

# Gaussian Phase-Space Representations IV

Vssup Lectures 2012

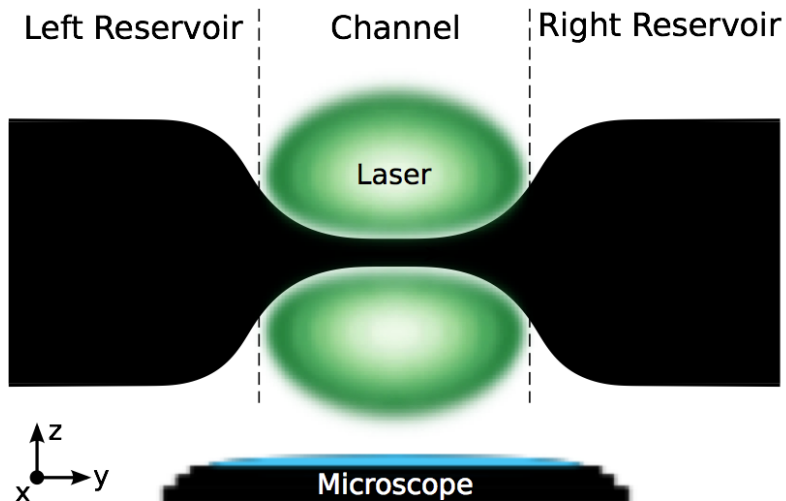
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July 6, 2012

# Outline

- 1 Fun with fermions
- 2 General Coherent States
- 3 General Gaussian Phase-space
- 4 Phase-space methods for finite temperature bosons
- 5 Phase-space methods for finite temperature fermions
- 6 Ground states of the Fermi-Hubbard model

# Mesoscopic cold atoms (Esslinger 2012)



## Universal quantized conductivity formula

What is the channel conductivity, ie the current in atoms per second per potential difference?



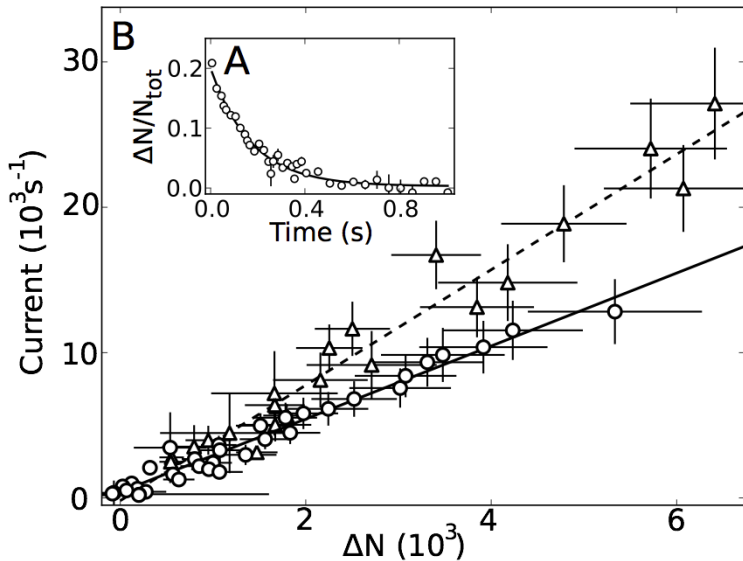
$$G = G_0 \sum_n t_n$$



$$G = 1/(\pi\hbar)$$

- This is a universal law found with mesoscopic electronics,  
**and now with mesoscopic atomtronics.**

# Mesoscopic cold atoms (Esslinger 2012)



# Dealing with atomic coherence in fermions

## How do we treat coherent phenomena with fermions?

- Is there a coherent state for fermions?
- Is there such a thing as a P-representation?
- Can we efficiently compute ground states?
- What about quantum transport?

