\mathbf{r}\tau) \equiv \frac{1}{2} \mathbf{\Omega}(\mathbf{r}\tau) \tag{59}$$

are the "bosonic" spins in the complex-projective (CP[1]) formulation, while the action, see Eq. (38), becomes

$$\mathcal{S}_J[\mathbf{\Omega}] \to J \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \int_0^\beta d\tau \left[\mathbf{S}_\zeta(\mathbf{r}\tau) \cdot \mathbf{S}_\zeta(\mathbf{r}'\tau) - \frac{1}{4} \right]. \tag{60}$$

Consequently, the complete spin-bosonic action $\mathcal{S}[\bar{\zeta}, \zeta] = \mathcal{S}_\theta[\bar{\zeta}, \zeta] + \mathcal{S}_J[\bar{\zeta}, \zeta]$ reads

$$\mathcal{S}_\theta[\bar{\zeta}, \zeta] = -2\theta \sum_{\mathbf{r}\alpha} (-1)^{\mathbf{r}} \int_0^\beta d\tau \bar{\zeta}_\alpha(\mathbf{r}\tau) \dot{\zeta}_\alpha(\mathbf{r}\tau),$$

$$\mathcal{S}_J[\bar{\zeta}, \zeta] = -J \sum_{\langle \mathbf{r}\mathbf{r}' \rangle} \int_0^\beta d\tau \bar{\mathcal{A}}(\mathbf{r}\tau\mathbf{r}'\tau) \mathcal{A}(\mathbf{r}\tau\mathbf{r}'\tau), \tag{61}$$

where $\theta = \frac{\Delta_c}{U}$ is the "theta angle" parameter in the Berry-phase term, while the AF-exchange term $\mathcal{S}_J[\bar{\zeta}, \zeta]$ we write with the help of the valence-bond operators $\mathcal{A}(\mathbf{r}\tau\mathbf{r}'\tau)$ for which the following relations hold:

$$\mathbf{S}_\zeta(\mathbf{r}\tau) \cdot \mathbf{S}_\zeta(\mathbf{r}'\tau) = -\bar{\mathcal{A}}(\mathbf{r}\tau\mathbf{r}'\tau) \mathcal{A}(\mathbf{r}\tau\mathbf{r}'\tau) + \tfrac{1}{4},$$

$$\mathcal{A}(\mathbf{r}\tau\mathbf{r}'\tau) = \frac{\zeta_\uparrow(\mathbf{r}\tau)\zeta_\downarrow(\mathbf{r}'\tau) - \zeta_\downarrow(\mathbf{r}\tau)\zeta_\uparrow(\mathbf{r}'\tau)}{\sqrt{2}}. \tag{62}$$

A. Hubbard-Stratonovich decoupling

In order to achieve a consistent representation of the underlying antiferromagnetic structure, it is unavoidable to explicitly split the degrees of freedom according to their location on sublattice A or B. Since the lattice is bipartite allowing one to make the unitary transformation

$$\zeta_\uparrow(\mathbf{r}\tau) \to -\zeta_\downarrow(\mathbf{r}\tau),$$

$$\zeta_\downarrow(\mathbf{r}\tau) \to \zeta_\uparrow(\mathbf{r}\tau), \tag{63}$$

for sites on one sublattice, so that

$$\mathcal{A}(\mathbf{r}\tau\mathbf{r}'\tau) \to \mathcal{A}'(\mathbf{r}\tau\mathbf{r}'\tau) = \sum_{\alpha=1}^{2} \frac{\zeta_\alpha(\mathbf{r}\tau)\zeta_\alpha(\mathbf{r}'\tau)}{\sqrt{2}}. \tag{64}$$

