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Magnetically Driven Superconducting Pairing Interaction in the Two-Dimensional Hubbard Model within a Spin-Rotationally Invariant Approach

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The spin-rotationally invariant SU(2) approach to the Hubbard model is extended to accommodate the charge degrees of freedom. Both U(1) and SU(2) gauge transformation are used to factorize the charge and spin contribution to the original electron operator in terms of the emergent gauge fields. It is shown that these fields play a similar role as phonons in the BCS theory: they provide the "glue" for fermion pairing. By tracing out gauge bosons the form of paired states is established and the role of antiferromagnetic correlations is explicated.

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1. Introduction

As a principal model describing the electronic correlation in the system, the Hubbard model has been used in many works to study the pairing instabilities which as usual are given by the second-order effective interaction with respect to the Coulomb interaction. In this context the structure of the pairing interaction, the two--dimensional (2D) Hubbard model, has been recently analyzed in [1–3], where the dynamical cluster Monte Carlo approximation is applied to two-dimensional Hubbard model with nearest-neighbors hopping and on-site Coulomb interaction. The Monte Carlo simulations have been also employed to study the phase separation and pairing in the doped two-dimensional Hubbard model [4]. Moreover, the charge-transfer nature of the cuprates plays an essential role in the doped systems [5], so that with discarding charge degrees of freedom an important part of the physics may be lost. In the same spirit a detour from the strict projection program was recently proposed in a form of the "gossamer" superconductor [6], recognizing the role of the double-occupancy charge configurations. In the present paper we construct a SU(2) spin-rotational and charge U(1) invariant theory using the electron operator factorization [7, 8]. Furthermore, we derive the low-energy fermionic action that rests on the SU(2)-invariant character of the Hamiltonian and a consistent scheme of coherent states within a functional--integral formulation. We show that U(1) and SU(2) gauge fields (the collective high energy modes in the SC system) take over the task which was carried out by phonons in BCS superconductors and play the role of the "glue" that is responsible for the formation of the electron pairs. In this sense the present work charts a route from the microscopic Hubbard model on the square lattice to an effective lower energy action that exhibits pairing potential.

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2. The model

Our starting point is the fermionic Hubbard Hamiltonian in the second-quantized form

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

Here, $\langle \boldsymbol{r}, \boldsymbol{r}'\rangle$ runs over the nearest-neighbor (n.n.) sites, t is the hopping amplitude, U stands for the Coulomb repulsion, while the operator $c^{\dagger}_{\alpha}(\boldsymbol{r})$ creates an electron with spin $\alpha = \uparrow\ (\equiv 1), \downarrow\ (\equiv 2)$ at the square lattice site $\boldsymbol{r}$. Furthermore, $n(\boldsymbol{r}) = n_{\uparrow}(\boldsymbol{r}) + n_{\downarrow}(\boldsymbol{r})$ is the number operator, where $n_{\alpha}(\boldsymbol{r}) = c^{\dagger}_{\alpha}(\boldsymbol{r})c_{\alpha}(\boldsymbol{r})$. Usually, working in the grand canonical ensemble a term $-\mu \sum_{\boldsymbol{r}} n(\boldsymbol{r})$ is added to $\mathcal{H}$ in Eq. (1) with μ being the chemical potential. We treat the problem of interacting fermions at finite temperature in the standard path-integral formalism [9] using Grassmann variables for the Fermi fields, $c_{\alpha}(\boldsymbol{r}\tau)$ depending on the "imaginary time" $0 \leq \tau \leq \beta \equiv 1/k_{\text{B}}T$ (with T being the temperature) that satisfy the antiperiodic condition $c_{\alpha}(\boldsymbol{r}\tau) = -c_{\alpha}(\boldsymbol{r}\tau + \beta)$, to write the path integral for the statistical sum $\mathcal{Z} = \int [\mathcal{D}\bar{c}\mathcal{D}c]\, \mathrm{e}^{-\mathcal{S}[\bar{c},c]}$ with the fermionic action

$$\mathcal{S}[\bar{c}, c] = \mathcal{S}_{\text{B}}[\bar{c}, c] + \int_0^{\beta} \mathrm{d}\tau \mathcal{H}[\bar{c}, c]\,, \tag{2}$$

that contains the fermionic Berry term

$$\mathcal{S}_{\mathrm{B}}[\bar{c},c]=\sum_{\boldsymbol{r}\alpha}\int_0^\beta \mathrm{d}\tau\bar{c}_\alpha(\boldsymbol{r}\tau)\partial_\tau c_\alpha(\boldsymbol{r}\tau)\,. \tag{3}$$

For the problem under study it is crucial to construct a covariant formulation of the theory, which naturally preserves the spin-rotational symmetry present in the Hubbard Hamiltonian. For this purpose, the density–density product in Eq. (1) can be written, following Ref. [10], in a spin-rotational invariant way

