Quantum Monte Carlo in Fermionic Models

Fakher F. Assaad (Field Theoretic Computer Simulations for Particle Physics and Condensed Matter, BU 8.5.2015)

<u>Outline</u>

Correlated electrons in bosonic and fermionic baths (CT-INT)

Electron-phonon interaction Correlated helical liquids

Determinantal quantum Monte Carlo for lattice models

Entanglement spectra for correlated topological insulators Mott transition

Conclusions





$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_{0}}\right]} = \sum_{n} \int_{0}^{\beta} d\tau_{1} \cdots \int_{0}^{\tau_{n-1}} d\tau_{n} \quad (-U)^{n} \det\left[M_{n}\left(\tau_{1}, \cdots, \tau_{n}\right)\right]$$

Sum with Monte Carlo Weight

Weight / Sign.

$$\succ H_U \rightarrow \frac{U}{2} \sum_{s=\pm 1} \left(n_{\uparrow}^d - \left[1/2 - s\delta \right] \right) \left(n_{\downarrow}^d - \left[1/2 + s\delta \right] \right) = -\frac{K}{2\beta} \sum_s e^{s\alpha \left(n_{\uparrow}^d - n_{\downarrow}^d \right)}$$

$$K = U\beta(\delta^2 - 1/4), \ \cosh(\alpha) - 1 = \frac{1}{2(\delta^2 - 1/4)}, \qquad \delta > 1/2$$

- → New dynamical variable s. Exact mapping onto CT-Hirsch-Fye, (i.e. CT-AUX) K. Mikelsons et al Phys. Rev. E 79, 057701 (2009) S. Rombouts et al. PRL 99, E. Gull et. al EPL (2008)
- → Sign problem behaves as in Hirsch-Fye.
 Absent for one-dimensional chains, particle-hole symmetry, impurity models
- → Spin polarized particle-hole symmetric problems (Fermion bag) E. Huffman, S. Chandrasekharan Phys. Rev. B 89, 111101 (2014)

$$\frac{\mathrm{Tr}\left[e^{-\beta H}\right]}{\mathrm{Tr}\left[e^{-\beta H_{0}}\right]} = \sum_{n} \int_{0}^{\beta} d\tau_{1} \sum_{s_{1}} \cdots \int_{0}^{\tau_{n-1}} d\tau_{n} \sum_{s_{n}} \left(-\frac{U}{2}\right)^{n} \det\left[M_{n}\left(\tau_{1}, s_{1} \cdots, \tau_{n}, s_{n}\right)\right]$$

Sum with Monte Carlo Weight

Sampling.



$$\frac{\operatorname{Tr}\left[e^{-\beta H}\right]}{\operatorname{Tr}\left[e^{-\beta H_{0}}\right]} = \underbrace{\sum_{n} \int_{0}^{\beta} d\tau_{1} \sum_{s_{1}} \cdots \int_{0}^{\tau_{n-1}} d\tau_{n} \sum_{s_{n}} \underbrace{\left(-\frac{U}{2}\right)^{n} \operatorname{det}\left[M_{n}\left(\tau_{1}, s_{1} \cdots, \tau_{n}, s_{n}\right)\right]}_{\operatorname{Sum with Monte Carlo}}$$
Weight
$$\underbrace{\operatorname{Measurements.}}_{G^{\sigma}{}_{C}}(\tau, \tau') = \frac{\left\langle T H_{U}\left[\tau_{1}, s_{1}\right] \cdots H_{U}\left[\tau_{n}, s_{n}\right] \hat{d}_{\sigma}^{+}(\tau) \hat{d}_{\sigma}(\tau') \right\rangle_{0}}{\left\langle T H_{U}\left[\tau_{1}, s_{1}\right] \cdots H_{U}\left[\tau_{n}, s_{n}\right] \right\rangle_{0}} = G^{\sigma}{}_{0}(\tau, \tau') - \sum_{\alpha, \beta=1}^{n} G^{\sigma}{}_{0}(\tau, \tau_{\alpha}) \left(M^{\sigma}{}_{n}^{-1}\right)_{\alpha\beta} G^{\sigma}{}_{0}(\tau_{\beta}, \tau')$$

Wick theorem applies for each configuration C of vertices.

