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Comparison of the non-crossing perturbative approach and the generalized projection method for strongly coupled spin-fermion systems at low doping

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Abstract. We analyse the two-dimensional spin-fermion model in the strong-coupling regime relevant to underdoped cuprates. We recall the set of general sum rules that relate the moments of spectral density and the imaginary part of the fermion self-energy to the static correlation functions. We show that the two-pole approximation of the projection method satisfies the sum rules for the first four moments of the spectral density and gives an exact upper bound for the quasiparticle energy near the band bottom. We prove that the non-crossing approximation that is often made in perturbative considerations of the model violates the sum rule for the third moment of the spectral density. This leads to incorrect positioning of the lowest quasiparticle band. On the other hand, the projection method is inadequate in the weak-coupling limit because of the approximate treatment of the kinetic energy term. We propose a generalization of the projection method that resolves this problem, and give a fermion self-energy that behaves correctly in both the weak- and strong-coupling limits.

1. Introduction

Over the past few years it has become increasingly clear that the anomalous normal- and superconducting-state properties of high-T_c cuprates are governed by their proximity to the transition into the antiferromagnetic Mott–Hubbard insulator state. The transition occurs for strongly underdoped systems. There are many indications that even overdoped cuprates are never far from being antiferromagnetic [1, 2]. Such kinds of incipient antiferromagnet at low temperatures have both fermionic and spin excitations that interact strongly. For the description of such interaction, the two-dimensional spin-fermion models (SFM) are used. They have a general form

$$\hat{H} = \hat{H}_{kin} + \hat{H}_s + \hat{H}_{int}. \tag{1}$$

Here the kinetic energy term

$$\hat{H}_{kin} = \sum_p \epsilon_p a_p^\dagger a_p \qquad a_p = N^{-1/2} \sum_r a_r \mathrm{e}^{-\mathrm{i}pr}$$

describes the bare-fermion propagation. We take, for definiteness, the simplest version of nearest-neighbour hopping, $\epsilon_p = -2t(\cos p_x + \cos p_y)$. The spin subsystem may be described by the microscopic Heisenberg Hamiltonian

$$\hat{H}_s = \frac{1}{2} I \sum_{rg} S^\alpha_{r+g} S^\alpha_r$$

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or quite generally by a phenomenological form of the dynamic susceptibility [3] $\chi(q,\omega)$, as long as we are only interested in the fermion spectrum. In the present work, we suppose that the spin subsystem is in the paramagnetic state $\langle S_r^\alpha \rangle = 0$ with strong antiferromagnetic correlations $C_g = \langle S_{r+g}^\alpha S_r^\alpha \rangle < 0$; the correlation function

$$C_q = N^{-1} \sum_r \exp(\mathrm{i}qr) \langle S_{\rho+r}^\alpha S_\rho^\alpha \rangle$$

is strongly peaked at wave vectors in the vicinity of $Q = (\pi, \pi)$.

The third term in its simplest form describes the Kondo interaction:

$$\hat{H}_{int} = J \sum_r a_r^\dagger \tilde{S}_r a_r = \frac{J}{\sqrt{N}} \sum_{pq} a_p^\dagger \tilde{S}_q a_{p+q} \qquad \tilde{S}_q = N^{-1/2} \sum_r \tilde{S}_r \mathrm{e}^{\mathrm{i}qr}. \quad (2)$$

In the above formulae the sums run over the sites r of a square lattice and over the nearest neighbours with the lattice spacing $|g| = 1$. For brevity, we discard the spin index for the creation ($a_{r\sigma}^+$) and annihilation ($a_{r\sigma}$) operators of the Fermi particles (we shall call them electrons), and in the Hamiltonian of the Kondo interaction H_{int} we use the notation $\tilde{S}_r = S_r^\alpha \sigma^\alpha$; summation over repeated indices is everywhere understood; the σ^α are the Pauli matrices. $\langle \cdots \rangle$ indicates thermodynamic averaging over the grand canonical ensemble.

In order to achieve a more realistic description, the interaction term may be generalized by the addition of nearest-neighbour coupling, $a_r^\dagger \tilde{S}_r a_{r+g} + \mathrm{HC}$ etc [4]. It is essential that in all cases $\hat{H}_{int}$ remains local in real space and does not couple directly to the excitations on sites separated by large distances.

