Quantum Monte Carlo and the Hubbard Model

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Abstract. Here we discuss quantum Monte Carlo and the Hubbard model. We note that while there is a fermion sign problem for the doped Hubbard model, Monte Carlo calculations have shown that the leading pairfield susceptibility has d-wave symmetry and that the pairing interaction is mediated by $S = 1$ particle-hole fluctuations.

Let me begin by thanking the Feenberg Memorial Metal Committee and the RPMBT for this award. It is of course an honor in light of Eugene Feenberg's seminal contributions to the strongly interacting quantum many-body problem. However, for me, it was particularly special because it brought back memories of attending Feenberg's course on "The Many-Body Problem" in 1961. At this time I was a graduate student at Stanford, so let me explain. In the late 50's the Stanford Mark IV electron accelerator was used to treat cancer patients during the day and I used it at night to study radiation produced free-radicals. Then in 1960 it was taken over for prototype design studies by Project M (which was to become SLAC). When this happened, I decided to switch to theory and Professor Edwin Jaynes agreed to become my advisor. Several months later, Ed informed me that he had accepted a Professorship at Washington University in St. Louis and encouraged me to come along. There in the physics building "Crow Hall" I shared an office with Feenberg's graduate students and attended his lectures. The warm reception by Feenberg and his students for an outsider from another graduate school is something that I will never forget.

Turning to physics, the award citation references Monte Carlo methods and superconductivity. After I left Washington University, I had the good fortune of learning about superconductivity working as a postdoc in 1962–64 with J.R. Schrieffer at the University of Pennsylvania. There along with John Wilkens, a PhD student of Bob's, we calculated the superconducting tunneling density of states for a model of Pb [1]. This was my first paper. In 1968 I moved to UCSB. There, in the first year of the ITP, 1979, Michael Creutz spoke about using Monte Carlo methods to study gluons on a lattice. Towards the end of his talk, he held up a stack of punchcards in one hand to illustrate how short the program was for these calculations. This made one wonder what might be possible for condensed matter lattice models. At that time the quarks were treated in the "quenched" approximation and there was interest in Monte Carlo methods that would include dynamic fermions. With Blankenbecler and Sugar, we developed a determinantal quantum Monte Carlo (DQMC) method [2] to treat fermions. Here the interacting problem was rewritten in terms of free fermions coupled to an auxiliary Hubbard-Stratonovich (HS) field. Using Wick's theorem, the fermions were integrated out leaving a determinant involving the HS field. The HS field was then summed over using a Monte Carlo method with the determinant giving the Boltzmann weight. We used this method to explore various electron-phonon models. Then in an insightful paper, J. Hirsch [3] introduced a discrete Hubbard-Stratonovich field and,

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combining a DQMC simulation with a finite scaling analysis, found that the groundstate of the half-filled Hubbard model had long range antiferromagnetic order. This work showed what could be done with the DQMC but at the same time set the bar very high for what was to come.

With the discovery of the high T_c cuprates [4] in 1986, there was intense interest in the doped 2D Hubbard model. There had been weak coupling predictions of d-wave superconductivity near the antiferromagnetic instability of the Hubbard model [5, 6]. However, little beyond RPA like calculations was known. It seemed like a perfect opportunity to apply the DQMC. However, for the doped Hubbard model the DQMC has what is called "a fermion sign problem". That is, the determinant of some HS field configurations can be negative. Furthermore, as the temperature is lowered relative to the bandwidth, the number of HS field configurations with positive determinants is found to be similar to the number with negative determinants. Then simple techniques, such as using the absolute value of the determinant as the Boltzmann weight and including the sign in the measurement, fail as the error grows exponentially at low temperatures.

So we do not have the same kind of DQMC results for the existence of long range d-wave superconductivity at low temperature for the doped 2D Hubbard model as we do for the zero temperature long range AF order of the 2D half-filled case. However, the results clearly show that the doped 2D Hubbard model contains d-wave pairing correlations [7] and that the pairing interaction responsible for these correlations is mediated by the exchange of $S = 1$ particle-hole fluctuations.