# Ways to define coherent states

- **Definition 1:** The coherent states  $|z\rangle$  are eigenstates of the annihilation operator  $a$ :  $\hat{a}|z\rangle = z|z\rangle$ .
- **Definition 2:** The coherent states  $|z\rangle$  are quantum states with a minimum uncertainty relationship:  $\Delta x \Delta p = \hbar/2$
- **Definition 3:** The coherent states  $|z\rangle$  can be obtained by applying a displacement operator  $D(z)$  on the ground state of harmonic oscillator:

$$|z\rangle = D(z)|0\rangle, D(z) = \exp(z\hat{a}^\dagger - z^*\hat{a})$$

# General coherent states from (3)

## Can we generalize coherent states?

- Consider  $\mathbf{T}$  as a set of operators closed under commutation - called a **LIE ALGEBRA**
- $\text{le } [T_i, T_j] = \sum_k C_{ijk} T_k$
- **Define a continuous Lie group** of operators  
 $g(\mathbf{z}) = \exp(\mathbf{T} \cdot \mathbf{z})$
- Let  $|\psi_o\rangle$  be some fixed vector - the *reference* state
- Then a general coherent state is the set of states  
 $|\mathbf{z}\rangle = \exp(\mathbf{T} \cdot \mathbf{z}) |\psi_o\rangle$
- Can get different coherent states from different  $|\psi_o\rangle$ .



# Coherent states for fermions

- **Definition 1:** Gives anticommuting Grassmann variables: if  $\hat{a}|z\rangle = z|z\rangle$ , then  $a$  anti-commutes  $\rightarrow z$  anti-commutes
- **Definition 2:** Not always unique, and not a complete set
- **Definition 3:**

## Coherent states for fermions?

- Consider  $|\psi_0\rangle = |1, \dots, 1, 0, \dots, 0\rangle$  as the **N-particle ground state**
- Let  $|z\rangle = \exp\left(\sum_{p,h} \hat{a}_p^\dagger z_{ph} \hat{a}_h\right) |\psi_0\rangle$
- For every created particle (p) we create a hole (h)

# General phase-space approach

Expand density matrix in a complete basis of operators

$$\hat{\rho} = \int P(\vec{\lambda}) \hat{\Lambda}(\vec{\lambda}) d\vec{\lambda}$$

Phase-space may be larger still!

- Here  $\hat{\Lambda}(\vec{\lambda})$  must be complete
- Quantum dynamics  $\rightarrow$  Trajectories in  $\vec{\lambda}$ .
- Different basis choice  $\hat{\Lambda}(\vec{\lambda}) \rightarrow$  different representation
- Eg, positive P-representation:  $\hat{\Lambda}(\vec{\lambda}) = |\alpha\rangle \langle \beta| / \langle \beta | \alpha \rangle$

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# Trade-offs: distribution vs basis

The diagram illustrates the relationship between a distribution  $\rho$  and its decomposition into two components,  $P$  and  $\Lambda$ . It consists of two rows of elements. The top row shows three bell-shaped curves: a purple curve labeled  $\rho$ , a red curve labeled  $P$ , and a blue curve labeled  $\Lambda$ . An equals sign  $=$  is placed between the purple and red curves, and a tensor product symbol  $\otimes$  is placed between the red and blue curves. The bottom row shows three mathematical symbols: a purple  $\sigma_\rho$ , a red  $\sigma_P$ , and a blue  $\sigma_\Lambda$ . A tilde symbol  $\sim$  is placed between the purple and red symbols, and a plus sign  $+$  is placed between the red and blue symbols.

$$\rho = P \otimes \Lambda$$
$$\sigma_\rho \sim \sigma_P + \sigma_\Lambda$$

# General Gaussian operator

General Gaussian operators give a complete basis in all cases

Normally-ordered exponential of a quadratic form in the  $2M$ -vector mode operator  $\delta\hat{\underline{a}} = (\hat{\underline{a}}, \hat{\underline{a}}^\dagger) - \underline{\alpha}$ , where  $\underline{\alpha}$  is a c-vector and  $\hat{\underline{a}}$  is the vector of annihilation operators. Used for either bosons or fermions:

$$\hat{\Lambda}(\vec{\lambda}) = \frac{\Omega}{\sqrt{|\underline{\sigma}|}} : \exp \left[ -\delta\hat{\underline{a}}^\dagger \underline{\sigma}^{-1} \delta\hat{\underline{a}}/2 \right] : .$$

**Quantum phase-space:**  $\vec{\lambda} = (\Omega, \underline{\alpha}, \underline{\sigma})$ .

# What is the covariance?

The covariance matrix acts as a 'stochastic Green's function'

$$\underline{\underline{\sigma}} = \begin{bmatrix} \mathbf{I} + \mathbf{n} & \mathbf{m} \\ \mathbf{m}^+ & \mathbf{I} + \mathbf{n}^T \end{bmatrix} \cdot$$

