

Coherence and Phase-space IV

VSSUP Lectures 2014

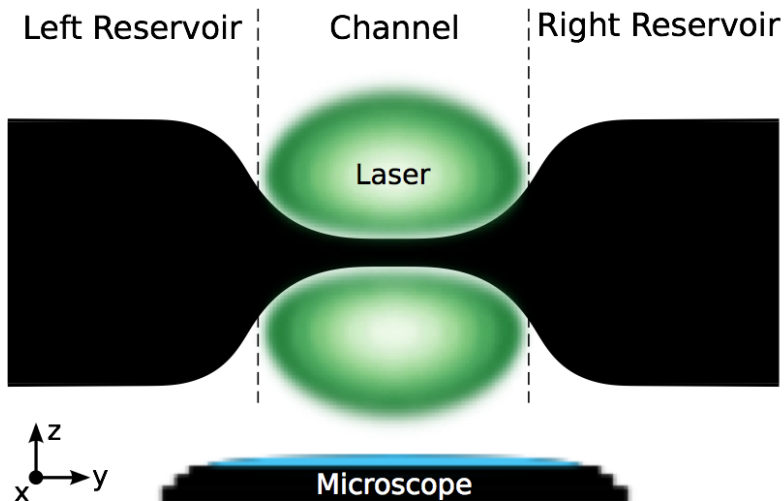
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January 23, 2014

Outline

- 1 Fun with fermions: General Coherent States
- 2 General Gaussian Phase-space
- 3 Phase-space for warm bosons and fermions
- 4 Ground states of the Fermi-Hubbard model

Mesoscopic cold atoms (Esslinger 2012)



Landauer Quantum Transport

Universal quantized conductivity formula

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



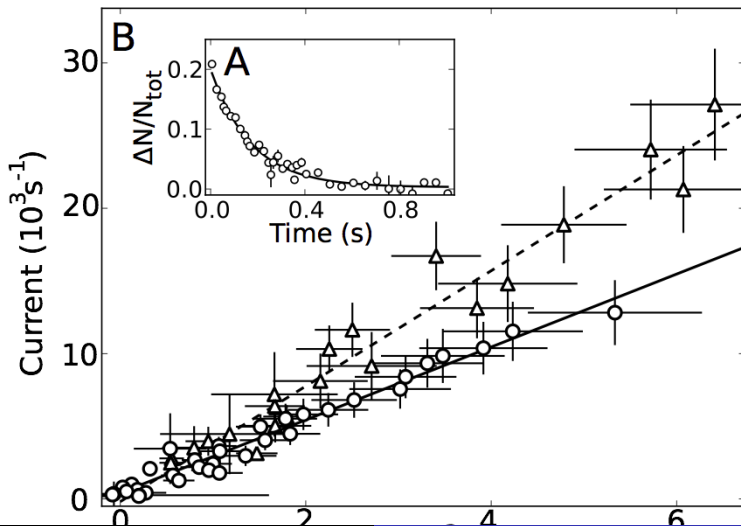
$$G = G_0 \sum_n t_n$$



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

- 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**
- I.e. $[T_i, T_j] = \sum_k C_{ijk} T_k$
- **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

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

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 $\delta\hat{\mathbf{a}} = (\hat{\mathbf{a}}, \hat{\mathbf{a}}^\dagger) - \underline{\alpha}$, where $\underline{\alpha}$ is a c-vector and $\hat{\mathbf{a}}$ is the vector of annihilation operators. Used for either bosons or fermions:

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

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

What is the covariance?

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

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

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

- Ω = 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:

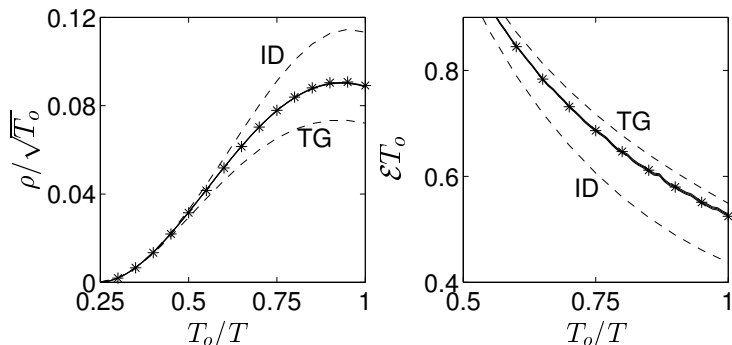
- $\hat{H}(\mathbf{a}, \mathbf{a}^\dagger) = \hbar \left[\sum \sum \omega_{ij} a_i^\dagger a_j + \sum : \hat{n}_j^2 : \right]$.
- ω_{ij} - nonlocal coupling, includes chemical potential.
- Boson number: $\hat{n}_i = a_i^\dagger a_i$.
- General approach also holds for quantum fields