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

where $S^a(\boldsymbol{r}\tau)=\frac{1}{2}\sum_{\alpha\alpha'}c^\dagger_\alpha(\boldsymbol{r}\tau)\hat{\sigma}^a_{\alpha\alpha'}c_{\alpha'}(\boldsymbol{r}\tau)$ denotes the vector spin operator ($a=x,y,z$) with $\hat{\sigma}^a$ being the Pauli matrices. The unit vector $\boldsymbol{\Omega}(\boldsymbol{r}\tau)=[\sin\vartheta(\boldsymbol{r}\tau)\cos\varphi(\boldsymbol{r}\tau),\sin\vartheta(\boldsymbol{r}\tau)\sin\varphi(\boldsymbol{r}\tau),\cos\vartheta(\boldsymbol{r}\tau)]$ written in terms of polar angles labels varying in space-time spin-quantization axis. The spin-rotation invariance is made explicit by performing the angular integration over $\boldsymbol{\Omega}(\boldsymbol{r}\tau)$ at each site and time. By decoupling spin- and charge-density terms in Eq. (4) using auxiliary fields $\varrho(\boldsymbol{r}\tau)$ and $\mathrm{i}V(\boldsymbol{r}\tau)$, respectively, we write down the partition function in the form

$$\mathcal{Z}=\int[\mathcal{D}\boldsymbol{\Omega}]\int[\mathcal{D}V\mathcal{D}\varrho]\int[\mathcal{D}\bar{c}\mathcal{D}c]\,\mathrm{e}^{-\mathcal{S}[\boldsymbol{\Omega},V,\varrho,\bar{c},c]}\,. \tag{5}$$

The effective action reads as

$$\begin{aligned}\mathcal{S}\left[\boldsymbol{\Omega},V,\varrho,\bar{c},c\right]=&\sum_{\boldsymbol{r}}\int_0^\beta\mathrm{d}\tau\left[\frac{\varrho^2(\boldsymbol{r}\tau)}{U}+\frac{V^2(\boldsymbol{r}\tau)}{U}\right.\\&\left.+\mathrm{i}V(\boldsymbol{r}\tau)n(\boldsymbol{r}\tau)+2\varrho(\boldsymbol{r}\tau)\boldsymbol{\Omega}(\boldsymbol{r}\tau)\cdot\boldsymbol{S}(\boldsymbol{r}\tau)\right]\\&+\mathcal{S}_{\mathrm{B}}[\bar{c},c]+\int_0^\beta\mathrm{d}\tau\mathcal{H}_t[\bar{c},c]\,.\end{aligned} \tag{6}$$

3. Gauge transformations of fermions

We switch now from the particle-number representation to the conjugate phase representation of the electronic degrees of freedom. To this aim the second-quantized Hamiltonian of the model is translated to the phase representation with the help of the topologically constrained path-integral formalism. To this end we write the fluctuating "imaginary chemical potential" $\mathrm{i}V(\boldsymbol{r}\tau)$ as a sum of a static $V_0(\boldsymbol{r})$ and periodic function $V(\boldsymbol{r}\tau)=V_0(\boldsymbol{r})+\tilde{V}(\boldsymbol{r}\tau)$ using the Fourier series,

$$\tilde{V}(\boldsymbol{r}\tau)=\frac{1}{\beta}\sum_{n=1}^{\infty}\left[\tilde{V}(\boldsymbol{r}\omega_n)\,\mathrm{e}^{\mathrm{i}\omega_n\tau}+\mathrm{c.c.}\right] \tag{7}$$

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

$$\dot{\phi}(\boldsymbol{r}\tau)\equiv\frac{\partial\phi(\boldsymbol{r}\tau)}{\partial\tau}=\tilde{V}(\boldsymbol{r}\tau)\,. \tag{8}$$

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

$$\begin{bmatrix}c_\alpha(\boldsymbol{r}\tau)\\ \bar{c}_\alpha(\boldsymbol{r}\tau)\end{bmatrix}=\begin{bmatrix}z(\boldsymbol{r}\tau)&0\\0&\bar{z}(\boldsymbol{r}\tau)\end{bmatrix}\begin{bmatrix}f_\alpha(\boldsymbol{r}\tau)\\ \bar{f}_\alpha(\boldsymbol{r}\tau)\end{bmatrix}, \tag{9}$$

where the unimodular parameter $|z(\boldsymbol{r}\tau)|^2=1$ satisfies $z(\boldsymbol{r}\tau)=\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{r}\tau)}$, we remove the imaginary term $\mathrm{i}\int_0^\beta\mathrm{d}\tau\tilde{V}(\boldsymbol{r}\tau)n(\boldsymbol{r}\tau)$ for all the Fourier modes of the $V(\boldsymbol{r}\tau)$ field, except for the zero frequency. The subsequent SU(2) transformation from $f_\alpha(\boldsymbol{r}\tau)$ to $h_\alpha(\boldsymbol{r}\tau)$ variables,

$$\begin{bmatrix}f_1(\boldsymbol{r}\tau)\\ f_2(\boldsymbol{r}\tau)\end{bmatrix}=\begin{bmatrix}\zeta_1(\boldsymbol{r}\tau)&-\bar{\zeta}_2(\boldsymbol{r}\tau)\\ \zeta_2(\boldsymbol{r}\tau)&\bar{\zeta}_1(\boldsymbol{r}\tau)\end{bmatrix}\begin{bmatrix}h_1(\boldsymbol{r}\tau)\\ h_2(\boldsymbol{r}\tau)\end{bmatrix} \tag{10}$$

with the constraint $|\zeta_1(\boldsymbol{r}\tau)|^2+|\zeta_2(\boldsymbol{r}\tau)|^2=1$ takes away the rotational dependence on $\boldsymbol{\Omega}(\boldsymbol{r}\tau)$ in the spin sector. This is done by means of the Hopf map,

$$\boldsymbol{R}(\boldsymbol{r}\tau)\hat{\sigma}^z\boldsymbol{R}^\dagger(\boldsymbol{r}\tau)=\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{\Omega}(\boldsymbol{r}\tau)\,, \tag{11}$$

