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Electron Spectral Functions in the Presence of the Antiferromagnetic Order in the Two-Dimensional Hubbard Model

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We use a recently proposed quantum $SU(2) \times U(1)$ rotor approach for the Hubbard model to calculate electronic spectral functions in a presence of an antiferromagnetic state for any value of the Coulomb interaction. We isolate the collective variables for charge and spin in the form of the space-time fluctuating U(1) phase field and SU(2) rotating spin quantization axis, respectively. As a result, the fermion Green function in the space-time domain becomes a product of a CP^1 propagator resulting from the SU(2) gauge fields, U(1) phase propagator and the pseudo-fermion correlation function. In turn, the spectral lines are obtained by performing the convolution of spin, charge and pseudo-fermion Green's functions. We observe an emergence of a sharp peak in the electron spectral functions within the antiferromagnetic phase, whose spectral weight is equal to the antiferromagnetic order parameter.

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1. Introduction

High-resolution angle-resolved photoemission spectroscopy (ARPES) is a powerful tool for study of the electronic structure of complex materials returning direct high-resolution momentum and energy dependent information about electronic states [1]. Since, it requires little or no modeling and experiments are performed in clean conditions (ultrahigh vacuum, no magnetic field), it can be straightforwardly used for comparison with theory. In the discussion of photoemission on solids, and in particular on the correlated electron systems, the most powerful and commonly used approach is based on the Green--function formalism. In this context, the propagation of a single electron in a many-body system is described by the time-ordered one-electron Green propagator. A common approach in describing strong electron correlations is based on consideration of the Hubbard model [2]. Since it envolves only few explicit parameters, it provides a great environment to test the power and quality of analytical [3–9] and numerical [10–17] methods. The inherent difficulty of dealing with Hamiltonians appropriate for strongly correlated electronic systems originates from the non-perturbative nature of the problem and the presence of several competing physical mechanisms. In the fermionic systems with spin and charge excitations the situation is even worse, because dynamic quantum fluctuations are important even in large dimensions. Thus, we use a recently developed quantum $SU(2) \times U(1)$ rotor approach method, which takes into account both spatial correlations and quantum fluctuations to calculate one--particle spectral function for the Hubbard model [7]. We isolate the collective variables for charge and spin 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 strongly interacting electrons appear as composite objects consisting of weakly interacting bare fermions with attached strongly fluctuating U(1) and SU(2) gauge fields. The collective spin and charge fluctuations are governed by the effective actions that are derived from the Hubbard model for any value of the Coulomb interaction. The fermion Green function in the space-time domain becomes the product of the complex-projective (CP^1) propagator (which results from the SU(2) gauge fields), U(1) phase propagator and the pseudo-fermion correlation function, while the fermion spectral lines are convolutions of spin, charge and pseudo-fermion Green's spectral functions.

The paper is organized as follows. After introduction of the model Hamiltonian in Sect. 2, we present in Sect. 3 the transformations to the phase and spin angular variables that reflect the basic symmetries of the Hubbard model. Section 4 is devoted to the derivation of Green's functions in the phase, spin-rotational and pseudo-fermion sectors. In Sect. 5 we present single electron spectral functions and finally conclude in Sect. 6.

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2. The model

We start with a Hubbard Hamiltonian $\mathcal{H} \equiv \mathcal{H}_t + \mathcal{H}_{\mathrm{U}}$:

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

where the Hubbard interaction term is given by

$$\mathcal{H}_{\mathrm{U}} = U \sum_{\boldsymbol{r}} n_{\uparrow}(\boldsymbol{r}) n_{\downarrow}(\boldsymbol{r}) \tag{2}$$

and $n(\boldsymbol{r}) = n_{\uparrow}(\boldsymbol{r}) + n_{\downarrow}(\boldsymbol{r})$ is the number operator. The summation $\langle \boldsymbol{r}, \boldsymbol{r}'\rangle$ runs over the nearest-neighbor (n.n.) sites of the two-dimensional (2D) square lattice, t is the hopping amplitude and U stands for the Coulomb repulsion, $c^{\dagger}_{\alpha}(\boldsymbol{r})$ and $c_{\alpha}(\boldsymbol{r})$ are operators of creation and annihilation of an electron with spin $\alpha = \uparrow (\equiv 1), \downarrow (\equiv 2)$ at the lattice site $\boldsymbol{r}$. The number of electrons with spin α is $n_{\alpha}(\boldsymbol{r}) = c^{\dagger}_{\alpha}(\boldsymbol{r})c_{\alpha}(\boldsymbol{r})$ and μ is the chemical potential controlling the average number of electrons. The partition function is written within the path integral formalism in the Grassmann fields, $c_{\alpha}(\boldsymbol{r}\tau)$ depending on the "imaginary time" $0 \leq \tau \leq \beta \equiv 1/k_{\mathrm{B}}T$ (with T being the temperature) that satisfy the anti-periodic condition $c_{\alpha}(\boldsymbol{r}\tau) = -c_{\alpha}(\boldsymbol{r}\tau + \beta)$:

$$\mathcal{Z} = \int [\mathcal{D}\bar{c}\mathcal{D}c]\, \mathrm{e}^{-\mathcal{S}[\bar{c},c]}, \tag{3}$$

where the fermionic action

$$\mathcal{S}[\bar{c},c] = \mathcal{S}_{\mathrm{B}}[\bar{c},c] + \int_0^{\beta} \mathrm{d}\tau \mathcal{H}[\bar{c},c] \tag{4}$$

contains the fermionic Berry term [18]

$$\mathcal{S}_{\mathrm{B}}[\bar{c},c] = \sum_{\boldsymbol{r}\alpha} \int_0^{\beta} \mathrm{d}\tau \bar{c}_{\alpha}(\boldsymbol{r}\tau)\partial_{\tau} c_{\alpha}(\boldsymbol{r}\tau) \tag{5}$$

that will play an important role in our considerations.

3. Spin-charge rotating reference frame

The Hubbard Hamiltonian contains the spin-rotational symmetry, which is crucial for its low energetic properties. Thus, it is important to use a theoretical approach that naturally preserves this symmetry. The Hubbard interaction term can be written in a spin-rotational form [19]:

$$\mathcal{H}_U = U \sum_{\boldsymbol{r}} \left\{ \frac{1}{4} n^2(\boldsymbol{r}\tau) - \left[\boldsymbol{\Omega}(\boldsymbol{r}\tau) \cdot \boldsymbol{S}(\boldsymbol{r}\tau)\right]^2 \right\}, \tag{6}$$

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 and $\boldsymbol{\Omega}$ is the spin-quantization axis that can be a priori arbitrary. Integration over all possible directions of $\boldsymbol{\Omega}(\boldsymbol{r}\tau)$ in the partition function at each site and time leads to an explicit spin-rotational invariance

$$\mathcal{Z} = \int [\mathcal{D}\boldsymbol{\Omega}] \int [\mathcal{D}\bar{c}\mathcal{D}c]\, \mathrm{e}^{-\mathcal{S}[\boldsymbol{\Omega},\bar{c},c]}. \tag{7}$$

Since the spin and charge density terms of the Hamiltonian in Eq. (6) are of the fourth order in fermionic operators, they must be decoupled using the Hubbard–Stratonovich (HS) formula [20] with auxiliary fields $\varrho(\boldsymbol{r}\tau)$ and $\mathrm{i}V(\boldsymbol{r}\tau)$, respectively. This leads to the following form of the partition function [21]:

$$\mathcal{Z} = \int [\mathcal{D}\boldsymbol{\Omega}] \int [\mathcal{D}V\mathcal{D}\varrho] \int [\mathcal{D}\bar{c}\mathcal{D}c]\, \mathrm{e}^{-\mathcal{S}[\boldsymbol{\Omega},V,\varrho,\bar{c},c]}, \tag{8}$$

while the effective action reads

$$\mathcal{S}\left[\boldsymbol{\Omega}, V, \varrho, \bar{c}, c\right] = \sum_{\boldsymbol{r}} \int_0^{\beta} \mathrm{d}\tau \left[\frac{\varrho^2(\boldsymbol{r}\tau)}{U} + \frac{V^2(\boldsymbol{r}\tau)}{U} + \mathrm{i}V(\boldsymbol{r}\tau)n(\boldsymbol{r}\tau) + 2\varrho(\boldsymbol{r}\tau)\boldsymbol{\Omega}(\boldsymbol{r}\tau)\cdot\boldsymbol{S}(\boldsymbol{r}\tau)\right] + \mathcal{S}_{\mathrm{B}}[\bar{c},c] + \int_0^{\beta} \mathrm{d}\tau \mathcal{H}_t[\bar{c},c]\,. \tag{9}$$

