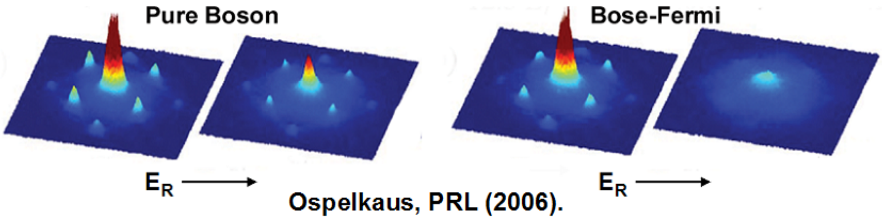
Auxiliary-Field Quantum Monte Carlo for Bose-Fermi Mixtures



Brenda Rubenstein,[1] **Shiwei Zhang**,[2] **and David Reichman**[1]
[1]Columbia University in the City of New York
[2]The College of William and Mary

Institute for Nuclear Theory, July 2013

Warning: The Mathy Version

This project is involved. However, since you are audience of experts, I will go through this project in all of its gory details. **Hold on tight.**

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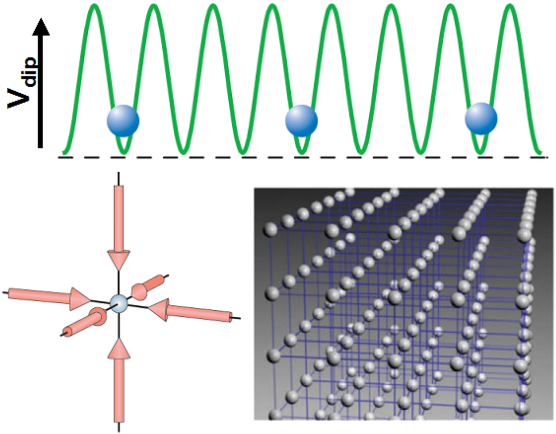
Introduction: Bose-Fermi Mixtures in Optical Lattices

Optical Lattices

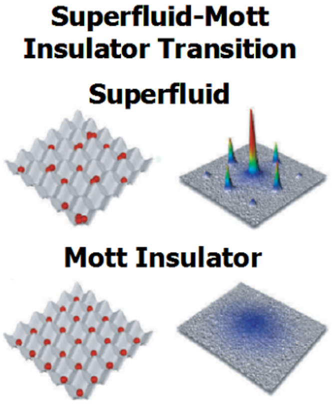
Optical lattices offer the possibility of simulating many of the fundamental models of physics with unprecedented control.



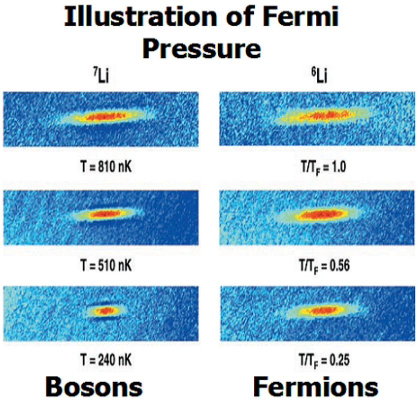
Bloch, Nature Physics (2005).

Optical Lattice Triumphs

Optical lattices have successfully simulated the Superfluid-Mott Insulator Transition and illustrated the effects of Fermi pressure.



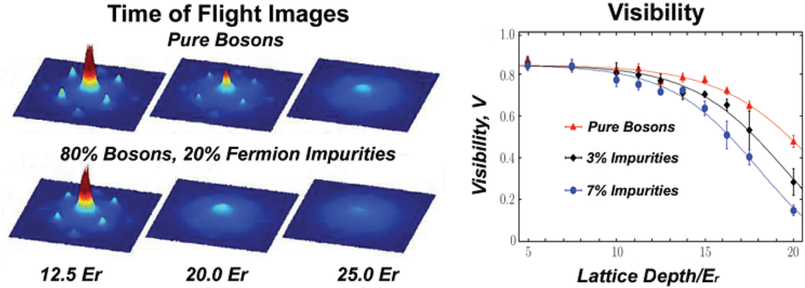
Greiner, Nature (2002).



Truscott, Science (2001).

Bose-Fermi Mixture Experiments

Successes studying pure Bose and Fermi gases have generated interest in Bose-Fermi mixtures. The first optical lattice experiments suggest that fermion impurities decrease boson coherence.

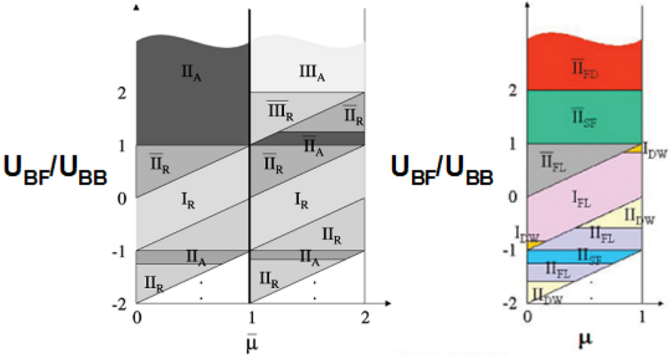


Ospelkaus, PRL (2006).

Key Question:

What can theory bring to the study of Bose-Fermi mixtures?

A Zoo of Theoretical Bose-Fermi Phases



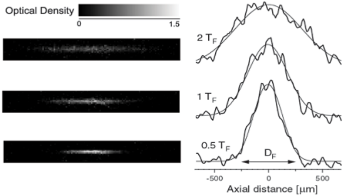
Lewenstein, PRL (2004).

Perturbation theory predicts a whole zoo of Bose-Fermi phases, including spin and charge density waves (DW), superfluids (SF), and Fermi liquids (FL) consisting of fermions paired with varying numbers of bosons or boson holes.

Why We REALLY Care About BF Mixtures

Sympathetic Cooling

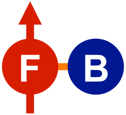
Onset of Fermi Degeneracy in Li-6 Cooled by Na-23



Column Density ***Axial Line Density***

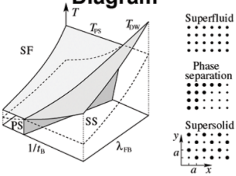
Hadzibabic, PRL (2002).

Dipolar Molecules



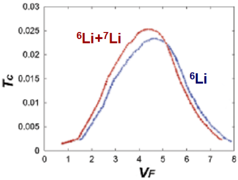
Supersolidity

Bose-Fermi Phase Diagram



Buchler, PRL (2003).

Enhanced Superfluidity



Illuminati, PRL (2004).

This Work's Motivating Question

Can We Develop a Method Capable of Determining the EXACT Phase Diagram and Properties of Bose-Fermi Mixtures at Finite Temperatures?

