

Research Interest

Niladri Gomes

May 2, 2017

1 Motivation

Determination of the mechanism of superconductivity (SC) in correlated electron superconductors is one of the most challenging problems in condensed matter physics. Recent discovery of an ubiquitous charge ordered (CO) state proximate to (SC) within the pseudo-gap phase of cuprates [5, 6, 7, 8] has given the problem a new complexity. A quantum critical transition that separates the under-doped and over-doped copper oxides has been proposed as well as debated [14, 15, 24]. It is highly relevant in this context that there exist other correlated-electron superconductors where also quantum criticality plays a crucial role; where SC is proximate to CO (with sometimes AFM a neighboring phase), but is reached not by doping but by application of pressure or chemical substitution that modifies the one-electron bandwidth. It is conceivable that the problem of determination of the mechanism of correlated-electron SC in these “cleaner” systems is simpler, and that they may provide fresh insight to the problem as a whole. With this motivation my research interests have been mostly to investigating on the mechanism and relationships between various broken symmetry phases, magnetism and SC in organic charge transfer solids (CTS).

2 Overview of organic CTS

CTS are hole carriers A_2X , where A is an organic molecule (TMTSF, BEDT-TTF, BETS, etc.) and X is an inorganic monovalent closed-shell anion (PF_6 , ClO_4 , $Cu(NCN)_2Cl$, $Cu(NCS)_2$, etc.); or electron-carriers $Z[Pd(dmit)_2]_2$, where Z is a closed-shell monovalent cation. In all cases electronically active 2D organic layers are separated by inactive inorganic layers. In my research I have focussed on hole carriers $(BEDT-TTF)_2X$. Depending on the anion, $(BEDT-TTF)_2X$ have different crystal structures, which are referred to as α , β , κ , θ etc. The common features shared by all superconducting CTS are quasi-two-dimensionality of the active organic layers, strong e-e repulsion, geometric lattice frustration and carrier density ($\rho=0.5$).

2.1 Broken symmetries and SC

The superconducting states in the CTS are often proximate to AFM, QSL or CO. Pressure-induced AFM-to-SC in κ -(BEDT-TTF) $_2X$, with $X = Cu(NCN)_2Cl$ and deuterated $Cu(NCN)_2Br$, and QSL-to-SC in $X = Cu_2(CN)_3$ have led to speculations that spin fluctuations are responsible for the SC [1, 11, 25]. However, CO-to-SC transitions are also common and are seen in the α , θ , β and β'' -(BEDT-TTF) compounds, as well as in the electron carrier $EtMe_3P[Pd(dmit)_2]_2$.

2.2 Effective e-e attraction and spin singlet states in $\rho=0.5$

It has often been surmised that correlated electron SC evolves upon doping a spin-gapped semiconductor, as would occur in toy models such as a 2D lattice consisting of weakly coupled even-leg ladders [4, 13]. Finding realistic 2D models with spin gap (SG) and enhanced pair correlations however has remained challenging. In the next section results of our recent numerical calculations [17] are presented, which is a numerical demonstration of enhanced SC pair correlation at $\rho \approx 0.5$.

2.3 Numerical demonstration of enhanced SC pair correlation at $\rho \approx 0.5$.

The standard singlet pair-creation operator is defined as

$$\Delta_i^\dagger = \frac{1}{\sqrt{2}} \sum_{\vec{v}} g(\vec{v}) (c_{i,\uparrow}^\dagger c_{i+\vec{v},\downarrow}^\dagger - c_{i,\downarrow}^\dagger c_{i+\vec{v},\uparrow}^\dagger). \quad (1)$$

The phases $g(\vec{v})$ determine the symmetry of the superconducting pairs. In our calculations we considered s , $d_{x^2-y^2}$, and d_{xy} pairing symmetries. We calculated [17] the equal-time pair-pair correlations $P_{ij} = \langle \Delta_i^\dagger \Delta_j \rangle$, for four different periodic anisotropic triangular lattices, 4×4 , 6×6 , 10×6 and 10×10 , with the widest possible carrier densities $0 < \rho < 1$, using four different numerical techniques. The complete

