Path Integral Monte Carlo for Quantum Boltzmannons

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Outline

1. What are boltzmannons?
   - Purpose of studying boltzmannon physics
2. Path Integral Monte Carlo (PIMC) method
3. PIMC method applied to 2-body system
4. Many boltzmannon system calculation

Quantum Boltzmannons

- When a system reaches sufficient conditions of density and temperature, particles of the same species are indistinguishable ($\lambda_T \approx \rho^{-1/3}$)

- For this case Bose-Einstein (bosons) or Fermi-Dirac (fermions) statistics are used in many-body calculations

- At higher temperatures or lower densities, Maxwell-Boltzmann statistics are obeyed, particles are distinguishable

- If particles belong to distinct species, M-B statistics are obeyed regardless of temperature/density (boltzmannons, still quantum mechanical!)

Quantum Boltzmannons

- Currently interest in cold-atom physics in experimentally probing systems with increasing number of species

- Theoretical limit: $N_{species} \rightarrow N_{particles}$, boltzmannon calculations may guide future experiments

- Boltzmannon calculations can attempt to disentangle the effects of statistics from that of interactions

Path Integral Monte Carlo

- Used to calculate thermodynamic properties of systems
- Use Feynman path integral formalism to describe partition function as integrals over coordinate space
- Use Monte Carlo methods to calculate these integrals
- We apply this method to distinguishable, quantum hard spheres

Path Integral Form of Partition Function

PIMC formalism begins with the thermal density matrix of the system:

$$\hat{\rho} = e^{-\beta \hat{H}} = \sum_i e^{-\beta E_i} |\psi_i><\psi_i|$$

The partition function is the trace of the thermal density matrix:

$$Z = Tr(\hat{\rho})$$

The trace can be performed in the position basis:

$$Z = \int dR < R|\hat{\rho}|R >$$

Note: R = {r1, r2, …, r N}

Path Integral Form of Partition Function

- Possible to expand partition function as path integral:

$$Z = \int dR < R|e^{\beta \hat{H}}|R >$$

$$Z = \int dR dR_2 < R|\, e^{-(\beta/2)\hat{H}}|R_2 >< R_2|e^{-(\beta/2)\hat{H}}|R >$$

$$Z \;=\; \int \dots \int dR dR_1 \dots dR_{M-1} \rho(\, R, R_1; \beta/M) \rho(R_1, R_2; \beta/M) \dots \rho(R_{M-1}, R; \beta/M)$$

- Made possible by:

$$e^{-(\beta_1+\beta_2)\hat{H}} = \; e^{-\beta_1 \hat{H}} e^{-\beta_2 \hat{H}}$$

$$\hat{1} = \int |R >< R| dr$$

Calculating Observables

- The full functional form of the partition function is now known

$$Z = \int d\boldsymbol{\mathcal{R}} \prod_{N=1}^{M} \left[\rho_{free}(R_N, R_{N+1}) \prod_{i,j} \rho_{ij}(r_{ij}, r'_{ij}) \right] \quad , \ \boldsymbol{\mathcal{R}} = \{R_N\}$$

- Splitting up 'free' and 2-body terms requires approximations that become more exact at larger values of ‘M’, smaller ‘thermal time step’

- Thermodynamic observables are functions of $\boldsymbol{\mathcal{R}}$ by taking the appropriate derivatives of the partition function

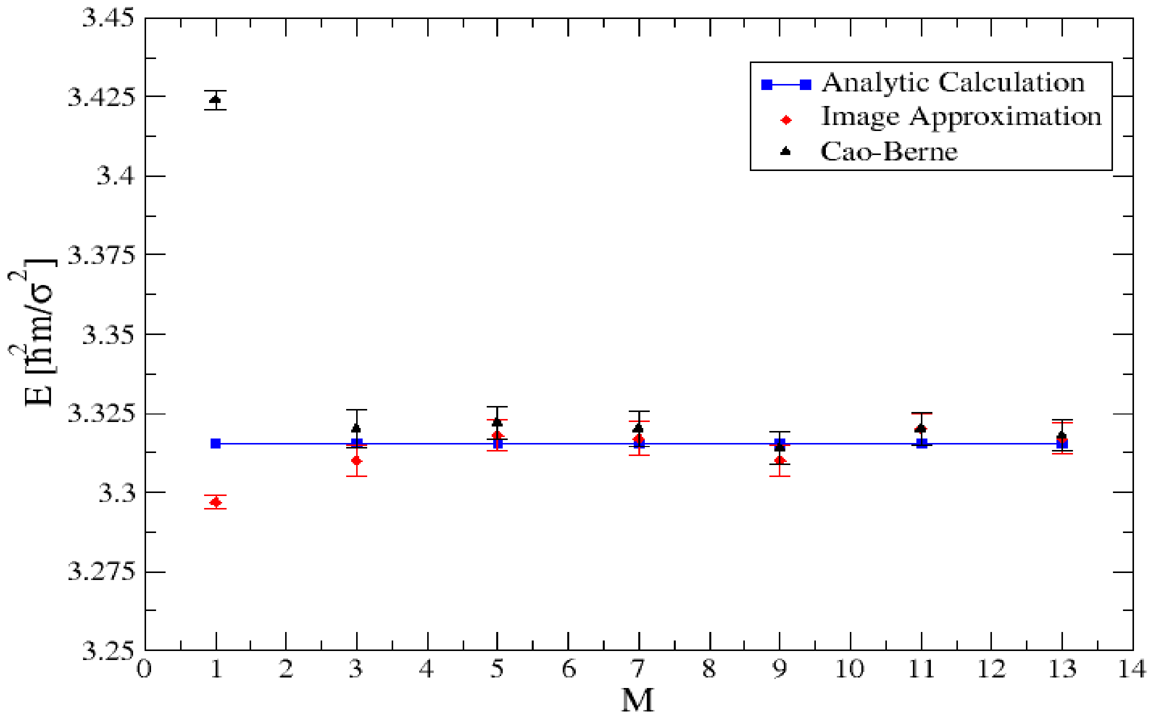
$$< \hat{O} > = Z^{-1} Tr(\hat{O}\hat{\rho}) \ = Z^{-1} \int d\boldsymbol{\mathcal{R}} O(\boldsymbol{\mathcal{R}}) W(\boldsymbol{\mathcal{R}})$$