Previous Approaches

Bose-Fermi Hubbard Hamiltonian

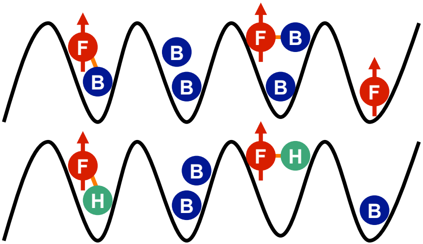
The starting point for most theoretical studies of Bose-Fermi mixtures is the Bose-Fermi-Hubbard Hamiltonian.

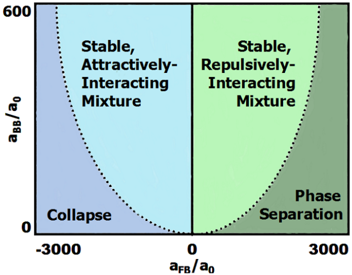
Bose-Fermi-Hubbard Hamiltonian

$$H_{BF} = -t_B \sum_{\langle ij \rangle} \left(\hat{b}_i^\dagger \hat{b}_j + H.c. \right) - t_F \sum_{\langle ij \rangle} \left(\hat{f}_i^\dagger \hat{f}_j + H.c. \right) + \frac{1}{2} U_B \sum_i \hat{n}_i (\hat{n}_i - 1) + U_{BF} \sum_i \hat{n}_i \hat{m}_i - \mu_B \sum_i \hat{n}_i - \mu_F \sum_i \hat{m}_i$$

$U_{BF}<0$

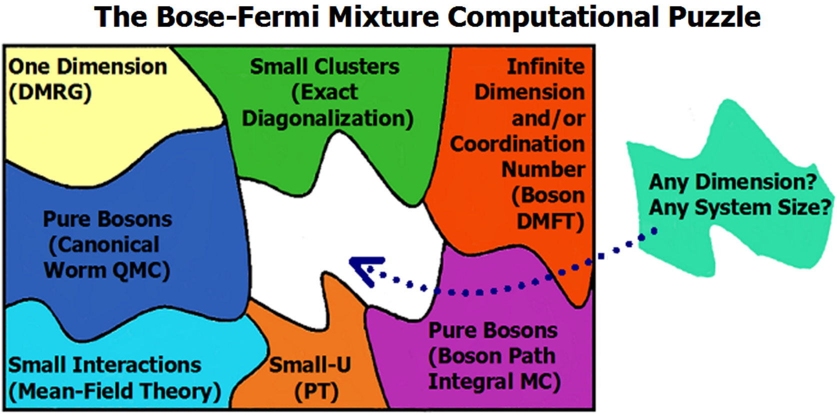
$U_{BF}>0$





Adapted from Ospelkaus, J.Phys.B (2008).

Previous Approaches



A number of approaches exist, but none are general.

Previous Theoretical and Computational Approaches

Previous Approaches	Applicability
Theoretical	
Mean-Field and Perturbation Theories	Good for Weak Interactions; Inaccurate for Strong Correlation
Bethe Ansatz	Exact in One Dimension
Computational	
DMRG	Exact in One Dimension
Exact Diagonalization	Exact, Useful for Small Clusters
QMC, Canonical Worm Algorithm	Exact, for Pure Bosons; How to Manage Sign Problem?
QMC, Path Integral Monte Carlo	Exact, for Pure Bosons; Nodal Surfaces for Mixtures?
Bose-Fermi DMFT	The Smaller the Dimension and/or Coord. #, The Less Exact

Can a technique be developed that can treat Bose-Fermi mixtures accurately in a computationally-tractable amount of time in any number of dimensions?

A Hint from the Original BSS Papers?

The seminal Auxiliary-Field Quantum Monte Carlo (AFQMC) paper aimed to study coupled boson-fermion systems...

PHYSICAL REVIEW D VOLUME 24, NUMBER 8 15 OCTOBER 1981

!!! **Monte Carlo calculations of coupled boson-fermion systems. I** !!!

R. Blankenbecler*

Laboratoire de Physique Théorique et Hautes Energies, University of Paris XI, 91405, Orsay, France

D. J. Scalapino and R. L. Sugar

Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara, California 93106

(Received 15 June 1981)

We present a formalism for carrying out Monte Carlo calculations of field theories with both boson and fermion degrees of freedom. The basic approach is to integrate out the fermion degrees of freedom and obtain an effective action for the boson fields to which standard Monte Carlo techniques can be applied. We study the structure of the effective action for a wide class of theories. We develop a procedure for making rapid calculations of the variation in the effective action due to local changes in the boson fields, which is essential for practical numerical calculations.

Perhaps, we can develop an algorithm to study Bose-Fermi mixtures based upon AFQMC?

Previous Auxiliary-Field Quantum Monte Carlo Approaches

There are AFQMC algorithms for bosons or fermions, but not for bosons, and therefore, mixtures at finite temperatures.

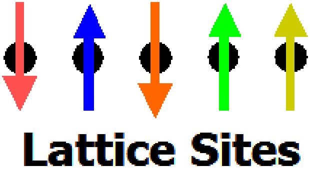
	Bosons	Fermions
T=0	Projector QMC	Ground State Constrained-Path QMC
T>0	?	Finite T Constrained-Path QMC

So, if we developed a finite-temperature boson algorithm, we'd have a general technique for mixtures.

Our Approach:
Bose-Fermi Auxiliary-Field Quantum Monte Carlo

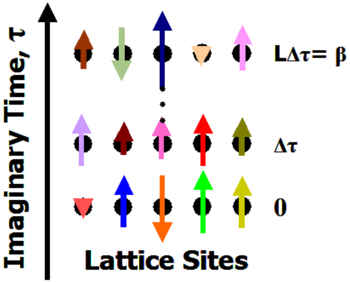
Basic Auxiliary-Field Quantum Monte Carlo

Classical Monte Carlo for Ising Model



- **Spins: Up or Down (+1/-1)**
- **Acceptance Criterion:** $e^{-\beta H(\vec{\sigma}_f)}/e^{-\beta H(\vec{\sigma}_i)}$
- **Principle Quantity Calculted: Energy,** $E(\vec{\sigma})$

Fermion AFQMC for Hubbard Model



- **Spins: Gaussian-Distributed**
- **Acceptance Criterion:** $Det\left[I + e^{-\beta H(\vec{\sigma}_f)}\right]/Det\left[I + e^{-\beta H(\vec{\sigma}_i)}\right]$
- **Principle Quantity Calculated: Green's Function,** $I/I + e^{-\beta H(\vec{\sigma})}$

Finite-Temperature AFQMC: A Mathful

First, the partition function is factored.

Finite-Temperature Averages

$$\langle \hat{O} \rangle \equiv \frac{Tr\left(\hat{O}e^{-\beta \hat{H}}\right)}{Tr\left(e^{-\beta \hat{H}}\right)}$$

Short-Time Breakup

$$Z \equiv Tr\left(e^{-\beta \hat{H}}\right) = Tr\left(e^{-\Delta\tau \hat{H}} e^{-\Delta\tau \hat{H}} ... e^{-\Delta\tau \hat{H}}\right) \qquad \Delta\tau = \beta / L$$

Suzuki-Trotter Factorization

$$e^{-\Delta\tau \hat{H}} \approx e^{-\Delta\tau \hat{K}/2} e^{-\Delta\tau \hat{V}} e^{-\Delta\tau \hat{K}/2}$$

The kinetic propagators are one-body terms and may be evaluated explicitly. The potential propagators are two-body terms and must be reexpressed as one-body terms.