Fig. 1 shows the d-wave pairfield susceptibility

$$P_d(T) = \int_0^\beta dt \langle \Delta_d(t) \Delta_d^+(0) \rangle \tag{1}$$

with

$$\Delta_d^+ = \frac{1}{2\sqrt{N}} \sum_{i,\delta} (-1)^\delta c_{\ell\uparrow}^+ c_{\ell+\delta\downarrow}^+ \tag{2}$$

for a doped Hubbard model with a site filling $\langle n \rangle = 0.875$. Here $c_{\ell s}^+$ creates an electron with spin s on the ℓth lattice site. The sum i is over the N lattice sites, δ sums over the four near-neighbor sites of ℓ and $(-1)^\delta$ gives the characteristic d-wave $+-+-$ alternation. Although this calculation involved only a 4×4 lattice and the fermion sign problem prevented one from going to low temperatures, it is clear that short range d-wave pairfield correlations are present in the doped 2D Hubbard model. It is also clear from Fig. 1 that it it important to keep track of the sign of the determinant [8]. The results which show a decrease of $P_d(T)$ at low temperatures were obtained in a calculation in which the absolute value of the determinant was used as a Boltzmann weight but the sign was not included in the measurement.

The pairing interaction is given by the irreducible particle-particle vertex $\Gamma^{pp}(k, k')$ shown on the left-hand side of Fig. 2. It consists of all Feynman diagrams that can not be cut into two parts by cutting just two particle lines. Both DQMC [9] and a more recently developed dynamic cluster approximation (DCA) [10] have shown that the leading pairfield eigenfunction associated with $\Gamma^{pp}(k, k')$ has d-wave symmetry. Using the DCA, the pairing interaction $\Gamma^{pp}(k, k')$ was decomposed into a fully irreducible vertex Λ_{irr} and $S = 1$ (spin) and $S = 0$ (charge) particle-hole contribution. Plots of Γ^{pp} and these various contributions are shown in Fig. 3. The peak in the pairing interaction at large momentum transfer is what favors the d-wave pairing. From the decomposition, one clearly sees that the interaction is mediated by the $S = 1$ channel. Thus in spite of the fermion sign problem, one has been able to determine that the dominant pairing correlations in the doped 2D Hubbard model have d-wave symmetry and the pairing interaction that is responsible for these correlations arises from the $S = 1$ particle-hole channel.
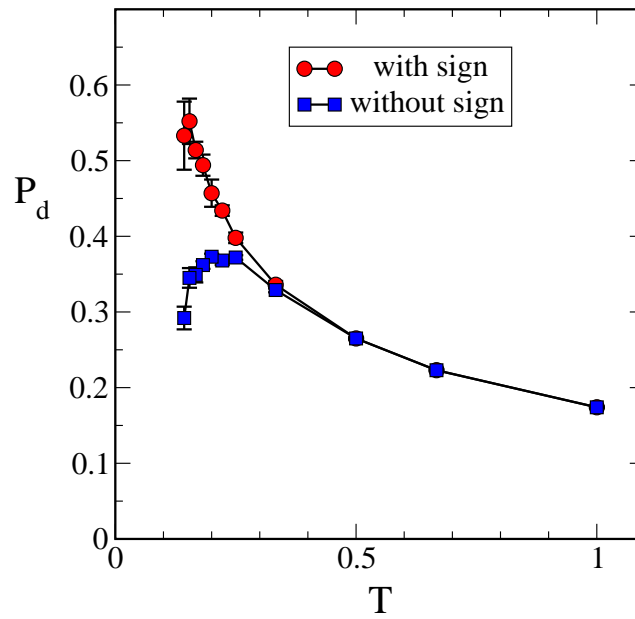
Figure 1. The d-wave pairfield susceptibility $P_d(T)$ (red circles) for a 4×4 lattice with $U = 4t$ and $\langle n \rangle = 0.875$ versus temperature T measured in units of the hopping t. The (blue squares) show the erroneous result that is found if the fermion sign is ignored (after Loh et al. [8]).
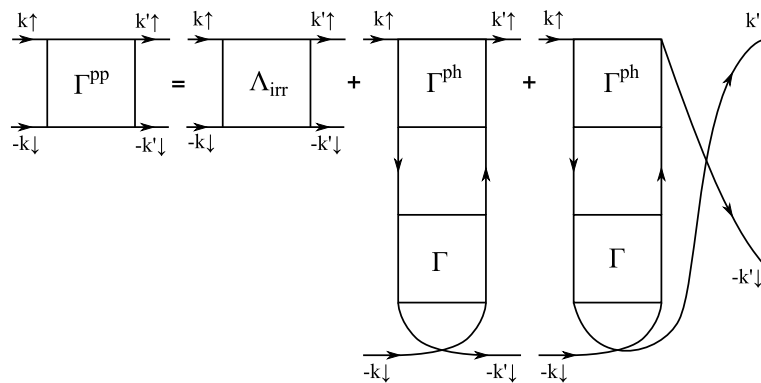

