Algebraic extraction of one-particle fields induced by repulsion on copper sites in the Emery model

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A model of free fermions is described, which embodies the strong local correlations on copper sites in the $CuO_2$ planes. One-particle fields induced by the correlations are extracted algebraically and found to renormalize the copper-oxygen hopping and change the band-widths of the effective one-particle Hamiltonian. The strength of these fields is adjusted through a single variational parameter, dependent on the band filling. It is found that additional hoppings appear among oxygen sites, even if only the copper-oxygen overlap was originally present.

## 1. Introduction

The normal state of electrons in high-$T_c$ superconductors has been the subject of considerable research. The principal problem, from the theoretical point of view, is how to reconcile two very different scales: the large Coulomb repulsion on the copper ions, and the physically interesting scale of $\sim 100K$. In other words, it is necessary to extract the long-wavelength behavior induced by a strongly localized correlation.

An early approach to problems of this type was the trial wave function of Gutzwiller [1,2], who derived an expression for the effective mass of the spin-up electrons, assuming the spin-down electrons to be static. The slave-boson approach [3] is of the same type, using the effective overlap integral as a variational parameter, subject to certain constraints. It is closely related to the Gutzwiller approach [4], although the latter computes the phase space available for hopping more precisely.

## 2. The high-temperature expansion

In calculating the trace of the density matrix for the Hubbard Hamiltonian $K+V$, with $V$ the on-site repulsion, it seems convenient to separate the interaction, which is diagonal in $R$-space:

$$e^{-\beta(K+V)} = e^{-\beta V/2} e^{-\beta \mathcal{K}} e^{-\beta V/2}\,, \qquad (1)$$

which may be considered as a definition of $\mathcal{K}$. Now, the approximation $\mathcal{K} \approx K$, which completely neglects the commutator series generated by $[K,V] \neq 0$, turns out to be precisely equivalent to the Gutzwiller trial wave function: the value of tr $a^\dagger_{i,\sigma} a_{j,\sigma} e^{-\beta V/2} e^{-\beta K} e^{-\beta V/2}$, calculated in the Gutzwiller approximation, goes over into the expression for $< g|a^\dagger_{i,\sigma} a_{j,\sigma}|g >$ in [2], under the correspondence $g \leftrightarrow e^{-\beta U/2}$, and

$$< \Phi|a^\dagger_{i,\sigma} a_{j,\sigma}|\Phi > \leftrightarrow \mathrm{tr}\; a^\dagger_{i,\sigma} a_{j,\sigma} e^{-\beta K}/\mathrm{tr}\; e^{-\beta K}\,. \qquad (2)$$

Neglecting $[K,V]$ is a high-temperature approximation, since the commutator is of order $\beta^2$. To improve it, assuming $V \gg K$, sum all the commutators $[V,[V,\ldots[V,K]\ldots]]$ to infinite order, to obtain

$$\mathcal{K} \approx \sum_{\substack{<i,j> \\ \sigma}} t_0 \left[\tau_1(U)(u+vn_{i,-\sigma}) a^\dagger_{i,\sigma} a_{j,\sigma} (u+vn_{j,-\sigma}) \right.$$

$$\left. + \tau_2(U)(-v+un_{i,-\sigma}) a^\dagger_{i,\sigma} a_{j,\sigma} (-v+un_{j,-\sigma})\right]\,. \qquad (3)$$

In the limit $U \to \infty$, one finds $u=-v=1/\sqrt{2}$, thus deriving the projected-hopping Hamiltonian. However, $\tau_1(U)$ and $\tau_2(U)$ diverge in this limit (they try to keep track of both Hubbard bands), and so one sets $\tau_2(U)=0$ and $t_0\tau_1(U)=t$, introducing a new (phenomenological) scale.