Finite-Temperature AFQMC: A Mathful

The potential propagators may be transformed into products of one-body terms times a weight via the Hubbard-Stratonovich Transformation.

Reexpression of $\hat{V}$ in Terms of One-Body Operators

$$\hat{V} = -\frac{1}{2}\sum_i \hat{v}_i^2$$

Hubbard-Stratonovich Transformation

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx e^{-x^2/2} e^{-xy} = e^{y^2/2}$$

$$e^{(1/2)\Delta\tau\hat{v}^2} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} d\sigma e^{-\sigma^2/2} e^{\sigma\sqrt{\Delta\tau}\hat{v}}$$

Reexpression of the Potential Propagator in Terms of One-Body Operators

$$e^{-\Delta\tau\hat{V}} = \prod_i \int_{-\infty}^{\infty} d\sigma_i \frac{e^{-\sigma_i^2/2}}{\sqrt{2\pi}} e^{\sigma_i\sqrt{\Delta\tau}\hat{v}_i} = \prod_i \int_{-\infty}^{\infty} d\sigma_i p(\sigma_i) e^{\sigma_i\sqrt{\Delta\tau}\hat{v}_i}$$

Finite-Temperature AFQMC: A Mathful

The potential propagators may now be recombined with the kinetic propagators.

Reexpression of the Short-Time Propagator

$$e^{-\Delta\tau\hat{H}} = e^{-\Delta\tau\hat{K}/2}\left[\prod_i \int_{-\infty}^{\infty} d\sigma_i p(\sigma_i) e^{\sigma_i\sqrt{\Delta\tau}\hat{v}_i}\right] e^{-\Delta\tau\hat{K}/2} + O(\Delta\tau^2)$$

Reexpression of the Partition Function

$$Z = Tr(e^{-\beta\hat{H}}) = \int_{-\infty}^{\infty} d\vec{\sigma}_L ... d\vec{\sigma}_1 P(\vec{\sigma}_L, ..., \vec{\sigma}_1) Tr\left(\hat{B}(\vec{\sigma}_L)...\hat{B}(\vec{\sigma}_1)\right)$$

Hirsch Expression for the Trace over Fermions

$$Tr_f\left(\hat{B}(\vec{\sigma})\right) = Det\left[I + B(\vec{\sigma})\right]$$

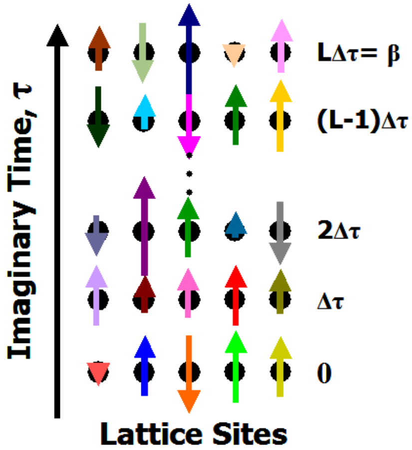
Final Expression for the Fermion Partition Function

$$Z = \int_{-\infty}^{\infty} d\vec{\sigma}_L ... d\vec{\sigma}_1 P(\vec{\sigma}_L, ..., \vec{\sigma}_1) Det\left[I + B(\vec{\sigma}_L)...B(\vec{\sigma}_1)\right]$$

What in the World Does This Mean?

Final Expression for the Fermion Partition Function

$$Z = \int_{-\infty}^{\infty} d\vec{\sigma}_L ... d\vec{\sigma}_1 P(\vec{\sigma}_L, ..., \vec{\sigma}_1) Det\left[I + B(\vec{\sigma}_L)...B(\vec{\sigma}_1)\right]$$



Translation

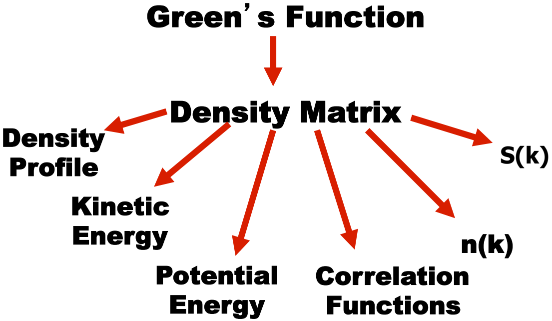
At each site and imaginary timeslice, you sample a field, $\sigma_{i,l}$, with a probability, $p(\sigma_{i,l})$. You then insert these fields into the $B(\vec{\sigma})$s and calculate the determinant.

Calculating Fermion Observables

With the expression for the partition function in hand, fields may be sampled. Based upon these fields, Green's Functions and most other observables may be evaluated.

Fermion Green's Function

$$G_{ij}^F = \langle \hat{f}_i \hat{f}_j^\dagger \rangle = \left[\frac{I}{I + B(\vec{\sigma}_L) \ldots B(\vec{\sigma}_2) B(\vec{\sigma}_1)} \right]_{ij}$$



Boson Auxiliary-Field Quantum Monte Carlo

The previous expressions yielded the partition function for fermions. For Bose-Fermi QMC, related expressions for the boson partition function had to be derived.

Boson Partition Function

$$Z_B \propto Det\left[(I - e^{-\beta H})^{-1}\right]$$

Fermion Parition Function

$$Z_F \propto Det\left[I + e^{-\beta H}\right]$$

Boson Green's Function

$$G^B_{ij} = \langle \hat{b}_i \hat{b}^\dagger_j \rangle = \left[\frac{I}{I - e^{-\beta H}}\right]_{ij}$$

Fermion Green's Function

$$G^F_{ij} = \langle \hat{f}_i \hat{f}^\dagger_j \rangle = \left[\frac{I}{I + e^{-\beta H}}\right]_{ij}$$

These are similar to their ideal gas forms.

Ideal Bose Gas Parition Function

$$Z^{IG}_B = \prod_k \left(\frac{1}{1 - e^{-\beta(\epsilon_k - \mu)}}\right)$$

Ideal Fermi Gas Partition Function

$$Z^{IG}_F = \prod_k \left(1 + e^{-\beta(\epsilon_k - \mu)}\right)$$

Bose-Fermi Auxiliary-Field Quantum Monte Carlo

To treat Bose-Fermi mixtures, the partition function must be reevaluated for the Bose-Fermi-Hubbard model.