where

$$\boldsymbol{R}(\boldsymbol{r}\tau)=\begin{bmatrix}\zeta_1(\boldsymbol{r}\tau)&-\bar{\zeta}_2(\boldsymbol{r}\tau)\\ \zeta_2(\boldsymbol{r}\tau)&\bar{\zeta}_1(\boldsymbol{r}\tau)\end{bmatrix} \tag{12}$$

that is based on the enlargement from two-sphere S_2 to the three-sphere $S_3\sim\mathrm{SU}(2)$. The unimodular constraint can be resolved by using the parametrization

$$\begin{aligned}\zeta_1(\boldsymbol{r}\tau)&=\mathrm{e}^{-\mathrm{i}/2[\varphi(\boldsymbol{r}\tau)+\chi(\boldsymbol{r}\tau)]}\cos\left(\frac{\vartheta(\boldsymbol{r}\tau)}{2}\right),\\ \zeta_2(\boldsymbol{r}\tau)&=\mathrm{e}^{\mathrm{i}/2[\varphi(\boldsymbol{r}\tau)-\chi(\boldsymbol{r}\tau)]}\sin\left(\frac{\vartheta(\boldsymbol{r}\tau)}{2}\right),\end{aligned} \tag{13}$$

with the Euler angular variables $\varphi(\boldsymbol{r}\tau),\vartheta(\boldsymbol{r}\tau)$ and $\chi(\boldsymbol{r}\tau)$, respectively. Here, the extra variable $\chi(\boldsymbol{r}\tau)$ represents the U(1) gauge freedom of the theory as a consequence of $S_2\to S_3$ mapping. One can summarize Eqs. (9) and (10) by the single joint gauge transformation exhibiting electron operator factorization

$$c_\alpha(\boldsymbol{r}\tau)=\sum_{\alpha'}z(\boldsymbol{r}\tau)R_{\alpha\alpha'}(\boldsymbol{r}\tau)h_{\alpha'}(\boldsymbol{r}\tau)\,, \tag{14}$$

where $\boldsymbol{R}(\boldsymbol{r}\tau)=\mathrm{e}^{-\mathrm{i}\hat{\sigma}_z\varphi(\boldsymbol{r}\tau)/2}\mathrm{e}^{-\mathrm{i}\hat{\sigma}_y\vartheta(\boldsymbol{r}\tau)/2}\mathrm{e}^{-\mathrm{i}\hat{\sigma}_z\chi(\boldsymbol{r}\tau)/2}$ is a unitary matrix which rotates the spin-quantization axis at site $\boldsymbol{r}$ and time τ.

The expectation value of the static (zero-frequency) part of the fluctuating potential $V_0(r)$ (in the charge sector) is calculated by the saddle-point method. As a result we obtain

$$V_0(r)=\mathrm{i}\left(\mu-\frac{U}{2}n_h\right)\equiv\mathrm{i}\bar{\mu}\,, \tag{15}$$

where $\bar{\mu}$ is the chemical potential with a Hartree shift originating from the saddle-point value of the static variable $V_0(\boldsymbol{r})$ with $n_h=n_{h\uparrow}+n_{h\downarrow}$ and $n_{h\alpha}=\langle\bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}\tau)\rangle$. Similarly in the magnetic sector, a saddle-point evaluation of $\rho(\boldsymbol{r})$ reproduces the conventional Hartree–Fock equations for a commensurate antiferromagnet

$$\rho(\boldsymbol{r}\tau)=(-1)^{\boldsymbol{r}}\Delta_{\mathrm{c}}\,, \tag{16}$$

where $\Delta_{\mathrm{c}}=U\langle S^z(\boldsymbol{r}\tau)\rangle$ sets the magnitude for the Mott-charge gap $\Delta_{\mathrm{c}}\sim U/2$ for $U/t\gg1$.

To summarize, the fermionic sector is governed by the effective Hamiltonian

$$\mathcal{H}_{\boldsymbol{\Omega},\phi} = \sum_{\boldsymbol{r}} \Delta_c(-1)^{\boldsymbol{r}}[\bar{h}_\uparrow(\boldsymbol{r}\tau)h_\uparrow(\boldsymbol{r}\tau) - \bar{h}_\downarrow(\boldsymbol{r}\tau)h_\downarrow(\boldsymbol{r}\tau)]$$
$$-t\sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle,\alpha\gamma} \bar{z}(\boldsymbol{r}\tau)z(\boldsymbol{r}'\tau)\left[\boldsymbol{R}^\dagger(\boldsymbol{r}\tau)\boldsymbol{R}(\boldsymbol{r}'\tau)\right]_{\alpha\gamma}\bar{h}_\alpha(\boldsymbol{r}\tau)$$
$$\times h_\gamma(\boldsymbol{r}'\tau) - \bar{\mu}\sum_{\boldsymbol{r}\alpha}\bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}\tau)\,. \tag{17}$$

The chief merit of the gauge transformation in Eq. (14) is that we have managed to cast the Hubbard problem into a system of h fermions submerged in the bath of strongly fluctuating U(1) and SU(2) gauge potentials (minimally coupled to fermions via hopping term) which mediate the interactions.