Biquadratic (four-variable) terms in the Lagrangian cannot be readily integrated in the path integral. Introducing a complex variable for each bond that depends on imaginary time $Q(\mathbf{r}\tau\mathbf{r}'\tau)$ we decouple the four-variable terms $\bar{\mathcal{A}}(\mathbf{r}\tau\mathbf{r}'\tau)\mathcal{A}'(\mathbf{r}\tau\mathbf{r}'\tau)$ using the formula

$$e^{\mathcal{S}_J[\bar{\zeta},\zeta]} = \int [\mathcal{D}^2 Q] e^{-\Sigma_{\langle \mathbf{r}\mathbf{r}' \rangle} \int_0^\beta d\tau (2/J|Q|^2 + Q\bar{\zeta}\cdot\bar{\zeta} + \bar{Q}\zeta\cdot\zeta)}, \tag{65}$$

where $\mathcal{D}^2 Q = \Pi_{\langle \mathbf{r}\mathbf{r}' \rangle_\tau} d^2 Q(\mathbf{r}\tau\mathbf{r}'\tau)$ and $d^2 Q = d\,\mathrm{Re}\,Q\, d\,\mathrm{Im}\,Q$. To handle the unimodularity condition one introduces Lagrange multipliers $\lambda(\mathbf{r}\tau)$ at each time and site. Then with the help of the Dirac-delta functional

$$\delta(|\boldsymbol{\zeta}(\mathbf{r}\tau)|^2-1)=\int\left[\frac{\mathcal{D}\lambda}{2\pi i}\right]e^{\Sigma_{\mathbf{r}}\int_0^\beta d\tau\lambda(|\boldsymbol{\zeta}|^2-1)}, \tag{66}$$

the variables $\zeta_1(\mathbf{r}\tau),\zeta_2(\mathbf{r}\tau)$ are now unconstrained bosonic fields. Thus, the local constraints are reintroduced into the theory through the dynamical fluctuations of the auxiliary λ field

$$\mathcal{Z}=\int[\mathcal{D}^2Q\mathcal{D}^2\boldsymbol{\zeta}\mathcal{D}\lambda]e^{-\Sigma_{\langle\mathbf{r}\mathbf{r}'\rangle}\int_0^\beta d\tau(2|Q|^2/J-\lambda\delta_{\mathbf{r}\mathbf{r}'}+\mathcal{H}_Q[\bar{\boldsymbol{\zeta}},\boldsymbol{\zeta}])}, \tag{67}$$

where

$$\mathcal{H}_Q[\bar{\boldsymbol{\zeta}},\boldsymbol{\zeta}]=\sum_{\langle\mathbf{r}\mathbf{r}'\rangle}\int_0^\beta d\tau(Q\bar{\boldsymbol{\zeta}}\cdot\bar{\boldsymbol{\zeta}}+\bar{Q}\boldsymbol{\zeta}\cdot\boldsymbol{\zeta}+\lambda\bar{\boldsymbol{\zeta}}\cdot\boldsymbol{\zeta}). \tag{68}$$

Furthermore, one then performs a saddle-point approximation over the Q and λ fields

$$Q_{\mathrm{sp}}(\mathbf{r}\tau\mathbf{r}'\tau)=-\frac{J}{2}\sum_{\alpha=1}^{2}\langle\bar{\zeta}_\alpha(\mathbf{r}\tau)\bar{\zeta}_\alpha(\mathbf{r}'\tau)\rangle=-\frac{J}{\sqrt{2}}\langle\mathcal{A}'(\mathbf{r}\tau\mathbf{r}'\tau)\rangle,$$

$$\frac{1}{2}=\frac{1}{2}\sum_{\alpha=1}^{2}\langle\bar{\zeta}_\alpha(\mathbf{r}\tau)\zeta_\alpha(\mathbf{r}\tau)\rangle, \tag{69}$$

by assuming the uniform solution $Q_{\mathrm{sp}}(\mathbf{r}\tau\mathbf{r}'\tau)\equiv Q$ we obtain for the Hamiltonian in the spin-bosonic sector

$$\mathcal{H}_Q[\bar{\boldsymbol{\zeta}},\boldsymbol{\zeta}]=\frac{1}{\beta N}\sum_{\mathbf{k}\omega_n}\sum_{\alpha=1}^{2}[\bar{\zeta}_\alpha(\mathbf{k},\omega_n),\zeta_\alpha(-\mathbf{k},-\omega_n)]\times\frac{\hat{\mathcal{G}}_\alpha^{-1}(\mathbf{k},\omega_n)}{2}\begin{bmatrix}\zeta_\alpha(\mathbf{k},\omega_n)\\ \bar{\zeta}_\alpha(-\mathbf{k},-\omega_n)\end{bmatrix}, \tag{70}$$

with

$$\hat{\mathcal{G}}_\alpha^{-1}(\mathbf{k},\omega_n)=\begin{pmatrix}2i\theta\omega_n+\lambda & -z\gamma_{\mathbf{k}}Q\\ -z\gamma_{\mathbf{k}}Q & -2i\theta\omega_n+\lambda\end{pmatrix}. \tag{71}$$