Bose-Fermi-Hubbard Hamiltonian

$$\hat{H}_{BF} = \hat{K}_B + \hat{K}_F + \frac{1}{2} U_B \sum_i \hat{n}_i(\hat{n}_i - 1) + U_{BF} \sum_i \hat{n}_i \hat{m}_i$$

Modified Bose-Fermi-Hubbard Hamiltonian

$$\hat{H}_{BF} = \hat{K}_B + \hat{K}_F + \frac{U_{BF}}{2} \sum_i (\hat{n}_i + \hat{m}_i)^2$$
$$+ \frac{U_B - U_{BF}}{2} \sum_i \hat{n}_i^2 - \frac{U_B}{2} \sum_i \hat{n}_i - \frac{U_{BF}}{2} \sum_i \hat{m}_i$$

Boson HS Transformation

$$e^{-\frac{\Delta\tau(U_B - U_{BF})}{2}\hat{n}_i^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\sigma_B^2/2} e^{-i\sigma_B \sqrt{\Delta\tau(U_B - U_{BF})}\hat{n}_i}$$

Bose-Fermi Coupling HS Transformation

$$e^{-\frac{\Delta\tau U_{BF}}{2}(\hat{n}_i + \hat{m}_i)^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\sigma_{BF}^2/2} e^{-i\sigma_{BF} \sqrt{\Delta\tau U_{BF}}(\hat{n}_i + \hat{m}_i)}$$

Bose-Fermi Auxiliary-Field Quantum Monte Carlo

The partition function may be evaluated as an integral over a weighted product of boson and fermion determinants.

Bose-Fermi Partition Function I

$$Z_{BF} = Tr_B \left(Tr_F \left(e^{-\beta \hat{H}_{BF}} \right) \right)$$

Bose-Fermi Partition Function II

$$Z_{BF} = \int_{-\infty}^{\infty} d\vec{\sigma}_{BF} d\vec{\sigma}_B P(\vec{\sigma}_{BF}, \vec{\sigma}_B)$$
$$Tr_B \left(B_B(\vec{\sigma}_{BF}, \vec{\sigma}_B) \right) Tr_F \left(B_F(\vec{\sigma}_{BF}) \right)$$

Final Bose-Fermi Partition Function

$$Z_{BF} = \int_{-\infty}^{\infty} d\vec{\sigma}_{BF} d\vec{\sigma}_B P(\vec{\sigma}_{BF}, \vec{\sigma}_B)$$
$$Det \left[\frac{I}{I - B_B(\vec{\sigma}_{BF}, \vec{\sigma}_B)} \right] Det \left[I + B_F(\vec{\sigma}_{BF}) \right]$$

Calculating Mixture Observables

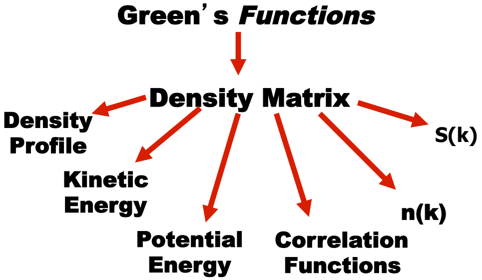
With the expression for the partition function in hand, multiple fields may be sampled. Based upon these fields, boson and fermion Green's Functions and most other observables may be evaluated.

Fermion Green's Function

$$G_{ij}^{F} = \left[\frac{I}{I+B_F(\vec{\sigma}_L)\ldots B_F(\vec{\sigma}_2)B_F(\vec{\sigma}_1)}\right]_{ij}$$

Boson Green's Function

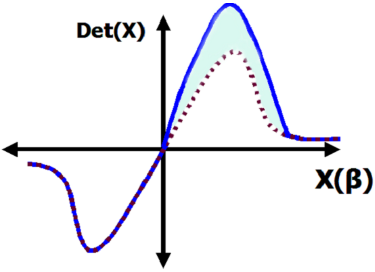
$$G_{ij}^{B} = \left[\frac{I}{I-B_B(\vec{\sigma}_L)\ldots B_B(\vec{\sigma}_2)B_B(\vec{\sigma}_1)}\right]_{ij}$$



Sign Problem and Constrained-Path Approximation

Sign Problem

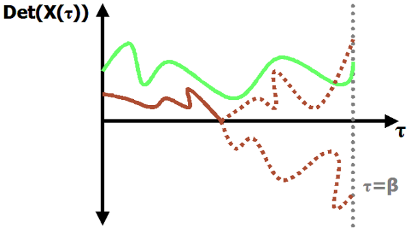
The sign problem arises when fermion determinants, $Det(\vec{X})$, acquire a negative sign as they traverse a path, $\vec{X}$, in auxiliary-field space.



Adapted from Zhang, PRL (1999).

Constrained-Path Approximation

Discard all walkers whose determinants become negative as they sample auxiliary-field space. These walkers ultimately contribute to noise.



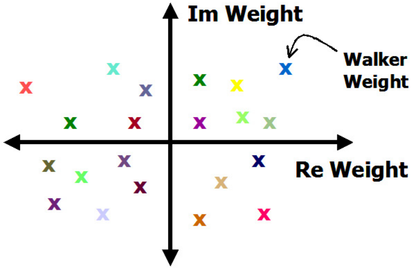
Adapted from Zhang, PRL (1999).

Phase Problem and Phaseless Approximation

Phase Problem

If $U_B > 0$, propagator is complex.

$$e^{-\Delta\tau \hat{V}_i} = e^{-\Delta\tau U_B \hat{n}_i^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\sigma_i e^{-\frac{1}{2}\sigma i^2} e^{\sigma_i \sqrt{-\Delta\tau U_B}\hat{n}_i}$$



Phaseless Approximation

Modify propagator so that fluctuations in the weights are minimized and then project weights onto real axis.

Projection of Weights, W

Let $\Delta\theta$ denote the phase angle:

$$\Delta\theta \equiv Im\left[ln\left(\frac{Det\left[\vec{X}_{(m+1)\Delta\tau}\right]}{Det\left[\vec{X}_{m\Delta\tau}\right]} \right)\right]$$

Assuming $|\Delta\theta| < \pi/2$, project the weights onto the real axis:

$$W' \leftarrow cos(\Delta\theta) W$$

Further Mitigating the Phase Problem

The phase problem may be mitigated by reducing the magnitude of the terms that multiply i in the complex propagators. This may be accomplished by subtracting off mean-field average densities from the true densities.

Bose-Fermi Hamiltonian with Mean-Field Densities Subtracted

$$H_{BF}^{MF} = \hat{K}_B + \hat{K}_F + \frac{U_{BF}}{2}\sum_i(\hat{n}_i + \hat{m}_i - \langle n \rangle - \langle m \rangle)^2$$
$$+\frac{U_B - U_{BF}}{2}\sum_i(\hat{n}_i - \langle n \rangle)^2 + \text{Other One-Body Terms}$$