4. Pairing interaction

Now we show that U(1) *and* SU(2) emergent gauge fields (the collective high-energy modes in the Hubbard system) take over the task which was carried out by phonons in BCS superconductors. In a way similar to phonons these gauge fields couple to the fermion density--type term via the amplitude t, see Eq. (17),

$$-t\sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle,\alpha\gamma} \bar{z}(\boldsymbol{r}\tau)z(\boldsymbol{r}'\tau)\left[\boldsymbol{R}^\dagger(\boldsymbol{r}\tau)\boldsymbol{R}(r'\tau)\right]_{\alpha\gamma}$$
$$\times\,\bar{h}_\alpha(\boldsymbol{r}\tau)h_\gamma(\boldsymbol{r}'\tau)\,. \tag{18}$$

Thus, in order to obtain an effective interaction among fermions we have to integrate out all the bosonic modes given by $\bar{z}(\boldsymbol{r}\tau), z(\boldsymbol{r}'\tau)$ and $\boldsymbol{R}^\dagger(\boldsymbol{r}\tau), \boldsymbol{R}(r'\tau)$ fields. To explicitly evaluate the effective interaction between fermions by tracing out the gauge degrees of freedom, we resort to the cumulant expansion. To this end we write the partition function as $\mathcal{Z} = \int[\mathcal{D}\bar{h}\mathcal{D}h]\mathrm{e}^{-\mathcal{S}[\bar{h},h]}$, where the effective fermionic action is

$$S_{\mathrm{eff}}[\bar{h},h] = -\ln\int[\mathcal{D}\phi\mathcal{D}\boldsymbol{\Omega}]\,\mathrm{e}^{-S[\boldsymbol{\Omega},\phi,\bar{h},h]}\,. \tag{19}$$

The expression Eq. (19) generates a cumulant series when expanded with respect to the hopping variable t. The relevant second-order term that contains the quartic fermionic term becomes

$$S^{(2)}\left[\bar{h},h\right] = -t^2\sum_{\langle \boldsymbol{r}_1\boldsymbol{r}_1'\rangle}\sum_{\langle \boldsymbol{r}_2\boldsymbol{r}_2'\rangle}\int_0^\beta \mathrm{d}\tau\,\mathrm{d}\tau'$$
$$\times\,\langle\bar{z}(\boldsymbol{r}_1\tau)z(\boldsymbol{r}_1'\tau)\bar{z}(\boldsymbol{r}_2\tau')z(\boldsymbol{r}_2'\tau')\rangle_{\mathrm{U}(1)}$$
$$\times\sum_{\alpha\alpha'}\sum_{\gamma\gamma'}\Big\langle\left[\boldsymbol{R}^\dagger(\boldsymbol{r}_1\tau)\boldsymbol{R}(\boldsymbol{r}_1'\tau)\right]_{\alpha\alpha'}$$
$$\times\left[\boldsymbol{R}^\dagger(\boldsymbol{r}_2\tau')\boldsymbol{R}(\boldsymbol{r}_2'\tau')\right]_{\gamma\gamma'}\Big\rangle_{\mathrm{SU}(2)}\bar{h}_\alpha(\boldsymbol{r}_1\tau)h_{\alpha'}(\boldsymbol{r}_1'\tau)$$
$$\times\bar{h}_\gamma(\boldsymbol{r}_2\tau')h_{\gamma'}(\boldsymbol{r}_2'\tau')\,, \tag{20}$$

where

$$\langle\ldots\rangle_{\mathrm{U}(1)} = \frac{\int[\mathcal{D}\phi]\ldots\mathrm{e}^{-S[\phi]}}{\int[\mathcal{D}\phi]\,\mathrm{e}^{-S[\phi]}} \tag{21}$$

is the averaging over U(1) phase field while

$$\langle\ldots\rangle_{\mathrm{SU}(2)} = \frac{\int[\mathcal{D}\boldsymbol{\Omega}]\ldots\mathrm{e}^{-S[\boldsymbol{\Omega}]}}{\int[\mathcal{D}\boldsymbol{\Omega}]\,\mathrm{e}^{-S[\boldsymbol{\Omega}]}} \tag{22}$$

is the averaging over spin-angular variables. The averaging in the charge sector is performed with the use of the U(1) phase action

$$S[\phi] = \sum_{\boldsymbol{r}}\int_0^\beta \mathrm{d}\tau\left[\frac{\dot{\phi}^2(\boldsymbol{r}\tau)}{U} + \frac{2\,\mu}{\mathrm{i}U}\dot{\phi}(\boldsymbol{r}\tau)\right] \tag{23}$$

that contains both the kinetic and Berry terms of the U(1) phase field in the charge sector. For the U(1) average in Eq. (20) we get

$$\langle\bar{z}(\boldsymbol{r}_1\tau)z(\boldsymbol{r}_1'\tau)\bar{z}(\boldsymbol{r}_2\tau')z(\boldsymbol{r}_2'\tau')\rangle_{\mathrm{U}(1)}$$
$$\approx\left(\delta_{\boldsymbol{r}_1\boldsymbol{r}_1'}\delta_{\boldsymbol{r}_2\boldsymbol{r}_2'} + \delta_{\boldsymbol{r}_1\boldsymbol{r}_2'}\delta_{\boldsymbol{r}_1'\boldsymbol{r}_2}\right)$$
$$\times\,\mathrm{e}^{-\frac{U}{2}\left[|\tau-\tau'|-\left(\tau-\tau'\right)^2/\beta\right]}\,. \tag{24}$$

Specializing to the low-temperature limit

$$\lim_{\tau\to0}\int_0^\beta \mathrm{d}\tau'\,\mathrm{e}^{-|\tau-\tau'|U/2}$$
$$= \lim_{\tau\to0}\left(\frac{2}{U} - \frac{2\mathrm{e}^{-\beta U}}{2}\right) = \frac{2}{U}\,, \tag{25}$$

we obtain the result for the U(1) phase average.