The usual approaches to the Hamiltonian (1) exploit its apparent similarity to that of the polaron problem. Various perturbative methods have the advantage of giving an exact treatment of the one-particle part, $\hat{H}_{kin}$. It is widely believed that the non-crossing approximation [2, 4–6] is appropriate for spin-fermion systems even in the strong-coupling regime, $J \gg t$. Below, we shall prove that in this regime the non-crossing approximation for the SFM violates the sum rule for the third moment of the spectral density; as a result, it gives incorrect positioning of the lowest 'singlet' band. An alternative is the Mori–Zwanzig projection technique [7]; due to the local nature of $\hat{H}_{int}$, it suffices to use a small number of basic operators to give an appropriate account of the local correlations. The obvious disadvantage of the technique is that the kinetic energy is treated in an approximate way; as a consequence, this technique fails to correctly describe the weak-coupling regime, $J \ll t$. In the present paper, we take the kinetic energy term into account exactly and use the projection method for the remaining terms. As a result, we obtain a fermion self-energy that behaves correctly in the weak-coupling limit and gives the correct lowest-band position in the strong-coupling limit.

2. Sum rules for the Green's function and the self-energy

The quantities that we calculate are the retarded fermion Green's function (GF)

$$G_{XY}(\omega) = \langle X | Y^\dagger \rangle \equiv -\mathrm{i} \int_{t'}^{\infty} \mathrm{d}t \, \mathrm{e}^{\mathrm{i}\omega(t-t')} \langle \{X(t), Y^\dagger(t')\} \rangle. \quad (3)$$

and the spectral density

$$A_{XY}(\omega) = -\frac{1}{\pi} \mathrm{Im}[G_{XY}(\omega + \mathrm{i}0)].$$

Here and below, $\{\ldots,\ldots\}, [\ldots,\ldots]$ stand for anticommutators and commutators respectively. For the diagonal GF, with $Y = X$, the spectral density is positive definite,

$A_{XX}(\omega) > 0$. The Mori–Zwanzig projection method allows us to represent $G_{XX}(z)$, for $\mathrm{Im}\, z > 0$, in the continued-fraction form [8, 9]:

$$G_{XX}(z) = \cfrac{b_0^2}{z - a_0 - \cfrac{b_1^2}{z - a_1 - \cdots - \cfrac{b_n^2}{z - a_n - \cdots}}} \tag{4}$$

where

$$b_0^2 = \int_{-\infty}^{+\infty} A_{XX}(\omega)\ \mathrm{d}\omega \qquad a_0 = \frac{1}{b_0^2}\int_{-\infty}^{+\infty} \omega A_{XX}(\omega)\ \mathrm{d}\omega. \tag{5}$$

The coefficients $b_n, a_n, n > 0$ are related to the spectral density $A_{XX}(\omega)$ via the set of orthogonal polynomials $P_n(\omega)$, satisfying the recurrence [10, 11]

$$\begin{aligned} &P_{-1}(\omega) = 0 \qquad P_0(\omega) = 1 \\ &P_{n+1}(\omega) = (\omega - a_n)P_n(\omega) - b_n^2 P_{n-1}(\omega) \end{aligned} \tag{6}$$

where

$$b_{n+1}^2 = \left(\int_{-\infty}^{+\infty} P_{n+1}^2(\omega)A_{XX}(\omega)\ \mathrm{d}\omega\right)\Big/\left(\int_{-\infty}^{+\infty} P_n^2(\omega)A_{XX}(\omega)\ \mathrm{d}\omega\right) \tag{7}$$

$$a_{n+1} = \left(\int_{-\infty}^{+\infty} \omega P_{n+1}^2(\omega)A_{XX}(\omega)\ \mathrm{d}\omega\right)\Big/\left(\int_{-\infty}^{+\infty} P_{n+1}^2(\omega)A_{XX}(\omega)\ \mathrm{d}\omega\right). \tag{8}$$

Here we have used the non-normalized form of the polynomials:

$$\int_{-\infty}^{+\infty} P_n(\omega)P_s(\omega)A_{XX}(\omega)\ \mathrm{d}\omega = \delta_{ns}\left(\prod_{m=1}^{m=n} b_m\right)^2.$$