Eg, fermion case: representation phase space is  $\vec{\lambda} = (\Omega, \mathbf{n}, \mathbf{m}, \mathbf{m}^+)$

- $\Omega$  = weight factor
- $\mathbf{n}$  = number correlation - OBSERVABLE
- $\mathbf{m}, \mathbf{m}^+$  = anomalous correlation - OBSERVABLE

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# Weighted stochastic gauge equations

Exponential quantum problems  $\rightarrow$  tractable stochastic equations

$$\begin{aligned}d\Omega/\partial t &= \Omega[U + \mathbf{g} \cdot \boldsymbol{\zeta}] \\d\boldsymbol{\alpha}/\partial t &= \mathbf{A} + \mathbf{B}(\boldsymbol{\zeta} - \mathbf{g})\end{aligned}$$

- Can be used for fermions AND bosons
- Can be used in imaginary time for finite temperatures
- $\mathbf{g}$  is a gauge chosen to stabilize trajectories
- A careful choice of basis, gauge and stochastic method is necessary



# BOSONIC INITIAL ENSEMBLES

Nonlinear interactions at each site + linear interactions coupling different sites:

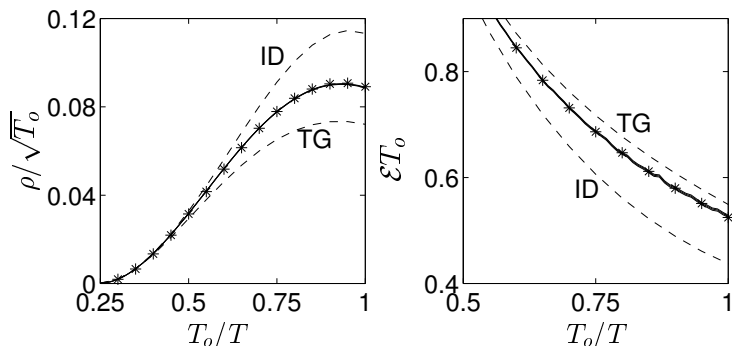
- $\hat{H}(\mathbf{a}, \mathbf{a}^\dagger) = \hbar \left[ \sum \sum \omega_{ij} a_i^\dagger a_j + \sum : \hat{n}_j^2 : \right]$ .
- $\omega_{ij}$  - nonlocal coupling, includes chemical potential.
- Boson number:  $\hat{n}_i = a_i^\dagger a_i$ .
- **General approach also holds for quantum fields**

# A: ONE-DIMENSION, FINITE TEMPERATURE

$$\begin{aligned}\frac{d\alpha}{d\tau} &= - [|\alpha\beta^*| + \omega - \nabla^2 + i\zeta_1(\tau)] \alpha \\ \frac{d\beta}{d\tau} &= - [|\alpha\beta^*| + \omega - \nabla^2 + i\zeta_2(\tau)] \beta \\ \frac{d\Omega}{d\tau} &= -H\Omega + \text{gauge terms}\end{aligned}$$

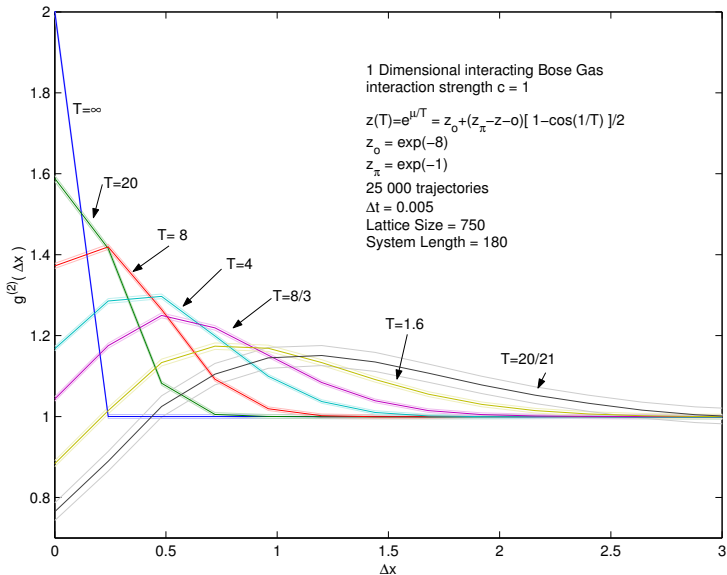
- **weighted** Gross-Pitaevskii equation + quantum noise