Besides noticing the spin-rotational invariance, one would also like to switch from the particle-number representation to the conjugate phase representation of the electronic degrees of freedom that is governed by the compact U(1) group, which can be done with the help of the topologically constrained path integral formalism [22]. 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

$$V(\boldsymbol{r}\tau) = V_0(\boldsymbol{r}) + \tilde{V}(\boldsymbol{r}\tau)\,, \tag{10}$$

where, using Fourier series

$$\tilde{V}(\boldsymbol{r}\tau) = \frac{1}{\beta}\sum_{n=1}^{\infty}\left[\tilde{V}(\boldsymbol{r}\omega_n)\mathrm{e}^{\mathrm{i}\omega_n\tau} + \mathrm{c.c.}\right] \tag{11}$$

with $\omega_n = 2\pi n/\beta$ ($n = 0, \pm 1, \pm 2$) being the (Bose) Matsubara frequencies. This allows us to introduce the U(1) *phase* field $\phi(\boldsymbol{r}\tau)$ via the Faraday-type relation [23]:

$$\dot{\phi}(\boldsymbol{r}\tau) \equiv \frac{\partial\phi(\boldsymbol{r}\tau)}{\partial\tau} = \mathrm{e}^{-\mathrm{i}\phi(\boldsymbol{r}\tau)}\frac{1}{\mathrm{i}}\frac{\partial}{\partial\tau}\mathrm{e}^{\mathrm{i}\phi(\boldsymbol{r}\tau)} = \tilde{V}(\boldsymbol{r}\tau)\,. \tag{12}$$

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

$$\begin{bmatrix} c_{\alpha}(\boldsymbol{r}\tau) \\ \bar{c}_{\alpha}(\boldsymbol{r}\tau) \end{bmatrix} = \begin{bmatrix} z(\boldsymbol{r}\tau) & 0 \\ 0 & \bar{z}(\boldsymbol{r}\tau) \end{bmatrix} \begin{bmatrix} \zeta_{\uparrow}(\boldsymbol{r}\tau) & -\bar{\zeta}_{\downarrow}(\boldsymbol{r}\tau) \\ \zeta_{\downarrow}(\boldsymbol{r}\tau) & \bar{\zeta}_{\uparrow}(\boldsymbol{r}\tau) \end{bmatrix} \times \begin{bmatrix} h_{\uparrow}(\boldsymbol{r}\tau) \\ h_{\downarrow}(\boldsymbol{r}\tau) \end{bmatrix}, \tag{13}$$

where the unimodular parameter $|z(\boldsymbol{r}\tau)|^2 = 1$ satisfies $z(\boldsymbol{r}\tau) = \mathrm{e}^{\mathrm{i}\phi(\boldsymbol{r}\tau)}$. The transformation to $\zeta_{\alpha}(r\tau)$ variables takes away the rotational dependence on $\boldsymbol{\Omega}(\boldsymbol{r}\tau)$ in the spin sector. This is done by means of the Hopf map [24]:

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

that is based on the enlargement from two-sphere S_2 to the three-sphere $S_3 \sim \mathrm{SU}(2)$. The variables fulfill the unimodularity condition

$$|\zeta_{\uparrow}(\boldsymbol{r}\tau)|^2 + |\zeta_{\downarrow}(\boldsymbol{r}\tau)|^2 = 1 \tag{15}$$

that can be resolved by using the parametrization of $\boldsymbol{\Omega}(\boldsymbol{r}\tau)$ with the Euler angular variables $\varphi(\boldsymbol{r}\tau), \vartheta(\boldsymbol{r}\tau)$:

$$\zeta_{1\uparrow}(\boldsymbol{r}\tau) = \mathrm{e}^{-\frac{\mathrm{i}}{2}[\varphi(\boldsymbol{r}\tau)+\chi(\boldsymbol{r}\tau)]}\cos\left(\frac{\vartheta(\boldsymbol{r}\tau)}{2}\right),$$

$$\zeta_{\downarrow}(\boldsymbol{r}\tau) = \mathrm{e}^{\frac{\mathrm{i}}{2}[\varphi(\boldsymbol{r}\tau)-\chi(\boldsymbol{r}\tau)]}\sin\left(\frac{\vartheta(\boldsymbol{r}\tau)}{2}\right). \tag{16}$$

The extra variable $\chi(\boldsymbol{r}\tau)$ represents the U(1) gauge freedom of the theory as a consequence of $S_2 \rightarrow S_3$ mapping from Eq. (14). As a result of the transformation in Eq. (13) the electrons emerge as composite particles consisting of spin-carrying neutral fermions and topological charged bosons in a form of "flux tubes" with the quantum phase variable dual to the local electron density.