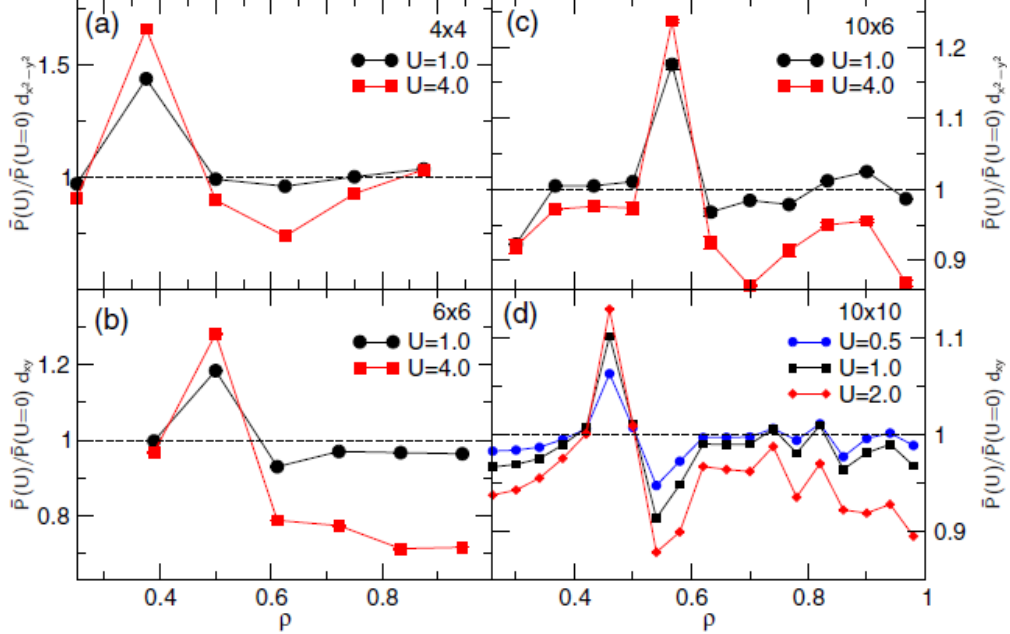


Figure 1: (color online) Average long range pair-pair correlation $\bar{P}(U)$ normalized by its uncorrelated value for (a) 4×4 , (b) 6×6 , (c) 10×6 and (d) 10×10 anisotropic triangular lattices, for $t_y = 0.9$ and $t_{x+y} = 0.8$. 4×4 results are exact; 6×6 and 10×6 results are obtained using the Path Integral Renormalization Group (PIRG) method; and 10×10 by the Constrained Path Monte Carlo (CPMC) method.

results, summarized in Fig. 1, are remarkable: Coulomb interactions enhance superconducting pair correlations only in a narrow density range close to $\rho = 0.5$. For each lattice $\bar{P}(U)/\bar{P}(U = 0) > 1$ for a single ρ that is either exactly 0.5 or one of two closest carrier fillings with closed shell Fermi level occupancy at $U = 0$. Pair correlations are suppressed by U at all other ρ , including the region $0.7 < \rho < 1$ that has been extensively investigated in the context of cuprate SC [24]. In three of four lattices in Fig. 1 enhancement of $\bar{P}(U)$ occurs for ρ slightly away from 0.5. Importantly, the deviation from 0.5 of the ρ at which $\bar{P}(U)$ is enhanced (excluding the 6×6 lattice where this deviation is zero) decreases monotonically with size.

The numerical ground state results have been further confirmed by finite temperature Determinantal Quantum Monte Carlo (DQMC) calculations.

3 Methods

Computational methods were an important part of our work. Here I briefly summarize the methods we adopted to carry out the research.