Subsequently, performing the sums over Matsubara frequencies one obtains

$$Q=\frac{J(\Delta_c)}{N}\sum_{\mathbf{k}}\frac{1}{2\theta}\frac{z\gamma_{\mathbf{k}}^2Q}{2\omega_{\mathbf{k}}}\coth\left(\frac{\beta\omega_{\mathbf{k}}}{4\theta}\right),$$

$$1=-\frac{1}{2\theta}+\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{2\theta}\frac{\lambda}{\omega_{\mathbf{k}}}\coth\left(\frac{\beta\omega_{\mathbf{k}}}{4\theta}\right), \tag{72}$$

where $\omega_{\mathbf{k}}=\sqrt{\lambda^2-(z\gamma_{\mathbf{k}}Q)^2}$ and z is the lattice coordination number.

VII. ANTIFERROMAGNETIC LONG-RANGE ORDER PARAMETER

A characteristic property of strongly correlated systems is the existence of local moments. Weak-coupling theories usually fail to properly describe these local moments. When electron correlation effects become stronger, in general, spin fluctuations have to be considered seriously. The HF transition temperature bears a physical meaning as a temperature below which the amplitude Δ_c of the AF order parameter takes a well-defined value. This is also interpreted as the appearance of local moments. However, a nonzero value of Δ_c does not imply the existence of AF long-range order. For this the angular degrees of freedom $\boldsymbol{\Omega}(\mathbf{r}\tau)$ have also to be ordered, whose low-lying excitations are in the form of spin waves. In the CP^1 representation (where the Néel field is represented by two Schwinger bosons) Bose-Einstein condensation of the Schwinger bosons at zero temperature signals the appearance of AF long-range order. The AF order parameter in terms of the original fermion operators is defined as

$$m_{AF}=\sum_{\mathbf{r}}(-1)^{\mathbf{r}}\langle S^z(\mathbf{r}\tau)\rangle=\sum_{\mathbf{r}}(-1)^{\mathbf{r}}\langle\boldsymbol{\Omega}(\mathbf{r}\tau)\rangle\cdot\langle\mathbf{S}_h(\mathbf{r}\tau)\rangle. \tag{73}$$

Owing the fact that $\langle S_h^a(\mathbf{r}\tau)\rangle=(-1)^{\mathbf{r}}\Delta_c\delta_{a,z}$ we obtain

$$m_{AF}=\Delta_c\sum_{\mathbf{r}}\langle\Omega^z(\mathbf{r}\tau)\rangle=\Delta_c\sum_{\mathbf{r}}[\langle\bar{\zeta}_\uparrow(\mathbf{r}\tau)\zeta_\uparrow(\mathbf{r}\tau)\rangle-\langle\bar{\zeta}_\downarrow(\mathbf{r}\tau)\zeta_\downarrow(\mathbf{r}\tau)\rangle]. \tag{74}$$

Furthermore, the order parameter for the CP^1 "boson condensate" is

$$\langle\bar{\zeta}_\alpha(\mathbf{k}\omega_n)\rangle=\langle\zeta_\alpha(\mathbf{k}\omega_n)\rangle=\sqrt{\frac{\beta N}{2}}m_0\delta_{0,\omega_n}\delta_{\uparrow,\alpha}(\delta_{\mathbf{k},0}+\delta_{\mathbf{k},\mathbf{Q}}). \tag{75}$$

This yields a macroscopic contribution (i.e., order 1) to the staggered magnetization and represents a macroscopic contribution to the CP^1 boson density, of the $\alpha=\uparrow$ bosons at the mode with $\mathbf{k}=0,\omega_n=0$ thus giving

$$m_{AF}=\frac{\Delta_c}{\beta UN}\sum_{\mathbf{k},\omega_n}[\langle\bar{\zeta}_\uparrow(\mathbf{k}\omega_n)\zeta_\uparrow(\mathbf{k}\omega_n)\rangle-\langle\bar{\zeta}_\downarrow(\mathbf{k}\omega_n)\zeta_\downarrow(\mathbf{k}\omega_n)\rangle]=\frac{\Delta_c}{U}m_0^2. \tag{76}$$

