Recent results on the Hubbard model by quantum Monte Carlo & Petaflop computers

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The Hubbard model has been a long standing model for too many years.

Experiments on optical lattices can solve fundamental questions about the model (soon?)

Quantum Monte Carlo can exploit massive parallelism in modern supercomputers, a factor $\sim 10000$ faster than 20 years ago.

Sampling the $<$Sign$>$ is the easiest task for parallelism, replicas and average!

More information (before optical lattices)?
Outline

From RVB insulator to High-Tc superconductivity with no electron-phonon coupling and repulsion (!)

Quantum Monte Carlo and Petaflop supercomputer: a new possibility to understand electron correlation

The honeycomb lattice $\rightarrow$ no spin liquid phase (contrary to previous claims)

How to survive with the sign problem?

Recent results by massive sampling/extrapolation: Small but non vanishing effect $\rightarrow$ Phase diagram?
Resonating valence bond (RVB)

In this theory the chemical valence bond is described as a singlet pair of electrons

\[
\frac{1}{\sqrt{2}} \left( |\uparrow \downarrow\rangle - |\downarrow \uparrow\rangle \right) \left[ \Psi_a(r) \Psi_b(r') + a \leftrightarrow b \right]
\]

spin up and spin down electrons in a spin singlet state

\(a\) and \(b\) are nuclear indexes

The true quantum state of a compound is a superposition or resonance of many valence bond states. The superposition usually improves the variational energy of the state.

L. Pauling, Phys. Rev. 54, 899 (1938)
Example of RVB

Benzene \( C_6H_6 \)

6 valence electrons in 6 sites (2p\(_z\) type) two ways to arrange nearest neighbor bonds (Kekule’ states)

**The rule:** two singlet bonds cannot overlap on the same Carbon atom otherwise two electrons feel a too large Coulomb repulsion.
\[
\frac{1}{\sqrt{2}} \left( |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right) [\Psi_a(r)\Psi_b(r') + a \leftrightarrow b]
\]

Kekule’ valence bonds

Dewar valence bond (believed less important)
Graphene layers can be experimentally prepared.
Definition of spin liquid

A spin state with

no magnetic order (classical trivial)
no broken translation symmetry (less trivial):

no Dimer state
(Read, Sachdev)

is a spin liquid
Recent development of supercomputers is based on an increased number of cores/node. But in this trend the bandwidth of the node increases much slower and the “delayed updates” technique becomes more and more crucial. Essentially one transforms matrix-updates (bandwidth limited) in matrix-matrix fast operations $LxK_{\text{rep}}$. 

![Graph showing speedup and speed in Petaflops per second vs. number of cores for different systems.](image)
Recent exciting result on the Hubbard model... Muramatsu group, Nature 2010.

No broken symmetry but a full gap at $U/t \sim 4$... this is an RVB phase...
The auxiliary field technique based on the Hubbard-Stratonovich (Hirsch) transformation provides a big reduction of the sign problem as:

The discrete HST (Hirsch '85):

\[
\exp[g(n_\uparrow - n_\downarrow)^2] = \frac{1}{2} \sum_{\sigma = \pm 1} \exp[\lambda \sigma (n_\uparrow - n_\downarrow)]
\]

\[
\cosh(\lambda) = \exp(g / 2)
\]
With this transformation the true propagator is a superposition of “'easy’” one-body propagators:

\[ |\psi_\tau\rangle = \exp(-H\tau) |\psi_T\rangle = \sum_{\{\sigma\}} U_\sigma(\tau,0) |\psi_T\rangle \]

and, if \( |\psi_T\rangle \) is a Slater determinant, \( U_\sigma(\tau,0) |\psi_T\rangle \) can be evaluated.

We can compute any correlation function \( O \) with standard MC with weight: \( W[\sigma] = \langle \psi_T | U_\sigma(\tau,0) |\psi_T\rangle \):

\[
\langle \psi_0 | O | \psi_0 \rangle = \frac{\langle \psi_{\tau/2} | O | \psi_{\tau/2} \rangle}{\langle \psi_\tau | \psi_T \rangle} = \sum_{\{\sigma\}} \frac{W[\sigma] O[\sigma]}{\sum_{\{\sigma\}} W[\sigma]}
\]

\[
O[\sigma] = \frac{\langle \psi_T | U_\sigma(\tau,\frac{\tau}{2}) O U_\sigma(\frac{\tau}{2},0) |\psi_T\rangle}{\langle \psi_T | U_\sigma(\tau,0) |\psi_T\rangle}
\]
Finite size scaling up to 2592 sites (previous 648)!