Note: Direct calculation of Matsubara Green functions.

$$G^{\sigma}_{C}(i\omega_{m}) = G^{\sigma}_{0}(i\omega_{m}) - G^{\sigma}_{0}(i\omega_{m})\sum_{\alpha,\beta=1}^{n} e^{-i\omega_{m}\tau_{\alpha}} \left(M^{\sigma}_{n}\right)_{\alpha\beta} G^{\sigma}_{0}(\tau_{\beta},0)$$

Average Expansion parameter.

$$\langle n \rangle = -\beta U \langle (n_{\uparrow}^{d} - 1/2)(n_{\downarrow}^{d} - 1/2) - \delta^{2} \rangle$$

> CPU time scales as $<n>^3$ \rightarrow $(\beta V)^3$



Histogram of expansion parameter.

<u>Bosonic Baths</u> \rightarrow Electron-phonon problems

F. F. Assaad and T. C. Lang Phys. Rev. B76, 035116 (2007).

Hubbard-Holstein:

$$\hat{H} = \sum_{i,j,\sigma} t_{i,j} \, \hat{c}_{i,\sigma}^{+} \hat{c}_{j,\sigma}^{-} + U \sum_{i} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}^{-} + g \sum_{i} \hat{Q}_{i}(\hat{n}_{i}-1) + \sum_{i} \frac{\hat{P}_{i}^{2}}{2M} + \frac{k}{2} \hat{Q}_{i}^{2}$$

Integrate out the phonons

$$Z = \int \left[dc^{+} dc \right] \exp \left[-S_{0} - U \int_{0}^{\beta} d\tau \ n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) + \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \sum_{i,j} \left[n_{i}(\tau) - 1 \right] D^{0}(i - j, \tau - \tau') \left[n_{j}(\tau') - 1 \right] \right]$$

$$D^{0}(i-j,\tau-\tau') = \delta_{i,j} \frac{g^{2}}{2k} P(\tau-\tau'), \quad \lambda = \frac{g^{2}}{Wk}$$
$$P(\tau) = \frac{\omega_{0}}{2(1-e^{-\beta\omega_{0}})} \Big[e^{-|\tau|\omega_{0}} + e^{-(\beta-|\tau|)\omega_{0}} \Big], \quad \omega_{0} = \sqrt{k/M}$$

Attractive, retarded interaction (time scale $1/w_0$).

Antiadiabatic limit: $\lim_{\omega_0 \to \infty} P(\tau) = \delta(\tau) \rightarrow \text{Attractive Hubbard.}$



$$Z = \int \left[dc^+ dc \right] \exp \left[-S_0 - U \int_0^\beta d\tau \ n_{i\uparrow}(\tau) n_{i\downarrow}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{i,j} \left[n_i(\tau) - 1 \right] D^0(i-j,\tau-\tau') \left[n_j(\tau') - 1 \right] \right]$$

QMC: Expand both in Hubbard and retarded phonon interaction.

Vertices:



Bosonic Baths → Electron-phonon problems M. Hohenadler, FFA. J. Phys.: Condens. Matter 25, 014005 (2013)

<u>Peierls to superfluid crossover in the one-dimensional quarter filled Holstein model @ λ =0.35</u> Charge correlation L=28, *β*t=40 s-wave pairing correlations (a) (b) 10 0.8 $\bigcirc \odot \omega_0 / t = 0.1$ (1) - 10^{-2 |} 0.6 $\gg \omega_0 / t = 0.25$ N(q) $\rightarrow \omega_0 / t = 0.5$ $\bigcirc \bigcirc \omega_0 / t = 0.1$ 0.4 10⁻³ ⊧ $\Rightarrow \Rightarrow \omega_0 / t = 1.0$ $\mu_{0} \omega_{0} / t = 0.5$ $\Delta \omega_0 / t = 4.0$ $\Rightarrow \omega_0 / t = 1.0$ 0.2 $\forall \forall \omega_0 / t = \infty$ 10⁻⁴ $\Delta \Delta \omega_0 / t = 4.0$ 0 0.5 1.5 2 1 10 20 0 q/π r

 $\omega_0 \ll t$ Pairs of electrons form a commensurate CDW (diagonal LRO).

 $\omega_0 >> t$ Pairs condense to form an s-wave superconductor (off diagonal LRO).

