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A squeezed-state approach for the spin polaron in the t–J model

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Abstract. The ground-state energy of spin polarons is investigated by means of squeezed states. The analytical theory developed by Barentzen for the intermediate-coupling region in the t–J model is improved by a procedure of diagonalization of quadratic terms in the effective Hamiltonian through a squeezing transformation.

1. Introduction

Ever since the discovery of cuprate superconductors, many concepts of condensed matter physics have been used in attempts to determine its mechanism [1]. Of these, spin-based models have received more attention because of the antiferromagnetic characters of these compounds. In the absence of doping, these materials are antiferromagnetic insulators, and after doping, the holes become charge carriers in the antiferromagnetic background, which form a strongly correlated system. Such systems are widely considered through the t–J model, which was originally suggested by Anderson [2].

The motion of a hole in an antiferromagnetic background causes a distortion of the spin system, whose quantization as virtual excitations (magnons) in turn acts back on the hole to form a quasiparticle, called a spin polaron. The spin-polaron concept was introduced into physics by de Gennes [3] and Nagaev [4], and applied to high-T_c superconductors by Wood and Cook [5], by Mott [6], and as the spin-bag mechanism by Schrieffer *et al* and Ramsak and Horsch [7]. However, a thorough examination of the spin polaron in connection with high-T_c superconductors was considered numerically in the self-consistent Born approximation by Martinez and Horsch [8], and analytically in a series of papers by Barentzen [9]. In the latter approach, the spin polaron in the t–J model is treated within the intermediate-coupling theory, where the Fröhlich approximations were employed in order to obtain the quasiparticle energy and bandwidth. A recent work on the subject investigates the spectral weight of a spin polaron using the same approach [10].

In the present work we follow Barentzen's approach and go one step further to diagonalize the quadratic terms that appear in the Hamiltonian after certain Bogoliubov transformations. This is achieved by means of another unitary transformation which essentially generates squeezed magnon states. The squeezed states, which play an important role in quantum optics [11], have now been successfully applied to the calculation of various ground-state energies involving boson systems, such as phonons [12]. The same method is to be adapted for the magnons surrounding a hole in the spin polaron.

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Our aim in the present work is firstly to produce an improvement over the existing intermediate-coupling results for the spin polarons and secondly to present an application where squeezed boson states are successfully used. In section 2, after giving a brief summary of Barentzen's approach, we introduce a unitary transformation that will diagonalize the quadratic terms in the Hamiltonian. This section contains calculations of the ground-state energy, the bandwidth, and the spectral weight of a spin polaron for intermediate coupling strength. We discuss the results in section 3.

2. Theory

The Hamiltonian used in the t–J model is obtained from the two-dimensional single-band Hubbard Hamiltonian with strong intra-atomic Coulomb correlation U. We start with the following effective Hamiltonian obtained by Barentzen in the linear spin-wave approximation:

$$H = -\frac{1}{8}NJz(1-c)^2 + 2t\sum_{\langle ij\rangle}(f_i^+ f_j b_i + \mathrm{HC}) + \frac{1}{2}J(1-c)^2\sum_{\langle ij\rangle}(b_i^+ b_j^+ + b_i b_i + \mathrm{HC}) \tag{1}$$

where $t > 0$ is the hopping integral and $J = 4t^2/U$ represents an antiferromagnetic coupling in the Heisenberg interaction, and f_i^+ and b_i^+ are the creation operators for the hole and spin waves, respectively. $c = \langle f_i^+ f_i\rangle = M/N$ is the concentration of holes, and M is unity for a single hole. A similar expression is derived in several other works [8, 13]. If $\alpha = 2t/J$ is introduced as a dimensionless coupling parameter, then equation (1) becomes reminiscent of the Fröhlich Hamiltonian, which describes an electron interacting with LO phonons in a polar crystal.