Modified Boson Propagator

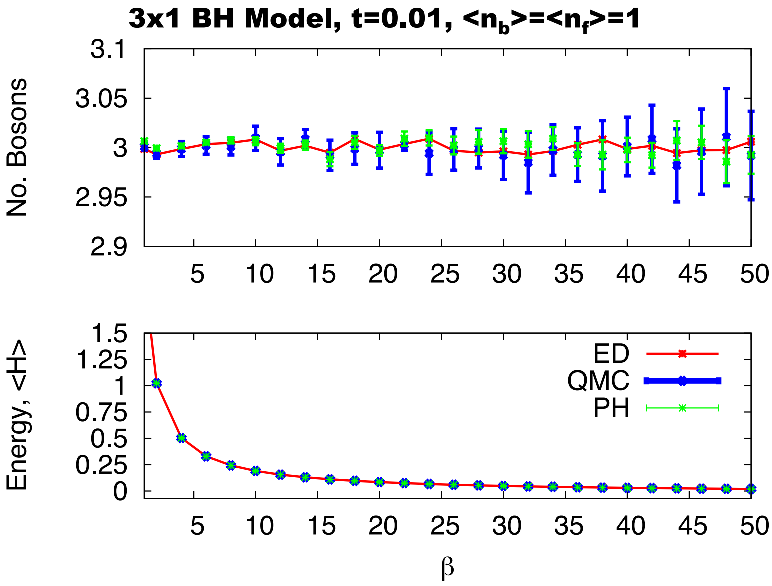
$$e^{-i\phi_B\sqrt{\Delta\tau(U_{BF}-U_B)}(n_i-\langle n \rangle)}$$

Modified Bose-Fermi Propagator

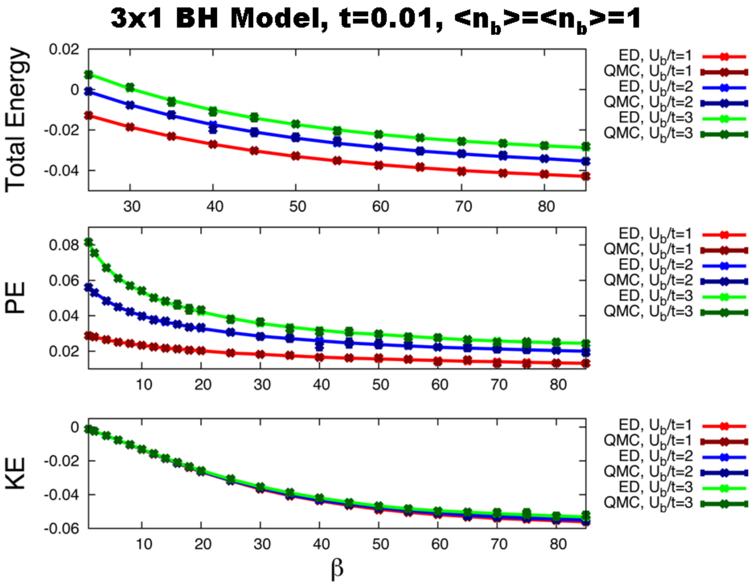
$$e^{-i\phi_{BF}\sqrt{-\Delta\tau U_{BF}}(n_i+m_i-\langle n \rangle-\langle m \rangle)}$$

Results:
Comparisons to Alternative Techniques

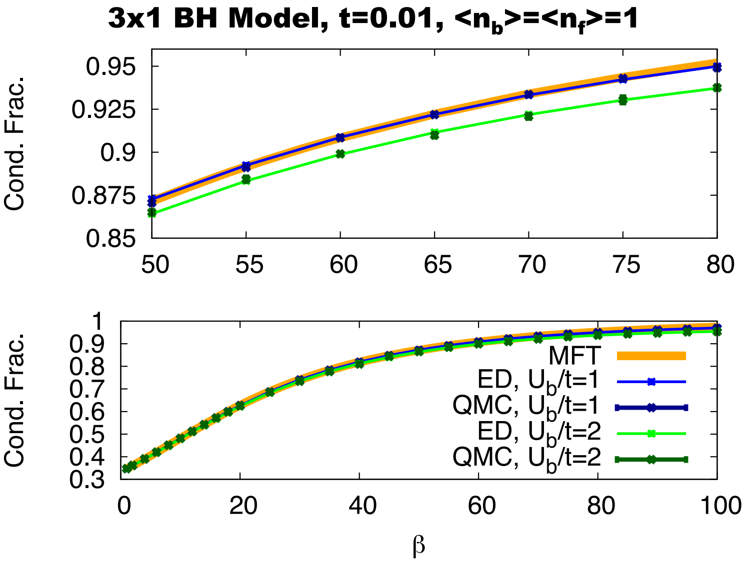
Comparison to ED: 3-Site Bose-Hubbard Model



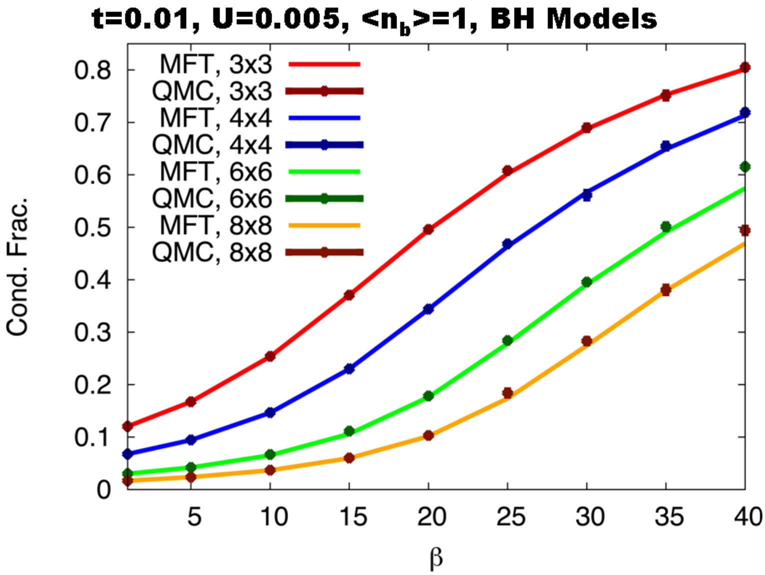
Comparison to ED: 3-Site Bose-Hubbard Model



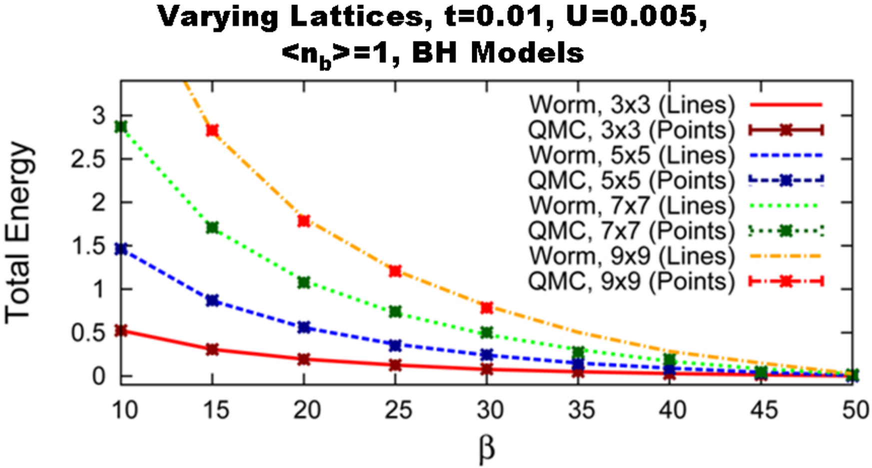
Comparison to ED: 3-Site Bose-Hubbard Model