A: ONE-DIMENSION, FINITE TEMPERATURE

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

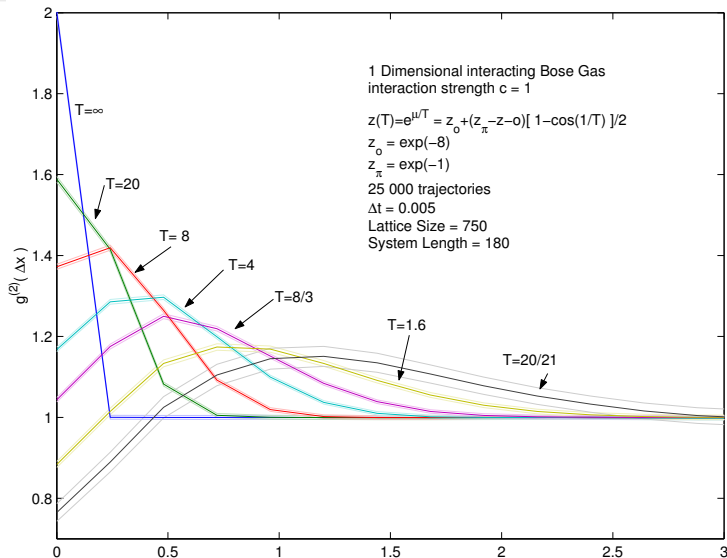
- **weighted** Gross-Pitaevskii equation + quantum noise

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** \rightarrow **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:

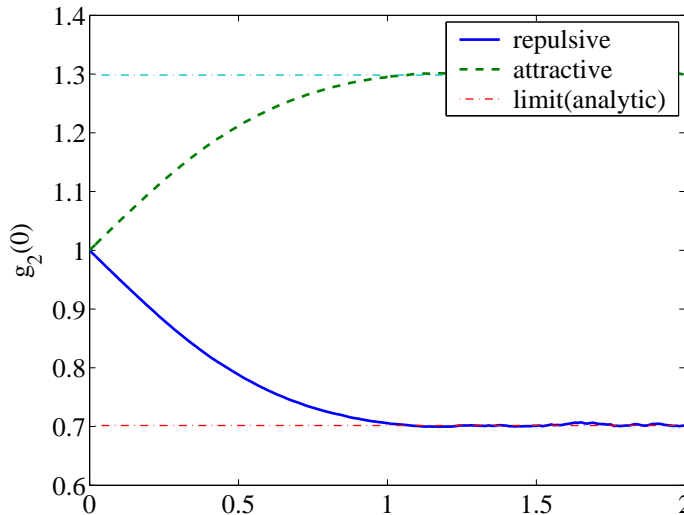
$$\langle A \rangle \sim \frac{\langle sA \rangle}{\langle s \rangle}$$

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

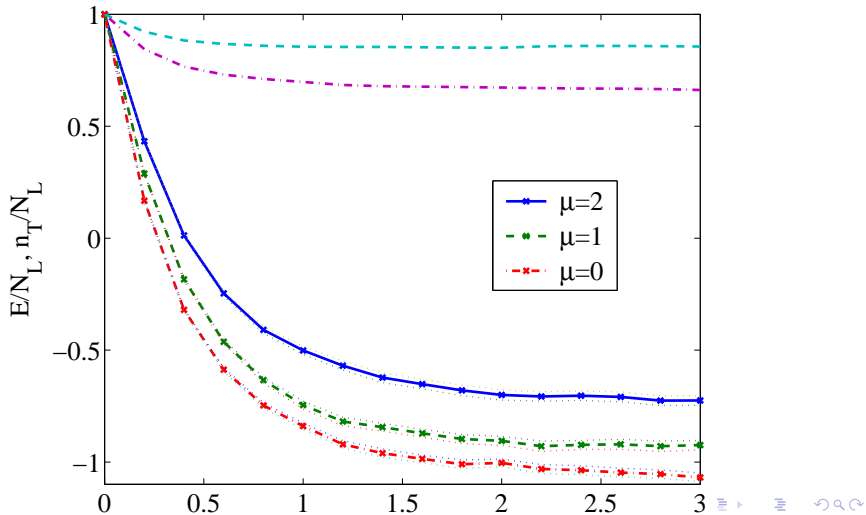
Finite-temperature phase-space equations