<u>Fermionic Baths</u> \rightarrow Correlation effects on edge state of quantum Spin Hall states S. Rachel & K. Le Hur, PRB 82, 075106, (2010) Phases of the Kane Mele Hubbard model M. Hohenadler et al. PRB 85 (2012) 8 **Magnetic Insulator Electronic Correlations** ←xyz AFM xy AFM 6 U/t2← Semimetal Quantum Spin Hall Insulator 0 0.0 0.10.2 λ/t Spin-orbit coupling









<u>Fermionic Baths</u> \rightarrow Correlation effects on edge state of quantum Spin Hall states



Single particle spectral function

Strong coupling: $\lambda / t = 0.05, U / t = 2$



→ Inelastic scattering between left (spin do) and right (spin up) movers reduces substantially the spectral weight of the helical edge state.

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For
$$H = H_0 + H_1$$

$$\lim_{L_\tau \to \infty, L_\tau \Delta \tau = \beta} \operatorname{Tr} \left[\left(e^{-\Delta \tau \hat{H}_0} e^{-\Delta \tau \hat{H}_1} \right)^{L_\tau} \right] = \operatorname{Tr} \left[e^{-\beta \hat{H}_0} T e^{-\int_0^\beta d\tau \hat{H}_1(\tau)} \right]$$





Implementation.

S. R. White, D. J. Scalapino, R. L. Sugar, E. Y. Loh, J. E. Gubernatis, and R. T. Scalettar. Phys. Rev. B40, 506 (1989)
S. Sorella, S. Baroni, R. Car, and M. Parrinello. Europhys. Lett., 8, 663, (1989)
G. Sugiyama and S. Koonin. Anals of Phys., 168, (1986)
M. Imada and Y. Hatsugai. J. Phys. Soc. Jpn., 58, 3752 (1989)

$$\operatorname{Tr}\left[\prod_{\tau=1}^{L_{\tau}} e^{-\Delta \tau \hat{H}_{KM}} e^{-\Delta \tau \sum_{\mathbf{i}} i \Phi(\mathbf{i}, \tau) \left[\hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{i}}^{-1}\right]}\right] = e^{i\Delta \tau \sum_{\mathbf{i}, \tau} \Phi(\mathbf{i}, \tau)} \operatorname{det}\left[1 + B_{L_{\tau}} \cdots B_{1}\right]$$

With
$$\hat{H}_{KM} = \hat{c}^{\dagger}T\hat{c}$$
 and $\sum_{i}i\Phi(i,\tau)\hat{c}_{i}^{\dagger}\hat{c}_{i} = \hat{c}^{\dagger}V(\tau)\hat{c}$ one obtains

$$B_{\tau} = e^{-\Delta \tau T} e^{-\Delta \tau V(\tau)}$$

Sampling. Single "spin-flip" sequential updating

Measurements.

$$\frac{\operatorname{Tr}\left[e^{-\beta\hat{H}}\hat{c}_{x}^{\dagger}\hat{c}_{y}\right]}{\operatorname{Tr}e^{-\beta\hat{H}}} = \int D\Phi \ P(\Phi) \ G_{x,y}(\Phi) \qquad P(\Phi) = \frac{e^{-S(\Phi)}}{\int D\Phi \ e^{-S(\Phi)}}, \quad G(\Phi) = (1+B_{L_{\tau}}\cdots B_{1})^{-1}$$

Wicks theorem holds for a given field configuration \rightarrow Any equal time observable can be computed from G

<u>Computational cost.</u> $V^{3}\beta$

Is it possible to better? In principle yes \rightarrow Hybrid molecular-dynamics hints to a V β scaling

R. T. Scalettar, D. J. Scalapino, R. L. Sugar, and D. Toussaint. Phys. Rev. B36, 8632 (1987). In practice?

<u>Recent developments</u>: Renyi entanglement entropies.