Figure 2. The pairing interaction is given by the irreducible particle-particle vertex Γ^{pp}. Here Γ^{pp} is decomposed into a fully irreducible two-fermion vertex Λ_{irr} plus contributions from the $S = 1$ and $S = 0$ particle-hole channels. Γ^{ph} are irreducible particle-hole vertices, Γ is the full vertex and the solid lines are fully dressed single particle propagators.
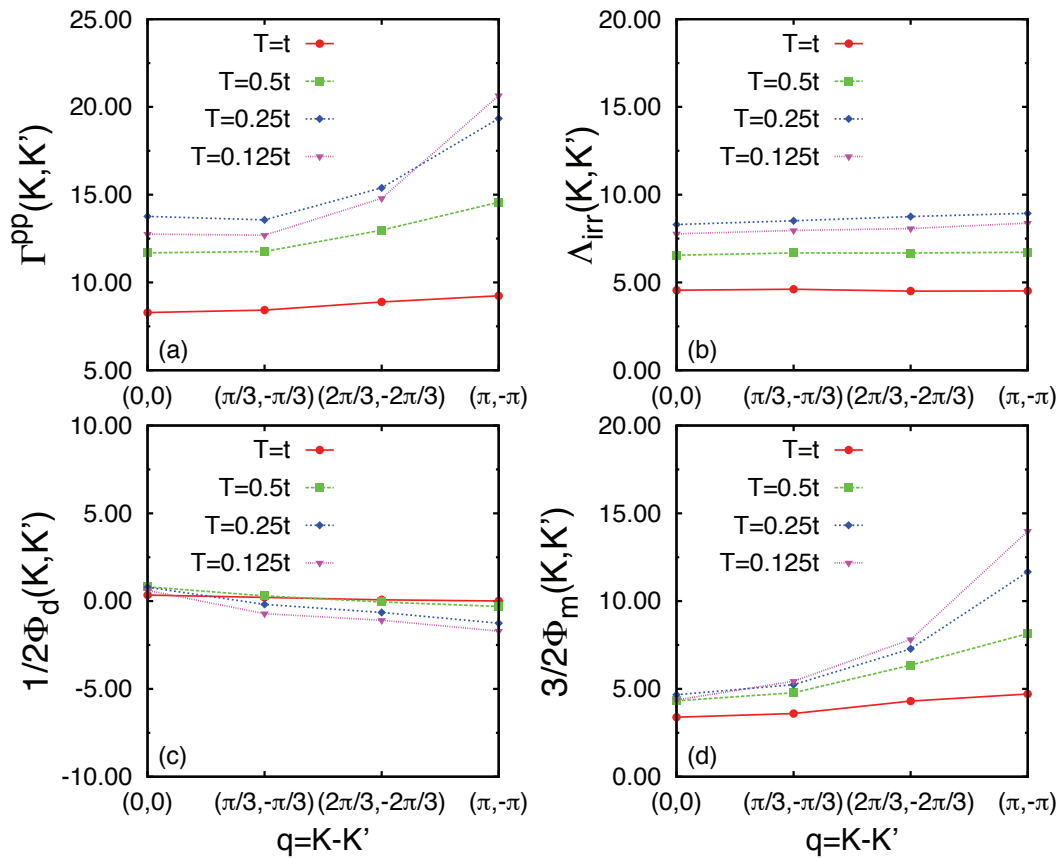
Figure 3. This figure illustrates the momentum dependence of the various contributions that make up the irreducible particle-particle pairing vertex Γ^{pp}. (a) The irreducible particle-particle vertex Γ^{pp} versus $q = K - K'$ for various temperatures with $\omega_n = \omega_{n'} = \pi T$. Note that the interaction increases with the momentum transfer as expected for a d-wave pairing interaction. (b) The q-dependence of the fully irreducible two-fermion vertex Λ_{irr}. (c) The q-dependence of the charge density ($S = 0$) channel for the same set of temperatures. (d) The q-dependence of the magnetic ($S = 1$) channel. Here, one sees that the increase in Γ^{pp} with momentum transfer arises from the $S = 1$ particle-hole channel (after Maier et al.[10]).

Although these results are for a single band Hubbard modeal, similar calculations have been carried out for the two-layer Hubbard model [11]. Here one finds that when the interlayer one-electron hopping becomes slightly larger than the intra layer hopping, the pairing shifts from d-wave to an $s^{\pm}$ state in which the gap switches sign between the bonding and anti-bonding Fermi surfaces, reminiscent of the Fe-pnictide/chalcogen superconductors. The Monte Carlo results for these models provide support for the idea that the unconventional, sign changing gap, superconductors share a common pairing mechanism mediated by the exchange of $S = 1$ spin-fluctuations.

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