On the other hand, from the equation of motion,

$$\omega\langle X|Y^\dagger\rangle = \langle\{X, Y^\dagger\}\rangle + \langle X\mathcal{L}|Y^\dagger\rangle \qquad X\mathcal{L} \equiv [X, \hat{H}] \tag{9}$$

the sum rule

$$\int_{-\infty}^{+\infty} F(\omega)A_{XY}(\omega)\ \mathrm{d}\omega = \left\langle\{XF(\mathcal{L}), Y^\dagger\}\right\rangle \tag{10}$$

follows for arbitrary functions $F(\mathcal{L})$. In particular, this establishes the relations of the coefficients a_n, b_n with the static correlation functions:

$$b_0^2 = \left\langle\{X, X^\dagger\}\right\rangle \qquad a_0 = \frac{\left\langle\{X\mathcal{L}, X^\dagger\}\right\rangle}{\left\langle\{X, X^\dagger\}\right\rangle} \tag{11}$$

$$b_1^2 = \frac{\left\langle\{X(\mathcal{L} - a_0)^2, X^\dagger\}\right\rangle}{\left\langle\{X, X^\dagger\}\right\rangle} \qquad a_1 = \frac{\left\langle\{X\mathcal{L}(\mathcal{L} - a_0)^2, X^\dagger\}\right\rangle}{\left\langle\{X(\mathcal{L} - a_0)^2, X^\dagger\}\right\rangle}. \tag{12}$$

Now, introducing the self-energy $\Sigma(z)$ through the relation

$$\left(z - \frac{\left\langle\{X\mathcal{L}, X^\dagger\}\right\rangle}{\left\langle\{X, X^\dagger\}\right\rangle} - \Sigma(z)\right)G_{XX}(z) = \left\langle\{X, X^\dagger\}\right\rangle \tag{13}$$

and comparing (4) and (13), we see that $\Sigma(z)$ is a continued fraction similar to $G(z)$. Thus we can introduce the spectral density

$$\rho(\omega) = -\mathrm{Im}[\Sigma(\omega + \mathrm{i}0^+)]/\pi$$

and obtain for it sum rules that follow from (10):

$$b_1^2 = \int_{-\infty}^{\infty} \rho(\omega)\ \mathrm{d}\omega \tag{14}$$

$$a_1 = \frac{1}{b_1^2}\int_{-\infty}^{+\infty} \omega\rho(\omega)\ \mathrm{d}\omega. \tag{15}$$

As follows from (12) and (8), the last equality relates the third moment of $A_{XX}(\omega)$, the first moment of $\rho(\omega)$, and the static correlation functions. For spin-fermion models in the limit of low doping, the spin–spin correlation functions are only involved in (12). Below, we show that non-crossing approximation violates sum rule (15) for the SFM, and is obviously incorrect in the strong-coupling limit, $J \gg t$.

3. The projection technique

In practice, projection technique calculations are possible only for a finite basis set, and only a finite number of continued-fraction levels can be calculated in (4).

In the framework of the SFM, we have

$$(\omega - \epsilon_p)\langle a_p|a_p^\dagger\rangle = 1 + J\sqrt{f_2}\langle b_p|a_p^\dagger\rangle \qquad b_p = N^{-1/2}\sum_r b_r \mathrm{e}^{-\mathrm{i}pr} \tag{16}$$

where

$$b_r = \frac{1}{\sqrt{f_2}}\tilde{S}_r a_r \qquad f_2 = \langle \tilde{S}_r \tilde{S}_r\rangle = \frac{3}{4}.$$

Thus, the 'bare'-electron operators a_r with the one-site spin-polaron operators b_r represent the natural basis set for giving an appropriate account of local correlations. It is important that this set is closed with respect to $\hat{H}_{int}$, i.e.

$$[a_r, \hat{H}_{int}] = J\sqrt{f_2}b_r \qquad [b_r, \hat{H}_{int}] = J(\sqrt{f_2}a_r - b_r). \tag{17}$$

