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Density of States in the $t'$-Hubbard Model: Exact Diagonalisation Results


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Abstract. — We calculated the density of states in a Hubbard model with nearest and next nearest neighbour hopping. Using an exact diagonalisation technique, we examined this model in a wide area of parameters. The density of states was calculated for different fillings and for positive and negative interaction $U$. The additional hopping to the next nearest neighbour sites has different effects on the gap between the particle and hole spectrum compared to the pure Hubbard model.

1. Introduction

There are several theories, which are actually favoured, to explain the high-temperature superconductors [1–4]. One of them is the van Hove scenario [4]. It states that the maximum of the critical temperature $T_c$ is, where the Fermi energy and a van Hove singularity in the density of states are at the same place. From the experiments we know [5] that the doping with maximum $T_c$ is not at half-filling for the high $T_c$ superconductors. On the other hand, the single-band Hubbard model has only a singularity in the density of states at half-filling [6]. Because of this reasons the single-band Hubbard model should be extended. One possibility is to allow, in addition to the hopping to the nearest neighbours, a hopping to the next nearest neighbours ($t'$). This $t'$-model is described by the Hamiltonian:

$$\mathcal{H} = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^+ c_{j\sigma} + t' \sum_{\langle\langle i,j \rangle, \sigma} c_{i\sigma}^+ c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where $t$ is the hopping parameter to the nearest neighbours (in the following we always set $t = 1$), $t'$ is the hopping parameter to the next nearest neighbours, $\langle i,j \rangle$ denotes the sum over all nearest neighbours and $\langle\langle i,j \rangle \rangle$ is the sum over the next nearest neighbours. $U$ is the interaction between the particles and $c_{i\sigma}^+$ creates a particle at the lattice site $i$ with spin $\sigma$ and $n_{i\sigma} = c_{i\sigma}^+ c_{i\sigma}$ is the particle number operator. In this model a van Hove singularity exists at $t' = 1 - \langle n \rangle$, if the interaction is zero, $U = 0$ [7].

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We use an exact diagonalisation technique to solve the model (1) (see Section 2). Because of the exponential growth of basis states with the system size, it is not possible to deal with large system sizes. This means that the density of states has individual peaks and is not a continuous spectrum. So the density of states cannot show singularities, which we would perhaps obtain in infinite system sizes. Nevertheless we can study the effects of the additionally $t'$ hopping to the density of states compared to the pure Hubbard model.

2. Calculation of the Spectral Density and the Density of States

As numerical technique we use the exact diagonalisation with the Lanczos method [8, 9]. One of the advantages of the Lanczos method is that one can easily calculate the Green functions with this method [10].

Within the Lanczos scheme it is not necessary to calculate all excited states of the model. The Green function to the state $|\Psi_t\rangle$ can be evaluated by the continued fraction expansion [10]:

$$
\langle \Psi_t | (x - H)^{-1} | \Psi_t \rangle = \frac{1}{x - \alpha_1 - \frac{\beta_1^2}{x - \alpha_2 - \frac{\beta_2^2}{x - \alpha_3 \cdots}},
$$

where $\alpha_i$ and $\beta_i$ are the diagonal and off-diagonal elements of the tridiagonal matrix $T_m$ from the Lanczos algorithm. The initial vector of the Lanczos algorithm is the state $|\Psi_t\rangle$.

The Green function $G^{(+)}(k, \omega)$ of the state $c^{(\pm)}_k |\Psi_0\rangle$ with the norm 1 is defined as:

$$
G^{(+)}(k, \omega) = \lim_{\delta \to 0} \langle \Psi_0 | c_k,\sigma (\omega + i\delta - H)^{-1} c^+_k,\sigma | \Psi_0 \rangle
$$

and

$$
G^{(-)}(k, \omega) = \lim_{\delta \to 0} \langle \Psi_0 | c^+_k,\sigma (\omega + i\delta - H)^{-1} c_k,\sigma | \Psi_0 \rangle,
$$

where $|\Psi_0\rangle$ is the norm 1 groundstate and $\delta$ is a small real number.

The spectral density $A^{(\pm)}(k, \omega)$ is connected with the Green function $G^{(\pm)}(k, \omega)$ of the same $k$-vector through the equation:

$$
A^{(\pm)}(k, \omega) = -\Im(G^{(\pm)}(k, \omega))
$$

Here $\Im$ is the imaginary part of the Green function. The spectral density $A^{(+)}$ is the particle part of the spectrum and $A^{(-)}$ gives the hole contribution to the spectrum.

