Continuous-Time Quantum Monte Carlo

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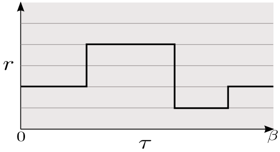
Outline

1. Overview of continuous-time quantum Monte Carlo methods
2. CT-INT for the Hubbard Hamiltonian
   Derivation of the algorithm.
3. Numerical implementation
   Updates, warmup, etc.
4. CT-INT for more general models
   Models defined by an action.
5. Application to electron-phonon models
   Fermionic model with retarded interaction.
6. Application to topological insulators
   Effective model of edge states.

Overview of continuous-time QMC methods

Continuous vs. discrete imaginary time

- D dimensional quantum systems live in D + 1 dimensions.
  The additional dimension is the imaginary time axis $\tau = it \in [0, \frac{1}{k_B T}]$.



- Discretizing $\tau = l\Delta\tau$ ($\Delta\tau = \frac{\beta}{L}$) permits the Suzuki-Trotter decomposition

$$e^{-\Delta\tau(\hat{H}_0+\hat{H}_1)} = e^{-\Delta\tau\hat{H}_0}\, e^{-\Delta\tau\hat{H}_1} + \mathcal{O}(\Delta\tau^2)$$

  useful to calculate expectation values of the form

$$\int dx \,\langle x|\, e^{-\beta\hat{H}}\,|x\rangle \;\approx \prod_{l=1}^{L} \int dx_l \int dy_l \,\langle x_l|\, e^{-\Delta\tau\hat{H}_0}|y_l\rangle\, \langle y_l|e^{-\Delta\tau\hat{H}_1}\,|x_l\rangle$$

  Examples: path integral (limit $\Delta\tau \to 0$), auxiliary-field QMC (finite $\Delta\tau$)
- Error: ignore if smaller than statistical errors, or extrapolate to $\Delta\tau = 0$.

Desirable to use continuous time.

Some milestones for continuous-time QMC methods

Gull et al., Rev. Mod. Phys. 2011

- Stochastic Series Expansion: Taylor expansion of $e^{-\beta \hat{H}}$ — Handscomb, Sandvik et al.
  Spins and bosons. $\Longrightarrow$ M. Troyer

- Diagrammatic Monte Carlo for bosons. — Prokof'ev, Svistunov, et al.
- Diagrammatic Monte Carlo in the thermodynamic limit. — Prokof'ev, Troyer, et al.
  $\Longrightarrow$ L. Pollet

- Continuous-time methods for fermions: — Rombouts

  – Interaction expansion (CT-INT) — Rubtsov et al.
  – Interaction expansion (CT-INT) — Rubtsov et al.
  – Hybridization expansion (CT-HYB) — Werner et al.
  – Interaction expansion with auxiliary fields (CT-AUX) — Gull et al.

- Discrete-time auxiliary-field QMC is central for lattice fermion models.
  Scales linearly with inverse temperature. — Blankenbecler et al.
  $\Longrightarrow$ F. Assaad

This talk: CT-INT, for CT-HYB and CT-AUX see Gull et al., RMP 2011

References

Key papers for the CT-INT method

- Rubtsov, Savkin, Lichtenstein, Phys. Rev. B **72**, 035122 (2005)
- Assaad & Lang, Phys. Rev. B **76**, 035116 (2007)

Review article

- Gull, Millis, Lichtenstein, Rubtsov, Troyer, Werner
  Rev. Mod. Phys. **83**, 349 (2011)

CT-INT for the Hubbard model

Starting point: partition function

We consider a system with Hamiltonian

$$\hat{H} = \underbrace{\hat{H}_0}_{\text{hopping}} + \underbrace{\hat{H}_1}_{\text{interaction}}$$

The grand-canonical partition function is given by ($\hat{H}_0$ includes $-\mu\hat{N}$)

$$Z = \text{Tr}\left[e^{-\beta\hat{H}}\right], \quad \beta = \frac{1}{k_B T}$$

A series expansion gives

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \ldots \int_0^\beta d\tau_n \left\langle T_\tau \hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n) \right\rangle_0$$

The time-dependent interaction operators are defined as

$$\hat{H}_1^{(D)}(\tau) = e^{\tau\hat{H}_0}\,\hat{H}_1\,e^{-\tau\hat{H}_0} \equiv \hat{H}_1(\tau)$$

Starting point for CT-INT

For simplicity, we assume an Hubbard interaction

$$\hat{H}_1(\tau) = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

To avoid a (trivial) sign problem, we rewrite $\hat{H}_1$ as

$$\hat{H}_1 = w \sum_i \underbrace{\sum_{s=\pm 1}}_{\text{Ising spins}} [\hat{n}_{i\uparrow} - \alpha_\uparrow(s)] [\hat{n}_{i\downarrow} - \alpha_\downarrow(s)] \,, \quad w = \frac{U}{2}$$

The dynamical Ising spins s are used to preserve the $SU(2)$ spin symmetry.
Static values α_σ are also possible.

