High-temperature superconductivity from quantum cluster methods

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Outline

1. Superconductivity
2. High-temperature superconductors
3. The Hubbard model
4. Quantum cluster methods
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1. Superconductivity
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Section 1

Superconductivity
A century ago…

Discovery of superconductivity in Mercury by Kammerlingh-Onnes (April 1911)
The Meissner effect (1933)

- Exclusion of magnetic flux upon cooling
- SC ≠ infinite conductivity
- Two types: I et II
London Equation (1935)

- **Hypothesis**: the SC has a *rigid* wavefunction at \( p = 0 \):
  \[
  \langle p \rangle = m\langle v_s \rangle + \frac{e}{c}A = 0
  \]

- **Supercurrent**
  \[
  J_s = n_s e\langle v_s \rangle = -\frac{n_s e^2}{mc}A
  \]

- **Ampere’s law** \( \Rightarrow \) penetration length
  \[
  \lambda_L = \sqrt{\frac{mc^2}{4\pi n_s e^2}}
  \]

  in which EM fields penetrate inside a superconductor
Landau-Ginzburg Theory (1950)

- **Order parameter** $\Psi$, such that $n_s = |\Psi(r)|^2$
- **Nonlinear equation**

\[
-\frac{\hbar^2}{2m^*} \left( \nabla - \frac{ie^*}{\hbar c} A \right)^2 \Psi + \beta |\Psi|^2 \Psi = -\alpha(T) \Psi
\]

- Is $\Psi$ the wavefunction of the superconductor? Rather: a boson field describing Cooper pairs (BCS)
Bardeen-Cooper-Schrieffer (BCS) Theory (1957)

- An attractive force binds electrons into Cooper pairs (bosons)
- The pairs condensate into a unique, coherent ground state
- Coherence length $\xi$: size of pairs
- Superconducting gap $\Delta$: Energy needed to break a pair ($\div 2$): $2\Delta = 3.528 \ T_c$
- Type I: $\xi > \lambda \sqrt{2}$
- Type II: $\xi < \lambda \sqrt{2}$
Electron-phonon interaction

- Electrons are attracted to each other via the exchange of virtual phonons.
- Effective retarded potential:

\[ V(q, \omega) = \frac{v_q}{\varepsilon(q)} \left[ 1 + \frac{\omega_q^2}{\omega^2 - \omega_q^2} \right] \]

Coulomb potential \( \leftarrow \)

Dielectric constant \( \leftarrow \)

Phonon frequency \( \rightarrow \)

Simpler description:

\[ V_q = \begin{cases} -V_0 & |\varepsilon_q| < \omega_D \\ 0 & |\varepsilon_q| > \omega_D \end{cases} \]

Electron energy \( \leftarrow \)

Debye frequency \( \leftarrow \)
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Section 2

High-temperature superconductors
Evolution of $T_c$
Superconducting cuprates

- April 1986: Discovery of SC in LBCO
- \(\text{CuO}_2\) planes with rare earth filling
- Superconducting upon doping

<table>
<thead>
<tr>
<th>Material</th>
<th>Formula</th>
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</thead>
<tbody>
<tr>
<td>LBCO</td>
<td>(\text{La}_{2-x}\text{B}_x\text{CuO}_4)</td>
</tr>
<tr>
<td>LSCO</td>
<td>(\text{La}_{2-x}\text{Sr}_x\text{CuO}_4)</td>
</tr>
<tr>
<td>YBCO</td>
<td>(\text{YBa}_2\text{Cu}<em>3\text{O}</em>{7-y})</td>
</tr>
<tr>
<td>BSSCO</td>
<td>(\text{Bi}_{2}\text{Sr}<em>2\text{Ca}<em>n\text{Cu}</em>{n+1}\text{O}</em>{2n+6+x})</td>
</tr>
<tr>
<td>NCCO</td>
<td>(\text{Nd}_{2-x}\text{Ce}<em>x\text{CuO}</em>{4-y})</td>
</tr>
<tr>
<td>PCCO</td>
<td>(\text{Pr}_{2-x}\text{Ce}<em>x\text{CuO}</em>{4-y})</td>
</tr>
</tbody>
</table>
Peculiarities of high-temperature superconductivity