4. Green's functions

The presented scheme allows us to transform the initial purely fermionic action of the Hubbard model into effective actions in spin, charge and fermionic sectors by performing the trace over selected set of variables. For more technical discussion we refer the readers to Ref. [7].

Charge (phase) action. In systems with the Coulomb interactions, the phase variable dual to the charge is an important collective field. We start with a partition function for charge sector

$$\mathcal{Z} = \int [\mathcal{D}\bar{z}Dz]\,\mathrm{e}^{-\mathcal{S}[\bar{z},z]}, \tag{17}$$

where the charge action with the topological contribution can be written as

$$\mathcal{S}_{\mathrm{eff}}[\bar{z},z] = \frac{1}{N\beta}\sum_{\boldsymbol{k},n}\bar{z}\left(\boldsymbol{k}\omega_n\right)G^{-1}_{z0\boldsymbol{k}}\left(\omega_n\right)z\left(\boldsymbol{k}\omega_n\right). \tag{18}$$

The inverse of the propagator reads

$$G^{-1}_{z0\boldsymbol{k}}\left(\omega_n\right) = \lambda_z + \gamma^{-1}\left(\omega_n\right), \tag{19}$$

while the phase correlator after the Fourier transform, can be written as

$$\gamma\left(\omega_n\right) = \frac{1}{\mathcal{Z}_0}\frac{4}{U}\sum_{m=-\infty}^{+\infty}\frac{\mathrm{e}^{-\frac{\beta U}{2}\left(m+\frac{\mu}{U}\right)^2}}{1-4\left(m+\frac{\mu}{U}-\frac{\mathrm{i}\omega_n}{U}\right)^2}, \tag{20}$$

where

$$\mathcal{Z}_0 = \sum_{m=-\infty}^{+\infty}\exp\left(-\frac{1}{2}\beta U\left(m+\frac{\mu}{U}\right)^2\right) \tag{21}$$

is the partition function for the set of non-interacting quantum rotors. Let us note that the presence of the integer winding numbers in Eqs. (20) and (21) renders the phase propagator periodic in the reduced chemical potential μ/U. The unimodular condition of the U(1) phase variables translates into the equation

$$1 = \frac{1}{N\beta}\sum_{\boldsymbol{k},n}\frac{1}{\lambda_{z0}+\gamma^{-1}\left(\omega_n\right)}, \tag{22}$$

which fixes the Lagrange multiplier λ_{z0}.

Fermionic action. Tracing out the gauge degrees of freedom we arrive at the effective action of pseudo-fermions. The partition function can be written as

$$\mathcal{Z} = \int \left[\mathcal{D}\bar{h}\mathcal{D}h\right]\mathrm{e}^{-\mathcal{S}[\bar{h},h]}, \tag{23}$$

where the fermionic action in a compact Nambu form reads

$$\mathcal{S}[\bar{h},h] = \frac{1}{\beta N}\sum_{\boldsymbol{k},n}\bar{\Lambda}_h\left(\boldsymbol{k}\omega_n\right)G^{-1}_{h0\boldsymbol{k}}\left(\omega_n\right)\Lambda_h\left(\boldsymbol{k}\omega_n\right), \tag{24}$$

where vectors $\overline{\Lambda}_h(\boldsymbol{k}\tau)$ are defined by

$$\bar{\Lambda}\left(\boldsymbol{k}\omega_n\right) = \left[\bar{h}_{\uparrow\boldsymbol{k}},\bar{h}_{\downarrow\boldsymbol{k}},\bar{h}_{\uparrow\boldsymbol{k}-\boldsymbol{\pi}},\bar{h}_{\downarrow\boldsymbol{k}-\boldsymbol{\pi}}\right]\left(\omega_n\right) \tag{25}$$

and the inverse propagator

$$G^{-1}_{h0\boldsymbol{k}}\left(\omega_n\right) = \begin{bmatrix}\omega^{-}_{h\boldsymbol{k}} & 0 & \Delta_{\mathrm{c}} & 0\\ 0 & \omega^{-}_{h\boldsymbol{k}} & 0 & -\Delta_{\mathrm{c}}\\ \Delta_{\mathrm{c}} & 0 & \omega^{+}_{h\boldsymbol{k}} & 0\\ 0 & -\Delta_{\mathrm{c}} & 0 & \omega^{+}_{h\boldsymbol{k}}\end{bmatrix}. \tag{26}$$