Rubtsov et al., PRB 2005

Short-hand notation

To lighten the notation, we introduce

$$v = \{x, y; s\}\,, \quad w(v) = U/2$$

For the Hubbard model

$$\underbrace{x = \{i, \tau, \uparrow\}, \quad y = \{i, \tau, \downarrow\}}_{\text{onsite, equal times, opposite spin}}, \qquad \underbrace{w = U/2}_{\text{independent of } v}$$

$$\begin{aligned} x &= \{i, \tau, \uparrow\} \\ y &= \{i, \tau, \downarrow\} \end{aligned}$$

With

$$\hat{h}_1(v) = [\hat{n}_{i\uparrow} - \alpha_\uparrow(s)]\,[\hat{n}_{i\downarrow} - \alpha_\downarrow(s)]$$

we can write the interaction as

$$\int_0^\beta d\tau\, \hat{H}_1(\tau) = \int_0^\beta d\tau \sum_i \sum_{s=\pm 1} w\, \hat{h}_1(v) = \underbrace{w}_{\text{vertex weight}} \sum_v \hat{h}_1(v)$$

Diagrammatic expansion of the partition function

Inserting the above form for the interaction, we have

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \dots \int_0^\beta d\tau_n \left\langle T_\tau \hat{H}_1(\tau_1) \cdots \hat{H}_1(\tau_n) \right\rangle_0$$
$$= \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} w^n \sum_{\nu_1} \cdots \sum_{\nu_n} \left\langle T_\tau \hat{h}_1(\nu_1) \cdots \hat{h}_1(\nu_n) \right\rangle_0$$

Each operator $\hat{h}_1(\nu)$ corresponds to a vertex, and we have to sum over all expansion orders n, and over the internal variables $\nu = \{x, y; s\}$ of the vertices.

Idea of CT-INT:

Stochastic summation of series by sampling vertex configurations.

Partition function as a sum over vertex configurations

We can write the diagrammatic expansion

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} w^n \sum_{v_1} \cdots \sum_{v_n} \left\langle T_\tau \, \hat{h}_1(v_1) \cdots \hat{h}_1(v_n) \right\rangle_0$$

as a sum over unordered vertex configurations C_n.

With the notation

$$\sum_n \sum_{v_1} \cdots \sum_{v_n} \quad \equiv \quad \sum_{C_n}$$

we obtain

$$\frac{Z}{Z_0} = \sum_{C_n} \underbrace{(-w)^n \left\langle T_\tau \, \hat{h}_1(v_1) \cdots \hat{h}_1(v_n) \right\rangle_0}_{\text{configuration weight}} = \sum_{C_n} W(C_n)$$

A configuration C_n is specified by the variables of all n vertices:

$$\{v_1, \ldots, v_n\}$$

Configuration weight as a determinant

Wick's Theorem:

$$\left\langle T_\tau \, \hat{h}_1(v_1) \cdots \hat{h}_1(v_n) \right\rangle_0 = \det M(C_n)$$

can be expressed in terms of contractions $\langle c_x^\dagger c_y \rangle_0$.
with the $2n \times 2n$ matrix $\alpha(v) = \alpha_\uparrow(s), \alpha_\downarrow(s)$

$$M(C_n) = \begin{bmatrix} G^0(x_1,x_1) - \alpha(v_1) & G^0(x_1,y_1) & \cdots & G^0(x_1,y_n) \\ G^0(y_1,x_1) & G^0(y_1,y_1) - \alpha(v_1) & \cdots & G^0(y_1,y_n) \\ \vdots & \vdots & \ddots & \vdots \\ G^0(x_n,x_1) & G^0(x_n,y_1) & \cdots & G^0(x_n,y_n) \\ G^0(y_n,x_1) & G^0(y_n,y_1) & \cdots & G^0(y_n,y_n) - \alpha(v_n) \end{bmatrix}$$

containing the non-interacting Green function $G^0(x,y) = \langle c_x^\dagger c_y \rangle_0$.