Finally, the fraction of condensed Schwinger bosons is given by

$$m_0^2=1+\frac{1}{2\theta_s}-\frac{1}{N}\sum_{\mathbf{k}}\frac{1}{2\theta_s}\frac{\lambda}{\omega_{\mathbf{k}}}\coth\left(\frac{\beta\omega_{\mathbf{k}}}{4\theta_s}\right), \tag{77}$$

which represents the extension of the saddle-point equation for the Lagrange multiplier to the region of the ordered state.

A. $d=2$ Hubbard model

In two dimensions, we expect no long-range AF order at finite temperatures due to Mermin and Wagner's theorem. This could be verified by explicitly performing two-dimensional momentum summations in Eq. (72) with the help of density of states for the two-dimensional square lattice $\rho_{2d}(\epsilon)=\int_{-\pi}^{\pi}[d^2\mathbf{k}/(2\pi)^3\ \delta[\epsilon-\epsilon(\mathbf{k})]$, where $\epsilon(\mathbf{k})=\epsilon_0(\cos k_x+\cos k_y)$ with

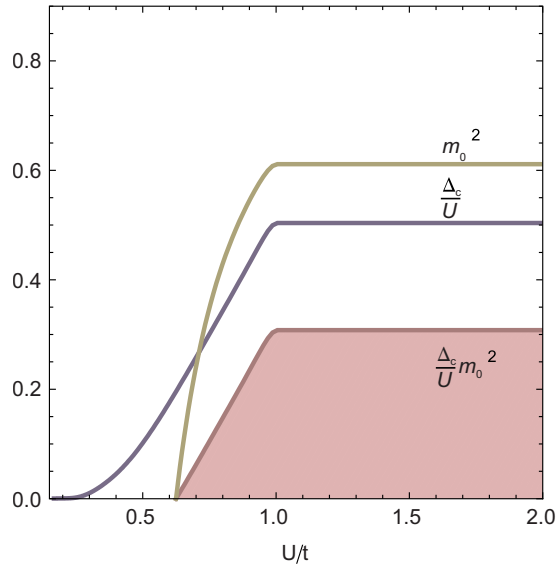

FIG. 3. (Color online) The Mott gap Δ_c, fraction of condensed Schwinger bosons m_0^2, and AF order parameter m_{AF} for the half-filled Hubbard two-dimensional model at zero temperature.

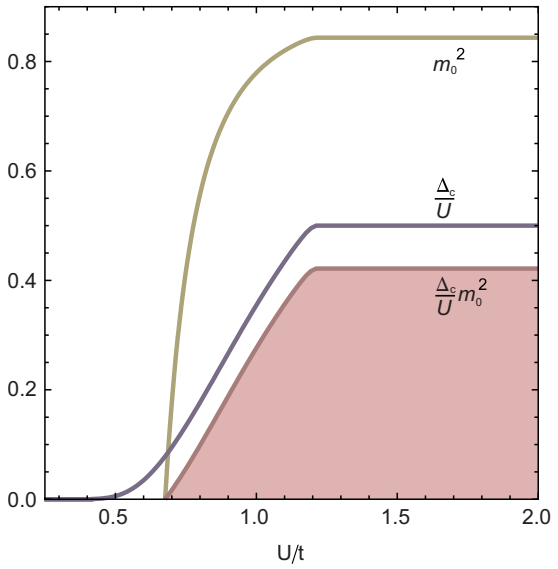

FIG. 4. (Color online) Same as in Fig. 2 but for three-dimensional Hubbard model.

$$\rho_{2d}(\epsilon) = \frac{1}{\pi^2 \epsilon} \Theta\left(1 - \frac{|\epsilon|}{2\epsilon_0}\right) \mathbf{K}\left[\sqrt{1 - \left(\frac{\epsilon}{2\epsilon_0}\right)^2}\right]. \quad (78)$$

