Particle Projection Using Complex Langevin

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June 22, 2017

Overview

Motivation: Ultracold Atoms, & Nuclei

We focus on non-relativistic Fermi systems:

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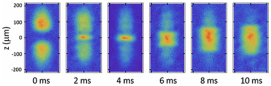
Ultracold Atoms

- Short-range, controllable interactions
- $T \geq 0$



- Controllable Parameters: temperature, coupling, polarization, mass imbalance, trap shape (harmonic, hard wall, lattices)
- Measurable Quantities: EoS, Hydrodynamic & Spin responses, Collective modes, etc

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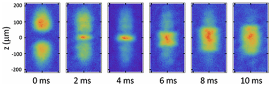

Nuclei

- Fixed Particle Number (N + P)
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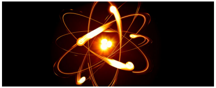

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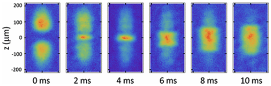

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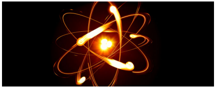

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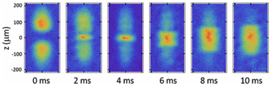

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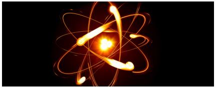

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- **We attempt to access the EoS using Particle Projection**

Grand Canonical Partition Function

- $\mathcal{Z} = \mathrm{tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\right] = \int \mathcal{D}\sigma \det M[\sigma, z_{\uparrow}] \det M[\sigma, z_{\downarrow}]$

Formalism

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$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 - g\sum_{i<j}\delta(x_i - x_j)$

g : bare coupling

$\delta(x_i - x_j)$: Contact Interaction

$M[\sigma, z]$: Fermion Matrix

$z = e^{\beta\mu}$: Fugacity

σ : Hubbard Stratonovich Auxiliary Field

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- $Q_{n,m} = \int_0^{2\pi} \frac{d\phi_\uparrow}{2\pi} \frac{d\phi_\downarrow}{2\pi} \mathcal{Z}[e^{i\phi_\uparrow}, e^{i\phi_\downarrow}] e^{-in\phi_\uparrow} e^{-im\phi_\downarrow}$
- $Q_{n,m} = e^{-\beta F_{n,m}}$

Complex Langevin Method

- Define $\Phi = (\sigma, \phi_\uparrow, \phi_\downarrow)$ & $S = \ln det^2 M[\sigma, z] + in\phi_\uparrow + im\phi_\downarrow$
- Langevin Eq: $\frac{\partial \Phi_x(\sigma)}{\partial \sigma} = -\frac{\delta S[\Phi]}{\delta \Phi_x(\sigma)} + \eta_x(\sigma)$
- $\Phi_a \rightarrow \Phi_a^R + i\Phi_a^I$
  - Real Part: $\Phi^R_{a,x}(n+1) = \Phi^R_{a,x}(n) + \epsilon K^R_{a,x}(n) + \sqrt{\epsilon}\eta_{a,x}(n)$
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  - $\eta_{a,x}(n)$: Noise s.t. $\langle \eta_{a,x} \rangle = 0$ & $\langle \eta_i \eta_j \rangle = \delta_{ij}$
  - ϵ: Time step
- Drift
  - $K^R_{a,x} = -\mathrm{Re}\left[\frac{\delta S}{\delta \Phi_{a,x}}\Big|_{\Phi_a \rightarrow \Phi_a^R + i\Phi_a^I}\right]$
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- Problems:

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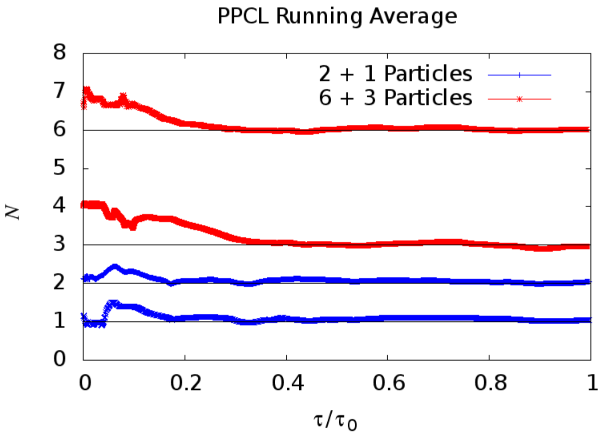
- Problems: Uncontrolled excursions in imaginary component, Singularities

Particle Projection Results

- Expectation of particle number operator.
  - $\langle \hat{N} \rangle = \langle \mathrm{tr}(M^{-1} \partial M / \partial z) \rangle$
- Average over Langevin time should converge to designated particle number, $n_\uparrow$, $n_\downarrow$
- Plot shows the running average over Langevin time.