The particle / hole $(+/\) -$ part of the density of states $N^{(\pm)}$ is the sum over all allowed momenta $k$ of the spectral densities $A^{(\pm)}(k, \omega)$:

$$
N^{(\pm)}(\omega) = \sum_k A^{(\pm)}(k, \omega)
$$

and the complete density of state is the sum of the particle $N^-$ and hole $N^+$ part of the spectrum:

$$
N(\omega) = N^{(+)}(\omega) + N^{(-)}(\omega)
$$

In the simulation it is of course not possible to determine the limits $\delta \to 0$, therefore we take a small value of $\delta = 0.05$ or 0.10.
3. Results

We have studied the $t'$–Hubbard model over a wide range of parameters. As the van Hove theory suggests the value of $t'$, to be near the doping [4], we take always positive values for $t'$ and fillings less or equal half filling. In the square 8-point system (see [11]) we studied the three different fillings $\langle n \rangle = 1.00$, $\langle n \rangle = 0.75$ and $\langle n \rangle = 0.50$, which belong to the number of particles $n_l = n_r = 4, 3$ and 2. The third parameter that we changed is the interaction $U$. We calculated the density of states for values between $U = -10$ and $U = 20$. But only in the range $U = -6$ to 6 we see changes in the evolution of the gap between the particle and hole spectrum.

In Figure 1 the evolution of the density of states is shown for $t' = +0.22$ for positive values of $U = 0, 1, \ldots, 6$. The spectra for $U > 0$ are shifted up for clarity. The spectrum for $U = 0$ is the spectrum that is expected by solving the non-interacting model exactly:

$$\varepsilon(k_x, k_y) = -2t(\cos(k_x) + \cos(k_y)) + 4t' \cos(k_x) \cos(k_y)$$  \hspace{1cm} (8)

and

$$N(\omega) = \frac{1}{n_0} \int dk_x \int dk_y \varepsilon(k_x, k_y)$$  \hspace{1cm} (9)

The delta peaks of the energy–axis are broadened by the finite imaginary part $\delta$.

For the interaction $U > 0$ the gap between the particle (solid line) and hole (dash–pointed line) spectrum does not open immediately with interaction $U \neq 0$ in contrast to the single-band Hubbard model. Spectra of the pure Hubbard model ($t' = 0$) can be found in [11].
Fig. 2. — Density of states $N^\pm(w)$ of the square 8 point system with the filling $\langle n \rangle = 1.00$, interaction $U = 2.0$ and the imaginary part $\delta = 0.10$ for several next nearest neighbour hopping parameter $t'$. Particle spectrum $N^-$. Solid line, hole spectrum $N^+$: dashed line. All curves, except for $t' = 0$, are shifted upwards for clarity.

There is obviously up to $U = 2$ no or only a very small gap between the particle $N^-$ and the hole $N^+$ spectrum. Only for $U \geq 3$ there is a clear gap. In a plot of the different spectra for constant interaction $U$ and various values of $t'$ (see Figure 2 with $U = 2.0$), one sees that for $t' = 0$ there is a gap of about 1.6, which reduces for increasing $t'$ ($t' = +0.10$ and $t' = +0.15$). The gap vanishes almost completely for still larger $t'$ ($t' = +0.22$ to $t' = +0.38$).

Plotting the gaps for different interactions and different values of $t'$ (see Fig. 3) we clearly see that the gap for the simple Hubbard model (solid line) at fixed interaction $U$ is the greatest. Increasing $t'$ it becomes smaller (dashed lines). On the other hand if the value of $t'$ is fixed, the gap for small interactions $U$ is about zero and increases at a certain value $U_g(t')$ dramatically. The value of $U_g(t')$ increases with the value of $t'$. For large interactions ($U \geq 6$) there is a nearly linear dependence between $U$ and $t'$ with about the same slope for all values of $t'$.

We can also see this transition in the spectral density. Therefore let us now consider Figure 4. Here we see the spectral density $A^{(\pm)}(k, \omega)$ for the momentum $k = (0, \pi)$ at different interactions $U$. At small interactions ($U \leq 2$) we see some huge peaks in the particle spectrum $A^-(k, \omega)$ and only relatively small peaks in the hole spectrum $A^+(k, \omega)$. For an interaction larger than $U = 3$ the situation changes. Here both the particle $A^-$ and the hole spectrum $A^+$ have an equivalent peak. A similar change in the weights of the spectral density occurs at the same interaction $U_g$, where the gap opens faster (compare Figs. 1 and 4). This change in the weights of the spectral density is seen for all allowed momenta $k$. For the $k$-vectors, which lie at the interaction $U = 0$ completely in the hole spectrum $A^+(k, \omega)$ (for example $k = (\pi, \pi)$),
Fig. 3. — Gap between the particle $N^-$ and the hole $N^+$ spectrum for the square 8 point system with the filling $\langle n \rangle = 1.00$ for different values of $t'$: $t' = 0.0$ ($\cdots$), $t' = +0.10$ ($\cdots$), $t' = +0.15$ ($\cdots$), $t' = +0.22$ ($\cdots$), $t' = +0.30$ ($\cdots$), $t' = +0.38$ ($\cdots$).