In Eq. (26) $\Delta_{\mathrm{c}} = U\langle S^z(\boldsymbol{r}\tau\rangle$ sets the magnitude for the Mott-charge gap. Furthermore, $\omega^{\pm}_{h\boldsymbol{k}} = \mathrm{i}\omega_n - \bar{\mu} \pm 2\chi\xi_{\boldsymbol{k}}$, where $\chi = t_J/2$, the effective hopping $t_J = Jv/4$ is proportional to the antiferromagnetic exchange constant $J = 4t^2/U$ and the v field can be fixed self-consistently using saddle-point method to give

$$v = \sum_{\alpha}\langle\bar{h}_{\alpha}(\boldsymbol{r}\tau)h_{\alpha}(r'\tau)\rangle\,. \tag{27}$$

Spin-angular action. Being interested in the magnetic properties of the system it is a natural step to obtain 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

$$\mathcal{Z} = \int \left[\mathcal{D}\bar{\boldsymbol{\zeta}}\mathcal{D}\boldsymbol{\zeta}\right]\mathrm{e}^{-\mathcal{S}[\bar{\boldsymbol{\zeta}},\boldsymbol{\zeta}]}, \tag{28}$$

where the action in the spin-bosonic sector

$$\mathcal{S}\left[\bar{\boldsymbol{\zeta}},\boldsymbol{\zeta}\right] = \frac{1}{2\beta N}\sum_{\boldsymbol{k}n\sigma}\bar{\Lambda}_{\zeta\sigma}\left(\boldsymbol{k}\omega_n\right)G^{-1}_{\zeta0\boldsymbol{k}}\left(\omega_n\right)\Lambda_{\zeta\sigma}\left(\boldsymbol{k}\omega_n\right) \tag{29}$$

with

$$\bar{\Lambda}\left(\boldsymbol{k},\omega_n\right) = \left[\bar{\zeta}_{\sigma\boldsymbol{k}},\zeta_{\sigma-\boldsymbol{k}},\bar{\zeta}_{\sigma\boldsymbol{k}-\boldsymbol{\pi}},\zeta_{\sigma-\boldsymbol{k}+\boldsymbol{\pi}}\right]\left(\omega_n\right) \tag{30}$$

and

$$G^{-1}_{\zeta0\boldsymbol{k}}\left(\omega_n\right) = \begin{bmatrix}\frac{\omega_n^2}{\mathcal{E}_s}+\lambda_\zeta & 2Q\xi_{\boldsymbol{k}} & -2\mathrm{i}\theta\omega_n & 0\\ 2Q\xi_{\boldsymbol{k}} & \frac{\omega_n^2}{\mathcal{E}_s}+\lambda_\zeta & 0 & 2\mathrm{i}\theta\omega_n\\ -2\mathrm{i}\theta\omega_n & 0 & \frac{\omega_n^2}{\mathcal{E}_s}+\lambda_\zeta & -2Q\xi_{\boldsymbol{k}}\\ 0 & 2\mathrm{i}\theta\omega_n & -2Q\xi_{\boldsymbol{k}} & \frac{\omega_n^2}{\mathcal{E}_s}+\lambda_\zeta\end{bmatrix}. \tag{31}$$

The kinetic energy scale for the SU(2) rotors is $\mathcal{E}_s = 1/(2\chi_{\mathrm{T}})$ with the transverse susceptibility behaving in weak and strong coupling limit as follows [25]:

$$\chi_{\mathrm{T}} \sim \begin{cases}\frac{1}{8J}, & t \ll U,\\ \frac{1}{2\pi}\frac{1}{t}\sqrt{\frac{t}{U}}, & t \gg U.\end{cases} \tag{32}$$

Also, decoupling of the fourth-order terms in the spin action leads to additional field Q, whose value is determined from the equation

$$Q = -\frac{J(\Delta_{\mathrm{c}})}{2}\langle\bar{\boldsymbol{\zeta}}(\boldsymbol{r}\tau)\cdot\bar{\boldsymbol{\zeta}}(\boldsymbol{r}'\tau)\rangle. \tag{33}$$

The AF-exchange coefficient

$$J(\Delta_{\rm c}) = \frac{4t^2}{U}\left(n_\uparrow - n_\downarrow\right)^2 \equiv \frac{4t^2}{U}\left(\frac{2\Delta_{\rm c}}{U}\right)^2 \tag{34}$$

behaves in the large-U limit ($U \to \infty$) like $J(\Delta_{\rm c}) \sim \frac{4t^2}{U}$ since $\frac{2\Delta_{\rm c}}{U} \to 1$. In general, the AF-exchange parameter persists as long as the charge gap $\Delta_{\rm c}$ exists. However, $J(\Delta_{\rm c})$ diminishes also in the weak coupling limit ($U/t \to 0$).

