Mesoscopics and the High $T_c$ Problem

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Abstract

Mesoscopic physics concerns itself with systems which are intermediate between a single atom and a bulk solid. Besides the many intrinsically interesting properties of mesoscopic systems, they can also provide physical insight into the physics of bulk systems. Here we discuss three examples of this from the field of high temperature superconductivity.
Many interesting electronic materials, especially those that exhibit high temperature superconductivity, lie in an intermediate coupling regime where the strength of the interaction is comparable to the electron bandwidth. The absence of any small parameter makes analytic approaches to such problems difficult. Conversely, in the absence of a small parameter there is every reason to expect the correlation lengths associated with any form of electronic order to be of order 1 in units of the lattice constant (barring an accident which places the system close to a critical point). Thus, with some sensible analysis (and with a little bit of luck), the properties of the system in the thermodynamic limit may be apparent in the properties of mesoscopic systems, even systems that are small enough that they can be studied by essentially exact numerical methods. Here we see how three such studies have provided insight into the high $T_c$ problem.

Following the discovery of the high $T_c$ cuprates there were various suggestions of ways in which the strongly repulsive Hubbard interaction, $U$, between two electrons on the same site could (paradoxically) produce high temperature pairing in a doped antiferromagnetic insulator. Numerous studies began with the $t-J$ model on a square lattice, which can be thought of as the strong coupling limit of the Hubbard model. Here it is assumed that $U$ is sufficiently large to prevent double occupancy of any site, leaving a one-electron near-neighbor hopping term $t$ and an exchange coupling $J$. An early argument for pairing was based upon the observation that if one adds two holes to the half-filled (one-electron per site) system, then eight exchange $J$ bonds are broken if the holes were well separated. However, if the two holes are placed on near neighbor sites, only seven exchange $J$ bonds are broken. Thus there is an effective near-neighbor attraction between the holes. This picture however was soon seen as more applicable to the phase separation regime [1]. Alternatively, in the context of the resonance-valence-bond [2] approach, variational calculations using Gutzwiller projected wavefunctions [3] and auxiliary-boson meanfield [4, 5] calculations found a superconducting state with $d$-wave symmetry in the $t-J$ model. From a more weak-coupling perspective, the idea of spin-fluctuation exchange mediated pairing near an antiferromagnetic instability [6] was also found to lead to $d$-wave pairing due to the increasingly positive strength of the pairing interaction at large momentum transfer. However, none of these approaches gave a simple, crisp real space picture, especially one that makes clear why $d$-wave rather than extended $s$-wave symmetry is preferred.

To address this, Trugman and one of the authors [7] decided to imagine that a 4-site
plaquette was extracted from the lattice. The “undoped” groundstate of the $t - J$ model on a plaquette with 4 electrons is a singlet having a wave function

$$|\psi_0(4)\rangle = (\Delta_{12}^+ \Delta_{34}^+ - \Delta_{23}^+ \Delta_{14}^+) |0\rangle. \quad (1)$$

Here, $\Delta_{ij}^+ = (c_{i\uparrow}^+ c_{j\downarrow}^+ - c_{i\downarrow}^+ c_{j\uparrow}^+)/\sqrt{2}$ creates a singlet pair on sites $ij$ and we have numbered the sites of the plaquette in a clockwise manner. This state is odd under a $\pi/2$ rotation. The two-electron groundstate

$$|\psi_0(2)\rangle = N(c_{2\uparrow}^+ c_{1\downarrow}^+ + c_{4\downarrow}^+ c_{1\uparrow}^+ + \cdots) |0\rangle \quad (2)$$

has spin 0 and is invariant under a $\pi/2$ rotation. Therefore the pairfield annihilation operator that connects the zero-hole (4-electron) and two-hole (2-electron) groundstates of the $2 \times 2$ plaquette must transform as $d_{x^2-y^2}$. The same calculation can be performed for the Hubbard model on a single plaquette; while the wave-functions are somewhat more complex, in this case, the symmetry of the 2 and 4 electron ground-states are invariant for any $U$ in the range $0 < U < \infty$. As Carlson et al. [8] noted, it showed the robustness of the $d$-wave character of the pairing in $t - J$ and Hubbard models.