The calculation of the SU(2) average is done with help of the effective action that involves the spin-directional degrees of freedom $\boldsymbol{\Omega}$, whose important fluctuations correspond to rotations. This can be done by integrating out fermions $\mathcal{Z} = \int[\mathcal{D}\boldsymbol{\Omega}]\mathrm{e}^{-\mathcal{S}[\boldsymbol{\Omega}]}$ where

$$\mathcal{S}[\boldsymbol{\Omega}] = -\ln\int[\mathcal{D}\phi\mathcal{D}\bar{h}\mathcal{D}h]\mathrm{e}^{-\mathcal{S}[\varphi,\phi,\vartheta,\bar{h},h]} \tag{26}$$

generates the low-energy action in the form $\mathcal{S}[\boldsymbol{\Omega}] = \mathcal{S}_0[\boldsymbol{\Omega}] + \mathcal{S}_{\mathrm{B}}[\boldsymbol{\Omega}] + \mathcal{S}_J[\boldsymbol{\Omega}]$. The interaction term with the spin stiffness becomes

$$\mathcal{S}_J[\boldsymbol{\Omega}] = \frac{J(\Delta)}{4}\sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle}\int_0^\beta \mathrm{d}\tau\,\boldsymbol{\Omega}(\boldsymbol{r}\tau)\cdot\boldsymbol{\Omega}(r'\tau)\,, \tag{27}$$

with the antiferromagnetic (AF) exchange coefficient

$$J(\Delta_c) = \frac{4t^2}{U}\left(n_\uparrow - n_\downarrow\right)^2 \equiv \frac{4t^2}{U}\left(\frac{2\Delta_c}{U}\right)^2. \tag{28}$$

From Eq. (28) it is evident that for $U\to\infty$ one has $J(\Delta_c)\sim\frac{4t^2}{U}$ since $\frac{2\Delta_c}{U}\to1$ in this limit. Thus, in the strong-coupling limit, the half-filled Hubbard model maps onto the quantum Heisenberg model. If we work in Dirac "north pole" gauge $\chi(\boldsymbol{r}\tau) = -\varphi(\boldsymbol{r}\tau)$ one recovers the familiar form

$$\mathcal{S}_{\mathrm{B}}[\boldsymbol{\Omega}] = \frac{\theta}{\mathrm{i}}\sum_{\boldsymbol{r}}\int_0^\beta \mathrm{d}\tau\dot{\varphi}(\boldsymbol{r}\tau)\left[1-\cos\vartheta(\boldsymbol{r}\tau)\right]. \tag{29}$$

Here, the integral on the right-hand side of Eq. (29) has a simple geometrical interpretation as it is equal to a solid angle swept by a unit vector $\boldsymbol{\Omega}(\vartheta,\varphi)$ during its motion [11]. 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 re-

alized the presence of an additional parameter with the topological angle or so-called theta term

$$\theta = \frac{\Delta_c}{U} \tag{30}$$

that is related to the Mott gap. In the large-U limit, one has $\Delta_c \to U/2$, so that $\theta \to \frac{1}{2}$ relevant for the half-integer spin. The kinetic-energy term in the spin sector becomes

$$\mathcal{S}_0[\boldsymbol{\Omega}] = \sum_{\boldsymbol{r}} \int_0^\beta \mathrm{d}\tau [\dot{\vartheta}^2(\boldsymbol{r}\tau) + \dot{\varphi}^2(\boldsymbol{r}\tau) + \dot{\chi}^2(\boldsymbol{r}\tau) + 2\dot{\varphi}(\boldsymbol{r}\tau)\dot{\chi}(\boldsymbol{r}\tau)\cos\vartheta(\boldsymbol{r}\tau)]/4\mathcal{E}_s, \tag{31}$$

where $\mathcal{E}_s = 1/(2\chi_T)$ and

$$\chi_T = \begin{cases} \dfrac{1}{8J}, & t \ll U, \\ \dfrac{1}{2\pi}\dfrac{1}{t}\sqrt{\dfrac{t}{U}}, & t \gg U, \end{cases} \tag{32}$$

is the transverse spin susceptibility.

Now we switch to the CP^1 representation for the SU(2) fields, so the spin-quantization axis can be conveniently written as

$$\boldsymbol{\Omega}(\boldsymbol{r}\tau) = \sum_{\alpha\alpha'} \bar{\zeta}_\alpha(\boldsymbol{r}\tau)\boldsymbol{\sigma}_{\alpha\alpha'}\zeta_{\alpha'}(\boldsymbol{r}\tau). \tag{33}$$