The AF order parameter in terms of the original fermion operators is defined as:

$$\begin{aligned} m_{\rm AF} &= \sum_{\boldsymbol{r}} (-1)^{\boldsymbol{r}} \langle S^z(\boldsymbol{r}\tau)\rangle \\ &= \sum_{\boldsymbol{r}} (-1)^{\boldsymbol{r}} \langle \boldsymbol{\Omega}(\boldsymbol{r}\tau)\rangle \cdot \langle \boldsymbol{S}_h(\boldsymbol{r}\tau)\rangle. \end{aligned} \tag{35}$$

Owing the fact that $\langle S^a_h(\boldsymbol{r}\tau)\rangle = (-1)^{\boldsymbol{r}}\Delta_{\rm c}\delta_{a,z}$ we obtain

$$\begin{aligned} m_{\rm AF} &= \Delta_{\rm c} \sum_{\boldsymbol{r}} \langle \Omega^z(\boldsymbol{r}\tau)\rangle \\ &= \Delta_{\rm c} \sum_{\boldsymbol{r}} \left[\langle \bar{\zeta}_\uparrow(\boldsymbol{r}\tau)\zeta_\uparrow(\boldsymbol{r}\tau)\rangle - \langle \bar{\zeta}_\downarrow(\boldsymbol{r}\tau)\zeta_\downarrow(\boldsymbol{r}\tau)\rangle\right] \\ &= \frac{\Delta_{\rm c}}{U} m_0^2 . \end{aligned} \tag{36}$$

It is clear that the existence of AF long-range order does not only require a nonzero value of $\Delta_{\rm c}$, but also the angular degrees of freedom $\boldsymbol{\Omega}(\boldsymbol{r}\tau)$ have to be ordered. In the CP^1 representation (where the Néel field is represented by two Schwinger bosons) it is signalled by the Bose–Einstein condensation of the Schwinger bosons at zero temperature. The CP^1 order parameter m_0^2 along with the Lagrange multiplier λ_ζ can be fixed from the uniformity condition in Eq. (15):

$$1 - m_0^2 = \frac{1}{\beta N} \sum_{\boldsymbol{k}n\sigma} G^\sigma_{\zeta\boldsymbol{k}}(\omega_n) .$$

5. Single electron spectral function

Within our construction, the electron Green function is a product of U(1) phase, SU(2) spin (in CP^1 representation) and pseudo-fermion Green's functions

$$\begin{aligned} G_{\alpha\alpha}(\boldsymbol{r}\boldsymbol{r}'\tau) = &- \sum_{\beta\gamma} \langle z_{\boldsymbol{r}}\bar{z}_{\boldsymbol{r}'}\rangle \left\langle R_{\alpha\beta}(\boldsymbol{r}\tau) R^\dagger_{\gamma\alpha}(\boldsymbol{r}'\tau)\right\rangle \\ &\times \langle h_\beta(\boldsymbol{r}\tau) h_\gamma(\boldsymbol{r}'\tau)\rangle \end{aligned} \tag{37}$$

where the Green functions in the respective sectors are defined as:

$$\begin{aligned} G_z(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') &= -\left\langle z(\boldsymbol{r},\tau)\,\bar{z}(\boldsymbol{r}',\tau')\right\rangle , \\ G^{\alpha\alpha'}_\zeta(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') &= -\left\langle \zeta_\alpha(\boldsymbol{r},\tau)\,\bar{\zeta}_{\alpha'}(\boldsymbol{r}',\tau')\right\rangle , \\ G^{\alpha\alpha'}_h(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') &= -\left\langle h_\alpha(\boldsymbol{r},\tau)\,\bar{h}_{\alpha'}(\boldsymbol{r}',\tau')\right\rangle . \end{aligned} \tag{38}$$

Since in the antiferromagnetic phase we allow for ordering in the spin sector, the averages over spin variables can be non-zero. This leads to the following expression for the spin-sector Green function:

$$\begin{aligned} G^{\alpha\alpha}_{\zeta\boldsymbol{k}}(\omega_n) = &-\beta N m_0^2 \delta_{\alpha\uparrow}\delta_{\boldsymbol{k}0}\delta_{\omega_n 0} \\ &+ (1 - 2\delta_{\alpha\uparrow}\delta_{\boldsymbol{k}0}\delta_{\omega_n 0})\, G^{\alpha\alpha}_{\zeta\boldsymbol{k}}(\omega_n) . \end{aligned} \tag{39}$$