The Hubbard model conserves spin, $\langle c_\uparrow^\dagger c_\downarrow \rangle_0 = \langle c_\downarrow^\dagger c_\uparrow \rangle_0 = 0$, so that

$$M(C_n) = \begin{bmatrix} M_\uparrow(C_n) & 0 \\ 0 & M_\downarrow(C_n) \end{bmatrix}$$

Therefore, $\det M(C_n) = \underbrace{\det M_\uparrow(C_n)}_{n\times n} \underbrace{\det M_\downarrow(C_n)}_{n\times n}$.

Determinants correspond to the sum over all Feynman diagrams

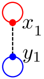
For the Hubbard model, the partition function can hence be written as

$$\frac{Z}{Z_0} = \sum_{C_n} \left(-\frac{U}{2}\right)^n \det M_\uparrow(C_n) \det M_\downarrow(C_n)$$

- The determinants correspond to a summation of all Feynman diagrams (connected and disconnected) for a given vertex configuration.

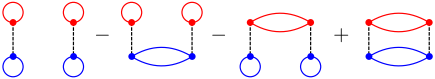
<u>$n = 1$:</u>

$$\det M_\uparrow(C_1) \det M_\downarrow(C_1) = G^0(x_1, x_1) G^0(y_1, y_1)$$



<u>$n = 2$:</u>

$$\det M_\uparrow(C_2) \det M_\downarrow(C_2) = [G^0(x_1, x_1) G^0(x_2, x_2) - G^0(x_1, x_2) G^0(x_2, x_1)] [(x \mapsto y)]$$



- The expansion converges for finite fermionic systems at $T > 0$.
- Although based on a weak-coupling expansion, the method is exact.

Stochastic summation using a Markov process

The sum over configurations can be carried out stochastically. In this way, we take into account configurations according to their statistical weight.

The variables appearing in

$$\sum_{C_n} \equiv \sum_n \sum_{\nu_1} \cdots \sum_{\nu_n} = \sum_n \sum_{x_1,y_1,s_1} \cdots \sum_{x_n,y_n,s_n}$$

can be carried out by adding/removing single vertices.

Monte Carlo updates:

- add a vertex $(n \mapsto n+1)$
- remove a vertex $(n \mapsto n-1)$

Optional:

- Move vertices in space and/or time.
- Flip Ising spins.
- Add/remove multiple vertices.

Configurations can be sampled using the Metropolis-Hastings algorithm

Partition function:

$$\frac{Z}{Z_0} = \sum_{C_n} \underbrace{W(C_n)}_{\text{configuration weight}}$$

Given a configuration C, we propose a new configuration C'.

In the Metropolis-Hastings algorithm, the acceptance probability is

$$P(C \mapsto C') = \min\left[1, \frac{W(C')}{W(C)}\right]$$

$$P(C \mapsto C') = \min\left[1, \frac{W(C')}{W(C)} \frac{T(C' \mapsto C)}{T(C \mapsto C)}\right]$$

- If $W(C') > W(C)$, the move is always accepted.
  If $W(C') < W(C)$, it is accepted with probability $P = W(C')/W(C)$.

- We also have to account for the proposal probabilities.

Update probabilities for the Hubbard model

Ratio of weights:

$$\frac{W(C_{n+1})}{W(C_n)} = \frac{\left(-\frac{U}{2}\right)^{n+1}}{\left(-\frac{U}{2}\right)^{n}} \prod_\sigma \frac{\det M_\sigma(C_{n+1})}{\det M_\sigma(C_n)} = -\frac{U}{2} \prod_\sigma \frac{\det M_\sigma(C_{n+1})}{\det M_\sigma(C_n)}$$

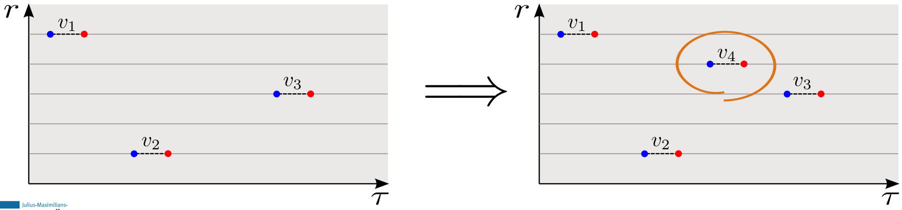
$$\frac{W(C_{n-1})}{W(C_n)} = \frac{\left(-\frac{U}{2}\right)^{n-1}}{\left(-\frac{U}{2}\right)^{n}} \prod_\sigma \frac{\det M_\sigma(C_{n-1})}{\det M_\sigma(C_n)} = -\frac{2}{U} \prod_\sigma \frac{\det M_\sigma(C_{n-1})}{\det M_\sigma(C_n)}$$