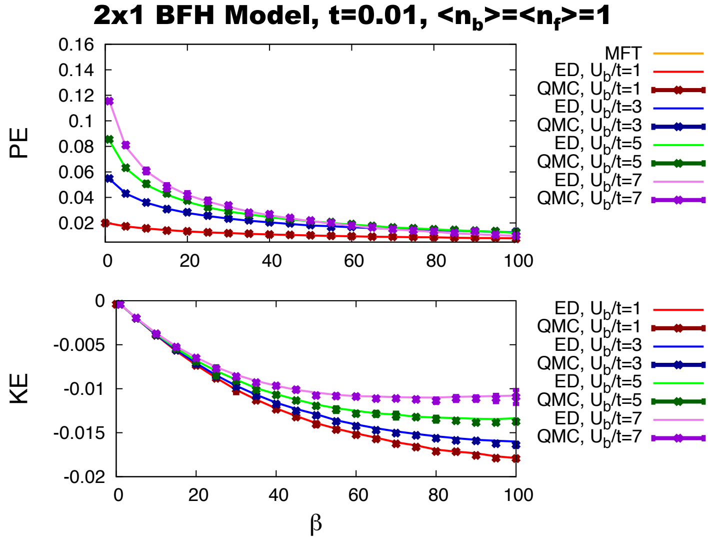
Comparison to MFT: 2D Bose-Hubbard Models



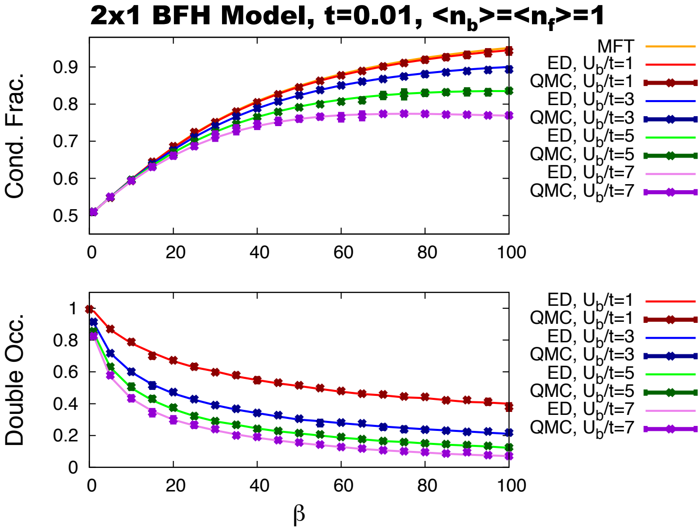
Comparison to Worm: 2D Bose-Hubbard Models



Comparison to ED: 2-Site Bose-Fermi-Hubbard Model



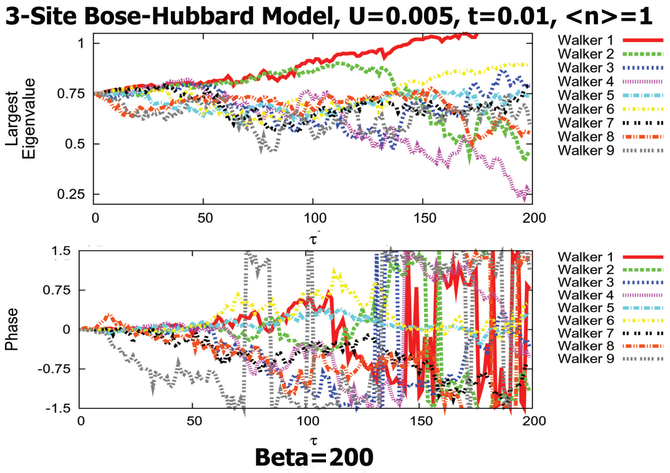
Comparison to ED: 2-Site Bose-Fermi-Hubbard Model



Discussion:
Challenges and Outlook

Key Challenge: "Rogue Eigenvalue Problem"

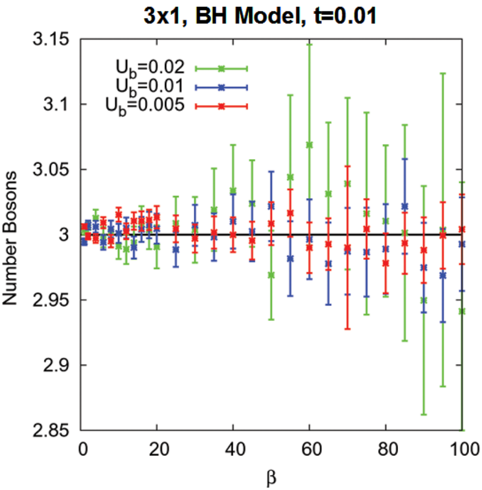
As the system condenses at low temperatures, it develops a "rogue eigenvalue" problem, where the dominant eigenvalue surpasses one, leading to large phase fluctuations.



Additional Challenges

- **Finding chemical potentials requires many graduate student hours!** Is there a way to readily calculate the chemical potential for a given boson occupancy?

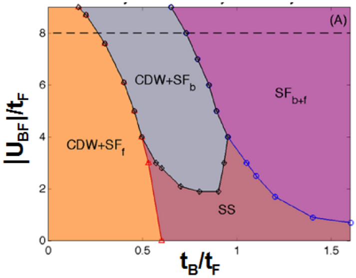
- For strong interactions, **BF-AFQMC experiences a bad phase problem that cannot be mitigated using the phaseless approximation.** Is there a better way of handling the phase problem?



Goals

- **To develop solutions to the "rogue eigenvalue problem."** We are currently testing a few candidates.
- **To determine exact mixture phase boundaries.** Where do the exact boundaries differ from those produced using MFT and DMFT?
- Can our technique say anything about enhanced superfluidity, sympathetic cooling, or supersolidity?

Phase Diagram for 3D BFH Model Using DMFT, $U_B/t_F=20$, $U_F/t_F=-10$, $T/t_F=0.2$, $\langle n_B \rangle=1$, $\langle n_F \rangle=.5$



Anders, PRL (2012).

Summary

Review

- Bose-Fermi AFQMC is a new Quantum Monte Carlo technique capable of simulating Bose-Fermi mixtures in any dimension and for any system size.
- BF-AFQMC is based upon a new finite-temperature QMC algorithm for bosons that can be combined with previous techniques for fermions.
- Results have been tested against those produced using Exact Diagonalization and Mean-Field Theory. Agreement was achieved in all cases.

Challenges

- BF-AFQMC is challenged at low temperatures and for strong interactions.

