

Particle Projection Using Complex Langevin

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 - Formalism
 - Results

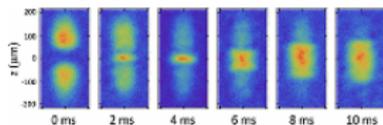
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- Short-range, controllable interactions
- $T \geq 0$



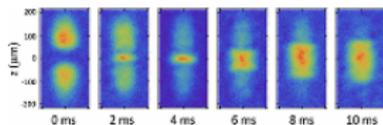
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- Measurable Quantities: EoS, Hydrodynamic & Spin responses, Collective modes, etc

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- Fixed Particle Number ($N + P$)
- $T = 0$



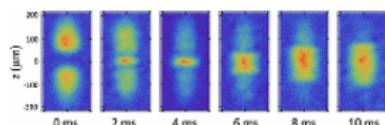
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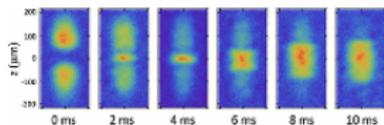


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- **We attempt to access the EoS using Particle Projection**

Grand Canonical Partition Function

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

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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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Expanding in powers of z_{\uparrow} and z_{\downarrow}

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 - This gives us access to the Fourier components of the Grand Canonical Partition Function, and therefore the **Canonical Partition Functions!**
- $Q_{n, m} = \int_0^{2\pi} \frac{d\phi_{\uparrow}}{2\pi} \frac{d\phi_{\downarrow}}{2\pi} \mathcal{Z}[e^{i\phi_{\uparrow}}, e^{i\phi_{\downarrow}}] e^{-in\phi_{\uparrow}} e^{-im\phi_{\downarrow}}$
- $Q_{n, m} = e^{-\beta F_{n, m}}$

- 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: $\Phi_{a,x}^R(n+1) = \Phi_{a,x}^R(n) + \epsilon K_{a,x}^R(n) + \sqrt{\epsilon} \eta_{a,x}(n)$
- Imaginary Part: $\Phi_{a,x}^I(n+1) = \Phi_{a,x}^I(n) + \epsilon K_{a,x}^I(n)$.
- $\eta_{a,x}(n)$: Noise s.t. $\langle \eta_{a,x} \rangle = 0$ & $\langle \eta_i \eta_j \rangle = \delta_{ij}$
- ϵ : Time step

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- Problems:

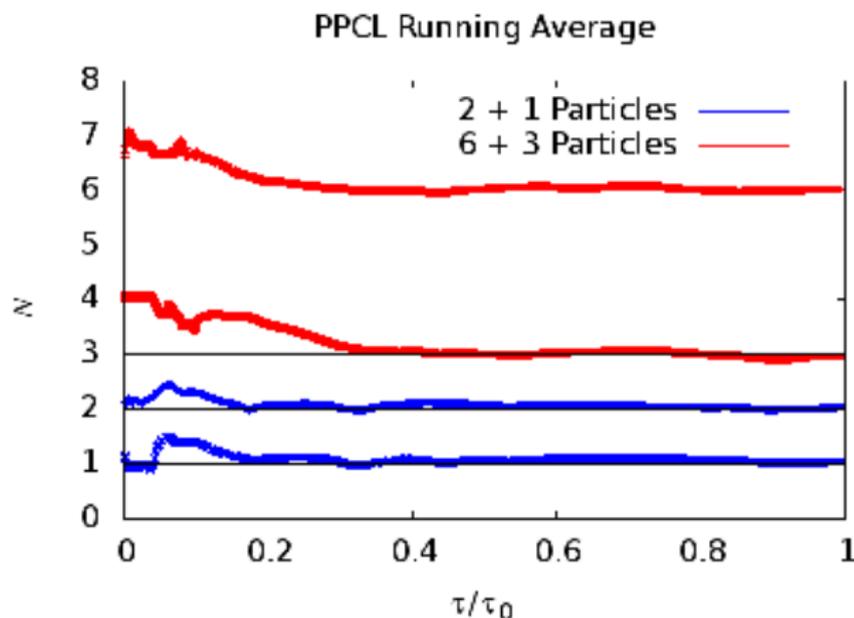
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- Problems: Uncontrolled excursions in imaginary component, Singularities

Particle Projection Results

- Expectation of particle number operator.
 - $\langle \hat{N} \rangle = \langle \text{tr}(M^{-1} \partial M / \partial z) \rangle$
- 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

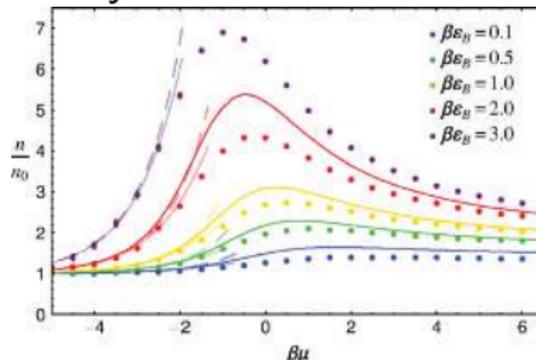


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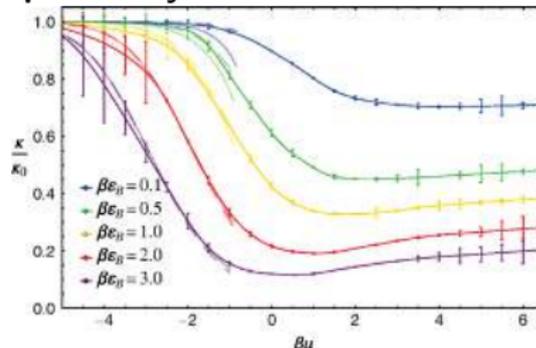
Virial Projection Motivation