Proposal probabilities:

$$T(C_n \mapsto C_{n+1}) = \frac{1}{L}\frac{1}{\beta}\frac{1}{2} \qquad T(C_{n+1} \mapsto C_n) = \frac{1}{n+1}$$

$$T(C_{n-1} \mapsto C_n) = \frac{1}{L}\frac{1}{\beta}\frac{1}{2} \qquad T(C_n \mapsto C_{n-1}) = \frac{1}{n}$$

$i_4 \in [1, L], \quad \tau_4 \in [0, \beta), \quad s_4 = \pm 1$



Measuring observables

Expectation value:

$$
\begin{aligned}
\langle \hat{O} \rangle &= \frac{1}{Z} \mathrm{Tr}\left[e^{-\beta \hat{H}} \hat{O} \right] \\
&= \frac{Z_0}{Z} \sum_{C_n} (-w)^n \langle T_\tau \hat{h}_1(v_1) \cdots \hat{h}_1(v_n)\, \hat{O} \rangle_0 \\
&= \frac{Z_0}{Z} \sum_{C_n} (-w)^n \det \widetilde{M}(C_n) \\
&= \frac{Z_0}{Z} \sum_{C_n} (-w)^n \det M(C_n)\, \underbrace{\frac{\det \widetilde{M}(C_n)}{\det M(C_n)}}_{\langle\langle \hat{O} \rangle\rangle_{C_n}} \\
&= \frac{Z_0}{Z} \sum_{C_n} W(C_n) \langle\langle \hat{O} \rangle\rangle_{C_n} \\
&= \frac{\sum_{C_n} W(C_n) \langle\langle \hat{O} \rangle\rangle_{C_n}}{\sum_{C_n} W(C_n)}
\end{aligned}
$$

Observables can be measured exploiting Wick's Theorem

Single-particle Green function:

$$G(x,y) = \langle c_x^\dagger c_y \rangle = \frac{\sum_{C_n} W_n \langle\langle G(x,y) \rangle\rangle_{C_n}}{\sum_{C_n} W_n}$$

$$\langle\langle G(x,y) \rangle\rangle_{C_n} = \frac{\det \begin{bmatrix} \multicolumn{3}{c}{\multirow{3}{*}{M(C_n)}} & G^0(x_1,y) \\ & & & G^0(y_1,y) \\ & & & \vdots \\ G^0(x,x_1) & G^0(x,y_1) & \dots & G^0(x,y) \end{bmatrix}}{\det M(C_n)}$$

For each configuration C_n, Wick's Theorem holds: Luitz & Assaad, PRB 2010

$$\langle\langle \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} \rangle\rangle_{C_n} = \langle\langle c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow} \rangle\rangle_{C_n} = \langle\langle c_{i\uparrow}^\dagger c_{i\uparrow} \rangle\rangle \langle\langle c_{i\downarrow}^\dagger c_{i\downarrow} \rangle\rangle - \langle\langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle\rangle \langle\langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle\rangle$$

$\Rightarrow$ Higher Green functions can be obtained from $\langle\langle c_x^\dagger c_y \rangle\rangle$.

Absence of a sign problem for the 1D Hubbard model

Assaad & Lang, PRB 2007

- At half filling, $SU(2)$ spin symmetry + particle-hole symmetry ensure absence of a sign problem, because

$$\det M_{\uparrow}(C_n) = (-1)^n \det M_{\downarrow}(C_n)$$

so that

$$W(C_n) = \left(-\frac{U}{2}\right)^n \det M_{\uparrow}(C_n) \det M_{\downarrow}(C_n) = \left(+\frac{U}{2}\right)^n [\det M_{\downarrow}(C_n)]^2$$

- For general filling $\langle n \rangle$, a sign problem can be avoided by setting

$$\alpha_{\uparrow} = \tfrac{1}{2}\langle n \rangle + \delta s$$
$$\alpha_{\downarrow} = \tfrac{1}{2}\langle n \rangle - \delta s$$

with $s = \pm 1$ and $\delta > 0$.

- A moderate sign problem can be handled by reweighting:

$$W(C_n) \mapsto |W(C_n)|\,, \quad \langle \hat{O} \rangle = \frac{\langle \hat{O}\,\mathrm{sgn}(W) \rangle}{\langle \mathrm{sgn}(W) \rangle}$$

Numerical implementation

Overview

Model: $G^0(x, y)$, vertex

- Use table of G^0 on a fine τ grid.
- Exploit translational symmetry in space and time.

$$G^0(x, y) = G^0(i - j, \tau - \tau')$$

Monte Carlo configuration: C_n

- List of vertices containing variables ν and α for each vertex.
- Associated with C_n is the matrix $M^{-1}(C_n)$, required to calculate acceptance probabilities and $G(x, y)$.

