Intermediate scale phenomena in cuprates

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Abstract

We present computations of cuprates which accurately describe the physics arising at scales of up to several lattice constants.

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After 20 years of research the low energy physics of cuprates remains a mystery. It is generally accepted that a three band Hamiltonian with Cu’s and O’s orbitals should contain the essential physics so we can say that there is consensus at the length scale of the Cu-O distance but there is disagreement when it comes to describe higher length scales or to set up a low energy model.

Much on the modeling in the field consists on guessing the low energy physics. We adopt a more conservative approach and try to move from the safe land of the atomic scale to the intermediate scale of a few atomic constants. An exact solution is not possible but a number of techniques allow to address the intermediate length scale physics with accuracy. Rather than guessing we can accurately compute what the model predicts at intermediate energies and length scales and compare in detail with experiments. This should considerably constrain the low energy physics. If our modeling is successful we should be able to describe spectroscopies from high energies up to some infrared cutoff (below which our ignorance sets in) and we should be able to describe short and intermediate length scale physics. This includes the ground state energy which, in a short range model, is essentially a short range property.

In the last years we have carried on this program pushing in some cases our “discerning cutoff” down to a few meV. We have based our computations on the Gutzwiller approximation and a time dependent extension\cite{1}. These techniques have revealed to be very accurate when compared with exact diagonalization\cite{2,3} and exact results in one\cite{1} and infinite\cite{1} dimensions. An accurate technique supplemented with an accurate model should produce results in accord with experiment and it does.

Within our approximations the lowest energy solutions consist of O centered stripes which have approximately a number of holes per lattice site along the stripe $\nu \sim 0.5$. These textures explain the behavior of the incommensurability, the chemical potential, some anomalous transport experiments\cite{5} and the optical conductivity as a function of doping\cite{6}. In order to get accurate parameters we have relied on LDA. New calculations in much larger systems which allow better resolution show small deviation from experiment. For example the filling of the stripes with the parameters of Ref. \cite{5} is $\nu = 0.56$ holes per site rather than $\nu = 0.5$ as found in experiment\cite{7}. This can be easily understand from the fact that the stripe filling is approximately given by $\nu \sim \sqrt{J/2C}$ with $C$ the inverse compressibility of

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{$\epsilon_h$ as a function of doping for vertical O centered stripes. We also show the result for Cu centered (CC) stripes for $d = 4$. The inset in reports the incommensurability as obtained from the present calculation (line) compared with experimental data from Ref. \cite{7}.}
\end{figure}
the stripe and $J$ the superexchange interaction\cite{8,5}. LDA parameters are well known to overestimate the value of $J$ so it is not surprising that the filling of the stripe is overestimated. To improve the agreement with experiment here we present new results with an empirical parameter set based on Ref. [9]. We use $\Delta = 3.3eV$ for Cu-O onsite energy splitting, $t_{pd} = 1.3eV$ ($t_{pp} = 0.7eV$) for Cu-O (O-O) hopping, $U_d = 8.8 eV$ ($U_p = 6.0 eV$) for onsite repulsion on Cu (O), $U_{pd} = 1.0 eV$ for Cu-O repulsion and $K_{pd} = -0.25$ for Cu-O direct exchange. The CuO interactions $U_{pd}$ and $K_{pd}$ where added by us. $K_{pd}$ has been recognized as essential to yield the correct value of $J$\cite{10} and so it plays an unsuspected role on fixing the filling of the stripe. We have found that the optical conductivity and the magnetic excitations computed within the time dependent Gutzwiller approximation\cite{1} for the undoped system are in excellent agreement with the experiment confirming the accuracy of the parameters.

Fig. 1 shows the energy per hole as a function of doping. Results are qualitatively similar as in Ref. [5] but now the stripes have $\nu \sim 1/2$ even for large systems. As discussed before\cite{4} for doping $x \leq 1/8$ the system responds to a change of doping by changing the periodicity $d$ whereas for $x \geq 1/8$ the periodicity gets fixed at $d = 4$ in a large doping range. The inset shows the resulting magnetic incommensurability compared with experiment.

Fig. 2 shows the charge and spin density at doping $x = 1/8$. A similar charge distribution was predicted in Ref. [4] and found to be in excellent agreement with a charge sensitive probe by Abbamonte and collaborators\cite{11}. They could not determine if the stripes were Cu centered or O centered. More recently Davis and collaborators\cite{12} have imaged glassy stripes which indeed are centered on O as predicted\cite{5}. Taken together these experiments give us amplitude and phase information of stripes in excellent agreement with Ref. [5] thus showing that it is possible to obtain and even predict realistic information on the intermediate scale physics of cuprates.

The Fourier transform of the charge and spin distribution determines Bragg peak weights ($\propto m^2_{Q}$) in scattering experiments (for the definitions see Ref. [13]) as shown in Fig. 3 Disregarding the difference in cross section for different processes (magnetic neutron scattering vs. X-ray or nuclear neutron scattering) we see that Bragg weights are practically 3 orders of magnitude smaller for charge than for spin. This is due to very soft charge distribution shown in Fig. 2 with respect to the spin distribution and explains why it has been so hard to detect charge ordering.

Optical excitation on top of these textures and magnetic excitations on top of similar textures in the one band Hubbard model have been found to be in excellent agreement with experiment confirming the validity of the intermediate scale physics found\cite{14,15}.

To conclude our computations are based on a mean-field like approach and therefore can not address subtle issues as the absence or presence of long range order, specially in the delicate magnetic channel, but we can reliably determine the behavior at intermediate length scales improving our understanding of these fascinating materials. Our results provide strong constrains on low energy theories.

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