3.1 Valence Bond (VB) diagonalization

The VB method used spin adapted VB diagram basis for studying correlated quantum systems [26, 18, 21]. The advantage of VB method over methods conserving only S_z are that it allows visualization of wavefunctions in terms of dominant VB diagrams.

3.2 Determinantal Quantum Monte Carlo (DQMC)

DQMC allows simulation of Hubbard-type models by integrating out the fermion degrees of freedom, replacing the Hubbard interaction with an auxiliary Hubbard-Stratonovich field [12, 16]. The method suffers from sign problem when used for fermion systems. Electron phonon-coupling can also be treated within DQMC [20].

3.3 Path Integral Renormalization Group (PIRG)

In the PIRG method, the wavefunction is expanded as a sum over L Slater determinants, and the projector operator $\exp(-\tau H)$ is used to project out the ground state from a random starting determinant [27]. The method is exact at $U = 0$ and for each L PIRG calculations are variational. The finite bias is removed by extrapolating quantities as a function of the energy variance ΔE . Importantly, PIRG doesn't suffer from sign problem.

Several additional techniques are essential to improve the accuracy of the PIRG. The use of lattice and spin symmetries using projection operators of the QP-PIRG has been shown to drastically lower the energy [28]. Second, it has been observed that PIRG method can get stuck in excited states. To prevent this, in addition to the PIRG projection operator, we used a random simulated annealing-like modification of the Slater determinants [23]. Furthermore, several starting states were chosen and their final energy were compared.

We have extensively benchmarked against the exact VB method and have found essentially perfect agreement [19]. The main disadvantage of PIRG compared to DQMC and CPMC is that it is much more computationally expensive.

3.4 Constrained Path Monte Carlo (CPMC)

CPMC is a ground-state projector QMC method [22]. Like PIRG, CPMC works in the space of Slater determinants. This space is overcomplete, which results in contributions to the ground state wavefunction that are both positive and negative. The Monte Carlo sampling is confined to the region where the overlap between each random walker $|\phi\rangle$ and a trial wavefunction $|\Psi_T\rangle$ is positive. This eliminates the loss of precision known as the fermion sign problem, but introduces an approximation into the method. A recent advance is the use of symmetry-adapted trial wavefunctions with CPMC, which greatly improves the accuracy [9]. We have used symmetry-adapted trial functions. The PIRG wavefunctions are ideal for this use.

4 Future Directions

While the pairing enhancement at a specific carrier density is intriguing and can have far reaching implications, our results miss two important aspects. First, in our calculation for the different lattices, the enhancement occurs in either the $d_{x^2-y^2}$ or d_{xy} channels, that is the pairing symmetry varies. Second, even as the density ρ where enhancement occurs tends to $\rho \approx 0.5$ as the lattice size increases, the precise ρ where the enhancement occurs is different on each lattice. The evolving phase diagram and continuous discovery of exotic phenomena in the unconventional superconductors has kept the field vibrant. The future scope of research thus, is many-fold. The CO state is known to be accompanied by giant phonon anomalies [29]. The effect of phonon could be studied as a combined effect of e-e and e-ph interactions in 2D systems within the Hubbard-Holstein model. Prior numerical calculations have been limited to $\rho = 1$ [3, 20]. Hubbard-Holstein model in 1D has been extensively studied using Stochastic Series Expansion (SSE) QMC [2, 10]. To add the effect of phonons, the variation of position coordinate of each oscillator will require an additional Monte Carlo sampling. The bare Hubbard model is sign-free at $\rho = 1$. Addition of e-ph interaction to the model has shown sign problem in the square lattice $\rho = 1$ limit [20]. Code development for the Hubbard-Holstein model to study pairing correlation and bond coupled e-ph model may be of interest. In the end, learning new algorithms and implementing them will keep me exploiting my code writing skills and take me deeper into numerical techniques. Given the absence of an analytical

solution of the problem, numerical methods has the ability to for an unbiased treatment of the strongly correlated problem.