Updates: addition/removal of vertices

- Explicit Ising spin flips are inexpensive and useful.

Warmup:

- Start with no vertices.
- Add/remove until equilibrium is reached.

Fast updates can be used to reduce numerical effort

- Direct calculation of

$$M^{-1}(C_n)\,, \quad \det M(C_n)\,, \quad \frac{\det M'}{\det M}$$

is numerically expensive, scaling with $(\dim M)^3$.

- Adding/removing a single vertex is a small change.
$M(C_n)$ and $M(C_{n\pm 1})$ only differ by one column and row.

- The smallness of the changes can be exploited using so-called fast updates.
FU's are at the heart of auxiliary-field QMC. $\Longrightarrow$ F. Assaad, Thursday

- FU's rely on formulas from matrix theory. Luitz, PhD Thesis, University of Würzburg

$$\det \begin{bmatrix} M & u \\ v^T & z \end{bmatrix} = \det M \det \left[z - v^T M^{-1} u\right] \; \det \begin{bmatrix} M & \vec{u} \\ \vec{v}^T & z \end{bmatrix} = \det M \det \left[z - \vec{v}^T\right.$$

M: $n \times n$, $u, v : n \times m$, z: $m \times m$; $m \ll n$ M: $n \times n$,
$\vec{u}, \vec{v} : n \times 1$, z: 1×1;

Simplest case: $m = 1$ (for example, in the Hubbard model).

Adding a vertex

We have to calculate

$$P(C_n \mapsto C_{n+1}) = \min\left[1, -\frac{UL\beta}{n+1} \underbrace{\prod_\sigma \frac{\det M_\sigma(C_{n+1})}{\det M_\sigma(C_n)}}_{\text{Hubbard model}}\right]$$

The matrix $M_\sigma(C_{n+1})$ is given by

$$M_\sigma(C_{n+1}) = \begin{bmatrix} M_\sigma(C_n) & \begin{matrix} G^0(x_1, x_{n+1}) \\ G^0(x_2, x_{n+1}) \\ \vdots \end{matrix} \\ G^0(x_{n+1}, x_1) \quad G^0(x_{n+1}, x_2) \quad \dots & G^0(x_{n+1}, x_{n+1}) - \alpha(v_{n+1}) \end{bmatrix}$$

which matches the structure of

$$\det \begin{bmatrix} M & \vec{u} \\ \vec{v}^T & z \end{bmatrix}$$

Consequently, we have

$$\frac{\det M_\sigma(C_{n+1})}{\det M_\sigma(C_n)} = \det\left[z - \vec{v}^T M_\sigma^{-1}(C_n)\, \vec{u}\right]$$

Removing a vertex

$$P(C_n \mapsto C_{n-1}) = \min\left[1, -\frac{n}{UL\beta}\prod_\sigma \frac{\det M_\sigma(C_{n-1})}{\det M_\sigma(C_n)}\right]$$

We consider removing the last vertex, and write

$$M_\sigma(C_n) = \begin{bmatrix} \multicolumn{3}{c}{M_\sigma(C_{n-1})} & \begin{matrix} G^0(x_1, x_n) \\ G^0(x_2, x_n) \\ \vdots \end{matrix} \\ G^0(x_n, x_1) & G^0(x_n, x_2) & \dots & G^0(x_n, x_n) - \alpha(v_n) \end{bmatrix}$$

to obtain

$$\frac{\det M_\sigma(C_{n-1})}{\det M_\sigma(C_n)} = \det\left[z - \vec{v}^T M_\sigma^{-1}(C_{n-1})\,\vec{u}\right] = [M_\sigma^{-1}(C_n)]_{nn}$$

Upon acceptance, M^{-1} can be updated efficiently [$\mathcal{O}(n^2)$] using the Sherman-Morrison formula:

$$(M + \vec{u}\,\vec{v}^T)^{-1} = M^{-1} - \frac{M^{-1}\,\vec{u}\,\vec{v}^T\,M^{-1}}{1 + \vec{v}^T\,M^{-1}\,\vec{u}}$$

Single-particle Green function

Knowledge of $G_\sigma(x,y)$ allows to calculate other observables via Wick's Theorem.

$$\langle\langle G_\sigma(x,y)\rangle\rangle = \frac{\det\begin{bmatrix} & M_\sigma(C_n) & & G^0(x_1,y) \\ & & & G^0(x_2,y) \\ & & & \vdots \\ G^0(x,x_1) & G^0(x,x_2) & \dots & G^0(x,y)\end{bmatrix}}{\det M_\sigma(C_n)}$$

$$= \det\left[z - \vec{v}^T M^{-1}\vec{u}\right]$$

$$= G^0(x,y) - \sum_{r,s=1}^{n} G^0(x,x_r)[M_\sigma^{-1}(C_n)]_{rs} G^0(x_s,y)$$

A similar equation can be obtained for the Matsubara Green function $G(k, i\omega_m)$, and makes CT-INT an excellent choice for DMFT calculations.

