Solution to sign problems in spin polarized fermion models interacting with quantum spins

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Hamiltonian Picture: CT-INT

- We will be working in the Hamiltonian picture and using the interaction expansion of the partition function.
- Additional symmetries may be recovered in a continuous time formulation, broadening the possibilities for solvable models.
- We set $H = H_0 + H_{\text{int}}$. Then we expand and get the following:

$$Z = \sum_k \int [dt]\,(-1)^k\, Tr\left(e^{-(\beta-t)H_0} H_{\text{int}} e^{-(t_1-t_2)H_0} H_{\text{int}} \ldots\right), \tag{1}$$

where there are k insertions of H_{int}.

Beard, Wiese(1996), Sandvik (1998), Prokof'ev, Svistunov (1998), Rubtsov, Savkin Lichtenstein (2005)

- We will see how, for some previously difficult models, this expansion leads directly to a calculation free of sign problems.

A General Model

- Specifically we will show, using the CT-INT expansion and the worldline representation, that this model has no sign problem:

$$H = -t\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) + V\sum_{\langle ij\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right) + \sum_{ij}\left(J_{\mathrm{perp}}\left(S_i^x S_j^x + S_i^y S_j^y\right) \pm J_z S_i^z S_j^z\right) - \sum_i h_i\left(n_i - \frac{1}{2}\right) S_i^x \qquad (2)$$

- Here, H_0^f is the tight-binding Hamiltonian.
- H_{int}^b is the fermion interaction term from the t-V model.
- Then H_0^b is a somewhat general spin model (includes Ising model, antiferromagnetic Heisenberg...).
- And H_{int}^{fb} allows interactions between the fermions and bosons.

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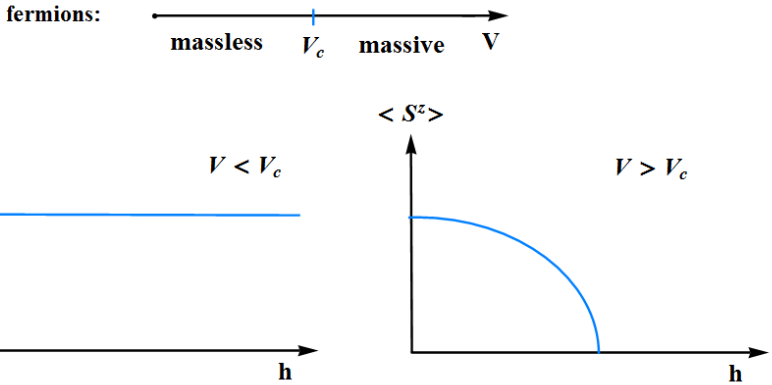
Physics Motivation

- Model suggests a phase transition for $H^{b}_{\rm int} = -J_z \sum_{\langle ij \rangle} S^z_i S^z_j$, $H^{fb}_{\rm int} = -\sum_i h_i \left(n_i - \frac{1}{2}\right) S^x_i$:



- What happens at the critical point V_c?

Fermion Bag approach to solving interacting fermion boson problems

- A key idea for this solution comes from *Solutions to sign problems in lattice Yukawa models* (Chandrasekharan 2012). In the paper, models containing fermionic and bosonic fields that interact with each other are solved using fermion bags and the worldline representation for bosons.
- While the bosonic and fermionic sectors may have sign problems on their own, **in combination the sign problem disappears**.
- The condensed matter community is already acquainted with fermion and boson interactive models. Methods are given in *Continuous-time QMC Solvers for Electronic Systems in Fermionic and Bosonic Baths* (Assaad 2014)
- We extend the analysis by considering models where the purely bosonic part of the theory is not free (as in the Yukawa models paper).

Reviewing The t-V Model

- We review why the t-V model has no sign problem in CT-INT.

$$H = -t \sum_{i,j} c_i^\dagger M_{ij} c_j + \sum_{\langle i,j \rangle} V \left(n_i - \frac{1}{2} \right) \left(n_j - \frac{1}{2} \right), \tag{3}$$

where

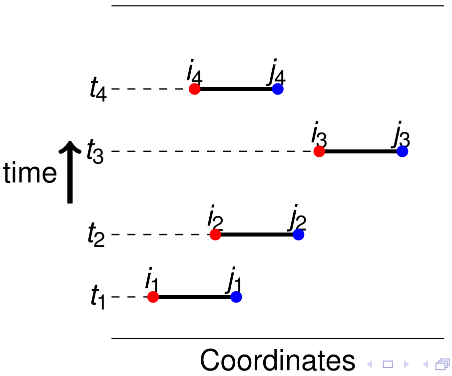
$$M_{ij} = \left(\delta_{i+\hat{e}_x,j} + \delta_{i-\hat{e}_x,j} \right) + \left(\delta_{i+\hat{e}_y,j} + \delta_{i-\hat{e}_y,j} \right), \tag{4}$$

- Similar model considered by: Gubernatis, Scalapino, Sugar, Toussaint. PRB (1985).