Introducing a spectral density function that is defined for fermions as follows:

$$G^{\alpha\alpha}_{{\rm X}\boldsymbol{k}}(\nu_n) = \int_{-\infty}^{+\infty} \frac{{\rm d}\omega}{2\pi} \frac{A^{\alpha\alpha}_{X\boldsymbol{k}}(\omega)}{{\rm i}\nu_n - \omega} \tag{40}$$

with $X = c, h$ for full system and pseudo-fermionic sector, respectively and, similarly, for bosonic sectors

$$G_{{\rm X}\boldsymbol{k}}(\omega_n) = \int_{-\infty}^{+\infty} \frac{{\rm d}\omega}{2\pi} \frac{A_{X\boldsymbol{k}}(\omega)}{{\rm i}\omega_n - \omega} , \tag{41}$$

where $X = z, \zeta$ for charge and spin part, one can calculate spectral density of the system

$$A^{\alpha\alpha}_{c\boldsymbol{k}}(\omega) = m_0^2 A^{\alpha\alpha}_{zh\boldsymbol{k}}(\omega) + \sum_\sigma A^{\sigma\sigma}_{zh\zeta\boldsymbol{k}}(\omega) . \tag{42}$$

Consequently, the density of states being a local spectral density

$$\rho^{\alpha\alpha}_X(\omega) = -\frac{1}{2\pi N} \sum_{\boldsymbol{k}} A^{\alpha\alpha}_{X\boldsymbol{k}}(\omega) , \tag{43}$$

can be written as

$$\rho^{\alpha\alpha}_{\rm c}(\omega) = m_0^2 \rho^{\alpha\alpha}_{zh}(\omega) + 2\rho^{\alpha\alpha}_{zh\zeta}(\omega) , \tag{44}$$

with

$$\begin{aligned} \rho^{\alpha\alpha}_{zh}(\omega) = &\int_{-\infty}^{+\infty} {\rm d}\omega' \rho_z(\omega')\, \rho^{\alpha\alpha}_h(\omega - \omega') \\ &\times \left[n_{\rm B}(-\omega') + n_{\rm F}(\omega - \omega')\right] , \\ \rho^{\alpha\alpha}_{zh\zeta}(\omega) = &\int_{-\infty}^{+\infty} {\rm d}\omega' \rho^{\alpha\alpha}_\zeta(\omega')\, \rho^{\alpha\alpha}_{zh}(\omega - \omega') \\ &\times \left[n_{\rm B}(-\omega') + n_{\rm F}(\omega - \omega')\right] . \end{aligned} \tag{45}$$

The single electron density of states in Eq. (44) contains then two terms. The first generates the coherence peak associated with the long-range AF order, which is a product of the condensate density m_0^2 and the pseudo-fermion spectral function convolved with phase spectral function $\rho^{\alpha\alpha}_{zh}(\omega)$. To the extent that the peak and the background are distinguishable objects, see Fig. 1, the weight under this quasi-particle peak should be equal to the condensate density m_0^2 of the CP^1 bosons. The second term $\rho^{\alpha\alpha}_{zh\zeta}(\omega)$ being the spectrum background is a double convolution of phase, spin-rotational and pseudo-fermion contributions. Since the density of states obeys the sum rule, the weight of this part of the spectrum is $1 - m_0^2$.

In Fig. 1 the evolution of the spectrum with variable coupling has been presented. For strong coupling limit the hopping is strongly renormalized leading to zero value of the v field in Eq. (27) and a non-dispersive spectrum. For lower interactions the spectrum becomes more complex and the long-range AF order disappears. Finally, in the weak coupling the density of states recovers the form usual for the 2D lattice with the logarithmic singularity at $\omega/t = 0$.

The details of disappearance of the long-range order and the corresponding coherence peaks in the spectrum have been presented in Fig. 2. The peaks located next to the gap decrease for weaker couplings until they finally

disappear for a critical value of $U/t = 1.18$. Since the spectrum obeys the sum rule, the spectral weight from the coherence peaks is relocated to the spectrum background. This behavior exhibits a great similarity to that, which is seen in the ARPES spectra in the underdoped high-temperature superconducting samples, however in this case the condensate density refers to the superconductor, not the antiferromagnet. The electron spectral function is very broad above the superconducting transition, but a sharp quasiparticle peak develops at the lowest binding energies, followed by a dip and a broader hump, giving rise to the so-called peak-dip-hump structure [26]. The evolution of the spectral density as a function of temperature is depicted in Fig. 3. At finite temperature there is no AF ordering according to the Mermin–Wagner theorem and consequently no coherence peak, but one observes the gap filling as the temperature increases.