- 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: $\left\langle \xi_j^{(r)}(\tau) \xi_{j'}^{(r')}(\tau') \right\rangle = 2U \delta(\tau - \tau') \delta_{j,j'} \delta_{r,r'}.$

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



B: 16x16 2D Lattice

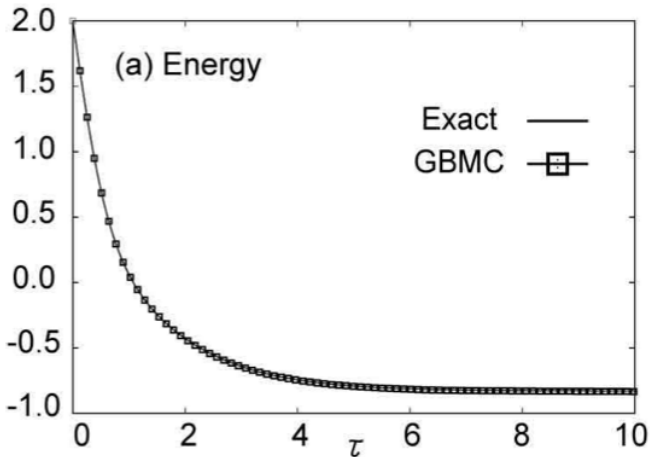


IMADA ALGORITHM

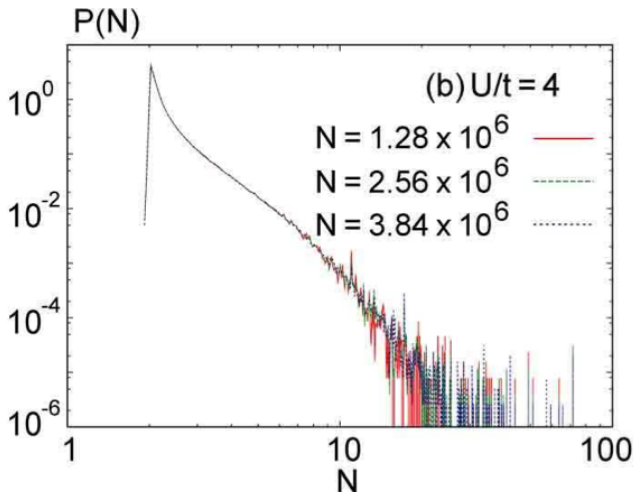
Imada improved on the original Gaussian method

- 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

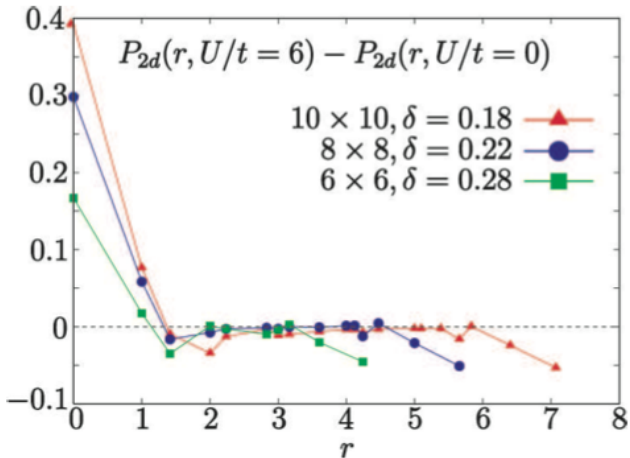
Imada algorithm test case - two sites



Imada algorithm test case - tail exponent = -4



Imada algorithm Hubbard model: no pairing



Summary

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