# ONE-DIMENSIONAL BEC



Uses imaginary time propagation to get a finite temperature  
Agreement of simulations with exact solutions

# Predicts: anomalous spatial correlations



# INTERACTING FERMIONS

$$\hat{H} = - \sum_{ij,\sigma} t_{ij} \hat{a}_{i,\sigma}^\dagger \hat{a}_{j,\sigma} + U \sum_j : \hat{n}_{j,j,\downarrow} \hat{n}_{j,j,\uparrow} :$$

- Hubbard model of an interacting Fermi gas on a lattice
- Ultracold gas in an optical lattice: experiments at ETH, Zurich
  - **Weak-coupling limit** → **BCS transitions**
  - **Relevance to high- $T_c$  superconductors?**
  - **Universal fermionic behavior - neutron star interiors?**

# QMC sign problem

- Traditional fermionic Quantum Monte Carlo (QMC) suffers from sign problems:

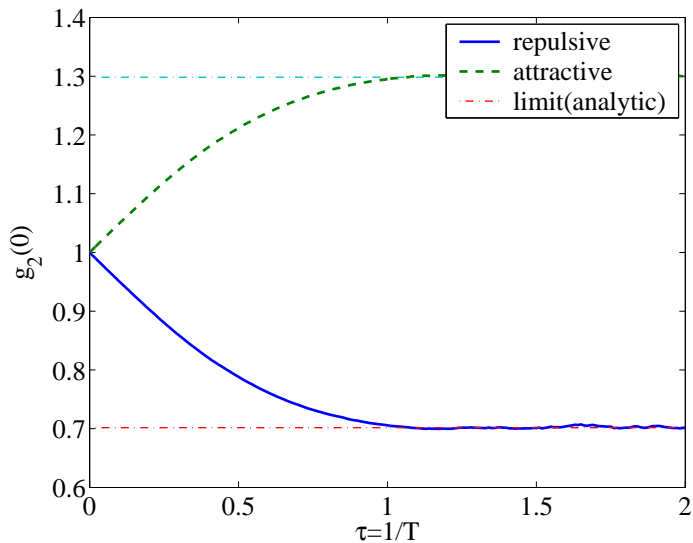
$$\langle A \rangle \sim \frac{\langle sA \rangle}{\langle s \rangle}$$

- sign problem increases with:
  - dimension,
  - lattice size,
  - interaction strength

# Finite-temperature phase-space equations

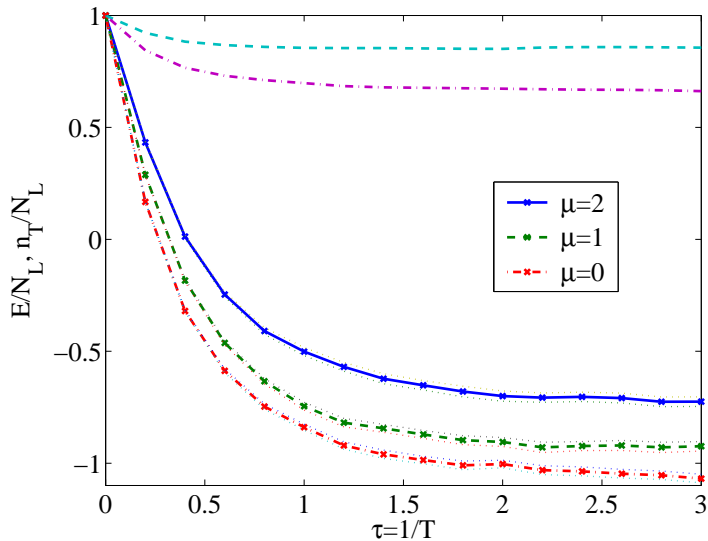
- Paths:  $\frac{dn_\sigma}{d\tau} = \frac{1}{2} \left\{ (1 - n_\sigma) T_\sigma^{(1)} n_\sigma + n_\sigma T_\sigma^{(2)} (1 - n_\sigma) \right\}$ .
- Weights:  $\frac{d\Omega}{d\tau} = -\Omega H(\mathbf{n}_1, \mathbf{n}_{-1})$ 
  - T-matrix:  
 $T_{i,j,\sigma}^{(r)} = t_{ij} - \delta_{i,j} \left\{ U(n_{j,j,-\sigma} - n_{j,j,\sigma} + \frac{1}{2}) - \mu + \sigma \xi_j^{(r)} \right\}$ .
  - Noises:  $\langle \xi_j^{(r)}(\tau) \xi_{j'}^{(r')}(\tau') \rangle = 2U \delta(\tau - \tau') \delta_{j,j'} \delta_{r,r'}$ .