Particle Projection Results

- 3D
- Unitarity
- $V = N_x^3 = 6^3$
- $N_\tau = 60$
- $\tau_0 = 2000$ steps

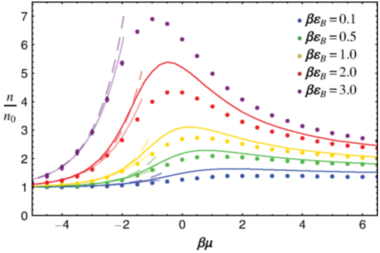


$$\hat{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 - g\sum_{i<j}\delta(x_i - x_j)$$

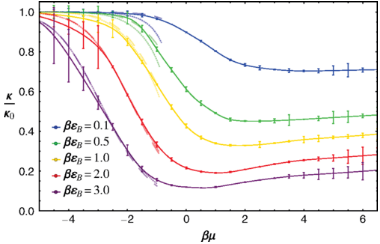
Virial Projection Motivation

- EoS gives us access to many measurable quantities in a system.
  - Density, Pressure, Contact, Compressibility...
- Conversely, virial coefficients tell us about the EoS.

Density EoS vs. Virial Coefficients



Compressibility EoS vs. Virial Coefficients



Phys. Rev. Lett. 115, 115301 (2015)

Virial Projection

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By taking $z \to ze^{i\phi}$, we may again utilize Fourier Projection to obtain **specific virial coefficients.**

- $b_n[z] = \frac{1}{\mathcal{Q}_1} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi n} \ln \mathcal{Z}[z \to ze^{-i\phi}] = b_n z^n$

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However, we cannot treat this as before by making $d\phi$ part of the random walk because of the ln and no obvious measure.

Virial Projection Continued

Now we differentiate with respect to z.

- $\frac{\partial b_n(z)}{\partial z} = \frac{1}{\mathcal{Q}_1} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi n} \int \mathcal{D}\sigma P[\sigma, z e^{-i\phi}] \mathrm{tr} \left[M^{-1} \partial M / \partial z \right]$

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where,

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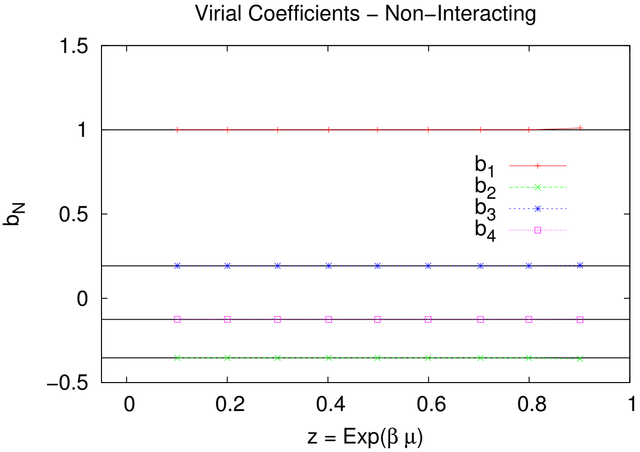
In practice it is best to use a **discretized** version of the Fourier integral,

- $\frac{\partial b_n(z)}{\partial z} = \frac{1}{\mathcal{Q}_1} \frac{1}{N_k} \sum_{k=0}^{N_k - 1} e^{i\phi_k n} \langle \mathrm{tr}\left[M^{-1} \partial M / \partial z\right] \rangle_{\phi_k, z} = n b_n z^{n-1}$
  - $\frac{1}{n z^{n-1}} \frac{\partial b_n(z)}{\partial z} = b_n$
  - N_k : Number of Fourier Points

Virial Projection Results

- We compute $\frac{\partial b_n(z)}{\partial z} = nb_n z^{n-1}$ for various z values.
- Dividing each by the respective nz^{n-1} yields a constant.
- Plot $\frac{1}{nz^{n-1}} \frac{\partial b_n(z)}{\partial z}$ vs. z

- 1D
- $N_x = 31$
- $N_\tau = 160$
- $N_k = 30$
- $\lambda^2 = \beta g^2 = 0.0$



Virial Projection Results - Interacting

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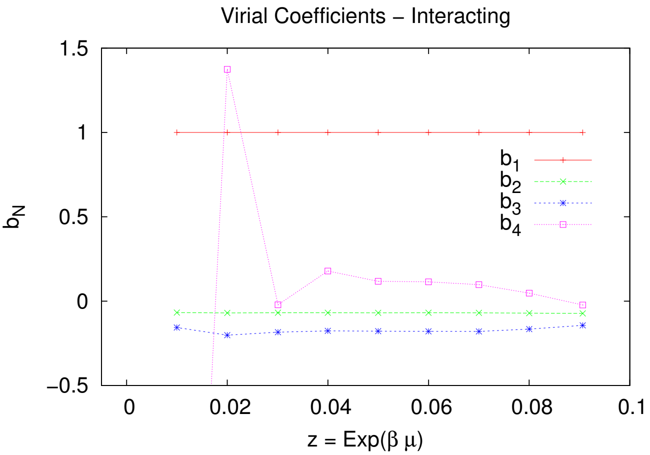
- $N_x = 31$
- $N_\tau = 160$
- $N_k = 45$
- $\lambda^2 = \beta g^2 = 1.0$



Summary & Outlook

- Goal: Use Fourier transforms to project onto subspace of fixed particle number.
- If successful, enable particle projection in 3D.
  - Access free energies for finite systems, and calculate virial coefficients
- Compute Free Energies for polarized systems such that $n_\uparrow \neq n_\downarrow$ (In progress)
- Compute higher order virial Coefficients (In progress)

Acknowledgments

Thank you for your attention!