Fig. 4. — Spectral density $A^\pm(k, \omega)$ of the square 8 point system with the filling $\langle n \rangle = 1.00$, different interactions $U$ and the imaginary part $\delta = 0.10$, the next nearest neighbour hopping $t' = +0.22$ and the k-vector $k = (0, \pi)$. Particle spectrum: solid line, hole spectrum: dashed line. All curves, except for $U = 0$, are shifted upwards for clarity.
Fig. 5. — Gap between the particle $N^-$ and the hole $N^+$ spectrum for the square 8 point system with the filling $\langle n \rangle = 0.75$ for different values of $t'$: $t' = 0.0$ ($\rightarrow$), $t' = +0.15$ ($\leftarrow$), $t' = +0.22$ ($\sim$), $t' = +0.25$ ($\blacksquare$), $t' = +0.30$ ($\triangle$), $t' = +0.50$ ($\ast$).

the distribution moves to the particle spectrum.

A possible explanation for this behaviour is that, in the pure Hubbard model, $t' = 0$, the Fermi surface is square and unstable against the metal insulator transition which occurs as soon as the Hubbard interaction $U$ is turned on. As $t'$ is increased, $t' > 0$, the Fermi surface in the free system, $U = 0$, is curved [4] and at small interaction $U$ no longer suitable for the metal insulator transition. Only at a larger value of $U$, depending on $t'$, the interaction is strong enough to mix the states and the metal insulator transition occurs.

To summarize, a metal insulator transition occurs in the $t'$-model at half filling, but delayed with respect to $U$. This transition at half filling is characteristic for models describing high-temperature superconductors. Therefore, this is another indication that the $t'$-model and the underlaying van Hove scenario describes the right physics of the high-temperature superconductors.

If we return to Figure 2, we see for the pure Hubbard model, $t' = 0$, only one central peak in the particle spectrum (at $\omega \approx -0.8$). For $t' > 0$ these peaks split into two parts (the peaks at $\omega = -0.8$ and $\omega \approx 1.2$ for $t' \approx 0.10$). The distance of these splitted peaks increases with increasing $t'$. These two peaks belong to two different momenta $k$. The lower one results from the spectral densities of $k = (0, \pi)$ and $k = (\pi, 0)$ and the upper one belongs to the momenta $k = (\pi/2, \pi/2)$ and degenerated momenta.

Now we reduce the filling and again plot the gap between the particle and the hole spectrum. Here we must distinguish between the filling $\langle n \rangle = 0.75$ and $\langle n \rangle = 0.50$ (Figs. 5 and 6). In the first case there is a gap between the particle and hole spectrum in the free system, because the Fermi energy lies between the two contributions at $\omega = -4t'$ and $\omega = 0$ in the density of states. One can see this gap of the free system ($U = 0$) in the lowest curve in Figure 1 (gap between the peaks by $\omega = -0.88$ and $\omega = 0$). In the second case the Fermi energy lies at $\omega = 4t'$, and not in a finite size gap of the free system. In both cases the gap for $0 < t' < 0.45$ is larger than for the pure Hubbard model. At the filling $\langle n \rangle = 0.75$ this increase of the gap with $t'$ is mainly caused by the increasing finite size gap of the free system (Fig. 5).

Also in the case of the filling $\langle n \rangle = 0.50$ (Fig. 6) the gap increases with increasing $t'$. But
Fig. 6. — Gap between the particle \( N^- \) and the hole \( N^+ \) spectrum for the square 8 point system with the filling \( \langle n \rangle = 0.50 \) for different values of \( t' \): \( t' = 0.0 \) \((\cdots\cdots)\), \( t' = +0.15 \) \((-\cdots-\cdots)\), \( t' = +0.22 \) \((-\square-)\), \( t' = +0.30 \) \((-\times-)\), \( t' = +0.38 \) \((-\cdot-\Delta-)\), \( t' = +0.45 \) \((-\cdot-\#-)\), \( t' = +0.50 \) \((-\cdot-\circ-)\).