Numerical effort

- Dominated by updates, which scale with $\mathcal{O}(n^2)$; n: expansion order
- To obtain independent configurations typically requires n updates.
  $\Longrightarrow$ CPU time scales as $\mathcal{O}(n^3)$.
- Average expansion order:

$$\langle n \rangle = \left\langle \sum_{\nu} w \hat{h}_1(\nu) \right\rangle = \int_0^\beta d\tau \langle \hat{H}_1(\tau) \rangle \sim \beta L U$$

$\Longrightarrow$ CPU time $\sim (\beta L U)^3$

– Auxiliary-field QMC scales linearly with β. $\Longrightarrow$ F. Assaad, Thursday
– Weak-coupling problems can be solved on large systems.

- As with other QMC methods, parallelization is straight forward.

CT-INT for more general models

Functional integral representation of the partition function

The partition function of a system with Hamiltonian $\hat{H}$ can be written as

$$Z = \int \mathcal{D}(\bar{c}, c) e^{-S[\bar{c}, c]}$$

with the action

$$S[\bar{c}, c] = \int_0^\beta d\tau [\bar{c}\, \partial_\tau\, c + H(\bar{c}, c)]$$

Assuming a Hamiltonian of the form

$$\hat{H}(c^\dagger, c) = \sum_{ij} (h_{ij} - \mu \delta_{ij}) c_i^\dagger c_j + \sum_{ijkl} V_{ijkl} c_i^\dagger c_j^\dagger c_k c_l$$

we have

$$S[\bar{c}, c] = \int_0^\beta d\tau \left[\sum_{ij} \bar{c}_i(\tau) [(\partial_\tau - \mu)\delta_{ij} + h_{ij}] c_j(\tau) + \sum_{ijkl} V_{ijkl} \bar{c}_i(\tau) \bar{c}_j(\tau) c_k(\tau) c_l(\tau) \right]$$

Hence, the interaction is nonlocal in space, but local in time.

General fermionic model defined in terms of an action

Rubtsov et al., PRB 2005

Instead of starting from a Hamiltonian, we consider a completely general action:

$$S = \underbrace{\iint dx dy \, \bar{c}(x) \, [G^0(x,y)]^{-1} \, c(y)}_{S_0} + \underbrace{\iiiint dx dx' dy dy' \, V(x,x',y,y') \, \bar{c}(x) c(x') \, \bar{c}(y) c(y')}_{S_1}$$

Most general case:

$$x = \{i, \tau, \sigma\}, \quad x' = \{i', \tau', \sigma'\}, \quad y = \{j, \bar{\tau}, \bar{\sigma}\}, \quad y' = \{j', \bar{\tau}', \bar{\sigma}'\}$$

Non-local interactions in space and time. In practice: $\tau = \tau'$, $\bar{\tau} = \bar{\tau}'$.

Applications:

- Effective, retarded interactions (phonons, downfolding).
- Impurity problems, and dynamical mean-field theory (bath encoded in G^0).

CT-INT based on perturbation expansion

Given the form

$$S = S_0 + S_1$$

we have

$$Z = \int \mathcal{D}(\bar{c}, c) e^{-S_0[\bar{c},c] - S_1[\bar{c},c]}$$
$$= Z_0 \langle e^{-S_1[\bar{c},c]} \rangle_0 \,, \quad \langle X \rangle_0 = \frac{1}{Z_0} \int \mathcal{D}(\bar{c}, c) e^{-S_0[\bar{c},c]} X$$

A perturbation expansion gives

$$\frac{Z}{Z_0} = \langle e^{-S_1[\bar{c},c]} \rangle_0 = \sum_n \frac{(-1)^n}{n!} \iiiint dx_1 dx_1' dy_1 dy_1' \cdots \iiiint dx_n dx_n' dy_n dy_n'$$
$$\times V(x_1, x_1', y_1, y_1') \cdots V(x_n, x_n', y_n, y_n')$$
$$\times \langle \bar{c}(x_1) c(x_1') \bar{c}(y_1) c(y_1') \cdots \bar{c}(x_n) c(x_n') \bar{c}(y_n) c(y_n') \rangle_0$$