The charge-charge correlation should decay as $1/r^4$ in the semimetal, as opposed to exponential in the insulator, thus by plotting $L^4 \rho(L_{\text{max}})$.

We clearly see a charge transition at $U/t \sim 3.75(5)$ consistent with the magnetic one $\rightarrow$ no spin liquid $\rightarrow$. 
The proposed spin liquid should have a spin gap …but no spin gap was found by direct evaluation.
First results on a model without sign problem:

Much larger size $\rightarrow$ no spin liquid in a model with no frustration.

As a consequence of the Murphy’s law “’No interesting results can be obtained with a fermionic model without sign problem….”” but this is under debate. There are exceptions, but have to be also tested on much larger sizes and lower temperatures.
Cuprates

quasi-2D structure

Phase diagram: temperature vs. doping

$J = 1500K >>$ Other materials

$\delta$ (doping) = 0.2 $<< 1$
The presence of holes (empty sites) allows charge (super-) current and superconductivity.
RVB \rightarrow \text{the actual order parameter } \sim x \text{ (doping)}

\[ \Phi = \left\langle \left( c^+ c^+ \right)_{d\text{-wave}} \right\rangle \neq 0 \text{ only for } x > 0 \]

This is the most important feature of an RVB superconductor
Is there superconductivity in the **square lattice** Hubbard $U>0$? At half-filling (as in the honeycomb) it is magnetic (not RVB).

From T. Maier et al. PRL ’05 $U/t=4$ Cluster DMFT
A very controversial results (see e.g. our VMC). Older paper by S. Zhang et al. PRL’97 by CPQMC

\[ \Delta_{i,j} = c_{i\uparrow}c_{i\downarrow} + c_{j\uparrow}c_{i\downarrow} \] destroys a singlet bond.

ODLRO if, for \(|i - j| \to \infty\):

\[ \langle \psi_0 | \Delta^{+}_{i,i+x} \Delta_{j,j+x(y)} | \psi_0 \rangle = (+ (d\text{-wave}) P_d^2 > 0 \]

\(|\psi_0\rangle\) is estimated by projection techniques:

\[ |\psi_0\rangle = \exp(-H\tau)|\psi_T\rangle \quad \text{for } \tau \to \infty \]

with constrained path approximation (CPQMC)
FIG. 2. Long-range behavior of the $d_{x^2−y^2}$ pairing correlation function versus distance for 0.85 filled $12 \times 12$ lattice at $U = 2$, 4, and 8. This behavior is shown for the free-electron and CPMC calculations. Also shown is the vertex contribution.

FIG. 3. Long-range behavior of the $d_{x^2−y^2}$ pairing correlation function versus distance for a 0.85 filled $16 \times 16$ lattice at $U = 2$ and 4. This behavior is shown for the free-electron and CPMC calculations. Also shown is the vertex contribution.

Note the huge scale of the pairing !!!!
For a lattice model we use here the Gutzwiller wf

$$\psi_{RVB} = \exp(-g \sum_i n_{i\uparrow} n_{i\downarrow}) \exp \sum_{i,j} f_{i,j} \left( c_{i\uparrow}^+ c_{j\downarrow}^+ + c_{j\uparrow}^+ c_{i\downarrow}^+ \right) |0\rangle$$

Singlet bond

where $f$ is determined by one parameter $\Delta^{BCS}_{x^2-y^2}$

$$H_{BCS} = \sum_{k,\sigma} \varepsilon_k c_{k,\sigma}^+ c_{k,\sigma} + \Delta^{BCS}_{x^2-y^2} \sum_k (\cos k_x - \cos k_y) c_{k\uparrow}^+ c_{-k\downarrow}^+ + h.c.$$  

and $\varepsilon_k = -2t(\cos k_x + \cos k_y) - \mu$, i.e. $f_k = \frac{\Delta_k}{\varepsilon_k + \sqrt{\varepsilon_k^2 + \Delta_k^2}}$

Use of Quantum Monte Carlo mandatory:
Gutzwiller approximation too poor in general, e.g. Mott transition in cubic lattices...etc.
Why we have to optimize $J(=g)$ and $\Delta^{BCS}_{x^2-y^2}$?