Of course studies of a 4-site model could not say anything about the possibility of superconducting order. However, it turned out that studies of 2-leg $t - J$ and Hubbard ladders yielded important insights concerning the character of the superconducting groundstate. The study of 2-leg ladders was motivated by a simple picture based upon the case in which the rung exchange interaction $J_r$ is large compared to the near neighbor leg exchange $J_\ell$. In this limit, for the undoped Heisenberg ladder, spin singlets tend to form on the rungs leading to a spin gapped groundstate. Then when holes are added, where $J_r > t$, they would occupy sites on either side of a rung so as to break only one exchange rung coupling. A measure of the spatial correlation of these rung hole pairs would then allow one to probe the superconducting order. Based on this large $J_r/J_\ell$ picture, it was initially a surprise when numerical calculations [9] showed that at half-filling the spin gap persisted to small values of $J_r/J_\ell$. In addition, for the hole doped ladder, despite the fact that $t > J_r$, the equal time pairfield-pairfield correlations appeared to have a power law decay, indicative of quasi-long-range “superconductivity”. In later work [10, 11], it was understood that the ladder would have a spin gap at half-filling for any finite $J_r/J_\ell > 0$, and that the groundstate of the doped ladder is a Luther-Emery [12] liquid. Furthermore, the pair structure is $d$-wave-like in the
sense that the rung and leg pairfield amplitudes have opposite signs. We now also know
that, in the limit as the length of the ladder tends to infinity, the $t - J$ ladder has perfect
Andreev reflection in response to an externally applied pairfield at one end of the ladder\cite{13}. The 2-leg $t - J$ and Hubbard ladders now represent some of the best understood models of
strongly correlated electron systems.

Admittedly, since the plaquette and the ladder are, respectively, zero and one dimensional
systems, neither can support a superconducting phase with a finite transition temperature.
However, in many cases it is possible to analyze the phase diagram of a higher dimensional
system constructed as an array of weakly coupled mesoscale structures, starting from the
exact numerical solution of the isolated structure, and treating the coupling between clusters
in the context of perturbation theory \cite{14}. Studies of arrays of weakly coupled two-leg
ladders\cite{15,16} and plaquettes\cite{17,18} (the “checkerboard Hubbard model”) lead to rather
complex phase diagrams with many competing phases, even where the above analysis shows
strong superconducting correlations on the isolated cluster. Nonetheless, among those phases
there are robust regions of $d$-wave, or $d$-wave-like superconductivity.

As a final example of insights gained from studies of small systems, we turn to calculations
on a 2-leg ladder model of an Fe-pnictide superconductor \cite{19}. Figure 1 shows the typical
Fermi surfaces of the Fe-pnictide materials in an unfolded (1 Fe/cell) Brillouin zone. There
are two-hole Fermi surfaces $\alpha_1$ and $\alpha_2$ around the $\Gamma$ point and two-electron Fermi surfaces $\beta_1$
and $\beta_2$ around $(\pi, 0)$ and $(0, \pi)$. The symbols indicate the dominant $d$-orbital contributing
to the Bloch state on the indicated portion of the Fermi surfaces. In weak coupling, RPA
\cite{20,21} and functional renormalization group \cite{22} calculations suggest that the pairing arises
from the scattering of time-reversed-pairs from the $d_{xz}$-dominated states on the $\alpha_1$ Fermi
surface to paired states with the same orbital character on the $\beta_2$ Fermi surface, and from
the analogous processes involving pairs in the $d_{yz}$ dominated states on the $\alpha_1$ and $\beta_1$ Fermi
surfaces. This is illustrated in Fig. 1 for the $d_{xz} - d_{xz}$ pair scattering.

In order to use numerical methods to study these processes in the intermediate to strong
coupling limit, the problem needs to be simplified. If we accept that the type of scattering
processes shown in Fig. 1 capture the essential physics, we can focus exclusively on pair
scattering involving two bands and only one orbital. The resulting two-leg Hubbard ladder
retains the $d_{xz}$ states along two cuts through the 2d BZ, $\mathbf{k} = (k_x, 0)$ which passes through
the $\alpha_1$ Fermi surface, and $\mathbf{k} = (k_x, \pi)$ which passes through $\beta_2$. This reduces the problem
FIG. 1: The Fermi surfaces for a five-orbital tight binding model of the Fe-pnictides. The main orbital contributions to the Bloch states are indicated: $d_{xz}$ (solid line), $d_{yz}$ (dashed line) and $d_{xy}$ (dotted line). The arrows illustrate the type of $d_{xz} - d_{xz}$ inter-Fermi surface scattering processes that lead to pairing in the spin-fluctuation-exchange calculations.

to that of the two-leg Hubbard ladder shown in Fig. 2b which can then be studied using the numerical density matrix renormalization group (DMRG) [23]. The one-electron hopping parameters $t_1 = -0.32$, $t_3 = -0.57$ in units of $t_2$, were chosen to reproduce the density functional bandstructure [24] near the Fermi surface for $k_y = 0$ and $\pi$. The repulsion $U$ between two electrons in the same orbital was varied in the range 3–4 in units of $t_2$.