One would expect α to take values around 5–6 in the high-T_c materials, which corresponds to an intermediate coupling strength. We can now make use of approximations employed in the Fröhlich polaron concept. The conservation of the total momentum for the hole system

$$\boldsymbol{K} = \sum_{\boldsymbol{k}} \boldsymbol{k} f_{\boldsymbol{k}}^+ f_{\boldsymbol{k}}$$

and the boson system

$$\boldsymbol{Q} = \sum_{\boldsymbol{q}} \boldsymbol{q} b_q^+ b_q$$

allows us to eliminate the momentum of the spin-wave system, through the first canonical transformation U introduced by Jost:

$$U = \sum_i \exp(-\mathrm{i}\boldsymbol{Q}\cdot\boldsymbol{R}_i) f_i^+ f_i. \tag{2}$$

Here $f_{\boldsymbol{k}}$ and $b_{\boldsymbol{k}}$ are the Fourier transforms of f_i and b_i, respectively.

The second transformation made by Barentzen is due to Bogoliubov:

$$V = \exp\left(\frac{1}{2}\sum_{\boldsymbol{q}} \theta_q (b_q^+ b_{-q}^+ - \mathrm{HC}\right) \tag{3}$$

where the parameters θ_q satisfy the relations

$$\sinh\theta_q = -\mathrm{sgn}(\gamma_q)\left(\frac{1-w_q}{2w_q}\right)^{1/2} \qquad \cosh\theta_q = \left(\frac{1+w_q}{2w_q}\right)^{1/2}. \tag{4}$$

In the preceding expressions $w_q = (1-\gamma_q^2)^{1/2}$ is the spin-wave dispersion relation for the square lattice and $\gamma_q = \frac{1}{2}(\cos q_x + \cos q_y)$ is the usual structure factor. A third transformation is achieved by means of the operator

$$W = \sum_{\boldsymbol{k}} \exp\left[N^{-1/2} \sum_{\boldsymbol{q}} \lambda_{\boldsymbol{q}}(\boldsymbol{k})(b_{\boldsymbol{q}} - b_{\boldsymbol{q}}^{+}) \right] f_{\boldsymbol{k}}^{+} f_{\boldsymbol{k}} \tag{5}$$

which generates coherent boson states.

With the help of these transformations, the Hamiltonian (1) becomes

$$H_{\boldsymbol{k}} = \sum_{\nu=0}^{\infty} H_{\boldsymbol{k}}^{(\nu)} \tag{6}$$

with

$$H_{\boldsymbol{k}}^{(0)} = -2\alpha\Omega(\boldsymbol{k}) + N^{-1} \sum_{\boldsymbol{q}} w_{\boldsymbol{q}} \lambda_{\boldsymbol{q}}^{2}(\boldsymbol{k}) \tag{7a}$$

$$H_{\boldsymbol{k}}^{(1)} = N^{-1/2} \sum_{\boldsymbol{q}} \left[\alpha F_{\boldsymbol{q}}(\boldsymbol{k}) - \epsilon_{\boldsymbol{q}}(\boldsymbol{k}) \lambda_{\boldsymbol{q}}(\boldsymbol{k}) \right] (b_{\boldsymbol{q}}^{+} + b_{\boldsymbol{q}}) \tag{7b}$$

$$H_{\boldsymbol{k}}^{(2)} = \sum_{\boldsymbol{q}} \epsilon_{\boldsymbol{q}}(\boldsymbol{k}) b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}} + \frac{\alpha}{2N} \sum_{\boldsymbol{q}\boldsymbol{q}'} \upsilon_{\boldsymbol{q}\boldsymbol{q}'} (b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}'}^{+} + b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}'} + \mathrm{HC}) \tag{7c}$$

where the unknown expressions are defined as follows:

$$\Omega(\boldsymbol{k}) = N^{-1} \sum_{\boldsymbol{q}} \lambda_{\boldsymbol{q}}(\boldsymbol{k}) F_{\boldsymbol{q}}(\boldsymbol{k}) \tag{8a}$$