Now the commutation relation

$$[\tilde{S}_{r+R}a_r, \hat{H}] = -t\sum_g \tilde{S}_{r+R}a_{r+g} + J\tilde{S}_{r+R}\tilde{S}_r a_r + [\tilde{S}_{r+R}a_r, \hat{H}_s] \tag{18}$$

is projected onto the basis set in order to decouple the equation of motion for the higher-order GFs $G_b(p,\omega) \equiv \langle b_p|a_p^\dagger\rangle$. In the following, we neglect the spin-excitation energy $I \ll t, J$:

$$\omega G_b = \langle [b_p, \hat{H}]|a_p^\dagger\rangle \simeq \left(\frac{C_g}{f_2}\epsilon_p - J\right)G_b + J\sqrt{f_2}G_a. \tag{19}$$

This gives both GFs in the two-pole approximation:

$$G^{(2)}_{a,b}(p,\omega) = \frac{|\alpha^S_{a,b}|^2}{\omega - \Omega_S} + \frac{|\alpha^T_{a,b}|^2}{\omega - \Omega_T} \qquad |\alpha^S_{a,b}|^2 + |\alpha^T_{a,b}|^2 = 1. \tag{20}$$

Here Ω_n, α_i^n, where $i = a, b$, and $n = ST$ $(\Omega_S < \Omega_T)$, are eigenvalues and eigenvectors of the problem

$$\begin{pmatrix} a_0 - \Omega_n & b_1 \\ b_1 & a_1 - \Omega_n \end{pmatrix}\begin{pmatrix} \alpha_1^n \\ \alpha_2^n \end{pmatrix} = 0 \tag{21}$$

where the matrix elements are

$$a_0 = \epsilon_p \qquad b_1 = J\sqrt{f_2} \qquad a_1 = \frac{C_g}{f_2}\epsilon_p - J. \tag{22}$$

If we take into account the normalization $b_0^2 = 1$, we see that the matrix elements correspond to continued-fraction coefficients of $G_a^{(2)}$ that coincide with the first two pairs of coefficients of the exact GF G_a. This means that $G_a^{(2)}$ automatically satisfies the sum rules (11), (14), and (15).

Near the band bottom, G_a and A_{aa} should have the forms

$$\begin{aligned} G_a(p,\omega) &= \frac{Z_a(p)}{\omega - E_p} + G_{inc} \\ A_{aa}(p,\omega) &= Z_a(p)\delta(\omega - E_p) + A_{inc}(p,\omega). \end{aligned} \tag{23}$$

Here E_p and $Z(p) < 1$ are the quasiparticle energy and the pole strength respectively. The incoherent part A_{inc} is not zero for $\omega > \omega_{min} > E_p$. Now it is easy to show that Ω_S represents an *exact upper bound* for E_p. Let us consider the eigen-operator for the lowest 'singlet' band:

$$\xi_S = \alpha_a^S a_p + \alpha_b^S b_p.$$

The GF

$$G_{\xi\xi} = \langle \xi_S | \xi_S^\dagger \rangle = \frac{Z_\xi(p)}{\omega - E_p} + G_{\xi\xi,inc}$$

has a pole at the same energy as the bare-fermion GF, G_a (in our model, $\alpha_a^S \neq 0$ for all p). On the other hand, from (5) and (21) we have

$$\Omega_S = Z_\xi(p)E_p + \int_{\omega_{min}}^{\infty} \omega A_{\xi\xi,inc}(p,\omega)\ \mathrm{d}\omega = Z_\xi(p)E_p + \left[1 - Z_\xi(p)\right]\Omega_{inc}. \tag{24}$$

Here,

$$\Omega_{inc} \equiv \left(\int_{\omega_{min}}^{\infty} \omega A_{\xi\xi,inc}(p,\omega)\ \mathrm{d}\omega\right) \Big/ \left(\int_{\omega_{min}}^{\infty} A_{\xi\xi,inc}(p,\omega)\ \mathrm{d}\omega\right) \geqslant \omega_{min}$$

is the centre of gravity of the incoherent part. As the pole strength lies in the range $0 \leqslant Z_\xi(p) \leqslant 1$, we have

$$E_p \leqslant \Omega_S \leqslant \Omega_{inc}. \tag{25}$$

That is, for any p close to the band bottom, the exact energy E_p is *always lower* than the energy given by the two-pole approximation.