As a result, there is no antiferromagnetic order at finite temperature in two-dimensional Hubbard model. Taking the zero-temperature limit in Eq. (72) and fixing the fermionic occupation number at $n=1$, in the limit $U/t \to \infty$ we find the order parameter value, $m_{AF}=0.308$ in the ground state (in agreement with the calculations from Ref. 15) that is less than the classical value $S=1/2$. Monte Carlo calculation on 2D Hubbard model[16] gave $m_{AF}=0.4$. This effect is due to the quantum zero-point motion, which has its origin in the noncommutability of the Hamiltonian and the staggered magnetization. In the opposite weak-coupling limit, $U/t \to 0$, the gap Δ_c persists at arbitrary small value of U/t; however, the true order parameter m_{AF}, which involves also the density of condensed Schwinger bosons, vanishes at $U/t \approx 0.621$ (see Fig. 3). The destruction of the AF order is due to the Berry-phase term θ whose coefficient, cf. Eq. (29), differs from the localized spin value $S=1/2$ while entering the weak-coupling limit. In particular, for $U/t \to 0$, which is in the weak-coupling limit, θ goes to zero along with the charge gap Δ_c [see Eq. (29)] and the self-consistency equation (72) predicts vanishing of the long-range AF order.

B. $d=3$ Hubbard model

In three dimensions, for a system with an ordered ground state, thermally excited states reduce the spin correlations at finite temperatures. When the temperature is much higher than the typical coupling energy scale J, we expect the spins to be uncorrelated at large distances and the magnetization m_{AF} to vanish in the absence of an ordering field. This requires a phase transition at some temperature T_c between the ordered and disordered phases. As in the previous case we employ the density of states for the cubic lattice $\rho_{3d}(\epsilon) = \int_{-\pi}^{\pi} [d^3\mathbf{k}/(2\pi)^3\ \delta[\epsilon - \epsilon(\mathbf{k})]$, where $\epsilon(\mathbf{k}) = \epsilon_0(\cos k_x + \cos k_y + \cos k_z)$, as follows:

$$\rho_{3d}(\epsilon) = \frac{1}{\pi^3 \epsilon} \int_{a_1}^{a_2} dx \Theta\left(1 - \frac{|\epsilon|}{3\epsilon_0}\right) \frac{\mathbf{K}\left[\sqrt{1 - \left(\frac{\epsilon}{2\epsilon_0} + \frac{x}{2}\right)^2}\right]}{\sqrt{1 - x^2}} \quad (79)$$

with $a_1 = \max(-1, -2 - \epsilon/\epsilon_0)$, $a_2 = \min(1, 2 - \epsilon/\epsilon_0)$.

The interaction dependence of the AF magnetic moment is depicted in Fig. 4. In the $U \to \infty$ localized limit it is $m_{AF} \approx 0.422$, i.e., less the mean-field value $\Delta_c/U = 1/2$, however, bigger than in the case of the 2D Hubbard model. Finally, Fig. 5 displays the calculated antiferromagnetic phase diagram as a function of temperature and interaction strength. At weak coupling our theory clearly describes a Slater antiferromagnet with an exponentially small AF gap. As U increases, the Slater antiferromagnet progressively evolves into a Mott-Heisenberg antiferromagnet with an AF gap of order U. In the weak interaction limit there is a destruction of the AF order at $U/t=0.676$ (see Fig. 6), due to the topological Berry-phase term whose coefficient, cf. Eq. (29), deviates from the from the localized spin value $S=1/2$ in the weak-coupling limit U/t. The AF critical temperature has a maximum at $U/t \approx 3.78$. It is worthwhile to compare our results with the previous work on the subject. Numerical methods such as dynamical cluster approximation (DCA)[17,18] give $U/t \approx 7.5$, whereas dynamical mean-field theory approximation (DMFA)[19] predicts $U/t \approx 10$. The methods based on a perturbation theory with respect to the interaction strength[20,21] are unable to reproduce the maximum in the AF critical temperature as a function of U/t. The significantly higher values of U/t resulting from DCA and DFMA have to be explained by the restricted ability of these methods while handling spatial fluctuations. Regarding the value of maximum of the critical temperature $T_c/t \approx 0.667$ found here,