$$\epsilon_{\boldsymbol{q}}(\boldsymbol{k}) = w_{\boldsymbol{q}} + 2\alpha\Omega(\boldsymbol{k}) \tag{8b}$$

$$\upsilon_{\boldsymbol{q}\boldsymbol{q}'}(\boldsymbol{k}) = \upsilon_{\boldsymbol{q}}(\boldsymbol{k}) \lambda_{\boldsymbol{q}'}(\boldsymbol{k}) + \boldsymbol{q} \leftrightarrow \boldsymbol{q}' \tag{8c}$$

$$\upsilon_{\boldsymbol{q}}(\boldsymbol{k}) = F_{\boldsymbol{q}}(\boldsymbol{k}) - \Omega(\boldsymbol{k}) \lambda_{\boldsymbol{q}}(\boldsymbol{k}) \tag{8d}$$

$$F_{\boldsymbol{q}}(\boldsymbol{k}) = F(\boldsymbol{k}) M_{\boldsymbol{q}}(\boldsymbol{k}) \tag{8e}$$

where $F(\boldsymbol{k})$ and $M_{\boldsymbol{q}}(\boldsymbol{k})$ are defined by the expressions

$$F(\boldsymbol{k}) = \exp\left(-N^{-1} \sum_{\boldsymbol{q}} \lambda_{\boldsymbol{q}}^{2}(\boldsymbol{k}) \right) \tag{9}$$

$$M_{\boldsymbol{q}}(\boldsymbol{k}) = \gamma_{\boldsymbol{k}} \sinh\theta_{\boldsymbol{q}} + \gamma_{\boldsymbol{k}-\boldsymbol{q}} \cosh\theta_{\boldsymbol{q}}. \tag{10}$$

In Barentzen's work, the first two terms in (6) have been considered by a variational method. In order to diagonalize $H_{\boldsymbol{k}}^{(2)}$ we now introduce a new unitary transformation:

$$S = \exp\left[\sum_{\boldsymbol{q} \neq \boldsymbol{q}'} \frac{\varphi_{\boldsymbol{q}\boldsymbol{q}'}}{N} (b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}'}^{+} - b_{\boldsymbol{q}} b_{\boldsymbol{q}'}) \right]. \tag{11}$$

This transformation generates squeezed boson states, and takes into account the correlation between two modes of the bosons. When applied to the ground state, it is therefore expected to give a more stable state. Here $\varphi_{\boldsymbol{q}\boldsymbol{q}'}$ is the squeezing angle depending on $\boldsymbol{q}$ and $\boldsymbol{q}'$, and defined as an element of a symmetrical 2×2 matrix with zero diagonal elements. Before applying the squeezing transformation it is convenient to rewrite the relevant Hamiltonian in the following symmetrical form:

$$H_{\boldsymbol{k}}^{(2)} = \frac{1}{2} \sum_{\boldsymbol{q}} \epsilon_{\boldsymbol{q}}(\boldsymbol{k}) b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}} + \frac{1}{2} \sum_{\boldsymbol{q}'} \epsilon_{\boldsymbol{q}'}(\boldsymbol{k}) b_{\boldsymbol{q}'}^{+} b_{\boldsymbol{q}'} + \frac{\alpha}{2N} \sum_{\boldsymbol{q}\boldsymbol{q}'} \upsilon_{\boldsymbol{q}\boldsymbol{q}'}(\boldsymbol{k}) (b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}'}^{+} + b_{\boldsymbol{q}}^{+} b_{\boldsymbol{q}'} + \mathrm{HC}). \tag{12}$$

