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Electron spectral density of the half-filled Hubbard model in the atomic limit at finite temperature

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Abstract: We have calculated the spectral function and density of states of half-filled two-dimensional Hubbard model in the Hubbard-I approximation assuming an antiferromagnetic long range order at low temperature and compared results to the QMC data. It occurs that calculated functions are in a qualitative agreement with the QMC one. We have also shown that Neel ordered state dispersion has the similar form to the spin density wave one.

Keywords: Hubbard model, half-filling, spectral function, density of states, redistribution of spectral weight
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1 Introduction

The Hubbard model, which takes into account both hopping of electrons and their interaction, is one of the basic models in the theory of strong electron correlations (SES) systems. The matter is that, despite the model's insufficiency for quantitative descriptions of any particular substance, it contains the important effects of SEC. There is certain interest to research an atomic limit $t \ll U$, since it is known that it's easier to describe such systems starting from the local approach instead of Hartry-Fock theory of a band limit. The Hubbard-I approximation in the $t \ll U$ limit yields the simplest description of the system as two energy bands divided by a gap [1]. With growth ratio it becomes obviously wrong, but apparently still is quite reasonable in a regime of SEC. In the diagram technique for the Hubbard X-operators [2, 3] the Hubbard-I solution is just a result

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of the Hartree-Fock approximation. A non-perturbative quantum Monte Carlo (QMC) method provides possibility to compare electronic properties of the Hubbard model at $t \ll U$ obtained in the Hubbard-I approximation to the QMC numerical results. Such comparison has been studied in [4], where a spectral density function $A\left(\vec{k},\omega\right)$ has been calculated at different temperatures. It occurs that at high temperature $T \sim t$ the functions $A\left(\vec{k},\omega\right)$ obtained by QMC and in Hubbard-I paramagnetic solution are very similar. With decreasing temperature, the difference between two $A\left(\vec{k},\omega\right)$ functions becomes larger. For low temperature, the spin density wave (SDW) solution has been used in [4] for comparison to QMC data. It is known that SDW solution is valid in the weak correlation band limit $U \ll W = zt$ and is not the appropriate solution in the SEC limit. In this paper, we calculated the spectral function $A\left(\vec{k},\omega\right)$ of the half-filled two-dimensional Hubbard model in the Hubbard-I approximation assuming an antiferromagnetic (AF) long range order at low temperature and compare it to the QMC data.

It occurs that calculated function $A\left(\vec{k},\omega\right)$ is in a rather reasonable agreement with the QMC one, in spite of all shortcomings of our approach. These shortcomings are the following:

(1) In the two-dimensional system, there is no Neel long range order at any finite temperature, so we should assume some anisotropy or interplane coupling.
Nevertheless,here it is not important because we compare our data to the finite system QMC one and the Mermin Wagner theorem does not hold in the finite system.

(2) The Hubbard-I approximation does not give the self-consistent description of the AF-state, the only solution for the sublattice magnetization m is zero. Thus, in the $t \ll U$ limit for $n_e = 1$ system, we construct the effective low-energy Heisenberg Hamiltonian with AF coupling $J = 4t^2/U$ and calculate the value of m in the Heisenberg model. For $T = 0$ it results in $m = 0.3$ with 40% spin reduction due to zero quantum spin fluctuation.

2 The electron spectrum in AFM state at half filling

The two-dimensional Hubbard model that we study has a Hamiltonian given by

$$\hat{H} - \mu\hat{N}_e = \sum_{f,\sigma}\left[\left(\varepsilon - \mu\right)n_{f,\sigma} + \frac{1}{2}Un_{f,\sigma}n_{f,\bar{\sigma}}\right] + \sum_{f,g,\sigma}\left(t_{f,g}a^{+}_{f,\sigma}a_{g,\sigma} + h.c.\right). \qquad (1)$$

Here μ is the chemical potential and ε is the single-electron energy, $a^{+}_{f,\sigma}$ ($a_{f,\sigma}$) are creation (destruction) operators of electron with spin $\sigma = \pm 1/2$ at lattice site f. The particle density at each site is given by $n_{f\sigma} = a^{+}_{f\sigma}a_{f\sigma}$. The second term describes an onsite Coulomb repulsion between particles with opposite spin. The third term for kinetic energy is restricted by the hopping matrix element t between only nearest neighbor sites.