In the strong-coupling limit, this gives

$$\Omega_S \approx -\frac{3}{2}J + \epsilon_p\left(\frac{1}{4} + C_g\right) \tag{26}$$

and from (24) it follows that the actual pole position is lower than Ω_S. It is not difficult to calculate the next continued-fraction coefficient:

$$b_2^2 = \frac{1}{f_2 N}\sum_q \left(\epsilon_{p+q} - \frac{4}{3}C_g\epsilon_p\right)^2 C_q \approx \left(\epsilon_{p+Q} - \frac{4}{3}C_g\epsilon_p\right)^2. \tag{27}$$

In the approximate equality we took into account the fact that the main contribution to the sum over q comes from the vicinity of Q, and $N^{-1}\sum_q C_q = f_2$. We see that b_2 is of the order of the kinetic energy $t \ll J$. This means that the small polaron formed by our basic operators interacts with the spin subsystem much more weakly than the bare hole. So, the expected polaron energy renormalization from Ω_S to E_p is of the order of t^2/J.

4. Exact treatment of the kinetic energy

From the above consideration, it follows that the two-pole expression (20) is useful in the strong-coupling limit. In the opposite case of $J \ll t$, it becomes inappropriate, because it gives the self-energy in the one-pole form

$$\Sigma^{(2)}(z) = b_1^2/(z - a_1) \tag{28}$$

and cannot describe the damping of quasiparticles. The reason for this lies in the approximate treatment of the kinetic energy term in the course of the projection of the equation for G_b, expression (19). Here we propose a generalization of the projection technique that completely removes this shortcoming, and makes it possible to take the kinetic energy term into account exactly.

We express b_p in the following form:

$$b_p = \frac{1}{\sqrt{Nf_2}} \sum_q \tilde{S}_q a_{p+q}. \tag{29}$$

The equation of motion for every term gives

$$(\omega - \epsilon_{p+q})\langle \tilde{S}_q a_{p+q} | a_{p_1}^\dagger \rangle = \langle [\tilde{S}_q a_{p+q}, \hat{V}] | a_{p_1}^\dagger \rangle. \tag{30}$$

Here and below, we use the notation $\hat{V} = \hat{H}_{int} + \hat{H}_s$. Now we project the higher-order operator on the right-hand side of (30) onto our basis operators $B_{1,p} \equiv a_p$, $B_{2,p} \equiv b_p$:

$$\begin{aligned}
\langle \{ [\tilde{S}_q a_{p+q}, \hat{V}], B_{i,p}^\dagger \} \rangle &= \frac{1}{N\sqrt{N}} \sum_{r_1 r_2 r_3} \langle \{ [\tilde{S}_{r_1} a_{r_2}, \hat{V}], B_{i,r_3}^\dagger \} \rangle \exp(\mathrm{i}qr_1 - \mathrm{i}(p+q)r_2 + \mathrm{i}pr_3) \\
&= \frac{1}{N\sqrt{N}} \sum_{r_1 r_2 r_3} \langle \{ [\tilde{S}_{r_1}, \hat{V}] a_{r_2} + \tilde{S}_{r_1} [a_{r_2}, \hat{V}], B_{i,r_3}^\dagger \} \rangle \exp(\mathrm{i}q(r_1 - r_2) + \mathrm{i}p(r_3 - r_2)) \\
&= \frac{1}{\sqrt{N}} \sum_R \langle \{ [\tilde{S}_{r+R}, \hat{V}] a_r + \tilde{S}_{r+R} [a_r, \hat{V}], B_{i,r}^\dagger \} \rangle \exp(\mathrm{i}qR) \\
&= \frac{1}{\sqrt{N}} \sum_R K_{i,R} \exp(\mathrm{i}qR) \equiv \frac{1}{\sqrt{N}} K_{i,q}
\end{aligned} \tag{31}$$

where $i = 1, 2$. We have used the local character of the operator $\hat{V}$ that gives δ_{r_2, r_3}. Thus equation (30) may be rewritten as

$$(\omega - \epsilon_{p+q})\langle \tilde{S}_q a_{p+q} | a_{p_1}^\dagger \rangle \simeq \frac{1}{\sqrt{N}} \sum_i K_{i,q} \langle B_{i,p} | a_{p_1}^\dagger \rangle. \tag{32}$$

Now, the equation for b_p is

$$\langle b_p | a_{p_1}^\dagger \rangle = \frac{1}{\sqrt{Nf_2}} \sum_q \langle \tilde{S}_q a_{p+q} | a_{p_1}^\dagger \rangle = \frac{1}{N\sqrt{f_2}} \sum_{i,q} \frac{K_{i,q}}{(\omega - \epsilon_{p+q})} \langle B_{i,p} | a_{p_1}^\dagger \rangle. \tag{33}$$