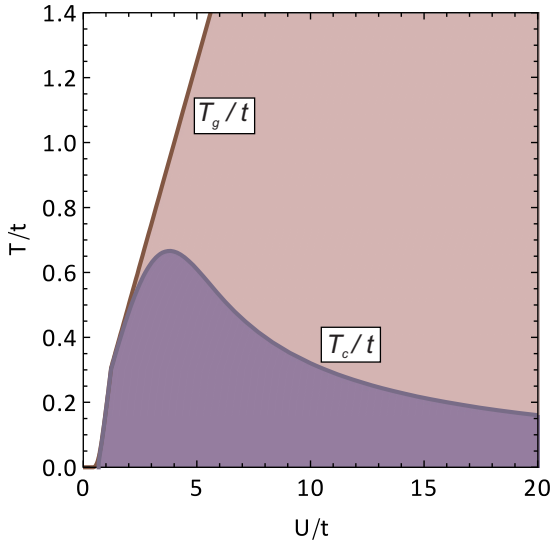

FIG. 5. (Color online) The temperature-interaction phase diagram for the three-dimensional Hubbard model at half-filling. Depicted is the temperature T_g for the vanishing of the gap parameter Δ_c as well as the true critical temperature T_c at which the long-range AF order ceases to exist, signaled by vanishing of m_{AF}.

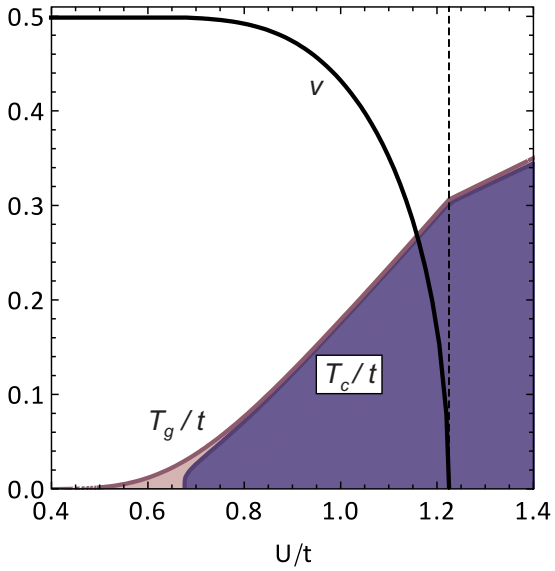

FIG. 6. (Color online) Details of the phase diagram from Fig. 5 in the weak-coupling regime. Depicted also is the interaction dependence of the kinetic parameter v that enters the effective, J-induced hopping parameter t_J. Note the vanishing of the true AF order for $U/t \approx 0.676$ and persistence of the gap Δ_c for arbitrary value of U/t.

it agrees with the result of Monte Carlo simulations by Scalettar *et al.*[22] $T_c/t \approx 0.72$ and by Hirsch[23] who obtained $T_c \approx W/18t$, where $W=12t$ is the bandwidth for the 3D Hubbard model, i.e., $T_c/t \approx 0.666$.

VIII. CONCLUSIONS

In conclusion, we have investigated the ground-state properties of the two-dimensional half-filled one band Hubbard model in the strong large U to intermediate-coupling limit, i.e., away from the strict Heisenberg limit and antiferromagnetic phase diagram of the three-dimensional Hubbard model using $SU(2) \times U(1)$ rotating reference frame description. Our focus on systems in the strong- to intermediate-coupling regime was motivated by the fact that weaker interactions are leading to increased electron mobility, which in turn should reduce the stability of magnetic phases. Calculations with the Hamiltonian for interacting electrons were reduced to calculation of functional integrals with a phase-angular action. Collective bosonic fields are introduced by means of a Hubbard-Stratonovich decoupling of the Hubbard interaction and subsequent gauge transformation. Our implementation for the Hubbard model is consistent with the spin rotation symmetry and simultaneously is able to reproduce the Hartree-Fock result. One important technical aspect arising in the construction of effective theories is that electron-defined operators in the bare high-energy theory are transformed into the composite particles subsequently employed in calculations within the effective low-energy theory. The inclusion of the quantum and spatial fluctuations has been shown to have a dramatic effect on transition temperatures and phase diagram. We have also compared the outcome of our calculations to a number of methods that were employed by other authors.

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