Further, the spatially non-uniform solution for electron spectral function in the two-dimensional square lattice with antiferromagnetic spin ordering is considered. (Near and at half filling the system has Neel order for $T = 0$ that is caused by a kinetic superex-

change.) Due to two sublattices the two-time temperature-dependent Green functions [5] read as

$$G\left(\vec{k},\omega\right)=\frac{1}{N}\begin{pmatrix}\sum\limits_{\vec{f}-\vec{f}'}e^{i\vec{k}(\vec{f}-\vec{f}')}\left\langle\left\langle a_f\mid a_{f'}^{+}\right\rangle\right\rangle_\omega & \sum\limits_{\vec{g}-\vec{f}}e^{i\vec{k}(\vec{g}-\vec{f})}\left\langle\left\langle a_g\mid a_{f'}^{+}\right\rangle\right\rangle_\omega\\ \sum\limits_{\vec{f}-\vec{g}}e^{i\vec{k}(\vec{f}-\vec{g})}\left\langle\left\langle a_f\mid a_g^{+}\right\rangle\right\rangle_\omega & \sum\limits_{\vec{g}-\vec{g}'}e^{i\vec{k}(\vec{g}-\vec{g}')}\left\langle\left\langle a_g\mid a_{g'}^{+}\right\rangle\right\rangle_\omega\end{pmatrix}, \tag{2}$$

where indexes f, f' correspond to the same sublattice, while f and g' correspond to different ones. The Fourier transform of Green function is a function of ω and is denoted by $\left\langle\left\langle a_f|a_g^{+}\right\rangle\right\rangle_\omega$.

Analytical expressions for Green functions are received in known Hubbard-I approach which corresponds to the following decoupling procedure

$$\left\langle\left\langle a_{f+h,\sigma}n_{f,\bar{\sigma}}\mid a_{f',\sigma}^{+}\right\rangle\right\rangle\rightarrow\left\langle n_{f,\bar{\sigma}}\right\rangle\left\langle\left\langle a_{f+h,\sigma}\mid a_{f',\sigma}^{+}\right\rangle\right\rangle. \tag{3}$$

In the atomic limit, a representation of the Hubbard X-operators is more convenient[6]. They are connected with usual Fermi-operators by a linear combination

$$a_{f\sigma}^{+}=X_f^{\sigma,0}+2\sigma X_f^{2,\bar{\sigma}},\quad a_{f\sigma}=X_f^{0,\sigma}+2\sigma X_f^{\bar{\sigma},2}. \tag{4}$$

Note that the single-electron Green function in the Hubbard operator representation is given by

$$G_{f,f'}=\left\langle\left\langle a_f\mid a_{f'}\right\rangle\right\rangle=\begin{pmatrix}\left\langle\left\langle X_f^{0,\sigma}\mid X_{f'}^{0,\sigma}\right\rangle\right\rangle & 2\sigma\left\langle\left\langle X_f^{\bar{\sigma},2}\mid X_{f'}^{\sigma,0}\right\rangle\right\rangle\\ 2\sigma\left\langle\left\langle X_f^{0,\sigma}\mid X_{f'}^{2,\bar{\sigma}}\right\rangle\right\rangle & \left\langle\left\langle X_f^{\bar{\sigma},2}\mid X_{f'}^{2,\bar{\sigma}}\right\rangle\right\rangle\end{pmatrix}. \tag{5}$$

Therefore we may write down in the X-representation the expressions for Green functions (A and B are sublattice indexes)

$$G_{AA}^{l}=F_A^{0,\sigma}\left((E-\varepsilon_1)\left[\nu^2-F_A^{\bar{\sigma},2}F_B^{\bar{\sigma},2}t^2(\vec{k})\right]+F_B^{0,\sigma}t(\vec{k})\left[\nu^2-F_A^{\bar{\sigma},2}t(\vec{k})\nu\right]\right)\Bigg/\prod_{i=1}^{4}(E-E_i),$$

$$G_{AB}^{l}=F_B^{0,\sigma}\left((E-\varepsilon_1)\left[\nu^2-F_A^{\bar{\sigma},2}F_B^{\bar{\sigma},2}t^2(\vec{k})\right]+F_A^{0,\sigma}t(\vec{k})\left[\nu^2-F_B^{\bar{\sigma},2}t(\vec{k})\nu\right]\right)\Bigg/\prod_{i=1}^{4}(E-E_i),$$