Explicit calculation gives ($I \approx 0$)

$$K_{1,q} = JC_q \qquad K_{2,q} = -\frac{J}{\sqrt{f_2}} C_q$$

and we obtain the following form for the fermion self-energy:

$$\Sigma(p, \omega) = \frac{J^2 f_2}{J + f_2 D_p^{-1}} \qquad D_p(\omega) \equiv \frac{1}{N} \sum_q \frac{C_q}{(\omega - \epsilon_{p+q})}. \tag{34}$$

In the weak-coupling limit, $J \ll t$, this expression coincides with the second-order result from perturbation theory:

$$\Sigma_{pert}(p,\omega) = J^2 D_p(\omega) \tag{35}$$

which corresponds to projecting (31) only on the first operator a_p. In this limit, a polaron of large radius is formed, and the bare fermion represents a slightly damped quasiparticle.

Now let us show that the self-energy (34) also gives the correct result in the strong-coupling limit. The pole position is given by $E_p - \epsilon_p - \Sigma(p, E_p) = 0$. For determination of the lowest-band position, we may neglect the $\epsilon_{p+q} \propto t$ compared with $\omega \propto -J$, and write $D_p(\omega) \approx f_2/\omega$; then,

$$\Sigma(p,\omega) \approx \frac{J^2 f_2}{J + f_2\omega/f_2}$$

$$E_p = \frac{\epsilon_p - J}{2} - \sqrt{\left(\frac{\epsilon_p + J}{2}\right)^2 + J^2 f_2} \approx -\frac{3}{2}J.$$

The perturbation theory result is

$$\Sigma_{pert}(p,\omega) \approx J^2 f_2/\omega$$

$$E_{pert} = \frac{\epsilon_p}{2} - \sqrt{\left(\frac{\epsilon_p}{2}\right)^2 + J^2 f_2} \approx -J\sqrt{\frac{3}{4}} > \Omega_S.$$

The reason that the perturbation theory fails is the violation of the sum rule (15) for the SFM. We have

$$\begin{aligned} \rho_{pert}(p,\omega) &= \frac{J^2}{N}\sum_q C_q \delta(\omega - \epsilon_{p+q}) \\ a_{1,pert} &= \frac{1}{b_1}\frac{J^2}{N}\sum_q C_q \int_{-\infty}^{+\infty} \omega\delta(\omega - \epsilon_{p+q})\ \mathrm{d}\omega = \frac{1}{f_2 N}\sum_q C_q \epsilon_{p+q} = \frac{C_g}{f_2}\epsilon_p. \end{aligned} \tag{36}$$

Comparing (36) with the exact value given by equation (22) we see that it is the absence of terms proportional to J that leads to the completely wrong result for $J \gg t$. It is not difficult to prove that summation of the infinite series of non-crossing diagrams for the self-energy does not change the value of $a_{1,pert}$ given by (36). Indeed, the non-crossing (self-consistent Born) approximation gives

$$\Sigma_{n-c}(p,\omega) = \frac{J^2}{N}\sum_q C_q G_a(p+q, \omega - \omega_q) \tag{37}$$

where ω_q is the energy of the spin excitations. We then have

$$a_{1,n-c} = \frac{1}{b_1}\frac{J^2}{N}\sum_q C_q \int_{-\infty}^{+\infty} \omega A_{aa}(p+q, \omega - \omega_q)\ \mathrm{d}\omega = \frac{1}{f_2 N}\sum_q C_q(\epsilon_{p+q} + \omega_q)$$

and obtain the same result (36) because ω_q is negligible, at least in the vicinity of $q = Q$.