As a consequence, all the terms in the spin action can be expressed as functions of unimodular $\zeta_\alpha(\boldsymbol{r}\tau)$ variables instead of angular variables, which are more complicated to be handled. Finally, the action assumes the form

$$\mathcal{S}[\bar{\boldsymbol{\zeta}}, \boldsymbol{\zeta}] = \sum_{\boldsymbol{r}} \int_0^\beta \mathrm{d}\tau \Big\{ 2\chi_T \dot{\boldsymbol{\zeta}}(\boldsymbol{r}\tau)\cdot\dot{\boldsymbol{\zeta}}(\boldsymbol{r}\tau) - \theta(-1)^r \left[\bar{\boldsymbol{\zeta}}(\boldsymbol{r}\tau)\cdot\dot{\boldsymbol{\zeta}}(\boldsymbol{r}\tau) - \dot{\bar{\boldsymbol{\zeta}}}(\boldsymbol{r}\tau)\cdot\boldsymbol{\zeta}(\boldsymbol{r}\tau)\right] \Big\} - J\sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle} \int_0^\beta \mathrm{d}\tau \bar{\mathcal{A}}(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\mathcal{A}(\boldsymbol{r}\tau\boldsymbol{r}'\tau) \tag{34}$$

with the bond operators

$$\bar{\mathcal{A}}(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\mathcal{A}(\boldsymbol{r}\tau\boldsymbol{r}'\tau) = -\frac{1}{4}\boldsymbol{\Omega}(\boldsymbol{r}\tau)\cdot\boldsymbol{\Omega}(\boldsymbol{r}'\tau) + \frac{1}{4},$$

$$\mathcal{A}(\boldsymbol{r}\tau\boldsymbol{r}'\tau) = \frac{\zeta_\uparrow(\boldsymbol{r}\tau)\zeta_\downarrow(\boldsymbol{r}'\tau) - \zeta_\downarrow(\boldsymbol{r}\tau)\zeta_\uparrow(\boldsymbol{r}'\tau)}{\sqrt{2}}. \tag{35}$$

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

$$\zeta_\uparrow(\boldsymbol{r}\tau) \to -\zeta_\downarrow(\boldsymbol{r}\tau), \quad \zeta_\downarrow(\boldsymbol{r}\tau) \to \zeta_\uparrow(\boldsymbol{r}\tau) \tag{36}$$

for sites on one sublattice, so that the antiferromagnetic bond operator becomes

$$\mathcal{A}(\boldsymbol{r}\tau r'\tau) \to \mathcal{A}'(\boldsymbol{r}\tau r'\tau) = \sum_{\alpha=1}^{2} \frac{\zeta_\alpha(\boldsymbol{r}\tau)\zeta_\alpha(\boldsymbol{r}'\tau)}{\sqrt{2}}. \tag{37}$$

This canonical transformation preserves the unimodular constraint of the CP^1 fields.

The calculation of the second-order contribution to the effective fermionic action in Eq. (20) is more involved since the SU(2) averages contain tensorial quantities of the form

$$\boldsymbol{M}_{\alpha\alpha',\gamma\gamma'}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau|\boldsymbol{r}'\tau, \boldsymbol{r}\tau) = \Big\langle \Big[\boldsymbol{R}^\dagger(\boldsymbol{r}_1\tau)\boldsymbol{R}(\boldsymbol{r}'_1\tau)\Big]_{\alpha\alpha'} \times \Big[\boldsymbol{R}^\dagger(\boldsymbol{r}_2\tau')\boldsymbol{R}(\boldsymbol{r}'_2\tau')\Big]_{\gamma\gamma'} \Big\rangle_{\mathrm{SU(2)}}. \tag{38}$$

The sublattice transformation of the CP^1 variables in Eq. (36) translates to the transformation of the rotation matrix $\boldsymbol{R}(\boldsymbol{r}\tau) \to \widetilde{\boldsymbol{R}}(\boldsymbol{r}\tau)$ matrix

$$\boldsymbol{R}(\boldsymbol{r}\tau) = (\mathrm{i}\hat{\sigma}_y)\widetilde{\boldsymbol{R}}(\boldsymbol{r}'\tau), \tag{39}$$

where $\widetilde{\boldsymbol{R}}(\boldsymbol{r}\tau)$ is the transformed form of the rotation matrix

$$\widetilde{\boldsymbol{R}}(\boldsymbol{r}\tau) = \begin{bmatrix} -\zeta_2(\boldsymbol{r}\tau) & -\bar{\zeta}_1(\boldsymbol{r}\tau) \\ \zeta_1(\boldsymbol{r}\tau) & -\bar{\zeta}_2(\boldsymbol{r}\tau) \end{bmatrix}. \tag{40}$$

It is convenient to define the following bond operator constructed from the CP^1 fields:

$$\mathcal{F}(\boldsymbol{r}\tau\boldsymbol{r}'\tau) = \frac{\bar{\zeta}_1(\boldsymbol{r}\tau)\zeta_1(\boldsymbol{r}'\tau) + \bar{\zeta}_2(\boldsymbol{r}\tau)\zeta_2(\boldsymbol{r}'\tau)}{\sqrt{2}}. \tag{41}$$