$$G_{AA}^{u}=F_A^{\bar{\sigma},2}\left((E-\varepsilon_1)^2\left(\nu+F_B^{\bar{\sigma},2}t(\vec{k})\right)-F_A^{0,\sigma}t^2(\vec{k})\left(E-\varepsilon_1-F_B^{0,\sigma}U\right)\right)\Bigg/\prod_{i=1}^{4}(E-E_i),$$

$$G_{AB}^{u}=F_B^{\bar{\sigma},2}\left((E-\varepsilon_1)^2\left(\nu+F_A^{\bar{\sigma},2}t(\vec{k})\right)-F_B^{0,\sigma}t^2(\vec{k})\left(E-\varepsilon_1-F_A^{0,\sigma}U\right)\right)\Bigg/\prod_{i=1}^{4}(E-E_i).$$

Here the following notations are used: $F_A^{0,\sigma}=\left\langle X_A^{0,0}+X_A^{\sigma,\sigma}\right\rangle$, $F_A^{\bar{\sigma},2}=\left\langle X_A^{2,2}+X_A^{\bar{\sigma},\bar{\sigma}}\right\rangle$ are the filling factors, $\varepsilon_1=(\varepsilon-\mu)$, $\nu=(E-\varepsilon_1-U)$. The upper indexes are related to lower (l) and upper (u) Hubbard bands. The bottom ones mark intra and inter

sublattice functions. The Green function poles E_i, determining quasiparticle dispersion, are the solution of the following equation of the fourth order:

$$\begin{aligned}
E^4 + & \; aE^3 + bE^2 + cE + d = 0, \\
a = & \; -2\left(2\varepsilon_1 + U\right), \\
b = & \; \left(2\varepsilon_1 + U\right)^2 + 2\varepsilon_1\left(\varepsilon_1 + U\right) - t^2(\vec{k}), \\
c = & \; -2\varepsilon_1\left(\varepsilon_1 + U\right)\left(2\varepsilon_1 + U\right) + 2\varepsilon_1 t^2(\vec{k}) + Ut^2(\vec{k})\left(2 - n_f\right), \\
d = & \; \varepsilon_1^2\left(\varepsilon_1 + U\right)^2 - \varepsilon_1^2 t^2(\vec{k}) - Ut^2(\vec{k})\left(2\varepsilon_1 + U\right)\left(1 - n_{f,\sigma}\right)\left(1 - n_{f,\bar{\sigma}}\right) \\
& -\varepsilon_1 Ut^2(\vec{k})\left(n_f - 2n_{f,\sigma}n_{f,\bar{\sigma}}\right).
\end{aligned}$$

Below, we shall restrict ourselves by half-filling case $n_e = 1$ where expression for chemical potential is known [7] for any values of model parameters and temperatures $\mu = \varepsilon + U/2$. In this case, the fourth order equation determining quasiparticle dispersion is reduced to a biquadratic one. And we at once receive a quasiparticle spectrum for the two-dimensional antiferromagnetic lattice in the Hubbard-I approximation

$$E_{\pm}^{l,u} = \pm\frac{1}{\sqrt{2}}\left(t^2(\vec{k}) \pm \sqrt{t^4(\vec{k}) + 4U^2t^2(\vec{k})n_{f,\sigma}n_{f,\bar{\sigma}}} - 2\varepsilon_1\left(\varepsilon_1 + U\right)\right)^{1/2}. \tag{6}$$

Due to two-fold reducing of the Brillouin zone in the AF state, each Hubbard subband of the paramagnetic phase is twice splitted. If these bands were conventional single electron bands with a number of states per atom being 1, the total number of states would be equal to 4. Here there are quasiparticle bands with a fractal spectral weight that is explicitly calculated by the QMC method. In our calculations, the fractal weights are controlled by the filling factor $F_f^{m,n} = \left\langle X_f^{m,m} + X_f^{n,n} \right\rangle$.