In the undoped, one electron per site, limit one finds the expected spin gapped ground-state. By applying a magnetic field to one of the end sites of the ladder, the resulting expectation value of the spin appears as shown in Fig. 2b. Here one sees “stripe”-like $(0, \pi)$ spin correlations which decay with a slow exponential due to the spin gap. Hole doping
FIG. 2: a) An Fe two-leg ladder with \( t_1 = -0.32 \), \( t_3 = -0.57 \) and \( U = 3 \) in units where \( t_2 = 1 \). These hopping parameters were chosen to fit the DFT calculation of the bandstructure for cuts with \( k_y = 0 \) and \( \pi \); b) The spin structure \( \langle S^z(\ell_x, \ell_y) \rangle \) induced on the undoped Fe ladder when an external magnetic field is applied to the lower left hand site.; c) The singlet pairfield \( \langle \Delta_{ij} \rangle \) induced across a rung, along a diagonal and along a leg at a distance 10 sites removed from the end of a 32 \( \times \) 2 Fe-ladder with a unit external pairfield applied to its end rung.

The stripe-like SDW pattern of the spin correlations in the undoped system as well as the structure of the pairfield are consistent with what is found in the RPA calculations \[20, 21\]. However, what we found most interesting was the relationship between the Fe-ladder and the previously studied 2-leg cuprate ladder. This is illustrated in Fig. 3. Here in Fig. 3a, every other rung has been twisted by 180° and the phase of the \( d_{xz} \)-orbit has been changed.
FIG. 3: a) Here every other rung of the ladder shown in Fig. 2a has been twisted by 180° and the phases of the orbitals denoted by the shaded sites have been changed by $e^{i\pi} = -1$.; b) The spin expectation values of Fig. 2b for the twisted ladder show the spin gapped $(\pi, \pi)$ antiferromagnetic behavior of the familiar cuprate ladder.; c) The induced pairfield correlations of Fig. 2c become the familiar $d$-wave-like pairing correlations seen for models of the cuprate ladders.

by $\pi$ on each of the sites of the twisted rung. In this way, the rung one-electron hopping matrix element remains $t_2$, but the leg and diagonal hoppings are changed to $-t_3$ and $-t_1$, respectively. The dominant hoppings on the twisted Fe-ladder are along the legs and rungs with only a weak diagonal hopping. The spin correlations shown in Fig. 3b, obtained by twisting every other rung of Fig. 2b, look just like the spin gapped AF correlations of the previously studied 2-leg Hubbard cuprate ladder. Because of the twist and the phase change $e^{i\pi} = -1$ of the orbitals on the sites of the twisted rungs, the pairfield correlations take on the $d$-wave-like form shown in Fig. 3c. In short, the twist maps $(\pi, 0)$ magnetic and sign-changing $s$-wave pairing correlations on the Fe-ladder into $(\pi, \pi)$ magnetic and $d$-wave-
like pairing correlations in the cuprate ladder! Finally, it turns out that the ratio of the leg-to-rung hopping 0.57 obtained from the fit to the Fe-pnictide DFT bandstructure is near the value which was previously found \[26\] to give the slowest pairfield decay for a cuprate ladder. Thus this Fe-ladder turns out to simply be a twisted version of the cuprate 2-leg Hubbard ladder with parameters near those which are optimal for pairing. This provides a direct link between the physics of these two materials.

Now, as noted by Joe in his book *Introduction to Mesoscopic Physics* \[27\], “the interest in studying systems in the intermediate size range between microscopic and macroscopic is not only in order to understand the macroscopic limit. Many novel phenomena exist that are intrinsic to mesoscopic systems.” Here we have only touched on some examples where strongly correlated mesoscopic models have been introduced in the hope that they can provide some insight into the macroscopic high $T_c$ problem. It is natural to ask whether there aren’t novel mesoscopic phenomena as well. Indeed, there are. For example, the difference between the even- and odd-legged Heisenberg ladders in which the even-leg ladders have a spin gap while the odd-leg ladders are gapless is a mesoscopic width effect \[15\]. It is also known that while the doped 2-leg ladder goes into a Luther-Emery phase \[12\], it takes a finite doping to bring the 3-leg ladder into this phase \[28, 29\]. Ladders also appear in the striped phase of the cuprates and, a better understanding of the mesoscopic properties of multi-leg ladders may shed light on the recently proposed $\pi$-phase shifted $d$-wave stripes \[30\].

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It is a pleasure to contribute to this volume in honor of Yoseph Imry’s 70th birthday. We know Joe as a scientist, teacher, co-worker and friend. DJS met Joe in the early seventies when Joe first came to UCSB. He remembers how they often talked about how one might gain insight into the basic physics of a macroscopic system from calculations on small subsystems and how these subsystems had their own interesting features. All of us are eager to recognize how much we have learned from Joe’s work, over the years concerning the intrinsic, subtle and beautiful physics one finds in the mesoscopic world. This work was supported in part by the National Science Foundation under the grant PHY05-51164 at the KITP. DJS acknowledges the Center for Nanophase Materials Science at ORNL, which is sponsored by
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