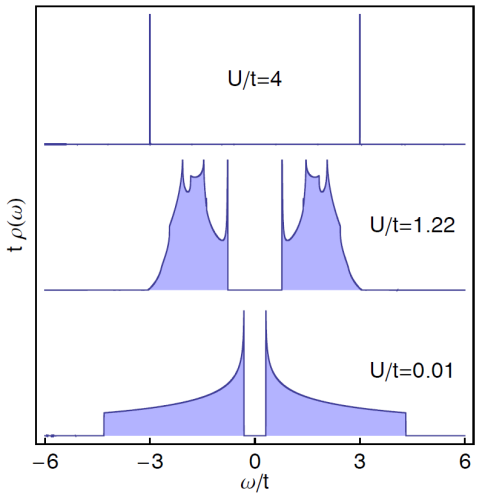

Fig. 1. Evolution of the density of states of the model for various interactions U/t from strong to weak--coupling limit.

6. Conclusions

In this paper we have presented a method of calculation of electron spectral densities for strongly correlated systems described by the Hubbard model in terms of a collective phase variable, the rotating quantization axis and the fermionic degrees of freedom. Our approach goes beyond purely local mean-field description by incorporating the effect of spatial correlations and in particular the influence of the ordered states on the spectral properties of the system. The inclusion of the antiferromagnetically ordered phase was done by resorting to the saddle--point analysis of the bosonic and fermionic effective actions, however the general architecture of the method is not resting on this assumption. The single-particle properties are obtained by writing the original fermion field in terms of a U(1) phase field related to the charge, CP^1 bosons that parametrize the variable spin quantization axis related to the rotational symmetry and pseudo--fermions. This decomposition in real space reduces the fermion Green function to the product of the phase, the Schwinger boson and the remaining fermionic propagators, respectively. Because the method takes into account spatial correlations, the effect of the ordered states on the electronic picture can be observed. The obtained density of states consists of two parts: one generating the coherence peak dependent on the density of condensed CP^1 bosons that represents the antiferromagnetic order and the second — with the remaining spectrum background. We notice a similarity of the situation to the behavior of the normal state ARPES spectra in the underdoped samples, where the the superconducting condensate produces the well-known peak-dip-hump structure.

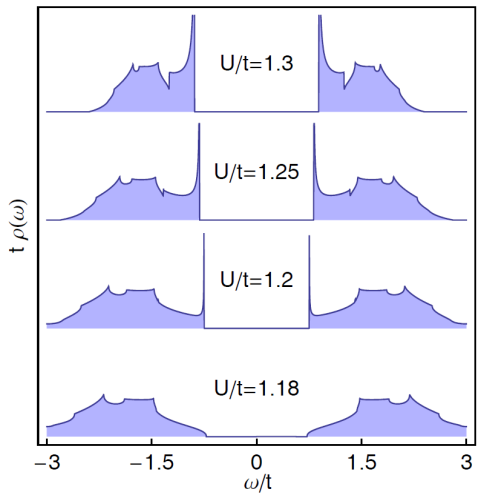

Fig. 2. Disappearance of the antiferromagnetic coherence peak density with variable interactions U/t from strong to weak-coupling limit.

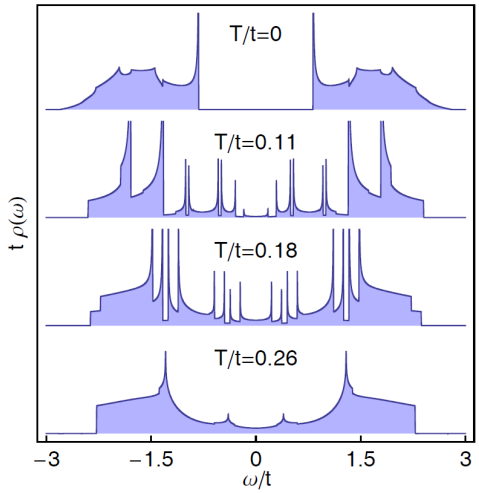

Fig. 3. Evolution of density of states as a function of the temperature (as indicated in the plot) for $U/t = 1.25$.

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