It is interesting to note that the obtained quasiparticle spectrum (6) can be rewritten through well known Hubbard-I paramagnetic solution. It turns out that the Neel ordered state dispersion has the similar form to the spin density wave one

$$E_{\pm}^{l,u} = \pm\sqrt{\left(\xi^{\pm}\right)^2 + \Delta^2}. \tag{7}$$

Where gap parameter $\Delta = Um$, sublattice magnetization $m = 1/2\left(n_{f,\sigma} - n_{f,\bar{\sigma}}\right)$ and $\xi_{\vec{k}}^{\pm}$ corresponds to dispersion of the upper and lower Hubbard bands in the paramagnetic phase with renormalized value of Coulomb repulsion $\tilde{U} = U\sqrt{1 - 4m^2}$:

$$\xi_{\vec{k}}^{\pm} = \frac{1}{2}\left(t\left(\vec{k}\right) \pm \sqrt{t^2\left(\vec{k}\right) + U^2}\right). \tag{8}$$

When $m = 0$ these bands are exactly the upper and lower Hubbard bands in the paramagnetic phase [1]. In the single electron SDW state the quasiparticle spectrum is given by the similar to Eq. (7) formulae with $\xi_{\vec{k}}^{\pm}$ being free electron dispersion.

Now we can calculate total spectral function of system as an imaginary part of one-electronic Green function:

$$\begin{aligned}
A\left(\vec{k},\omega\right) &= -\frac{1}{\pi}\hat{S}p\left(\mathrm{Im}G\left(\vec{k},\omega\right)\right) \\
&= -\frac{1}{\pi}\mathrm{Im}\left(G_{AA}^{l}\left(\vec{k},\omega\right) + G_{AB}^{l}\left(\vec{k},\omega\right) + G_{AA}^{u}\left(\vec{k},\omega\right) + G_{AB}^{u}\left(\vec{k},\omega\right)\right)
\end{aligned} \tag{9}$$

and the single electron density of states (DOS)

$$N(\omega) = \frac{1}{N} \sum_{\vec{k}} A\left(\vec{k}, \omega\right). \tag{10}$$

The accepted approach does not contain any information on a line-width (spectral density expression includes usual delta-functions). To compare obtained results to the calculated by a quantum Monte Carlo method, we approximate delta-functions by a Lorentzian line shape with a suitably chosen temperature-dependent parameter δ. Such weight and width renormalization of the quasiparticle spectral lines assumes some nonzero imaginary part of a self-energy value $\Sigma(\vec{k}, \omega)$, and means a phenomenological output beyond the Hubbard-I approximation.

It is necessary to note that there is no unequivocal conformity between temperature and parameter δ. However, at temperature reduction, this parameter also aspires to zero. And despite the fact that the Mermin-Wagner theorem prevents a long-rang Neel ordered state in a two dimensional system for finite temperature, it is commonly believed that a system is effectively ordered if the spin correlation length becomes comparable to the system size.

In figures 1-3 angle-resolved spectral function are plotted simultaneously with the data of numerical QMC calculations taken from the work [4]. The following values of parameters are used: $U = 8t$, $\varepsilon - \mu + U/2 = 0$ and $t(\vec{k}) = -2t\left(\cos(k_x) + \cos(k_y)\right)$. In the low-temperature region we take the parameter of sublattice magnetization $m = 0.3$.

Starting from the high-temperature range (fig.1,2), we found that Hubbard-1 approximation, which neglects all spin correlations effects, approximates weight and positions of spectral peaks given by the upper and lower Hubbard bands. It is not surprising since these effects are not essential at the paramagnetic state ($m = 0$) when all relevant spin degrees of freedom are thermally exited.

For $T = 1.00t$ the QMC data [4] have revealed very weak satellites at $k = (0, 0)$ for unoccupied and $k = (\pi, \pi)$ for occupied states. These satellites correspond to our bands E^u_+ and E^l_- with very small spectral weights. Of course there is no long magnetic order at such high temperature but there is short magnetic order that evidently results in these weak satellites.

At media and low temperatures (fig.3,4) both Hubbard bands of the paramagnetic state are split in two subbands $E^{l,u}_{\pm}$. For the largest part of the Brillouin zone one of the subbands both below and above the Fermi level has larger spectral weight the other looks like a weak satellite. The non-trivial result obtained in the QMC method as well as in our calculation is the redistribution of spectral weight between strong and weak peaks. This is most clearly seen in the fig.4 for $T = 0.1t$.