With the definition in Eq. (41) the matrix $\boldsymbol{M}_{\alpha\alpha',\gamma\gamma'}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau|\boldsymbol{r}'\tau, \boldsymbol{r}\tau)$ will be written in a compact form as

$$\boldsymbol{M}_{\alpha\alpha',\gamma\gamma'}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau|\boldsymbol{r}'\tau, \boldsymbol{r}\tau) = \left\langle \begin{bmatrix} \mathcal{F}\bar{\mathcal{F}} & \mathcal{F}\bar{\mathcal{A}} & -\mathcal{F}\mathcal{A} & \mathcal{F}\mathcal{F} \\ -\bar{\mathcal{A}}\bar{\mathcal{F}} & -\bar{\mathcal{A}}\bar{\mathcal{A}} & \bar{\mathcal{A}}\mathcal{A} & -\bar{\mathcal{A}}\mathcal{F} \\ \mathcal{A}\bar{\mathcal{F}} & \mathcal{A}\bar{\mathcal{A}} & -\mathcal{A}\mathcal{A} & \mathcal{A}\mathcal{F} \\ \bar{\mathcal{F}}\bar{\mathcal{F}} & \bar{\mathcal{F}}\bar{\mathcal{A}} & -\bar{\mathcal{F}}\mathcal{A} & \bar{\mathcal{F}}\mathcal{F} \end{bmatrix}_{\alpha\alpha',\gamma\gamma'} \right\rangle_{\mathrm{SU(2)}} \tag{42}$$

where $\alpha\alpha', \gamma\gamma' = \{11, 12, 21, 22\}$. Now, we can rewrite the second-order fermionic action taking into account the non-vanishing averages over CP^1 fields to get

$$S^{(2)}[\bar{h}, h] = -\frac{t^2}{\mathcal{U}}\int_0^\beta \mathrm{d}\tau \sum_{\langle \boldsymbol{r}\boldsymbol{r}'\rangle} M_{11,11}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau|\boldsymbol{r}'\tau, \boldsymbol{r}\tau) \sum_\alpha \bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}'\tau)\bar{h}_\alpha(\boldsymbol{r}'\tau)h_\alpha(\boldsymbol{r}\tau)$$

$$+ M_{11,22}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau|\boldsymbol{r}'\tau, \boldsymbol{r}\tau) \left[\sum_{\alpha\beta} \bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}'\tau)\bar{h}_\beta(\boldsymbol{r}'\tau)h_\beta(\boldsymbol{r}\tau) - \sum_\alpha \bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}'\tau)\bar{h}_\alpha(\boldsymbol{r}'\tau)h_\alpha(\boldsymbol{r}\tau)\right]$$

$$+ M_{12,21}(\boldsymbol{r}\tau,\boldsymbol{r}'\tau|\boldsymbol{r}'\tau,\boldsymbol{r}\tau)\left[\sum_{\alpha\beta}\bar{h}_\alpha(\boldsymbol{r}\tau)h_\beta(\boldsymbol{r}'\tau)\bar{h}_\beta(\boldsymbol{r}'\tau)h_\alpha(\boldsymbol{r}\tau)-\sum_\alpha\bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}'\tau)\bar{h}_\alpha(\boldsymbol{r}'\tau)h_\alpha(\boldsymbol{r}\tau)\right]$$

$$+ M_{12,12}(\boldsymbol{r}\tau,\boldsymbol{r}'\tau|\boldsymbol{r}'\tau,\boldsymbol{r}\tau)\left[\sum_{\alpha\beta}\bar{h}_\alpha(\boldsymbol{r}\tau)h_\beta(\boldsymbol{r}'\tau)\bar{h}_\alpha(\boldsymbol{r}\tau')h_\beta(\boldsymbol{r}\tau)-\sum_\alpha\bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}'\tau)\bar{h}_\alpha(\boldsymbol{r}'\tau)h_\alpha(\boldsymbol{r}\tau)\right]. \tag{43}$$

In deriving the above result, we made the observation that the dynamics of spin variables is slower as compared to the charge counterparts, allowing to treat SU(2) variables as local in time $\boldsymbol{R}(\boldsymbol{r}\tau')=\boldsymbol{R}(\boldsymbol{r}\tau)+(\tau'-\tau)\partial_\tau\boldsymbol{R}(\boldsymbol{r}\tau)+\mathrm{O}[(\tau'-\tau)^2]$. Furthermore, we can reduce Eq. (43) to a compact form

$$S^{(2)}[\bar{h},h]=\frac{t^2}{U}\int_0^\beta \mathrm{d}\tau\sum_{\langle\boldsymbol{r}\boldsymbol{r}'\rangle}\left[\gamma_1 n(\boldsymbol{r}\tau)n(\boldsymbol{r}'\tau)+\gamma_2\bar{\mathcal{A}}'_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\mathcal{A}'_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)+\gamma_3\boldsymbol{S}_h(\boldsymbol{r}\tau)\cdot\boldsymbol{S}_h(\boldsymbol{r}'\tau)+\gamma_4 n(r\tau)\right], \tag{44}$$

where the interaction coefficients

$$\gamma_1=f^2(\boldsymbol{0})+2g^2(\boldsymbol{0})+g^2(\boldsymbol{d})+4f^2(\boldsymbol{d})>0\,,$$

$$\gamma_2=-2[6f^2(\boldsymbol{d})+2f^2(\boldsymbol{0})]<0\,,$$

$$\gamma_3=4[f^2(\boldsymbol{0})-g^2(\boldsymbol{d})]\,,$$

$$\gamma_4=2g^2(\boldsymbol{d})+2f^2(\boldsymbol{d})+4g^2(\boldsymbol{0})>0 \tag{45}$$

are given in terms of the CP^1 normal (g) and anomalous (f) correlation functions

$$g(\boldsymbol{r}-\boldsymbol{r}')=-\left\langle\zeta_\alpha(\boldsymbol{r}\tau)\bar{\zeta}_\alpha(\boldsymbol{r}'\tau)\right\rangle_{\mathrm{SU}(2)}\,,$$

$$f(\boldsymbol{r}-\boldsymbol{r}')=\langle\zeta_\alpha(\boldsymbol{r}\tau)\zeta_\alpha(\boldsymbol{r}'\tau)\rangle_{\mathrm{SU}(2)}\,. \tag{46}$$