- 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



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Grand Potential

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

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

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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 .

$$\bullet \frac{\partial b_n(z)}{\partial z} = \frac{1}{Q_1} \int_0^{2\pi} \frac{d\phi}{2\pi} e^{i\phi n} \int \mathcal{D}\sigma P[\sigma, z e^{-i\phi}] \text{tr} [M^{-1} \partial M / \partial z]$$

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where,

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

$$\bullet \frac{\partial b_n(z)}{\partial z} = \frac{1}{\mathcal{Q}_1} \frac{1}{N_k} \sum_{k=0}^{N_k-1} e^{i\phi_k n} \langle \text{tr} [M^{-1} \partial M / \partial z] \rangle_{\phi_k, z} = n b_n z^{n-1}$$

$$\bullet \frac{1}{n z^{n-1}} \frac{\partial b_n(z)}{\partial z} = b_n$$

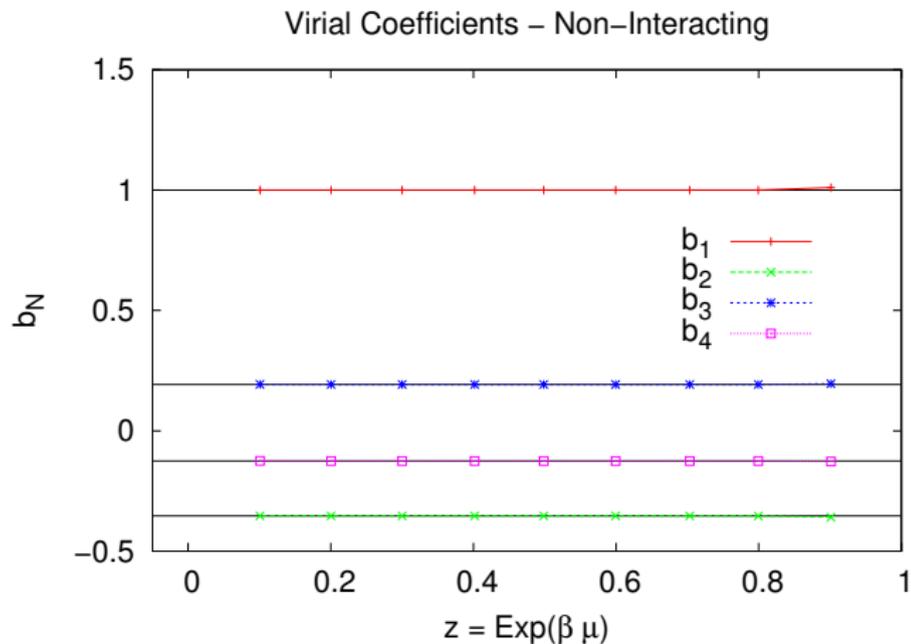
• N_k : Number of Fourier Points

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

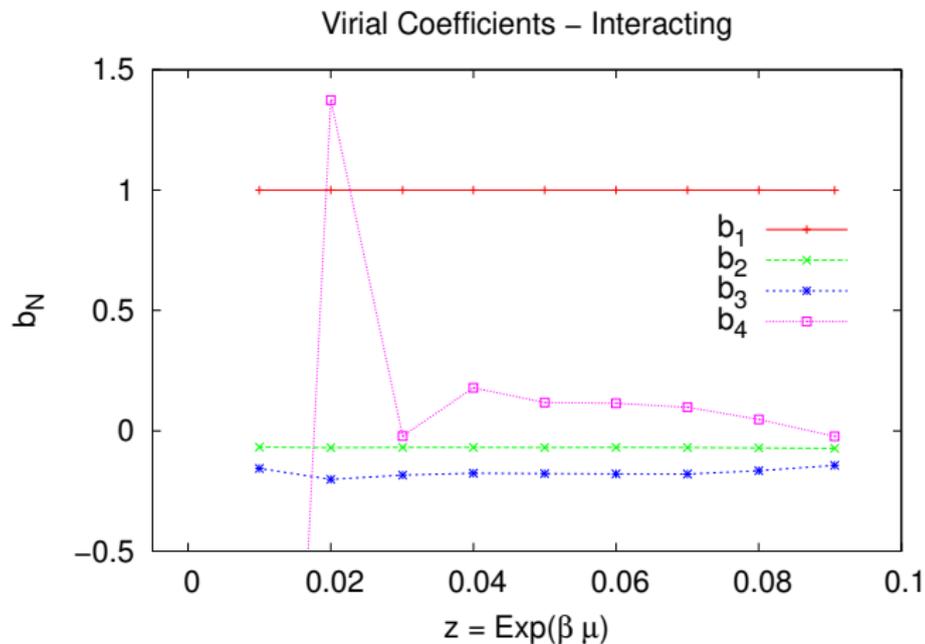
Virial Projection Results - Non Interacting

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



Virial Projection Results - Interacting

- 1D
- $N_x = 31$
- $N_\tau = 160$
- $N_k = 45$
- $\lambda^2 = \beta g^2 = 1.0$



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)

Thank you for your attention!