- Bad conductors in the normal phase
- Strongly type II ($\xi \ll \lambda_L$)
  YBCO: $\xi_{ab} \sim 2\text{nm}$, $\lambda_{ab} \sim 150\text{ nm}$
- Close to antiferromagnetic phase
- $d$-wave gap symmetry

Opening of $d$-wave gap at Fermi surface
Phase diagram: doping vs. temperature

$La_{2-x}Sr_xCuO_4$  $R_{2-x}Ce_xCuO_4$

Temperature (K) vs. doping (electron or hole) diagram showing regions of overdoped, underdoped, and pseudogap phases. $T^*$ indicates a critical temperature.
Much of the Physics resides in the CuO$_2$ planes

- $d$ Cu orbitals are hybridized with $p$ O orbitals
- Two electrons on the same Cu orbital: costs an energy $U$
Band theory for undoped LSCO

The usual DFT methods predict that undoped cuprates should be metals...

In fact: An antiferromagnetic insulators

... whereas they are antiferromagnetic insulators!

and probably Mott insulators underneath...

Antiferromagnetism may be the key to superconductivity.
Cartoon of a possible pairing mechanism

Propagating a single hole leaves a costly trail in an AF background

Not so for the propagation of a pair of holes!
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The Hubbard model
The Hubbard model

\[ H = \sum_{\mathbf{r}, \mathbf{r}', \sigma} t_{\mathbf{r}, \mathbf{r}'} c^\dagger_{\mathbf{r} \sigma} c_{\mathbf{r}' \sigma} + U \sum_{\mathbf{r}} n_{\mathbf{r} \uparrow} n_{\mathbf{r} \downarrow} - \mu \sum_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma} \]

- Hopping amplitude \( t_{\mathbf{r}, \mathbf{r}'} \)
- Creation operator \( c^\dagger_{\mathbf{r} \sigma} \)
- Number of spin \( \uparrow \) electrons at \( \mathbf{r} \)
- Repulsion term \( U \)
- Electron number \( n_{\mathbf{r}, \sigma} \)

\( w(x) \) is a function of \( x \).
Non-interacting limit

- $U = 0$: back to band theory.

\[ \varepsilon(k) = \frac{1}{N} \sum_{i,j} t_{ij} e^{-i(n_i - n_j) \cdot k} \]

- Square lattice with hopping to 1st, 2nd and 3rd neighbors ($t$, $t'$ et $t''$)

\[ \varepsilon(k) = -2t(\cos k_x + \cos k_y) - 2t'(\cos(k_x + k_y) + \cos(k_x - k_y)) - 2t''(\cos 2k_x + \cos 2k_y) \]

Hopping amplitudes

Fermi surface $t' = -0.3t$, $t'' = 0.2t$
**Strong $U$ limit**

- At half-filling (undoped), electrons localize to minimize the potential energy
- Ground state is $2^N$-fold degenerate when $U \to \infty$
- Effective Hamiltonian at large $U$: the quantum Heisenberg model

\[ H \to J \sum_{i,j} S_i \cdot S_j \quad J = \frac{4t^2}{U} \quad S = \frac{1}{2} c^\dagger_\alpha \sigma_{\alpha \beta} c_\beta \]

- Drive towards antiferromagnetism
  Simple argument (2nd order perturbation theory) ($H_{\text{kin.}} \ll H_{\text{pot.}}$):

\[ E_0 = \varepsilon_0 + \langle 0 | H_{\text{kin.}} | 0 \rangle + \sum_n \left| \frac{\langle n | H_{\text{kin.}} | 0 \rangle}{\varepsilon_0 - \varepsilon_n} \right|^2 \sim 0 < \varepsilon_0 \]
The Hubbard model

An exponential problem

- A band structure computation involves the iterated solution of a **one-body** problem: An eigenvalue problem of dimension
  \[ D \sim 10^3 - 10^4. \]