Moreover, the self-energy (37) leads to the absence of quasiparticles. We may write

$$\Sigma_{n-c}(p,\omega) \approx J^2 f_2 G_a(p+Q,\omega).$$

Then,

$$\begin{aligned} G_a(p,\omega) &= \left[\omega - \epsilon_p - J^2 f_2 G_a(p+Q,\omega)\right]^{-1} \\ &= \left[\omega - \epsilon_p - \frac{J^2 f_2}{\omega - \epsilon_{p+Q} - J^2 f_2 G_a(p,\omega)}\right]^{-1}. \end{aligned}$$

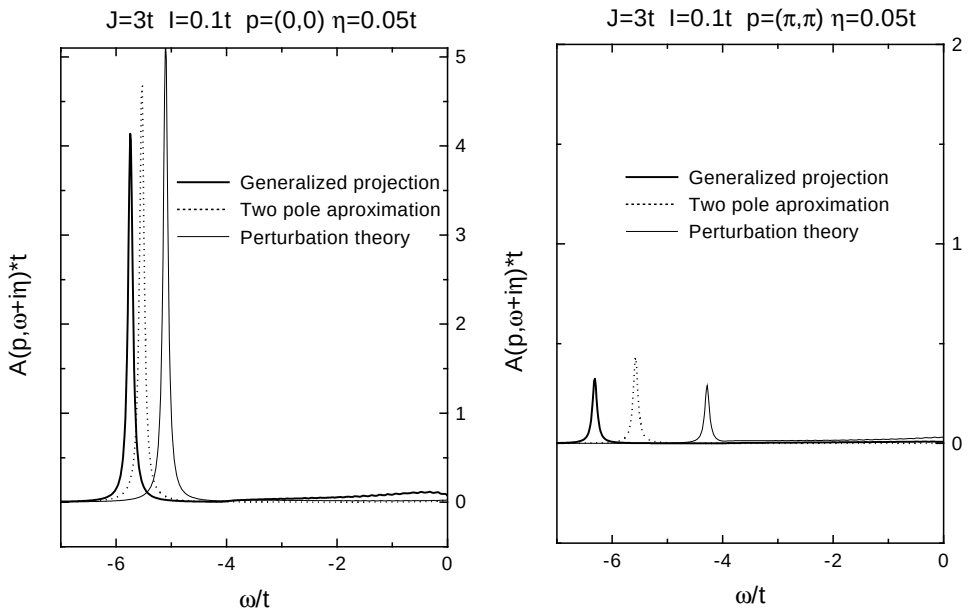

Figure 1. The spectral density of the one-particle Green's function with the self-energy obtained in three different ways: from the two-pole approximation, (28); from the generalized projection method, equation (34); and from second-order perturbation theory, equation (35).

Solution of the quadratic equation gives the expression for the Green's function:

$$G_a(p,\omega) = \frac{(\omega-\epsilon_p)(\omega-\epsilon_{p+Q}) - \sqrt{(\omega-\epsilon_p)^2(\omega-\epsilon_{p+Q})^2 - 4J^2 f_2(\omega-\epsilon_p)(\omega-\epsilon_{p+Q})}}{2J^2 f_2(\omega-\epsilon_p)}$$

which has no poles. An analogous result was obtained previously in reference [4].

5. Numerical results

In figure 1, we present the spectral densities $A_{aa}(p,\omega+\mathrm{i}\eta)$, $\eta = 0.05t$, that correspond to three different representations of the fermion self-energy: the two-pole approximation, equation (28); the generalized projection method, equation (34); and second-order perturbation theory, equation (35). We took the value $J/t = 3$, which is typical for underdoped cuprates [1–3]. For the spin–spin correlation function, we used the expression

$$C_q = \sqrt{\frac{3|C_g|(1-\gamma_q)}{2\alpha_1(1+\gamma_q)}}$$

which is provided by the spherically symmetric theory for the Heisenberg model on a square lattice [12, 13] ($\gamma_q \equiv (\cos q_x + \cos q_y)/2$, $C_g \approx -0.35$, $\alpha_1 \approx 2.35$). We calculate the function $D_p(\omega)$ by direct summation over $n \times n$ q-points in the Brillouin zone (the results for $n = 32$ and $n = 80$ are almost indistinguishable). From figure 1 we see that the lowest-pole position obtained by the generalized projection method satisfies the relation (25), in contrast to that given by perturbation theory.