The form of the quadratic operators under the squeezing transformation is given in reference [12]. Now, the ground-state energy $E(\boldsymbol{k})$ is obtained from the expectation value

$$E(\boldsymbol{k}) = w\langle 0|(H_{\boldsymbol{k}}^{(0)} + \tilde{H}_{\boldsymbol{k}}^{(2)})|0\rangle \tag{13}$$

where $|0\rangle$ is the vacuum state of the bosons, $w = zJ/2$, and $\tilde{H}_{\boldsymbol{k}}^{(2)} = S^{-1}H_{\boldsymbol{k}}^{(2)}S$. The energy in the dimensionless form becomes

$$\begin{aligned}\frac{E(\boldsymbol{k})}{w} &= -2\alpha\Omega(\boldsymbol{k}) + \frac{1}{2N}\sum_q w_q\lambda_q^2 + \frac{1}{2N}\sum_{q'} w_{q'}\lambda_{q'}^2 \\ &\quad + \frac{1}{2}\sum_{q,q'}\epsilon_q(\boldsymbol{k})\sinh^2\left(\frac{\varphi_{qq'}}{N}\right) + \frac{1}{2}\sum_{q,q'}\epsilon_q(\boldsymbol{k})\sinh^2\left(\frac{\varphi_{qq'}}{N}\right) \\ &\quad + \frac{\alpha}{2N}\sum_{q,q'}\left\{\upsilon_{qq'}(\boldsymbol{k})\sinh\left(\frac{\varphi_{qq'}}{N}\right)\cosh\left(\frac{\varphi_{qq'}}{N}\right)\right. \\ &\quad \left. + \upsilon_{qq'}^*(\boldsymbol{k})\sinh\left(\frac{\varphi_{qq'}}{N}\right)\cosh\left(\frac{\varphi_{qq'}}{N}\right)\right\}.\end{aligned} \tag{14}$$

It should be mentioned that there is no contribution to the energy from $H_k^{(1)}$ and the $b_q^+b_{q'}$ term of $H_k^{(2)}$. Furthermore, certain approximations have been made as regards the transformed operators $S^{-1}b_q^+b_{q'}^+S$ and $S^{-1}b_qb_{q'}S$, as discussed in the appendix of reference [12].

The minimization of this energy with respect to $\lambda_{q''}$ and $\varphi_{qq'}$ gives

$$\begin{aligned}&-2\alpha F_{q''} + 2\lambda_{q''}\epsilon_{q''}(k) + 2\alpha(F_{q''} - 2\Omega\lambda_{q''})\sum_{q,q'}\sinh^2\left(\frac{\varphi_{qq'}}{N}\right) \\ &\quad + \alpha\sum_q(F_q - 2\Omega\lambda_q)\sinh\left(\frac{2\varphi_{qq'}}{N}\right) = 0\end{aligned} \tag{15}$$

and

$$(\epsilon_q + \epsilon_{q'})\sinh\left(\frac{2\varphi_{qq'}}{N}\right) + \frac{\alpha}{N}\upsilon_{qq'}\cosh\left(\frac{2\varphi_{qq'}}{N}\right) = 0. \tag{16}$$

In (15), the higher-order terms of $\lambda_{q''}$ are neglected as an approximation. Furthermore, $\lambda_{q''}$ is obtained from (15) by taking

$$\lambda_q = \alpha\frac{F_q(\boldsymbol{k})}{\epsilon_q(\boldsymbol{k})}$$

in the last sum of this equation. The two coupled equations are to be solved self-consistently for the parameters λ_q and $\varphi_{qq'}$ at certain points $\boldsymbol{k}$ of the Brillouin zone. The use of these parameters in (14) gives us the ground-state energy of the spin polaron. Since N is large, $\varphi_{qq'}/N$ is small; therefore one can take $\sinh(\varphi_{qq'}/N) \simeq \varphi_{qq'}/N$ and $\cosh(\varphi_{qq'}/N) \simeq 1$ in (15) and (16). It is not possible to obtain the energy relation (14) in a closed form by eliminating λ_q or $\varphi_{qq'}$; therefore the calculation will be carried out numerically. We write the three related equations to be solved self-consistently as follows:

$$\Omega(\boldsymbol{k}) = F^2(\boldsymbol{k})X(\boldsymbol{k}) \tag{17a}$$

$$X(\boldsymbol{k}) = \frac{\alpha}{N}\sum_{q''}\left[\left\{M_{q''} - \frac{M_{q''}w_{q''}}{\epsilon_{q''}}\sum_{q,q'}(\varphi_{qq'})^2 - \sum_q\frac{M_qw_q}{\epsilon_q}\varphi_{qq''}\right\}\frac{M_{q''}}{\epsilon_{q''}}\right] \tag{17b}$$

$$\ln F(\boldsymbol{k}) = -\frac{\alpha^2}{N}\sum_{q''}\left\{\left[M_{q''} - \frac{M_{q''}w_{q''}}{\epsilon_{q''}}\sum_{q,q'}(\varphi_{qq'})^2 - \sum_q\frac{M_qw_q}{\epsilon_q}\varphi_{qq''}\right]\frac{F(\boldsymbol{k})}{\epsilon_{q''}}\right\}^2. \tag{17c}$$

We choose an initial value for Ω and calculate X and F from (17b) and (17c), respectively, from which we then obtain a new value for Ω through (17a). This process is carried out until their differences reach a given accuracy. The final values so found are to be used in (14) to obtain energies.

We now turn to the calculation of the spectral weight $Z_{\boldsymbol{k}}$ of the hole at the momentum $\boldsymbol{k}$, which is defined as [10]

$$Z_{\boldsymbol{k}} = \left|\langle\phi_{\boldsymbol{k}}^{(0)}|\phi_{\boldsymbol{k}}\rangle\right|^2. \tag{18}$$

Here $|\phi_{\boldsymbol{k}}^{(0)}\rangle = |f_{\boldsymbol{k}}^{+}0\rangle$ and $|\phi_{\boldsymbol{k}}\rangle = UWVS|f_{\boldsymbol{k}}^{+}0\rangle$ denote the unperturbed ground state and the ground state of the full Hamiltonian. Then, the spectral weight $Z_{\boldsymbol{k}}$ becomes

$$Z_{\boldsymbol{k}} = \exp\left[-\frac{1}{2N}\sum_{\boldsymbol{q}}\lambda_{\boldsymbol{q}}^2 - \sum_{\boldsymbol{q}\boldsymbol{q}'}\left(\frac{\varphi_{\boldsymbol{q}\boldsymbol{q}'}}{N}\right)^2\right] \tag{19}$$

where the Baker–Campbell–Hausdorff formula is used [14] and the first term in the squeezing parameter has been considered.

3. Results and discussion

The ground-state energy of the spin polaron is obtained from (17a), (17b), (17c), together with equations (8) by solving self-consistently at certain points $\boldsymbol{k}$ of the Brillouin zone. Figure 1 shows the quasiparticle energy dispersion along the direction ΓMXΓ of the BZ. Our result does indeed give a more stable ground-state energy comparing with the Barentzen's work; in particular the difference is more pronounced around the points $\overline{\mathrm{M}}$ and X. At $\overline{\mathrm{M}}$, for which