- The Hubbard model poses a **many-body** problem:
  - The Hilbert space dimension increases exponentially with the number \( L \) of sites.
  - For a half-filled system:
    \[ D \sim 4^L \frac{2}{\pi L} \]

- Numerically limited to small systems \((L \leq 16)\) if performing an exact diagonalization

<table>
<thead>
<tr>
<th>( L )</th>
<th>dimension ( D )</th>
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<tr>
<td>2</td>
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</tr>
<tr>
<td>4</td>
<td>36</td>
</tr>
<tr>
<td>6</td>
<td>400</td>
</tr>
<tr>
<td>8</td>
<td>4,900</td>
</tr>
<tr>
<td>10</td>
<td>63,504</td>
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<tr>
<td>12</td>
<td>853,776</td>
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<tr>
<td>14</td>
<td>11,778,624</td>
</tr>
<tr>
<td>16</td>
<td>165,636,900</td>
</tr>
</tbody>
</table>
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Quantum cluster methods
Cluster kinematics

- Solve an effective model on a finite cluster of sites
- Patch up the clusters together
- CPT: extends the cluster self-energy to the whole system
1D example: spectral function with increasing $U/t$
A cluster’s environment is represented by a bath of uncorrelated sites.

Follows the Anderson impurity model, the cluster being the impurity.

Bath parameters are determined by a self-consistency procedure.
Interlude: The one-particle Green function

- Contains information about one-particle excitations
- Appears naturally in Many-Body theory
- At zero temperature:

\[ G_{\alpha\beta}(\omega) = \langle \Omega | c_\alpha \frac{1}{\omega - H + E_0} c_\beta^\dagger | \Omega \rangle + \langle \Omega | c_\beta^\dagger \frac{1}{\omega + H - E_0} c_\alpha | \Omega \rangle \]

- For non interacting electrons ($U = 0$):

\[ G(\omega) = \frac{1}{\omega - t + \mu} \quad \text{ou} \quad G(k, \omega) = \frac{1}{\omega - \varepsilon_k + \mu} \quad (\alpha = \beta = k) \]

- If $U \neq 0$, one defines the self-energy $\Sigma$:

\[ G(\omega) = \frac{1}{\omega - t + \mu - \Sigma(\omega)} \quad \text{ou} \quad G(k, \omega) = \frac{1}{\omega - \varepsilon_k + \mu - \Sigma(k, \omega)} \]
CDMFT (cont.)

\[ H = \sum_{\alpha, \beta} t_{\alpha \beta} c_{\alpha}^\dagger c_{\beta} + \sum_{\alpha, \mu} \left( \theta_{\alpha \mu} c_{\alpha}^\dagger a_{\mu} + \text{c.h.} \right) + \sum_{\mu} \epsilon_{\mu} a_{\mu}^\dagger a_{\mu} + \text{interaction} \]

Cluster Green function:

\[ G^{-1}(\omega) = \omega - t - \Gamma(\omega) - \Sigma(\omega) \]

Hybridation function:

\[ \Gamma_{\alpha \beta}(\omega) = \sum_{\mu} \frac{\theta_{\alpha \mu} \theta_{\beta \mu}^*}{\omega - \epsilon_{\mu}} \]

Self-consistency:

\[ G(\omega) = \int_{\tilde{k}} \left[ \omega - t(\tilde{k}) - \Sigma(\omega) \right]^{-1} \]
CDMFT (cont.)

Initial guess for $\Gamma$

Cluster Solver: Compute $G$

$$\tilde{G} = \frac{L}{N} \sum_{\tilde{k}} \left[ G_0^{-1}(\tilde{k}) - \Sigma(\omega) \right]^{-1}$$

$G_0^{-1} = \tilde{G}^{-1} + \Sigma$

update $\Gamma$ by minimizing $d$

$\Gamma$ converged? Exit

Yes

No
Cluster Dynamical Impurity Approximation

- Same systems as CDMFT
- But bath parameters are determined by minimizing an energy functional
- more accurate, but harder

\[ \Omega() = \Omega' - \int \frac{d\omega}{\pi} \sum_{\tilde{k}} \ln \text{det} \left[ 1 - V(\tilde{k}, i\omega) G(\tilde{k}, i\omega) \right] \]