  $V \geq 2t$: Chandrasekharan, Cox, Holland, Wiese. Nucl. Phys. (1999).
- Key property for M_{ij}-matrix: $M^T = -DMD$, ($D_{ij} = \sigma_i \delta_{ij}$). Encodes particle-hole symmetry for the free part of the Hamiltonian. (Puts M in $SO(n,n)$.)
- Also, $-V(n_i - \frac{1}{2})(n_j - \frac{1}{2})$ can be written as proportional to $\sum_{\sigma=\pm} e^{\sum_{ij} \sigma \lambda c_i^\dagger \kappa_{ij} c_j}$, where κ_{ij} is in $SO(n,n)$. Wang et. al. 2015

The Partition Function

$$Z = Z_0 \sum_k \sum_{[b]} \int [dt] \, (-V)^k \, Tr \left(e^{-(\beta - t_k)H_0} \left(n_{\mathbf{i}_k} - \frac{1}{2} \right) \left(n_{\mathbf{j}_k} - \frac{1}{2} \right) \right.$$
$$\left. \ldots e^{-(t_3 - t_2)H_0} \left(n_{\mathbf{i}_2} - \frac{1}{2} \right) \left(n_{\mathbf{j}_2} - \frac{1}{2} \right) e^{-(t_2 - t_1)H_0} \left(n_{\mathbf{i}_1} - \frac{1}{2} \right) \left(n_{\mathbf{j}_1} - \frac{1}{2} \right) e^{-t_1 H_0} \right) \quad (5)$$



The G-Matrix Elements

- This trace can be evaluated exactly in terms of the determinant of a $2k \times 2k$ matrix, $A([b,t])$.
- Thus we have:

$$Z = Z_0 \sum_k \sum_{[b,s]} \int [dt] \, (-V)^k \det A([b,t]) \tag{6}$$

- For the matrix A, the following identity holds: $a_{ji} = -\sigma_i a_{ij} \sigma_j$. A takes the form of:

$$A = \left(\begin{array}{c|c} A_1 & S \\ \hline S^T & A_2 \end{array} \right). \tag{7}$$

- Here $A_1 = -A_1^T$, and $A_2 = -A_2^T$.
- All blocks are squares because each bond contains one even site and one odd site.

Positivity of the determinants

- Now notice that:

$$A\tilde{D} = \left(\begin{array}{c|c} A_1 & S \\ \hline S^T & A_2 \end{array}\right)\left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -1 \end{array}\right) = \left(\begin{array}{c|c} A_1 & -S \\ \hline S^T & -A_2 \end{array}\right) \quad (8)$$

- This matrix is antisymmetric, so $\det\left(A\tilde{D}\right) = \det A \det \tilde{D} \geq 0$.
- But

$$\det \tilde{D} = \det \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -1 \end{array}\right) = (-1)^k \quad (9)$$

for $2k$ bonds.

- Thus $(-1)^k \det A \geq 0$. No sign problem!

Subsequent Work

- Another solution has since been found by using the Majorana representation of the fermions. Li, Jiang, Yao. Phys. Rev. B (2015)
- Both methods have been used to obtain critical exponents for the quantum phase transition from massless to massive fermions.
  CT-INT: Wang, Corboz, Troyer. New J. Phys. (2014)
  Majorana: Li, Jiang, Yao. New J. Phys. (2015)
- Guiding principle unifying both methods for solving t-V model found. Wang, Liu, Iazzi, Troyer, Harcos. arXiv:1506.05349
- Beyond this guiding principle: staggered chemical potential.

Staggered Chemical Potential Extension

- In general, respecting a *staggered reference configuration* of particles on one sublattice and holes on the other is a guiding principle for avoiding sign problems. Consider:

$$\sum_i h_i n_i^{s_i}. \tag{10}$$

  Here $h_i \geq 0$, s_i is $+1$ on the even sublattice and -1 on the odd sublattice.
- Up to a constant, this potential is equivalent to

$$\sum_i \sigma_i h_i \left(n_i - \frac{1}{2} \right) \tag{11}$$

- As long as $A\tilde{D}$ remains real and symmetric, the sign problem is solved. Notice that insertions of this term extend the matrix. The σ_i factors give us the right $\tilde{D}$ for the extended matrix.
- We are inserting $n_i - \frac{1}{2}$ alone now. Can't be rewritten in terms of $e^{\sum_{ij} \sigma \lambda c_i^\dagger \kappa_{ij} c_j}$ with $\kappa_i \in SO(n, n)$, so violates $SO(n, n)$ guiding principle.