While the trends for spectral weight redistribution are similar in our Hubbard-I calculations and in the QMC data, in some regions of the Brillouin zone (near $\vec{k} = (0, 0)$ and $\vec{k} = (\pi, \pi)$) there is a reasonable agreement in the shape and position of peaks in $A\left(\vec{k}, \omega\right)$ and there are regions in a k-space (near $\vec{k} = (\pi/2, \pi/2)$ and $\vec{k} = (\pi, 0)$) with rather large deviations of our and QMC data.

The single electron DOS (fig.5) at low temperature shows two peak structure corresponding to the occupied (l) and unoccupied (u) Hubbard bands. Weak satellites in the spectral density resulted in the shoulders for both peaks. Our data for DOS are in a qualitative agreement to the QMC data by [8].

3 Conclusions

Summarizing we have shown that the spectral function at the low temperature consists of four peaks corresponding to the AFM Hubbard-I subbands similar to the QMC data. The general trend of the spectral weight redistribution is also in agreement to the QMC. Nevertheless for some regions in the k-space there are quantitative disagreements. The DOS in Hubbard-I solution is similar to the DOS in QMC.

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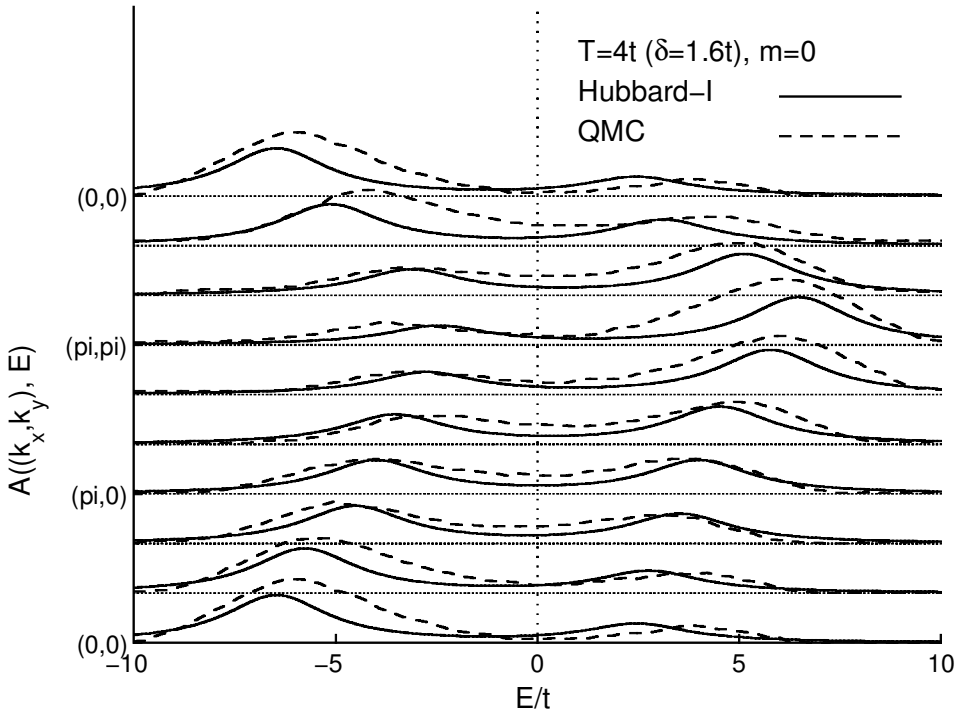

Fig. 1 The angle-resolved spectral function for half filled Hubbard model at low temperature, T=4t. The QMC data are taken from the work[4].