- G.S. energy of cluster
- inter cluster hopping + hybridization
- cluster Green function
CDIA : The Mott transition

M. Balzer et al., Europhys. Lett. 85 (2009), 17002
Early CDMFT results for the cuprate problem

Left: $t' = t'' = 0$. Right: more realistic model

- $U = 4t$
- $U = 8t$
- $U = 12t$
- $U = 16t$
- $U = 24t$

- $M, \psi$
- $\psi/J$

- $U = 8t$
- $t' = -0.3t$
- $t'' = 0.2t$

ψ (10×)
Early CDMFT results for the cuprate problem (cont.)

- Local repulsion $U$ favors $d$-wave superconductivity.
- SC order parameter seems to scale like $J = 4t^2/U$.
- Close to half-filling: more pairing, but less density of states (close to Mott insulator).
- Particle-hole asymmetry due to band structure ($t' \neq 0$).
- Simple model (and small clusters) lead to homogeneous AF-dSC coexistence.

But: *What can we say about the pairing mechanism?*
Digression: Dynamical spin susceptibility

Contains information about spin excitations

At zero temperature:

\[ \chi_{ab}(\omega) = \langle \Omega | S_a^z \frac{1}{\omega - H + E_0} S_b^z | \Omega \rangle \]

\[ \chi_q(\omega) = \langle \Omega | S_q^z \frac{1}{\omega - H + E_0} S_q^z | \Omega \rangle \]

The imaginary part \( \chi''_q(\omega) \) contains the magnon spectrum.

Can be measured by neutron diffraction

Reminder:

\[ \lim_{\eta \to 0^+} \text{Im} \frac{1}{\omega - \omega_0 + i\eta} = \pi \delta(\omega - \omega_0) \]
The intensity of the first peak of $\chi''(\pi, \pi)$ is correlated to the presence of superconductivity.


La$_{2-x}$Sr$_x$CuO$_4$, $x = 0.16$
Effect of long-range interactions

- Coulomb interaction (nearest neighbors):

\[ H = \sum_{r,r',\sigma} t_{r,r'} c_{r\sigma}^\dagger c_{r'\sigma} + U \sum_r n_{r\uparrow} n_{r\downarrow} + V \sum_{\langle rr'\rangle} n_r n_{r'} - \mu \sum_{r,\sigma} n_{r,\sigma} \]

- \( V \) is generally larger than \( J \):

\[ J = \frac{4t^2}{U-V} \lesssim V \ll U \]

- Can Superconductivity survive \( V \)?

- Yes! The key is the retarded nature of the effective attraction. (like the electron-phonon interaction in conventional superconductivity)
Effect of long-range interactions (cont.)

- $V$ is detrimental to SC in the overdoped region
- ...but not in the underdoped region
  - Two compensating effects:
    - $V$ breaks pairs by itself
    - but $V$ increases $J \rightarrow$ increases pairing
- Quite different at small coupling (below the Mott transition)

Sénéchal, Tremblay, Day, Bouliane (in progress)
Finite-frequency contribution to SC order

\[ I_F(\omega) = \int_0^\infty \frac{d\omega'}{2\pi} \int F(\mathbf{k}, \omega') \psi = I_F(\infty) \]

In Nambu representation:

\[ G(\mathbf{k}, \omega) = \begin{pmatrix} G_\uparrow(\omega) & F(\omega) \\ F^\dagger(\omega) & G_\downarrow(-\omega) \end{pmatrix} \]

- The low-frequency contribution comes from magnetic fluctuations (scales like $J$)
- High-frequencies show the pair-breaking effect of $V$. 

Sénéchal, Tremblay, Day, Bouliane (in progress)
Quantum cluster methods support a pairing mechanism via magnetic fluctuations.

The spectral features of the order parameter are correlated with the AF susceptibility.

This magnetic interaction is retarded, which makes SC robust against longer-range Coulomb repulsion.

At low doping: $V$ increases $J$, which compensates $V$’s pair breaking effect.