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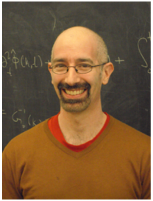

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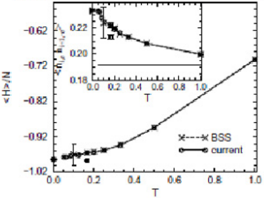
Accuracy of Constrained-Path and Phaseless Approximations

Hubbard Model CPMC, 4x4 Lattice, U=4.0, <n>=.875



β		$\langle s \rangle$	$G(1,0)$	$G(2,2)$	$P_d(2,1)$
3	current		0.1631(1)	−0.0415(1)	0.0625(2)
	BSS	0.99	0.1631(1)	−0.0418(1)	0.0630(3)
6	current		0.1663(3)	−0.0470(4)	0.077(2)
	BSS	0.44	0.1662(2)	−0.0465(2)	0.083(3)
20	current		0.166(1)	−0.050(1)	0.078(2)
∞	exact		0.167	−0.051	0.078(2)

Zhang, PRL (1999).

Bose-Hubbard Model Phaseless QMC, 13x1, <n>=.31, U=1.538, t=2.676, κ=.35, T=0

Type	E	$\langle \hat{T} \rangle$	$\langle \hat{V}_{\text{trap}} \rangle$	$\langle \hat{V}_{2\text{AB}} \rangle$	$\langle N_0/N \rangle$
Exact	4.244	1.183	1.793	1.268	98.5%
QMC	4.242(8)	1.182(6)	1.799(1)	1.262(3)	98.4%
GP	4.429	1.029	1.800	1.599	100.0%

Bose-Hubbard Model Phaseless QMC, 24x24x24, <n>=.007, T=0

Type	E/N	$\langle \hat{T} \rangle/N$	$\langle \hat{V}_{\text{trap}} \rangle/N$	$\langle \hat{V}_{2\text{B}} \rangle/N$
a_s=80 Å				
phaseless	1.7943(3)	0.5984(3)	0.96029(9)	0.23562(8)
unconstrained	1.7947(2)	0.5987(2)	0.96006(4)	0.23594(4)
GP	1.7924	0.5947	0.95649	0.24121
a_s=500 Å				
phaseless	2.6777(2)	0.500(3)	1.5638(6)	0.591(1)
unconstrained	2.6811(4)	0.511(7)	1.563(2)	0.614(3)
GP	2.620	0.408	1.4901	0.721

Purwanto, PRA (2005). ·

Derivation of Boson Partition Function I

Desired Expression for the Boson Partition Function

$$Tr_B\left[e^{-b_i^\dagger A_{ij} b_j} e^{-b_i^\dagger B_{ij} b_j}\right] = Det\left[\frac{I}{I - e^{-A}e^{-B}}\right]$$

In deriving this expression for bosons, we follow the analogous derivation for fermions by Hirsch (1985).

Identity We Seek to Prove

$$e^{-b_i^\dagger A_{ij} b_j} e^{-b_i^\dagger B_{ij} b_j} = e^{-\sum_\nu b_\nu^\dagger l_\nu b_\nu}, \quad \lambda_\nu = e^{-l_\nu}$$

Desired Result from This Identity

$$\begin{aligned} Tr_B\left[e^{-\sum_\nu b_\nu^\dagger l_\nu b_\nu}\right] &= Tr_B\left[\prod_\nu e^{-b_\nu^\dagger l_\nu b_\nu}\right] \\ &= \prod_\nu \sum_{n_\nu} e^{-n_\nu l_\nu} \\ &= \prod_\nu \left[1 - e^{-l_\nu}\right]^{-1} \\ &= Det\left[\left[I - e^{-A}e^{-B}\right]^{-1}\right] \end{aligned}$$

Derivation of Boson Partition Function II

First Consider the Trace of a General One-Body Operator

$$Tr_B\left[e^{b_i^\dagger C_{ij} b_j}\right] = Tr_B\left[e^{-\sum_i \bar{b}_i^\dagger c_i \bar{b}_i}\right]$$
$$= \prod_i \sum_{n_i} e^{-n_i c_i}$$
$$= \prod_i [1 - e^{-c_i}]^{-1}$$
$$= Det\left[\left[I - e^{-C}\right]^{-1}\right]$$

We then show that $e^{-b_i^\dagger A_{ij} b_j} e^{-b_i^\dagger B_{ij} b_j}$ acts on all excitations the same way that $e^{-b_i^\dagger C_{ij} b_j}$ does.

Acting a One-Body Operator on a Single Excitation

$$e^{-b_i^\dagger C_{ij} b_j} \sum_n c_n b_n^\dagger |0\rangle = \sum_n c_n \left[e^{-b_i^\dagger C_{ij} b_j} b_n^\dagger\right] |0\rangle$$
$$= \sum_n c_n b_n^\dagger - c_n b_i^\dagger C_{ij} b_j b_n^\dagger + 1/2 c_n b_i^\dagger C_{ij} b_j b_\alpha^\dagger C_{\alpha\beta} b_\beta b_n^\dagger + ... + |0\rangle$$
$$= \sum_n c_n \left[b_n^\dagger - b_i^\dagger C_{in} + 1/2 b_i^\dagger C_{i\alpha} C_{\alpha n} + ...+\right] |0\rangle$$
$$= \sum_i \sum_{i'} \left[e^{-C}\right]_{ii'} c_{i'} b_i^\dagger |0\rangle = \sum_i \tilde{c}_i b_i^\dagger |0\rangle$$

Derivation of Boson Partition Function III

Acting a Product of One-Body Operators on a Single Excitation

$$e^{-b_i^\dagger A_{ij} b_j} e^{-b_i^\dagger B_{ij} b_j} \sum_n c_n b_n^\dagger |0\rangle$$
$$= \sum_n c_n \left[e^{-b_i^\dagger A_{ij} b_j} \left(b_n^\dagger - \sum_i b_i^\dagger B_{in} + 1/2 \sum_{i\alpha} b_i^\dagger B_{i\alpha} B_{\alpha n} + \ldots \right) \right] |0\rangle$$
$$= \sum_n c_n \left[b_n^\dagger + \left(- \sum_i b_i^\dagger B_{in} + 1/2 \sum_{i\alpha} b_i^\dagger B_{i\alpha} B_{\alpha n} + \ldots \right) + \ldots \right] |0\rangle$$
$$\sum_i \left[\sum_{i'} [e^{-A} e^{-B}]_{ii'} c_{i'} \right] b_i^\dagger |0\rangle = \sum_i \tilde{c}_i b_i^\dagger |0\rangle$$

This is the same result as when a single one-body operator was applied to the same excitation. Applying to any number of excitations, one finds that this result holds generally.