References

- [1] D. Sénéchal A. H. Nevidomskyy, C. Scheiber and A.-M. S. Tremblay. *Phys. Rev. B*, 77:064427, 2008.
- [2] R. T. Clay and S. Mazumdar. *Phys. Rev. Lett.*, 94:207206, 2005.
- [3] B. Moritz R. T. Scalettar E. A. Nowadnick, S. Johnston and T. P. Devereaux. *Phys. Rev. Lett.*, 109:246404, 2012.
- [4] E. Fradkin E. Arrigoni and S. A. Kivelson. *Phys. Rev. B*, 69:214519, 2004.
- [5] G. Ghiringhelli et al. *Science*, 337:821, 2012.
- [6] J. Chang et al. *Nature Physics*, 8:871, 2012.
- [7] R. Comin et al. *Science*, 343:390, 2014.
- [8] T. Wu et al. *Nat. Commun.*, 4:2113, 2013.
- [9] R. Rodriguez-Guzman G. E. Scuseria H. Shi, C. A. Jimenez-Hoyos and S. Zhang. *Phys. Rev. B*, 89:125129, 2014.
- [10] R. P. Hardikar and R. T. Clay. *Phys. Rev. B*, 75:245103, 2007.
- [11] H. Kino and H. Kontani. *J. Phys. Soc. Jpn.*, 67:3691, 1998.
- [12] E. Y. Loh and J. E. Gubernatis. *Elsevier*, pages 177–235, 1992.
- [13] Hirokazu Tsunetsugu Matthias Troyer and T. M. Rice. *Phys. Rev. B*, 53:251, 1996.
- [14] N. Nagaosa P. A. Lee and X. G. Wen. *Rev. Mod. Phys.*, 78:17, 2006.
- [15] M. Randeria-T. M. Rice N. Trivedi P. W. Anderson, P. A. Lee and F. C. Zhang. *J. Phys.: Condens. Matter*, 16:R755, 2004.
- [16] D. J. Scalapino R. Blankenbecler and R. L. Sugar. *Phys. Rev. D*, 24:2278, 1981.
- [17] N. Gomes R. T. Clay, W. De Silva and S. Mazumdar. *Phys. Rev. B*, 93:165110, 2016.
- [18] S. Ramasesha and Z. G. Soos. *Int. J. Quant. Chem.*, XXV:1003, 1984.
- [19] H. Li S. Dayal, R. T. Clay and S. Mazumdar. *Phys. Rev. B*, 83:245106, 2011.
- [20] Y. F. Kung-B. Moritz R. T. Scalettar S. Johnston, E. A. Nowadnick and T. P. Devereaux. *Phys. Rev. B*, 87:235133, 2013.
- [21] J. Carlson S. Zhang and J. E. Gubernatis. *Chem. Phys. Lett*, 130:522, 1986.
- [22] J. Carlson S. Zhang and J. E. Gubernatis. *Phys. Rev. B*, 69:7464, 1997.
- [23] P. Sahebsara and D. Sénéchal. *Phys. Rev. Lett.*, 97:257004, 2006.
- [24] D. J. Scalapino. *Rev. Mod. Phys.*, 84:1383, 2012.
- [25] J. Schmalian. *Phys. Rev. Lett.*, 81:4232, 1998.
- [26] Z. G. Soos and S. Ramasesha. *Phys. Rev. B*, 29:5410, 1984.
- [27] Kashima T and Imada M. *J. Phys. Soc. Jpn.*, 70:2287–99, 2001.

- [28] T.Mizusaki and M.Imada. *Phys. Rev. B*, 74:014421, 2006.
- [29] T.M. Rice Ye-Hua Liu, Robert M. Konik and Fu-Chun Zhang. *Nat. Commun.*, 7:10378, 2015.