# A: 1D Lattice - 100 sites vs: exact result





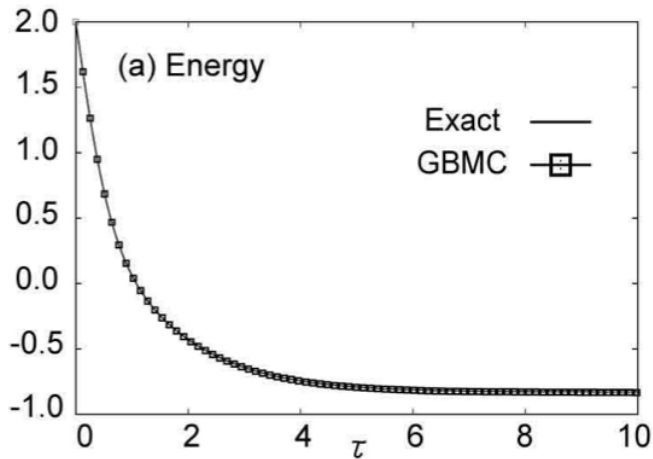
## B: 16x16 2D Lattice



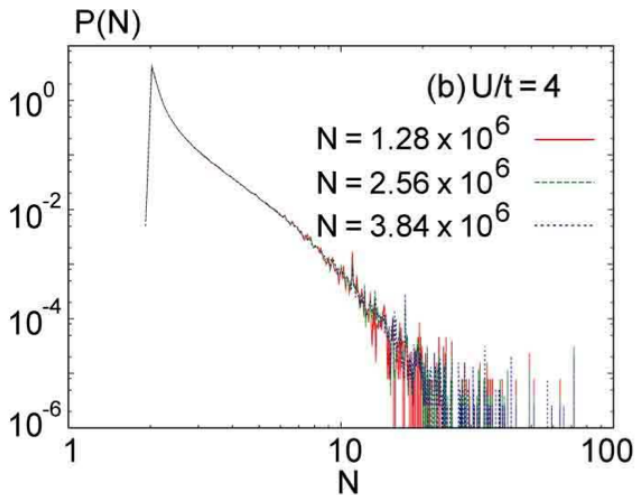
## Imada improved on the original Gaussian method

- Used number projections to reduce the size of Hilbert space
  - Importance sampling helps to improve statistics
  - No evidence of a Fermi 'sign' problem
  - No evidence of boundary term problems

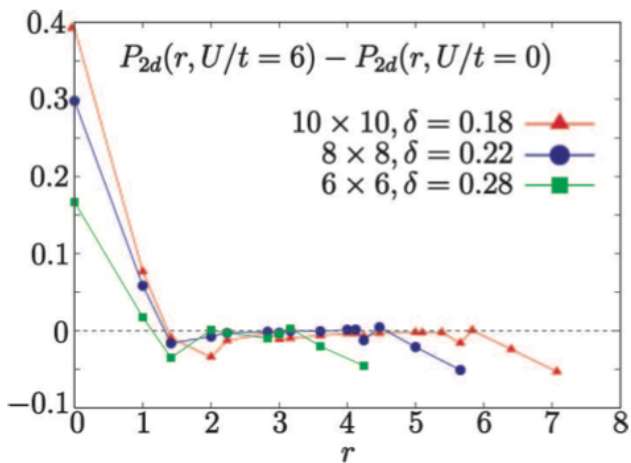
## Imada algorithm test case - two sites



# Imada algorithm test case - tail exponent = -4



# Imada algorithm Hubbard model: no pairing



## Gaussian phase-space extends to fermions

- Provides a new way to treat strongly correlated systems
  - Predicts no long-range order in Hubbard model
  - Apparently NOT the explanation of high  $T_c$  superconductors
  - To be tested in atomic Fermi gas experiments