Conclusion

If $e^{-b_i^\dagger A_{ij} b_j} e^{-b_i^\dagger B_{ij} b_j} = e^{-b_\nu^\dagger I_\nu b_\nu}$**, then**

$$Tr_B \left[e^{-b_i^\dagger A_{ij} b_j} e^{-b_i^\dagger B_{ij} b_j} \right] = Det \left[\left[I - e^{-A} e^{-B} \right]^{-1} \right]$$

Derivation of Boson Green's Function

Definition of Boson Green's Function

$$G_{ij}^B = \langle b_i b_j^\dagger \rangle = \frac{Tr_B\left[b_i b_j^\dagger \prod_\nu e^{-b_\nu^\dagger l_\nu b_\nu}\right]}{\prod_\nu (1-e^{-l_\nu})^{-1}}$$

Final Form for Boson Green's Function

$$G_{ij}^B = \frac{Tr_B\left[(\delta_{ij}+b_i^\dagger b_j) \prod_\nu e^{-b_\nu^\dagger l_\nu b_\nu}\right]}{\prod_\nu (1-e^{-l_\nu})^{-1}} = I + \frac{Tr_B\left[b_i^\dagger b_j \prod_\nu e^{-b_\nu^\dagger l_\nu b_\nu}\right]}{\prod_\nu (1-e^{-l_\nu})^{-1}}$$

$$= I + \sum_{\nu'} \langle \nu' | i \rangle \langle j | \nu' \rangle \frac{Tr_B\left[b_{\nu'}^\dagger b_{\nu'} \prod_\nu e^{-b_\nu^\dagger l_\nu b_\nu}\right]}{\prod_\nu (1-e^{-l_\nu})^{-1}}$$

$$= I - \sum_{\nu'} \langle \nu' | i \rangle \langle j | \nu' \rangle \frac{d}{dl_{\nu'}} ln Tr_B \left[e^{-b_\nu^\dagger l_\nu b_\nu}\right]$$

$$I + \sum_{\nu'} \langle \nu' | i \rangle \langle j | \nu' \rangle \frac{e^{-l_{\nu'}}}{1-e^{-l_{\nu'}}} = I + \left[\frac{e^{-C}}{I-e^{-C}}\right]_{ij} = \left[\frac{I}{I-e^{-C}}\right]_{ij}$$

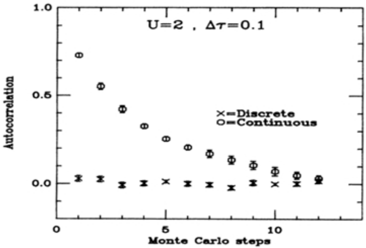
Discrete vs. Continuous HS Transformations

Discrete HS Transformation (Assumes Spin Up or Down)

$$e^{-U\Delta\tau(\hat{m}_\uparrow - 1/2)(\hat{m}_\downarrow - 1/2)} = \frac{1}{2} e^{-U\Delta\tau/4} \sum_{\sigma=\pm 1} e^{\nu\sigma(\hat{m}_\uparrow - \hat{m}_\downarrow)}$$
$$\cosh(\nu) = e^{\nu} + e^{-\nu}$$

Continuous HS Transformation

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx e^{-x^2/2} e^{-xy} = e^{y^2/2}$$
$$e^{(1/2)\Delta\tau\hat{v}^2} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} d\sigma e^{-\sigma^2/2} e^{\sigma\sqrt{\Delta\tau}\hat{v}}$$



Autocorrelation Times for Hubbard Model Using Discrete vs. Continuous HS Transforms
Buendia, PRB (1986)

Local Updating for Bosons

Previous and Updated Matrices

$$M_1 = I - FV_1$$
$$M_2 = I - FV_2$$

Difference Between Matrices

$$V_1^{-1} V_2 = I + \alpha e_1 e_1^T$$
$$\alpha \equiv \frac{V_2(1,1)}{V_1(1,1)} - 1$$

Expressing Updated Matrix in Terms of Previous

$$M_1 = I - FV_1 - FV_1(V_1^{-1} V_2 - I)$$
$$= M_1 - \alpha F V_1 e_1 e_1^T$$
$$= M_1[I + \alpha(I - M_1^{-1}) e_1 e_1^T]$$

Local Updating for Bosons (Contd.)

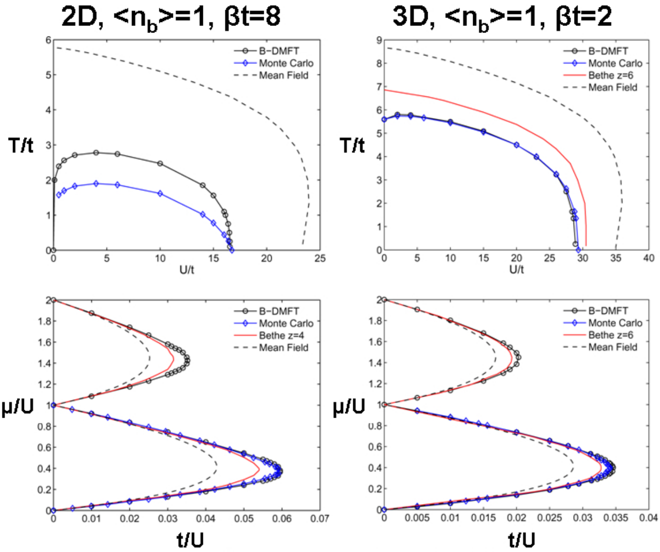
Ratio of Determinants

$$r^b = \frac{Det[I/M_2]}{Det[I/M_1]} = \frac{Det[M_1]}{Det[M_2]}$$
$$1/r^b = Det[M_2]/Det[M_1]$$
$$= Det[I + \alpha(I - M_1^{-1})e_1 e_1^T]$$
$$= 1 + \alpha(1 - e_1^T M_1^{-1} e_1)$$
$$r^b = \frac{1}{1+\alpha(1-e_1^T M_1^{-1} e_1)}$$

Updated Matrix Inverse

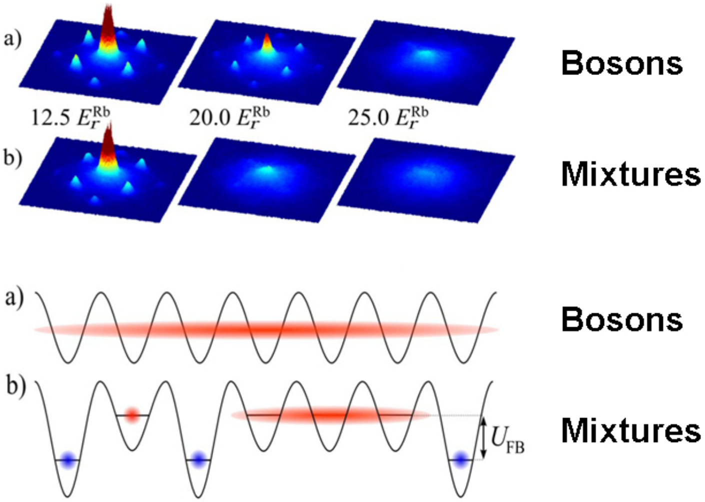
$$M_2^{-1} = [I + \alpha(I - M_1^{-1})e_1 e_1^T]^{-1} M_1^{-1}$$
$$= \left[I - \frac{\alpha(I-M_1^{-1})e_1 e_1^T}{1+\alpha e_1^T (I-M_1^{-1})e_1} \right] M_1^{-1}$$
$$= M_1^{-1} - \frac{\alpha}{r^b}(I - M_1^{-1})e_1 e_1^T M_1^{-1}$$

Boson Dynamical Mean Field Theory



Anders, New J. Phys. (2011).

Bose-Fermi Experiments



Ospelkaus, PRL (2006).