A different way of writing Wick's theorem. T. Grover Phys. Rev. Lett., 111, 130402, (2013).

$$\hat{\rho} \equiv \frac{e^{-\beta\hat{H}}}{Z} = \int d\Phi P(\Phi)\hat{\rho}(\Phi), \qquad \hat{\rho}(\Phi) = \det\left[1 - G(\Phi)\right]e^{-\hat{c}^{\dagger}\ln\left[G^{-1}(\Phi) - 1\right]\hat{c}}$$

 S_n

6.5

6

5.5

5

1

2

3

5

4

п

6

7

8



$$\hat{\rho}_{A} = \operatorname{Tr}_{B}\hat{\rho} \equiv \int d\Phi P(\Phi)\hat{\rho}_{A}(\Phi) \qquad \hat{\rho}_{A}(\Phi) : G \to G_{A}$$
n-replicas
$$\operatorname{Tr}\hat{\rho}_{A}^{n} = \int d\Phi^{1} \cdots d\Phi^{n} P(\Phi^{1}) \cdots P(\Phi^{n}) \operatorname{Tr}\left[\hat{\rho}_{A}(\Phi^{1}) \cdots \hat{\rho}_{A}(\Phi^{n})\right]$$
(b)
$$U/t = 2, L = 6, W_{A} = 4, \Lambda = 5 \times 10^{-6}$$

$$S_{n} = -\frac{1}{n-1} \ln \operatorname{Tr}\hat{\rho}_{A}^{n} \qquad \overset{7.5}{7}$$

F. F. Assaad, T. C. Lang, and F. Parisen Toldin Phys. Rev. B, 89, 125121, (2014)

Peter Bröcker and Simon Trebst arXiv:1404.3027

<u>**Recent developments</u></u>: Entanglement spectrum \hat{\rho}_A = e^{-\hat{H}_E}</u>**

$$\left\langle a_x^{\dagger}(\tau_E)a_y \right\rangle_E = \frac{\operatorname{Tr}\left[\hat{\rho}_A^{\ n-\tau_E}a_x^{\dagger}\hat{\rho}_A^{\ \tau_E}a_y\right]}{\operatorname{Tr}\left[\hat{\rho}_A^{\ n}\right]} \qquad \Rightarrow \qquad \left\langle a_x^{\dagger}(\tau_E)a_x \right\rangle_E = \int d\omega \ \frac{e^{-\tau_E\omega}}{1+e^{-n\omega}}A^E(x,\omega)$$

Example: Single particle entanglement spectral function for dimerized Kane-Mele Hubbard model.





The Mott transition

Measuring the magnetic moment

FFA & I. Herbut PRX 3, 031010 (2013)

Steven R. White and A. L. Chernyshev Phys. Rev. Lett. 99, 127004

Introduce pinning fields

$$H = H_{tU} + h_0(n_{0,\uparrow} - n_{0,\downarrow})$$

$$m = \lim_{R \to \infty} \lim_{L \to \infty} \left\langle S^{z}(R) \right\rangle e^{i\mathbf{Q} \cdot \mathbf{R}}$$
$$m = \lim_{L \to \infty} \frac{1}{L^{2}} \sum_{i} e^{i\mathbf{Q} \cdot \mathbf{i}} \left\langle S^{z}(i) \right\rangle$$



Measuring the single particle gap





The Mott transition



Gross-Neveu Yukawa

I. Herbut, V. Juričić, O. Vafek PRB 80, 075432, (2009)

$$L_0 = \sum_{\sigma} \overline{\psi}_{\sigma}(\mathbf{x}, \tau) \partial_{\mu} \gamma_{\mu} \psi_{\sigma}(\mathbf{x}, \tau) \qquad \text{Dirac fermions}$$

$$L_{b} = \vec{\psi}_{t}(\mathbf{x},\tau) \cdot \left[-\partial_{\tau}^{2} - v^{2} \vec{\nabla}^{2} + t \right] \vec{\psi}_{t}(\mathbf{x},\tau) + \lambda \left(\vec{\psi}_{t}(\mathbf{x},\tau) \cdot \vec{\psi}_{t}(\mathbf{x},\tau) \right)^{2}$$

$$L_{y} = g \ \vec{\psi}_{t}(\mathbf{x},\tau) \cdot \sum_{\sigma,\sigma'} \vec{\psi}_{\sigma}(\mathbf{x},\tau) \vec{\sigma}_{\sigma,\sigma'} \psi_{\sigma'}(\mathbf{x},\tau) \qquad \text{Yukawa coupling}$$

$$\Delta_{sp} \propto g \left| \left\langle \vec{\psi}_t \right\rangle \right|$$

Upper critical dimension d=3 \rightarrow ϵ -expansion





Conclusion

Correlated electrons in bosonic and fermionic baths (CT-INT)



Correlation effects in helical liquids



Determinantal quantum Monte Carlo for lattice models



Mott transition. Fermionic criticality



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F. Parisen Toldin



I. Herbut