## 3. The free fermion model

The above considerations can be applied to the Emery model, obtaining first the projected-hopping model,

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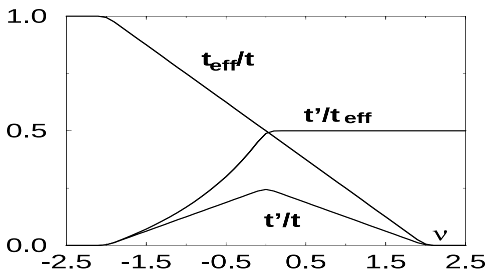


Figure 1. Dependence of the effective hoppings on $\nu$.

$$H = \sum_{i,\sigma} \Big[ t_0(u + v n_{i,-\sigma}) A_{i,\sigma} + \epsilon_d n_{i,\sigma} + \tag{4}$$

$$+ \epsilon_p (p^\dagger_{i+\hat{x}/2,\sigma} p_{i+\hat{x}/2,\sigma} + p^\dagger_{i+\hat{y}/2,\sigma} p_{i+\hat{y}/2,\sigma}) \Big] ,$$

where $A_{i,\sigma}$ is the hopping over the four bonds impinging on copper site $i$, and $n_{i,\sigma}$ is the number operator for the coppers. In the $U \to \infty$ limit, the scale is again reset by hand, $t_0 u = -t_0 v \equiv t$. Treating (4) in the high-temperature spirit of the preceding section, the commutator between its spin-up and spin-down part is neglected, thus losing the '$J$' part of the $t - J$ model. One is then left with the interaction

$$v\, n_{i,-\sigma} A_{i,\sigma} \tag{5}$$

between the down-spin density and the up-spin '$CuO_4$ molecule' $A_{i,\sigma}$. The single-particle contribution of this interaction to the Hamiltonian is extracted from the site and bond terms in a cluster expansion. The thermodynamic limit in the number of 'molecules', equal to the number of down-spins, is taken through a variational parameter $\nu$, the chemical potential for the band of down-spins, which are kept static. The principal effect of (5) is found to be the renormalization of the copper-oxygen overlap, $t \to t_{eff} = t - b/\beta$, and the appearance of an oxygen-oxygen overlap $t' = a/2\beta$, where (writing $v$ for $vt_0$)

$$a = \frac{1}{4}\left[ \ln\left( \frac{1 + e^{\beta(\nu - 2v)}}{1 + e^{\beta\nu}} \right) + \ln\left( \frac{1 + e^{\beta(\nu + 2v)}}{1 + e^{\beta\nu}} \right) \right] \tag{6}$$

$$b = \frac{1}{4}\left[ \ln\left( \frac{1 + e^{\beta(\nu - 2v)}}{1 + e^{\beta(\nu + 2v)}} \right) \right] . \tag{7}$$

The dependence of these terms on $\nu$ is shown in the figure. As $\nu$ increases, $t_{eff}$ goes from $ut_0$ to $(u+v)t_0$, *i.e.* from $t$ to zero, while $t'$ is zero for both large and small $\nu$. Their ratio saturates at one-half. The figure is taken for the 'electron situation' (large $U_d$ limit in the electron picture [5]), with the bands narrowing as the concentration of fermions increases. The 'hole situation' corresponds to $u = 0$, $v = 1$, leading to $\nu \to -\nu$ in the figure, *i.e.* it is mirrored around the vertical axis.

## 4. Discussion

Placing the Gutzwiller and, by implication, slave-boson, approach in the context of a class of high-temperature approximations — those which try to calculate the operator $\mathcal{K}$ in (1) by neglecting (large) parts of the Baker-Campbell-Hausdorff series — it has been possible to arrive at a new model of strong local correlations. Formally, it is a model of free fermions, containing an additional variational parameter. Physically, it embodies much of the same physics as the older approaches. However, due to a systematic formal implementation of these physical ideas through a cluster expansion, many new terms appear. The model shall have to be judged on two counts: whether it can treat the electronic sector in more complex models, which could include effects of crystal structure, with sufficient simplicity, and by the importance of the new terms themselves.

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