FINAL REPORT

Competing Phases and Basic Mechanisms in Strongly-interacting Electron Systems

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I. SUMMARY OF COMPLETED PROJECT

The goal of this work was to continue our effort to develop numerical tools in order to understand the properties of strongly-correlated electron materials.

Towards this goal, we developed new stochastic series Monte Carlo techniques to study the phases of a two-dimensional quantum XY model with ring exchange in an external magnetic field [1]. We determined the zero-temperature phase diagram of this model and found two quantum phase transitions. The first was between an XY-ordered phase and a striped valence-bond phase. The second was between the valence-bond phase and a staggered Neel antiferromagnetic phase. With the external field as an additional control parameter we were able to conclude that this system did not show a quantum spin liquid phase.

We extended the study of the XY model with ring exchange to study its behavior in the 3 dimensions [2]. We find that in three dimensions, the superfluid phase persists to asymptotically large values of the ring exchange K. We do find exotic fractionalized phases in three dimensions.

The role of the electron-phonon coupling in the cuprates remains open. We have studied the effect of an onsite Hubbard U Coulomb interaction on the electron-phonon vertex [3]. We found that at strong coupling, Coulomb interaction caused the electron-phonon interaction to be suppressed at large momentum transfers leading to an effective peaking of the interaction in the forward direction while for weaker values of U, the electron-phonon interaction was simply suppressed at all q values. This behavior could favor d-wave pairing, although the effective pairing strength of the phonons remains weak in this model.

The dynamics of the pairing interaction is reflected in the frequency dependence of the gap. We have used exact diagonilazation to study the frequency dependence of the gap for a two-leg t-J ladder [4]. We were able to determine both the real and imaginary parts of the gap. Our key observation was that the weight of the imaginary part was sufficient to account for most all of $Re\Delta\left(k,\omega=0\right)$, implying that the dynamics of the interaction is not set by the Mott-Hubbard gap (which is infinite for the t-J model).

II. PUBLICATIONS

1. Two-dimensional Quantum XY Model with Ring Exchange and External Field (w/R.G. Melko & A.W. Sandvik), *Phys. Rev. B* **69**, 100408 (2004); cond-mat/0311080.

2. Persistent Superfluid Phase in a Three-dimensional Quantum XY Model with Ring Exchange (w/R.G. Melko), *Phys. Rev. B* **71**, 094511 (2005); cond-mat/0408373.

3. Electron-phonon Vertex in the Two-dimensional One-band Hubbard Model (w/Z.B. Huang, W. Hanke, & E. Arrigoni), *Phys. Rev. B* **68**, 220507 (2003).

4. Superconducting Gap for a Two-leg t-J Ladder (w/D. Poilblanc & S. Capponi), Phys. Rev. Lett. 91, 137203 (2003); cond-mat/0303605.

III. PERSONNEL

The following personnel, in addition to the Principal Investigators, received support from DOE Grant DE-FG02-03ER46048.

Graduate Student:

R.G. Melko received his PhD in September 2005. His thesis title was *Quantum Monte Carlo Simulations of Spin* $\frac{1}{2}$ *XY Models with Ring Exchange.* He is now a Wigner Fellow at Oak Ridge National Laboratory, Tennessee.