CT-INT can in principle be applied to a general fermionic action

The partition function can be cast into the form

$$\frac{Z}{Z_0} = \sum_{C_n} (-1)^n w(v_1) \cdots w(v_n) \langle h_1(v_1) \cdots h_1(v_n) \rangle_0$$
$$= \sum_{C_n} (-1)^n w(v_1) \cdots w(v_n) \det M(C_n)$$

A vertex is characterized by $w(v) = V(x, x', y, y')$, $v = \{x, y, x', y'; s\}$, and

$$h(v) = [\bar{c}(x)c(x') - \alpha(x, x', s)][\bar{c}(y)c(y') - \alpha(y, y', s)]$$

- The Monte Carlo sampling is over all variables of the vertex, and n.
- Addition/removal of vertices is sufficient.
- Updates and measurements (almost) independent of model.

Application to electron-phonon models

Example for a problem with a retarded interaction

The Holstein model describes the coupling of electrons to harmonic oscillators:

$$H = \underbrace{-t \sum_{\langle ij \rangle \sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.} \right)}_{\text{free electrons}} + \underbrace{\sum_i \left(\frac{1}{2M} \hat{P}_i^2 + \frac{K}{2} \hat{Q}_i^2 \right)}_{\text{free oscillators}} - g \sum_i \hat{Q}_i \left(\hat{n}_i - 1 \right)$$

Phonon frequency: $\omega_0 = \sqrt{\frac{K}{M}}$.

Partition function as path-integral:

$$Z = \underbrace{\int \mathcal{D}(\bar{c}, c) e^{-S_0[\bar{c}, c]}}_{\text{electrons}} \underbrace{\int \mathcal{D}(q) e^{-S_{\text{ep}}[\bar{c}, c, q]}}_{\text{electron}-\text{phonon}}$$

$$S_{\text{ep}}[\bar{c}, c, q] = \int_0^{\beta} d\tau \sum_i \left[\frac{M}{2} \{\partial_\tau q_i(\tau)\}^2 + \frac{K}{2} q_i^2(\tau) + g q_i(\tau) \{n_i(\tau) - 1\} \right]$$

More general fermion-boson models can also be considered.

CT-INT for the Holstein model

Assaad & Lang, PRB 2007

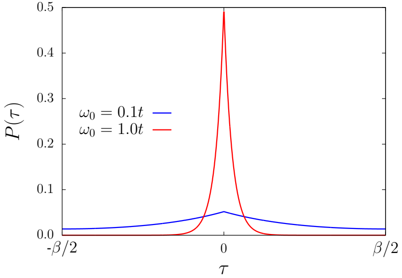
Integration over phonon coordinates $q_i(\tau)$ gives the fermionic action

$$S_1(\bar{c}, c) = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_i [n_i(\tau) - 1] D(\tau - \tau') [n_i(\tau') - 1]$$

corresponding to a retarded (non-local in time) electron-electron interaction

$$H_1(\tau) = -\frac{g^2}{4K} \int_0^\beta d\tau' \sum_i \sum_{\sigma\sigma'} \sum_s P(\tau - \tau') \left[n_{i\sigma}(\tau) - \alpha(s)\right] \left[n_{i\sigma'}(\tau') - \alpha(s)\right]$$

- interaction range: $\Delta \sim \frac{1}{\omega_0}$
- $\omega_0 \to \infty$: $P(\tau) \to \delta(\tau)$,
  Hubbard interaction $U = -\frac{g^2}{K}$.



Structure of the vertices

Vertex variables:

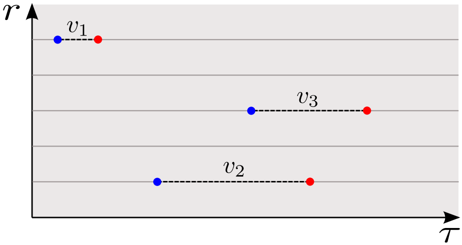
$$v = \{i, \tau, \tau', \sigma, \sigma'; s\}$$

Weight depends on v:

$$w(v) = -\frac{g^2}{4K} P(\tau - \tau')$$

Sample $\tau - \tau'$ according to $P(\tau - \tau') \implies T(C_n \mapsto C_{n+1}) \sim P(\tau - \tau')$.