Factoring the Fermionic and Bosonic Pieces

- Now let's calculate Z using a model with both fermionic and bosonic parts.
- The expansion in terms of interaction operator insertions will consist of terms of the form

$$(-1)^k \,\mathrm{Tr}\left(e^{-(\beta-t_1)H_0} H_{\mathrm{int}} e^{-(t_1-t_2)H_0} H_{\mathrm{int}} \ldots H_{\mathrm{int}} e^{-t_k H_0}\right), \qquad (12)$$

Where $H_0 = H_0^f + H_0^b$ and $H_{\mathrm{int}} = H_{\mathrm{int}}^f + H_{\mathrm{int}}^{fb}$.
- A subset of the terms will be given by

$$h_i\,(-1)^{2+1}\,\mathrm{Tr}\left(e^{-(\beta-t_1)H_0} H_{\mathrm{int}}^f e^{-(t_1-t_2)H_0}\left(n_i - \frac{1}{2}\right) S_i^x e^{-t_2 H_0}\right). \qquad (13)$$

- This expression may then be rewritten as the product

$$h_i\,(-1)^{2+1}\,\mathrm{Tr}\left(e^{-(\beta-t_2)H_0^b} S_i^x e^{-t_2 H_0^b}\right) \mathrm{Tr}\left(e^{-(\beta-t_1)H_0^f} H_{\mathrm{int}}^f e^{-(t_1-t_2)H_0^f}\left(n_i - \frac{1}{2}\right) e^{-t_2 H_0^f}\right). \qquad (14)$$

- The fermionic sector has $(n_i - \frac{1}{2})$ instead of $\sigma_i(n_i - \frac{1}{2})$. **Sign problem.**

Bosonic Terms

- The bosonic factors are of the form

$$\mathrm{Tr}\left(e^{-(\beta-t_1)H_0^b}S_{i_1}^x e^{-(t_1-t_2)H_0^b}S_{i_2}^x \ldots S_{i_m}^x e^{-t_m H_0^b}\right), \qquad (15)$$

where here we assume m insertions from H_{int}^{fb}.

- We expand the trace in the S^z basis:

$$\sum_{\{S(t)\}} \langle S^z(t_0)|\, e^{-(\beta-t_1)H_0^b}S_{i_1}^x\, |S^z(t_1)\rangle \langle S^z(t_1)|\, e^{-(t_1-t_2)H_0^b}\ldots$$
$$\ldots S_{i_m}^x\, |S^z(t_m)\rangle \langle S^z(t_m)|\, e^{-t_m H_0^b}\, |S^z(t_0)\rangle , \qquad (16)$$

- Remembering that $S_i^x = \frac{1}{2}\left(S_i^+ + S_i^-\right)$, we note the function of S_i^x is to flip the spin state at site i.
- We will see how this works using a couple of examples.

First Example: Ising Model Coupled with Fermions

- We begin with an Ising model interaction between bosons, using

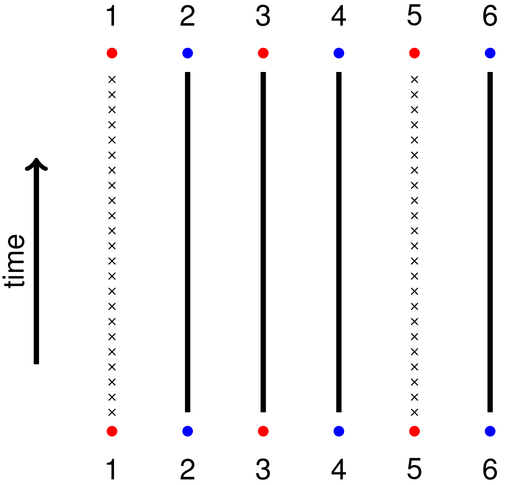
$$H_0^b = \pm J \sum_{\langle ij \rangle} S_i^z S_j^z . \tag{17}$$

- In the z-spin basis, this Hamiltionian simply measures and does not flip any spins.
- We will see that using this Hamiltonian piece in combination with the fermion pieces removes any sign problems.

Worldline Approach: Without Insertions

The picture below represents $\langle\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow|\, e^{-\beta H_0^b}\, |\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow\rangle$.

- $\uparrow$-states are particles, $\downarrow$-states are holes.
- H_0^b does not flip s^z.
- The time evolution with no S_z insertions just consists of straight lines.