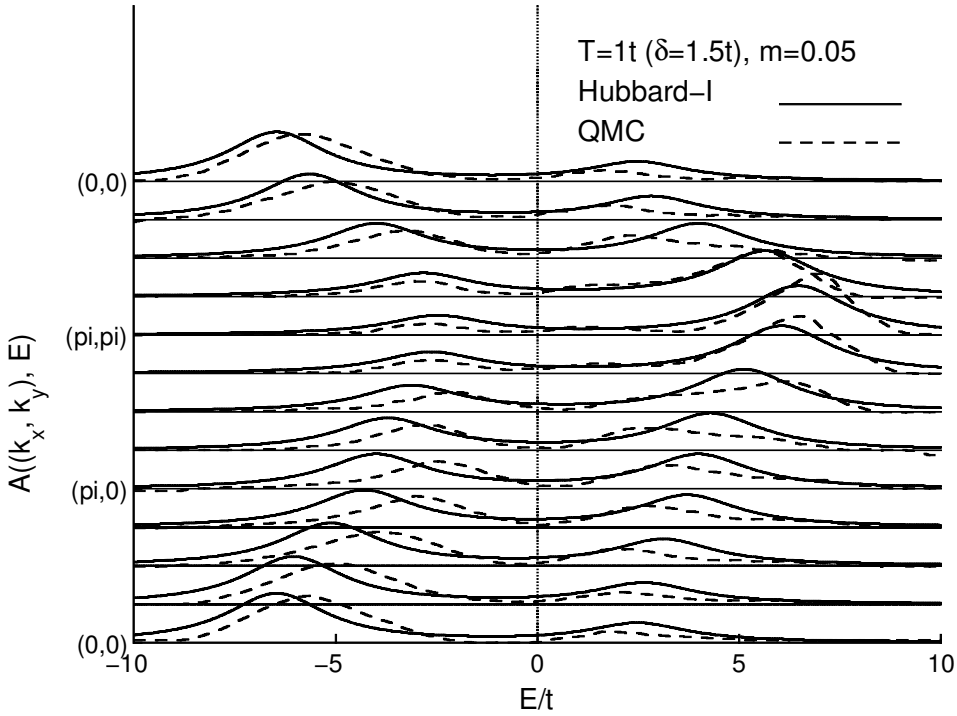

Fig. 2 The angle-resolved spectral function for half filled Hubbard model at low temperature, T=1t. The QMC data are taken from the work[4].

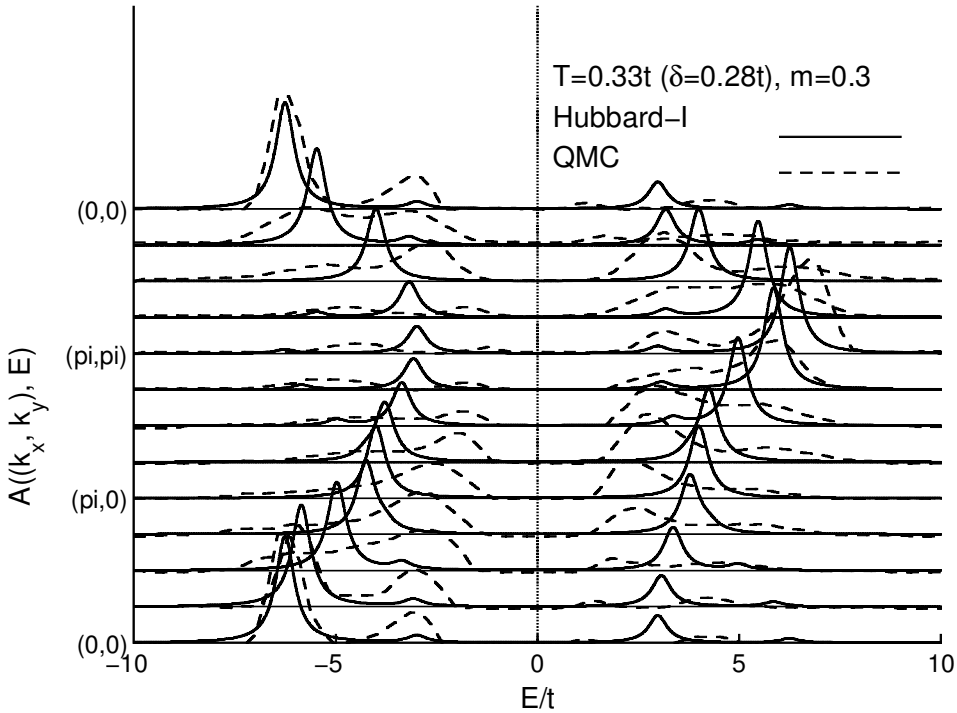

Fig. 3 The angle-resolved spectral function for half filled Hubbard model at media temperature. The QMC data are taken from the work[4].