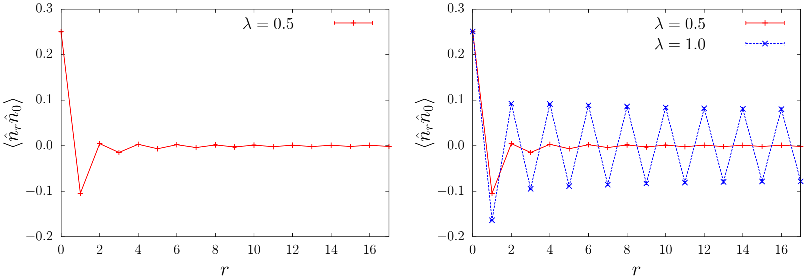
Vertices are non-local in time:



Peierls transition in the spinless Holstein model

Hohenadler, Fehske, Assaad, PRB 2011

Density-density correlations $\langle \widehat{n}_r \widehat{n}_0 \rangle$:



$\lambda < \lambda_c$: (metallic phase)

$$\langle n_r n_0 \rangle = -\frac{K_\rho}{2\pi^2 r^2} + \frac{A}{r^{2K_\rho}} \cos(2k_F x)$$

$\lambda > \lambda_c$: (Peierls phase)

Long-range charge order at $T = 0$, $K_\rho = 0$.

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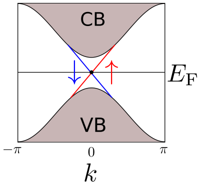
Application to topological insulators

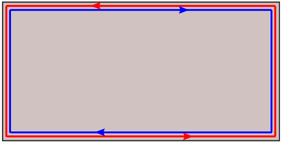
Topological insulators in two dimensions

Hasan & Kane, RMP 2010

Spin-orbit coupling gives rise to topological insulators.

Kane and Mele, PRL 2005; Bernevig et al., PRL 2006



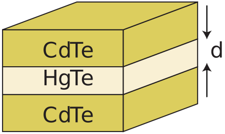


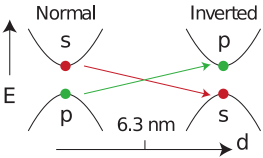
- Bulk band gap.
- $\sigma_s^{xy} = \nu \frac{e^2}{2\pi}$.
- Helical edge states.

Protected/stable against disorder & weak interactions.

Experimental realisation:

Bernevig et al., PRL 2006; König et al., Science 2007

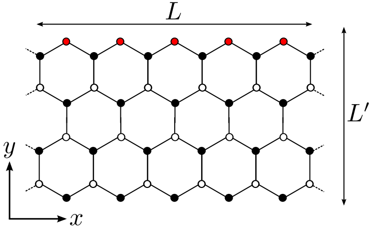




CT-INT study of correlated edge states

Hohenadler, Lang, Assaad, PRL 2011

Bulk is gapped; edge states determine low-energy physics
$\Longrightarrow$ consider electronic interactions only at the edge.



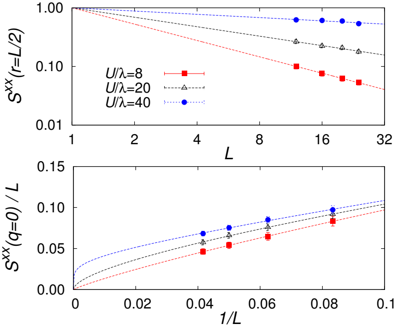
Effective, 1D action can be simulated using CT-INT, $\langle n \rangle \sim (\beta L U)^3$.

$$S = \underbrace{- \sum_{r r' \sigma} \iint_0^\beta d\tau d\tau' \, \bar{c}_{r\sigma}(\tau) \left[G^0_\sigma(r - r', \tau - \tau') \right]^{-1} c_{r'\sigma}(\tau')}_{S_0}$$

$$\underbrace{+ U \sum_{r} \int_0^\beta \left[n_{r\uparrow}(\tau) - \tfrac{1}{2} \right] \left[n_{r\downarrow}(\tau) - \tfrac{1}{2} \right]}_{S_1}$$

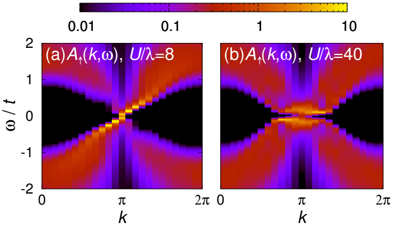
Correlation effects on helical edge states

Hohenadler & Assaad, PRB 2012



Transverse spin correlations strongly enhanced, but no long-range order.

Edge states remain metallic, but there is a pronounced transfer of spectral weight.



Summary

- CT-INT is based on a series expansion in the interaction H_1. Series convergent for finite systems at $T > 0$.
- Action-based formalism permits application to a variety of models.
- Configuration space consists of vertices. Updates: addition/removal.
- Method scales as $(\beta L V)^3$.
- Sign problem depends on the model.

Thank you for your attention.