At higher doping: $V$ hinders superconductivity.
Acknowledgements

Collaborators in Sherbrooke (last 5 years):
QUESTIONS ?
Three-band model

- Hubbard model involving one Cu and two O orbitals (Emery 1987)

\[
H = (\varepsilon_d - \mu) \sum_{i,\sigma} n_{i\sigma}^{(d)} + (\varepsilon_p - \mu) \sum_{j,\sigma} n_{j\sigma}^{(p)}
+ t_{pd} \sum_{\langle i,j \rangle} (p_{i\sigma}^{\dagger} d_{i\sigma} + d_{i\sigma}^{\dagger} p_{j\sigma}) + t_{pp} \sum_{\langle j,j' \rangle} (p_{j\sigma}^{\dagger} p_{j'\sigma} + \text{H.c.})
+ U_d \sum_{i} n_{i\uparrow}^{(d)} n_{i\downarrow}^{(d)} + U_p \sum_{j} n_{j\uparrow}^{(p)} n_{j\downarrow}^{(p)} + U_{pd} \sum_{\langle i,j \rangle} n_{i\sigma}^{(d)} n_{j\sigma}^{(p)}
\]

- Parameters (eV)

<table>
<thead>
<tr>
<th>(\varepsilon_p - \varepsilon_d)</th>
<th>(t_{pd})</th>
<th>(t_{pp})</th>
<th>(U_d)</th>
<th>(U_p)</th>
<th>(U_{pd})</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.6</td>
<td>1.3</td>
<td>0.65</td>
<td>10.5</td>
<td>4</td>
<td>1.2</td>
</tr>
</tbody>
</table>
Variational Cluster Approximation: results

M. Guillot (mémoire MSc)
BCS Theory (cont.)

- Effective Hamiltonian:

\[ H_{\text{cin.}} = \sum_{\mathbf{k}, \sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma} \quad H_{\text{pot.}} = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', q, \sigma, \sigma'} V_q c_{\mathbf{k}+q, \sigma}^\dagger c_{\mathbf{k}'-q, \sigma'}^\dagger c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} \]

- Mean-field factorization:

\[ H_{\text{pot.}} = \frac{1}{2} \sum_{\mathbf{k}, \mathbf{k}', q, \sigma, \sigma'} V_q \left\{ \left\langle c_{\mathbf{k}+q, \sigma}^\dagger c_{\mathbf{k}'-q, \sigma'}^\dagger \right\rangle c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} + c_{\mathbf{k}+q, \sigma}^\dagger c_{\mathbf{k}'-q, \sigma'}^\dagger \left\langle c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} \right\rangle \right\} \]

- One sets

\[ \left\langle c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma} \right\rangle \propto \delta_{\mathbf{k}, -\mathbf{k}'} \delta_{\sigma, -\sigma'} \]

Pairs have zero spin and zero momentum.
BCS Theory (cont.)

- Define

\[ \Delta_k = \sum_q V_{q-k} \langle c_q \downarrow c_{-q} \uparrow \rangle \]

- Mean-field Hamiltonian:

\[ H = \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_k \Delta_k^* c_{-k\downarrow} c_{k\uparrow} + \Delta_k c_{-k\uparrow}^\dagger c_{k\downarrow}^\dagger \]

- Quasi-particles with energy

\[ E_k = \sqrt{\varepsilon_k^2 + |\Delta_k|^2} \] above a ground state made of condensed Cooper pairs.
Hubbard model: methods of solution

The more difficult the problem, the more methods to solve it!

- Perturbation theory in $U/t$ or in $t/U$ (more difficult)
- Self-consistent schemes based on perturbation theory
- Self-consistent two-particle theory [Tremblay et al.]
- Variational methods on the ground state (e.g. Gutzwiller)
- Various approximate reductions to a 1-body problem:
  - Mean-field theory built on an ordered state
  - slave bosons
- Quantum Monte-Carlo simulations (various schemes)
- Exact diagonalizations of small systems in periodic boundary conditions
- Dynamical Mean Field Theory (DMFT)
- Quantum cluster methods: CPT, DCA, CDMFT, VCA, CDIA