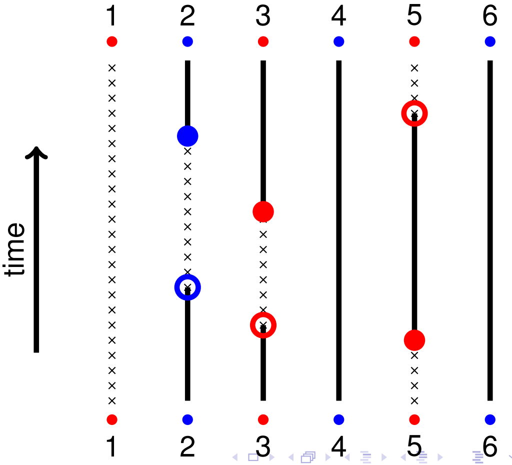


Worldline Approach: With Insertions

$$\langle\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow|\, e^{-(\beta-t_6)H_0^b} S_5^x e^{-(t_6-t_5)H_0^b} S_2^x e^{-(t_5-t_4)H_0^b} S_3^x e^{-(t_4-t_3)H_0^b}$$

$$\times S_2^x e^{-(t_3-t_2)H_0^b} S_3^x e^{-(t_2-t_1)H_0^b} S_5^x e^{-(t_1)H_0^b} |\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow\rangle$$

- If we flip a spin, we must flip it back again.
- We need an even number of every S_i^x operator.



No Sign Problem

- However,

$$S_i^x S_i^x = \sigma_i \sigma_i S_i^x S_i^x. \tag{18}$$

- Thus it is as if our $H_{\rm int}^b$ insertion is really

$$\sum_i h_i \sigma_i \left(n_i - \frac{1}{2}\right) S_i. \tag{19}$$

- And thus most generally the Ising model coupled with fermions

$$\begin{aligned} H = & -t \sum_{\langle ij \rangle} \left(c_i^\dagger c_j + c_j^\dagger c_i\right) + V \sum_{\langle ij \rangle} \left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right) \\ & \pm J \sum_{ij} S_i^z S_j^z - \sum_i h_i \left(n_i - \frac{1}{2}\right) S_i^x \end{aligned} \tag{20}$$

has no sign problem for any h_i.

Example 2: Antiferromagnet

- We now see how these techniques can help us solve a Heisenberg antiferromagnet coupled with fermions, where

$$\begin{aligned} H = &- t\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) + V\sum_{\langle ij\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right) \\ &+ J\sum_{ij}\left(\vec{S}_i\cdot\vec{S}_j - \frac{1}{4}\right) - \sum_i h_i\left(n_i - \frac{1}{2}\right)S_i^x \end{aligned} \tag{21}$$

- We begin by seeing how the antiferromagnetic term affects the states in the z-spin basis.

The Boson-Boson interaction

- For two nearest neighbors, using the basis states $(\uparrow\uparrow, \uparrow\downarrow, \downarrow\uparrow, \downarrow\downarrow)$, we have

$$H = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -J/2 & J/2 & 0 \\ 0 & J/2 & -J/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{22}$$

- At the infinitesimal level, we get for $e^{-\epsilon H}$: (limiting ourselves to the $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ states)

$$\left(1 + \frac{\epsilon J}{2}\right) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \frac{\epsilon J}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{23}$$

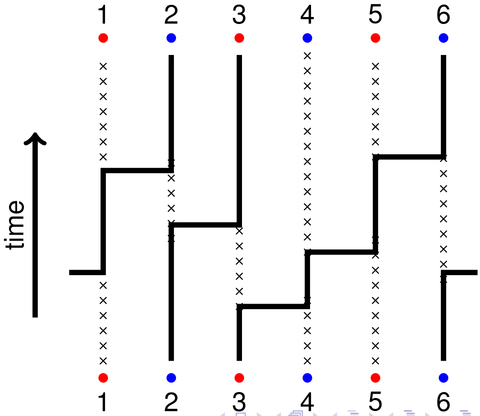
- Therefore, every time the Hamiltonian flips a nearest neighbor spin pair, the overall matrix element takes on an extra minus sign.