From the result in Eq. (43) we can deduce the spin-singlet pairing possibility in the fermionic sector. To bring the kinetic-energy term to a standard form, one performs a rotation of the fermionic variables on one of the sublattices in a manner similar to the bosonic transformation in Eq. (36):

$$h_\uparrow(\boldsymbol{r}'\tau)\to-h_\downarrow(\boldsymbol{r}'\tau)\,,$$

$$h_\downarrow(\boldsymbol{r}'\tau)\to h_\uparrow(\boldsymbol{r}'\tau)\,. \tag{47}$$

As a result the hopping term assumes the conventional form that is diagonal in the spin indices

$$S_t^{(1)}[\bar{h},h]=-\tilde{t}\sum_{\langle\boldsymbol{r}\boldsymbol{r}'\rangle,\alpha}\int_0^\beta\bar{h}_\alpha(\boldsymbol{r}\tau)h_\alpha(\boldsymbol{r}'\tau)\,, \tag{48}$$

while the second-order term is given by

$$S^{(2)}[\bar{h},h]=\sum_{\langle\boldsymbol{r}\boldsymbol{r}'\rangle}\int_0^\beta\mathrm{d}\tau\big[\gamma_1 n(\boldsymbol{r}\tau)n(\boldsymbol{r}'\tau)$$

$$-\gamma_2\bar{\mathcal{A}}_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\mathcal{A}_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\big], \tag{49}$$

where

$$\mathcal{A}_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)=\frac{h_\uparrow(\boldsymbol{r}\tau)h_\downarrow(\boldsymbol{r}'\tau)-h_\downarrow(\boldsymbol{r}\tau)h_\uparrow(\boldsymbol{r}'\tau)}{\sqrt{2}}\,,$$

$$\bar{\mathcal{A}}_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)=\frac{\bar{h}_\downarrow(\boldsymbol{r}'\tau)\bar{h}_\uparrow(\boldsymbol{r}\tau)-\bar{h}_\uparrow(\boldsymbol{r}'\tau)\bar{h}_\downarrow(\boldsymbol{r}\tau)}{\sqrt{2}} \tag{50}$$

are the bond operators relevant for a singlet pairing. The rotational invariance of the right-hand side in Eq. (49) is manifested since

$$-\bar{\mathcal{A}}_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\mathcal{A}_h(\boldsymbol{r}\tau\boldsymbol{r}'\tau)$$

$$=\boldsymbol{S}_h(\boldsymbol{r}\tau)\cdot\boldsymbol{S}_h(r'\tau)-\frac{1}{4}n_h(\boldsymbol{r}\tau)n_h(r'\tau)\,. \tag{51}$$

The coefficients γ_1 and γ_2 are given by Eq. (45). By noting that $g(\boldsymbol{d})=0$ and $f(\boldsymbol{0})=0$ one obtains

$$\gamma_1=\frac{4t^2}{U}\left[f^2(\boldsymbol{d})+\frac{1}{2}g^2(\boldsymbol{0})\right],$$

$$\gamma_2=\frac{4t^2}{U}\left[3f^2(\boldsymbol{d})\right]=J\left[\frac{3Q^2}{J^2(\Delta)}\right]. \tag{52}$$

The effective nonretarded interaction containing γ_2 in front of the $\bar{\mathcal{A}}(\boldsymbol{r}\tau\boldsymbol{r}'\tau)\mathcal{A}(\boldsymbol{r}\tau\boldsymbol{r}'\tau)$ term is negative and therefore constitutes the attractive potential for fermion pairing. The result is plotted in Fig. 1. Let us note that the pairing interaction survives in rather narrow range of the Coulomb interaction $1.17<U/t<1.41$. This result suggests that superconductivity in the Hubbard model, if possible, represents a rather delicate balance between kinetic energy and Coulomb interaction. Moreover, the form of the effective fermionic action suggests that other competing ordered phases can occur simultaneously, which can quench the superconductivity substantially. Therefore, the issue of pairing interaction is not settling the question about the long-range superconducting order in the Hubbard model. As far as modeling of cuprates is concerned, there is also a problem of interplane interaction, entirely omitted in the present work, which can affect the bulk superconductivity considerably.

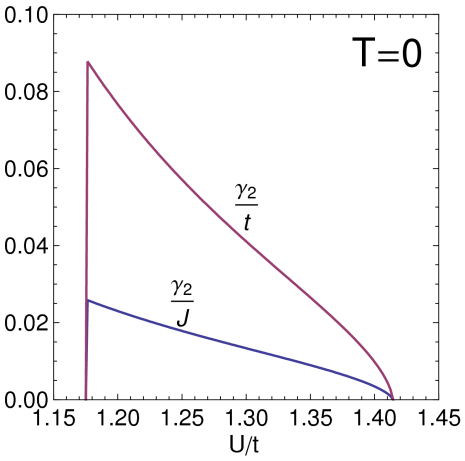

Fig. 1. Pairing interaction γ_2 normalized to the hopping parameter t (upper curve) and the antiferromagnetic-exchange parameter $J = 4t^2/U$ (lower curve) as a function of the Coulomb interaction U/t calculated at zero temperature and half filling $\bar{\mu} = 0$ for the two-dimensional Hubbard model with nearest-neighbors hopping.

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