In contrast to the filling \( \langle n \rangle = 0.75 \) there is no finite size gap at the Fermi level. Moreover, the gap tends to a constant value for huge interactions \( U \) (e.g. at \( t' = +0.22 \) the gap tends to 0.36, dashed line with boxes in Fig. 6). The situation changes dramatically for \( t' \geq +0.45 \) and large interactions \( U \geq 4 \). At \( t' = +0.45 \) the gap has its maximum at \( U = 4 \) and decreases for larger \( U \). If we increase \( t' \) to \( t' = +0.50 \), then we see a sudden breakdown of the gap between \( U = 5.0 \) and \( U = 5.3 \). For \( U > 5.3 \) there is no longer a gap between the particle \( N^- \) and hole spectrum \( N^+ \) of the density of states. The reasons for this sudden breakdown of the gap are not yet clear.

There are some possible explanations: the breakdown may be a result of the degeneration of the \( k \)-vectors \( k = (0, \pi) \), \( k = (\pi, 0) \) and \( k = (\pi, \pi) \) for \( t' = +0.50 \) or of the special system size. Another possibility is, that the accumulation of different \( k \)-vectors at the Fermi energy as in the van Hove scenario causes this breakdown.

Dagotto et al. found a similar breakdown for a superconducting order parameter in the \( t-J \) model with the same filling [12]. Their explanation is a phase transition.

In addition to the positive \( U \) case, we have also calculated the density of states and the gap between the particle and the hole spectrum of the density of states for negative interactions \( U \). The resulting gap for several fillings are plotted in Figure 7. Here we see the gaps for the three possible fillings, \( \langle n \rangle = 1.00 \) \((7 (a))\), \( \langle n \rangle = 0.75 \) \((7 (b))\) and \( \langle n \rangle = 0.50 \) \((7 (c))\). In the cases of \( \langle n \rangle = 1.00 \) and \( \langle n \rangle = 0.50 \) the gap decreases with increasing \( t' \). In the case of \( \langle n \rangle = 0.75 \) the situation is a little more complicated. As above, there is a finite size gap between the particle and the hole spectrum in the free system, \( U = 0 \), with \( t' \neq 0 \). Therefore we see in Figure 7 (b) that the gap increases with increasing \( t' \) for small interactions \( 0 > U > -1 \). But at large interaction \( U > 4 \) the gap shows the same behaviour at the fillings \( \langle n \rangle = 1.00 \) \((a)\) and \( \langle n \rangle = 0.50 \) \((c)\). So for huge interactions there is a decrease of the gap with increasing \( t' \) for all fillings. Similar to the positive \( U \) case and half filling the increase of the gap is almost linear with the interaction \( U \) for large interactions \( U > 4 \), for all fillings and for all values of \( t' \).

Given only the density of states \( N^{(\pm)}(\omega) \) and the spectral density \( A^{(\pm)}(k, \omega) \), it is impossible
Fig. 7. — Gap between the particle $N^-$ and the hole $N^+$ spectrum for the square 8 point system for negative interaction $U$ and different values of $t'$: $t' = 0.0$ (---), $t' = +0.15$ (--), $t' = +0.30$ (---). Subplot a) filling $\langle n \rangle = 1.00$, b) $\langle n \rangle = 0.75$ and c) $\langle n \rangle = 0.50$. 
to clarify what is the origin of the gap. Therefore we must calculate additional observables like correlation functions. Projector quantum Monte Carlo results [13] indicate that the $t'$-model in the negative $U$ regime is superconducting away from half filling.

4. Conclusions

Within the positive $U$ range for half filling $t'$ retards the opening of the gap with respect to $U$. This retardation increases with increasing $t'$. So the metal insulator transition seems to be delayed through a finite value of $t'$. This transition supports the $t'$-model and the van Hove scenario as possible explanations for the high-temperature superconductors.

At the filling $\langle n \rangle = 0.75$ the increasing value of the gap with increasing $t'$ is dominated by the finite size gap in the free system, $U = 0$. For that reason the gap increases with increasing $t'$. And at the next possible filling, $\langle n \rangle = 0.50$, there is a huge magnification with increasing $t'$, until $t'$ reaches the value $t' = +0.45$. Here we see a maximum of the gap at $U = 4$. Finally at $t' = +0.50$ there is a sudden breakdown of the gap at the interaction $U \approx 5$. The origin of this behaviour is not yet clear. Additional calculations are in progress.

In the case of negative interactions $U$ there are no large changes in the evolution of the gap for various fillings observed. Here the additional hopping $t'$ decreases the gap with increasing $t'$. The only exception is the case of the filling $\langle n \rangle = 0.75$ with small interactions $|U| < 1$, there the finite size gap for $t' \neq 0$ dominates.

In order to decide on the origin of this gap in the negative $U$ regime, it is necessary to calculate other observables like correlation functions. But results obtained with the projector quantum Monte Carlo [13] indicate that the negative $U$ $t'$-model is superconducting away from half filling.

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References