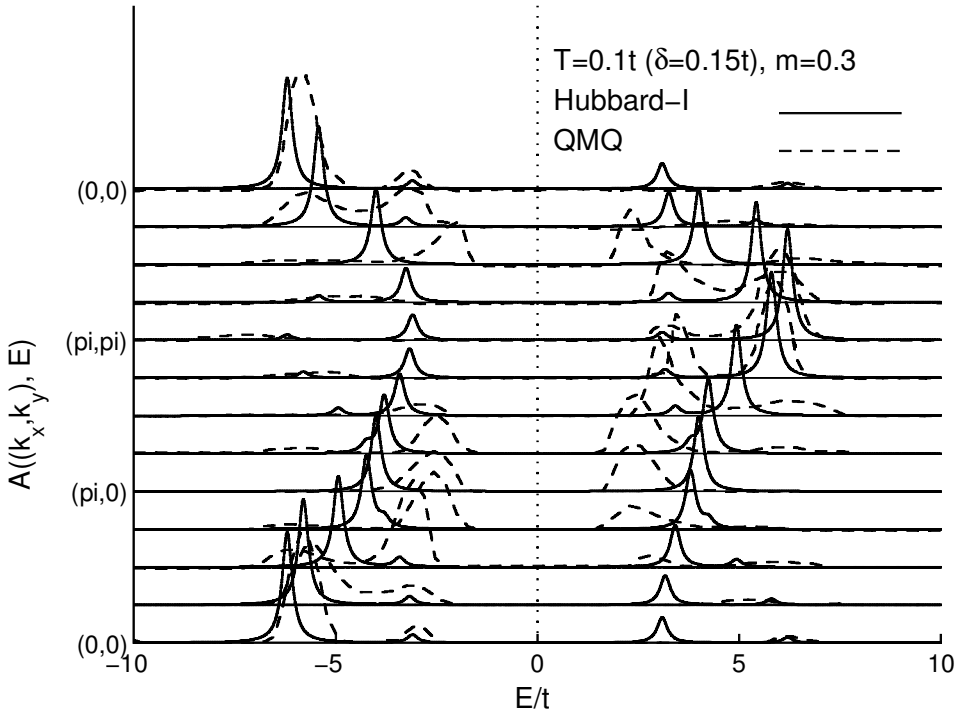

Fig. 4 The angle-resolved spectral function for half filled Hubbard model at low temperature. The QMC data are taken from the work[4].

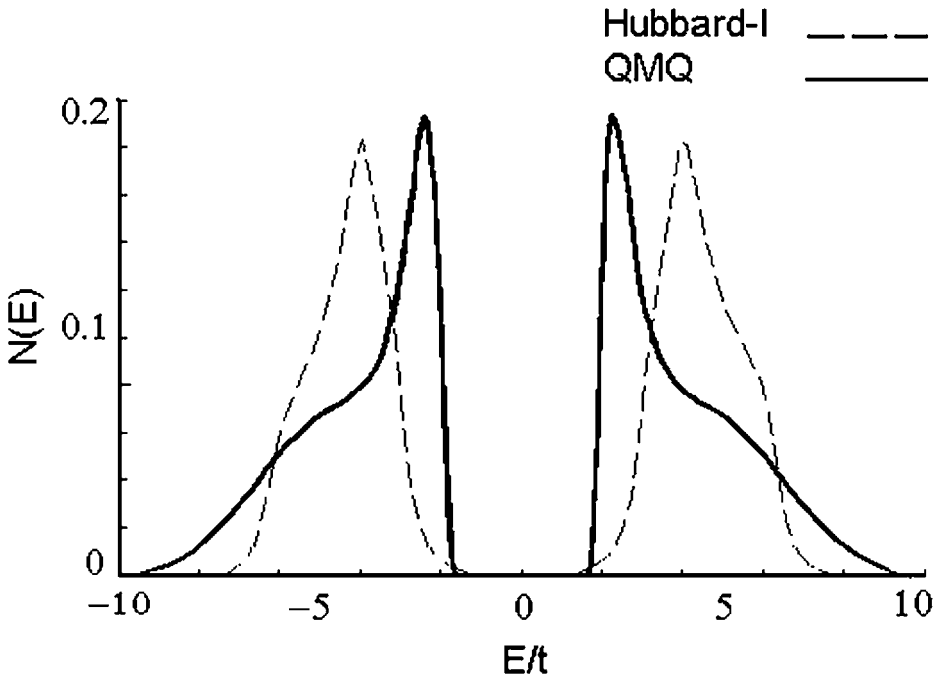

Fig. 5 The single-particle density of states for half-filled Hubbard model. The QMC data are taken from the work[8].