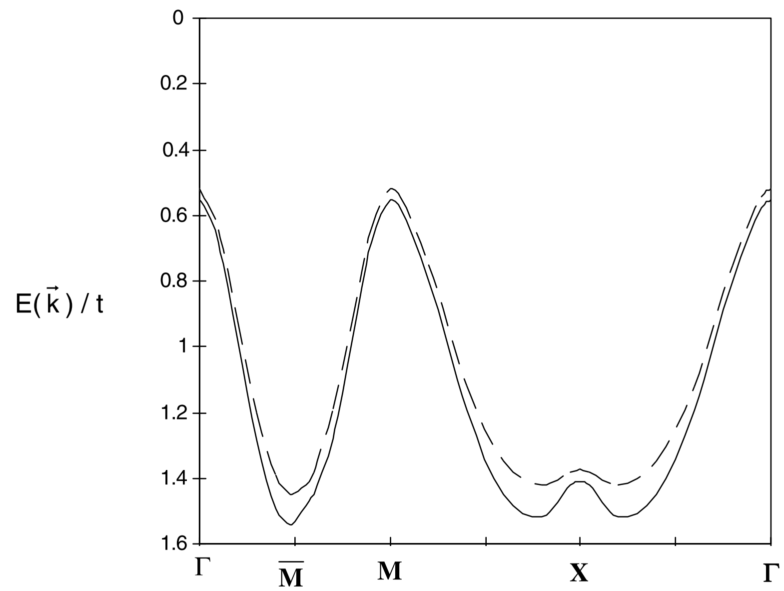
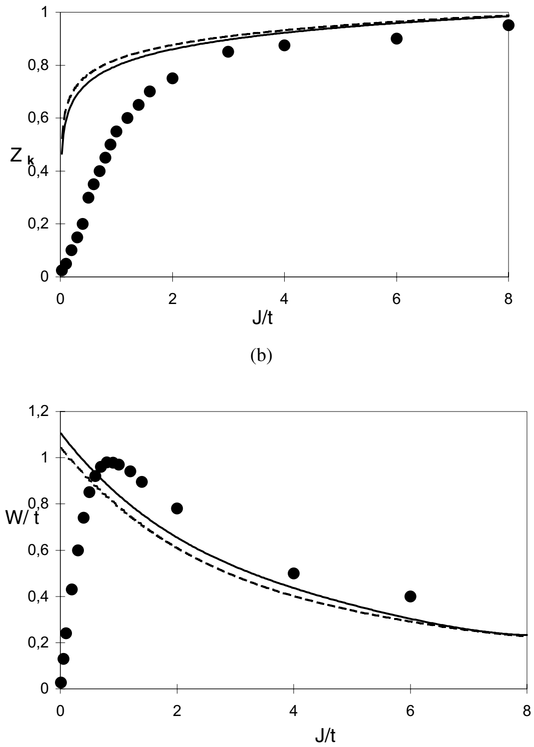


Figure 1. The dispersion relation of a spin polaron for $J/t = 0.4$ plotted in the Brillouin zone. The solid line is the present result and the dashed line is that of Barentzen.

$\boldsymbol{k} = (\pi/2, \pi/2)$, the present result is noticeably lower, but still above that of Martinez and Horsch [8]. The band minimum turns out to be at the same point $\overline{\mathrm{M}}$ as in the other works; consequently the bandwidth W is defined as $W = E(\Gamma) - E(\overline{\mathrm{M}})$. Figure 2(a) shows the bandwidth against the coupling constant J/t, where it seems that our result slightly improves on that of Barentzen. Another improvement can be seen in the spectral weight curve, which is plotted as a function of J/t in figure 2(b).



(a)

Figure 2. The bandwidth W/t (a) and the spectral weights $Z_{\boldsymbol{k}}$ calculated at $\boldsymbol{k} = (\pi/2, \pi/2)$ (b) as functions of J/t. The solid line is the present result and the dashed line is that of Barentzen. Dots are the results of the self-consistent Born approximation for a 16×16 lattice [8].

The range of validity of this approach is in the weak- and intermediate-coupling regions, i.e. for $J/t \geqslant 0.4$. Below this value a different approach is required to overcome the drawbacks inherent in this theory. One of these is the behaviour of the bandwidth towards the strong-coupling region where the self-consistent Born approximation gives a completely different result, which decreases to zero as α increases, instead of reaching a constant value as in the intermediate-coupling theory. Secondly, the energy dispersion of this theory gives rise to a finite gap $2\alpha\Omega(\boldsymbol{k})$ at a given $\boldsymbol{k}$ as $q \to 0$. In our approach, as $q \to 0$, $\varphi_{qq'}$ vanishes and $\Omega(\boldsymbol{k})$ takes a finite value as before.

In summary, we have made a small correction to the ground-state energy, the bandwidth, and the spectral weight of the spin polaron developed by Barentzen in the intermediate-coupling theory. We have used two-mode squeezed states in which the correlation between spin excitations is involved; this slightly improved on the previous results, as expected in view of results for squeezed states which are employed in other areas of condensed matter physics.

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