Hubbard Model: $H = -t \sum_{<ij>,\sigma} c^+_i c_j + U \sum_i n_i^\uparrow n_i^\downarrow$

In mean field (BCS) no way to have $BCS>0$ for $U>0$

Theorem Lieb ‘90

Qualitative new features appear if $J$ and BCS are optimized together: RVB insulator or supercond.
There are “’huge’” finite size effects and
\[
\Delta_{x^2-y^2}^{BCS} \sim 0.01 \div 0.001 \text{ for } \#\text{Sites} \rightarrow \infty
\]
\[
P_d^2 \sim (\Delta_{x^2-y^2}^{BCS})^2 \sim 10^{-4} \div 10^{-6} \text{ almost unmeasurable by QMC}
\]
The pairing is almost unmeasurable for $U < \sim 5t$

Gutzwiller wave function

\[
\Delta_{x^2-y^2}
\]

\[
U / t
\]
Converged computations can be done by sampling Sign $\sim 0.01$ and by extrapolation (see later).
e.g. for the smallest U=0 pairing we start with Several different trial functions with different $\Delta^{BCS}_{x^2-y^2}$

Extrapolated
e.g. for the smallest U=0 pairing we start with

Several different trial functions with different $\Delta^{BCS}_{x^2-y^2}$

We use that all wf’s for $\tau \rightarrow \infty$ converge to the same value. Notice also non monotonic…
Test on an 18 sites where exact results known

By extrapolating consistently up to $\tau t=1$ with 3wf’s
The right scale is different and caught by the GW

In general the “right” pairing are much smaller than $U=0$ but much flatter (see blue), showing short coherence.
Why much smaller?

Correlation (U) makes a strong renormalization of the quasiparticle weight: 
\[ c_{kF}^+ \rightarrow Z_{kF} \tilde{c}_{kF}^+ \text{ with } Z_{kF} \ll 1 \]

The pairing correlations contains 4 c’s→ 
\[ Z_K^4 \sim 1/100 \]
\[ \left| \psi_{\tau/2} \right\rangle = \exp(-H \tau / 2) \left| \psi_T \right\rangle = \sum_i a_i \exp(-E_i \tau / 2) \left| \psi_i \right\rangle \]

where \( a_i = \langle \psi_T | \psi_i \rangle \) and \( H \left| \psi_i \right\rangle = E_i \left| \psi_i \right\rangle \)

\[
\frac{\langle \psi_{\tau/2} | O | \psi_{\tau/2} \rangle}{\langle \psi_{\tau} | \psi_T \rangle} = \sum_{i,j} a_i a_j \langle \psi_i | O | \psi_j \rangle \exp[-(E_i + E_j) \tau / 2] \sum_i a_i^2 \exp(-E_i \tau)
\]

\[
\sim \langle \psi_0 | O | \psi_0 \rangle + \sum_i b_i(O, \psi_T) \exp(-\Delta_i) \quad \Delta_i = | E_i - E_0 |
\]

By using two \( \Delta \) and two \( "b" \) for each \( O \) and \( \psi_T \) 
\( \rightarrow \) stable fits for estimating accurately \( \langle \psi_0 | O | \psi_0 \rangle \)
We have considered several closed shell fillings. Studying the evolution for $U>0$ of the pairing correlation, the smallest one for $U=0$. $P_d$ can be estimated by subtracting the "small" $U=0$ contribution (vertex correction).
Superconductivity from strong correlation t-J model

\[ P_d = 2 \sqrt{\left| \langle \psi_0 | \Delta^+_i \Delta^-_j \Delta^-_k \Delta^+_l | \psi_0 \rangle \right|} \]

at the largest distance

\[ J/t = 0.4 \]

8x8 empty
242 full

S. Sorella et al. PRL ‘02

\[ P_d \text{ is an order of magnitude larger than Hubbard!} \]
Conclusions

No spin liquid phase in the Honeycomb lattice. No spin liquid without sign problem?

Gutwiller wavefunction predicts d-wave pairing in the $U>0$ Hubbard model, but is indeed very small for $U<4t$ (if not zero at all).

By sampling the sign reasonably converged/extrapolated ground state properties can be obtained in closed shell #Sites $\sim 100$.

Good evidence of d-wave pairing, phase diagram possible by assuming small size effects in vertex corr.