Figure 2 shows the spectral function in the generalized projection method for various values of p along the diagonal of the Brillouin zone. Quasiparticle poles exist throughout

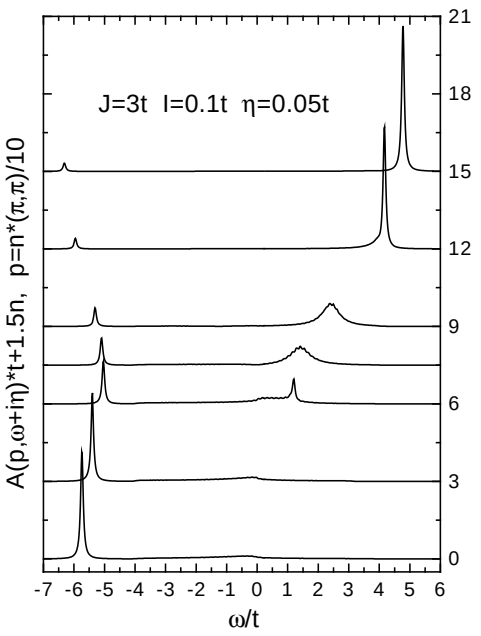

Figure 2. The spectral density in the generalized projection method as a function of the quasimomentum p in the strong-coupling regime, where $J/t = 3$.

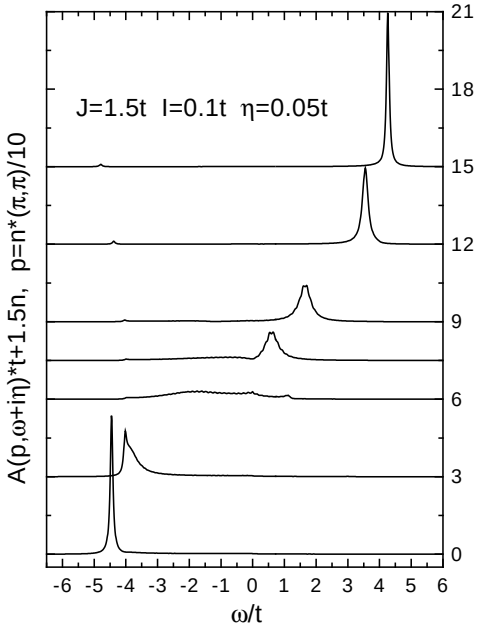

Figure 3. The spectral density in the intermediate-parameter regime.

the whole Brillouin zone. The quasiparticle dispersion E_p has only approximate symmetry relative to the boundary of the antiferromagnetic Brillouin zone. The strong asymmetry of the spectral weight in the generalized projection method is the consequence of the sum rule (5)—the centre of gravity $A_{aa}(p, \omega)$ should coincide with $a_0 = \epsilon_p$. So, near the point $p = (\pi, \pi)$, where the quasiparticle peak is far from ϵ_p, its weight is small.

We have shown above that the expression (34) gives reasonable solutions in both the weak- and strong-coupling limits. Thus we may expect it to be valid in the intermediate regime where $J \sim t$. Figure 3 shows the fermion spectral density for $J = 1.5t$. In this regime the quasiparticle solution exists only near the two band minima $p = (\pi, \pi)$ and $p = (0, 0)$. At other points (for which we can say that the quasiparticle pole lies within the band of bare fermions), the interaction mixes solutions with different p. For $p = 0.2(\pi, \pi)$ and $p = 0.8(\pi, \pi)$, we have resonant solutions near the bottom ($\epsilon_{min} = -4t$) and the top ($\epsilon_{max} = 4t$) of the bare-fermionic band respectively. Near $p = (\pi/2, \pi/2)$, we have a purely incoherent spectrum.

6. Conclusions

We have considered the spin-fermion model that is often used for the description of strongly correlated systems. We have compared two popular approaches to the calculation of the fermionic Green's function: the non-crossing approximation of perturbation theory and the Mori–Zwanzig projection technique. We have shown that the first of these is valid only in the weak-coupling regime while the second is valid only in the strong-coupling regime. For the model, the non-crossing approximation gives an incorrect position for the lowest quasiparticle band. The reason for this is the rough violation of the sum rule for the

third moment of the spectral density. The summation of the infinite series of non-crossing diagrams for the self-energy does not alter this result. We have proposed a generalized version of the projection method that treats the kinetic energy term that is quadratic in the fermion fields exactly. The resulting expression for the self-energy coincides with that of perturbation theory in the weak-coupling limit, and provides the correct quasiparticle pole position in the strong-coupling limit. We thus consider it as a good starting point for the investigation of the intermediate-coupling regime that is believed to be relevant for optimally doped cuprate compounds.

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