Worldline Approach: Without H_{int}^{fb} Insertions

One contribution to $\langle\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow|\, e^{-\beta H_0^b}\, |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle$ is

$$(-\epsilon J/2)^6 \langle\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow|\, e^{-(\beta-t_6)E_0^b(t_6)}\, S_6^+ S_5^-\, e^{-(t_6-t_5)E_0^b(t_5)}\, S_2^+ S_1^-\, e^{-(t_5-t_4)E_0^b(t_4)}\, S_3^+ S_2^-$$
$$\times\, e^{-(t_4-t_3)E_0^b(t_3)}\, S_5^+ S_4^-\, e^{-(t_3-t_2)E_0^b(t_2)}\, S_1^+ S_6^-\, e^{-(t_2-t_1)E_0^b(t_1)}\, S_4^+ S_3^-\, e^{-t_1 E_0^b(0)}\, |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle :$$

- Even to even or odd to odd site: even number of hops (flips).
- We follow the worldline in one continuous loop from even to even or odd to odd. Positive weight.

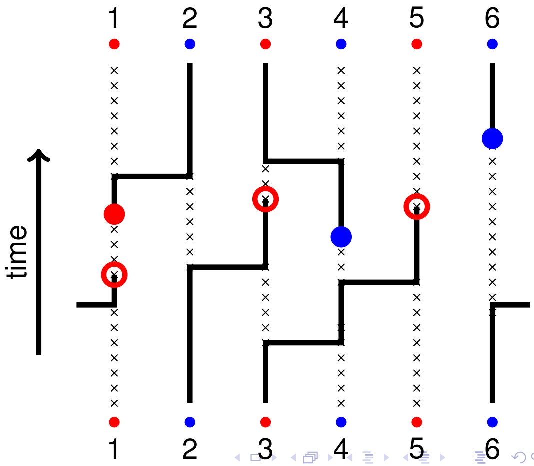


Worldline Approach: With $H_{\rm int}^{fb}$ insertions

Contribution to $\langle\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow|\, e^{-(\beta-t_6)H_0^b} S_6^x\, e^{-(t_6-t_5)H_0^b} S_3^x\, e^{-(t_5-t_4)H_0^b} S_5^x$

$\times e^{-(t_4-t_3)H_0^b} S_1^x\, e^{-(t_3-t_2)H_0^b} S_4^x\, e^{-(t_2-t_1)H_0^b} S_1^x\, e^{-t_1 H_0^b}\, |\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\rangle$

- Every even and odd insertion pair of S_i and S_j produces (-) sign.
- Every even and even (odd and odd) insertion pair of S_i and S_j (S_i and S_j) produces (+) sign.



Sign Problem in Antiferromagnet?

- What does this do for us?
- If we have an $\left(n_i - \frac{1}{2}\right) S_i^x$, $\left(n_j - \frac{1}{2}\right) S_j^x$ pair, we get a negative sign from the bosonic sector.
- If we have an $\left(n_i - \frac{1}{2}\right) S_i^x$, $\left(n_j - \frac{1}{2}\right) S_j^x$ pair ($\left(n_i - \frac{1}{2}\right) S_i^x$, $\left(n_j - \frac{1}{2}\right) S_j^x$ pair), we get a positive sign from the bosonic sector.
- Thus we are encoding a σ_i factor into

$$\left(n_i - \frac{1}{2}\right). \tag{24}$$

- The antiferromagnet coupled with fermions has no sign problem in the CT-INT expansion.

Conclusions

- Generally, models of this form:

$$H = -t\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) + V\sum_{\langle ij\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right)$$
$$+\sum_{ij}\left(J_{\mathrm{perp}}\left(S_i^x S_j^x + S_i^y S_j^y\right) \pm J_z S_i^z S_j^z\right) - \sum_i h_i\left(n_i - \frac{1}{2}\right)S_i^x, \quad (25)$$

  where $t, V, J_{\mathrm{perp}}, J_z, h_i \geq 0$ are solvable.
- The staggered reference configuration is a useful guiding principle for solvable models.
- The staggered chemical potential goes beyond the $SO(n,n)$ guiding principle.
- We have shown that we can violate this configuration by combining the fermionic sector with a specific type of bosonic sector. We see this using the worldline representation for bosons.

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Conclusions

- Generally, models of this form:

$$H = -t\sum_{\langle ij\rangle}\left(c_i^\dagger c_j + c_j^\dagger c_i\right) + V\sum_{\langle ij\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right) + \sum_{ij}\left(J_{\mathrm{perp}}\left(S_i^x S_j^x + S_i^y S_j^y\right) \pm J_z S_i^z S_j^z\right) - \sum_i h_i\left(n_i - \frac{1}{2}\right) S_i^x, \quad (25)$$

  where $t, V, J_{\mathrm{perp}}, J_z, h_i \geq 0$ are solvable.
- The staggered reference configuration is a useful guiding principle for solvable models.
- The staggered chemical potential goes beyond the $SO(n,n)$ guiding principle.
- We have shown that we can violate this configuration by combining the fermionic sector with a specific type of bosonic sector. We see this using the worldline representation for bosons.