Two Particle Hard Sphere, Hard Cavity System

- The first system we studied was an infinite spherical well in the separation distance ($\sigma < r < r_{cav}$)
- Two different previously derived two-body density matrices used in calculations (Image Approximation, Cao-Berne)
- Test convergence vs 'M' to analytically solved energy of system for both
- Convergence studies important to test effectiveness of density matrix approximation

Convergence in Energy of Two Hard Sphere Particles Inside Hard Cavity

- Convergence seems to be similar between density matrices
- Same calculation performed at varying temperature
- Convergence behaviour very similar over varying temperature



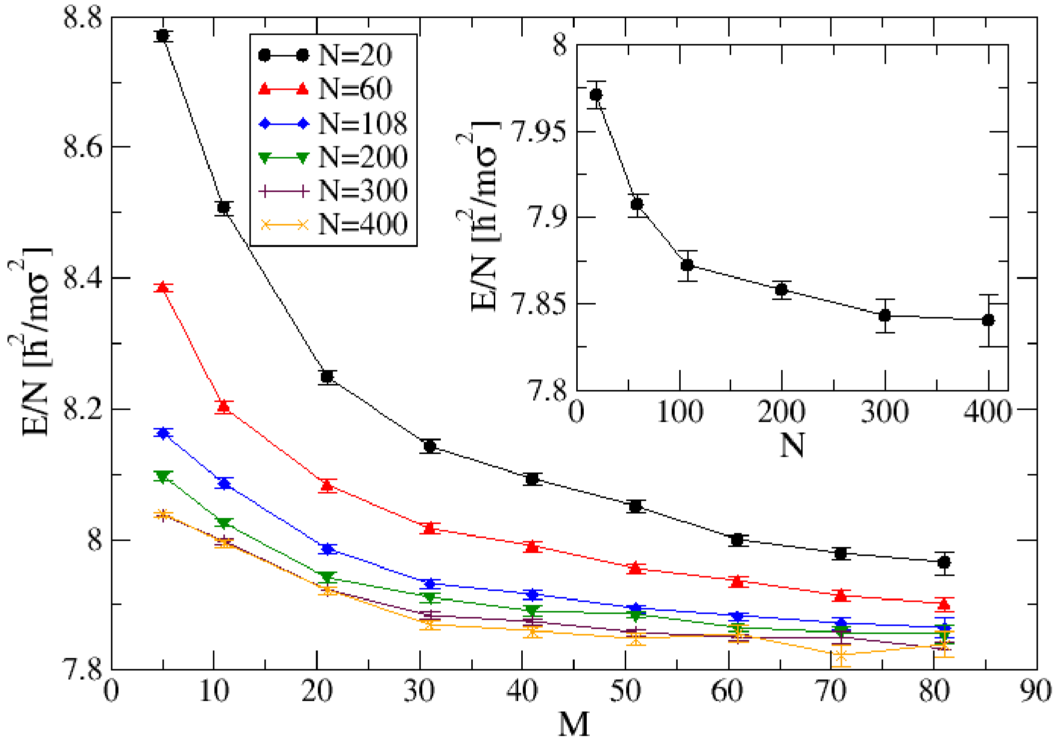
$T(\hbar^2/m\sigma^2 k_B)^{-1} = 1.0,\ r_{cav} = 6.0\sigma$

Many-Particle System

- Next, we studied a many-body boltzmannon system
- The particles’ interactions were taken to be a hard sphere repulstion
- The Cao-Berne two body density matrix was used
- Study was done in periodic simulation box, finite-size effects must be considered

Many Particle System

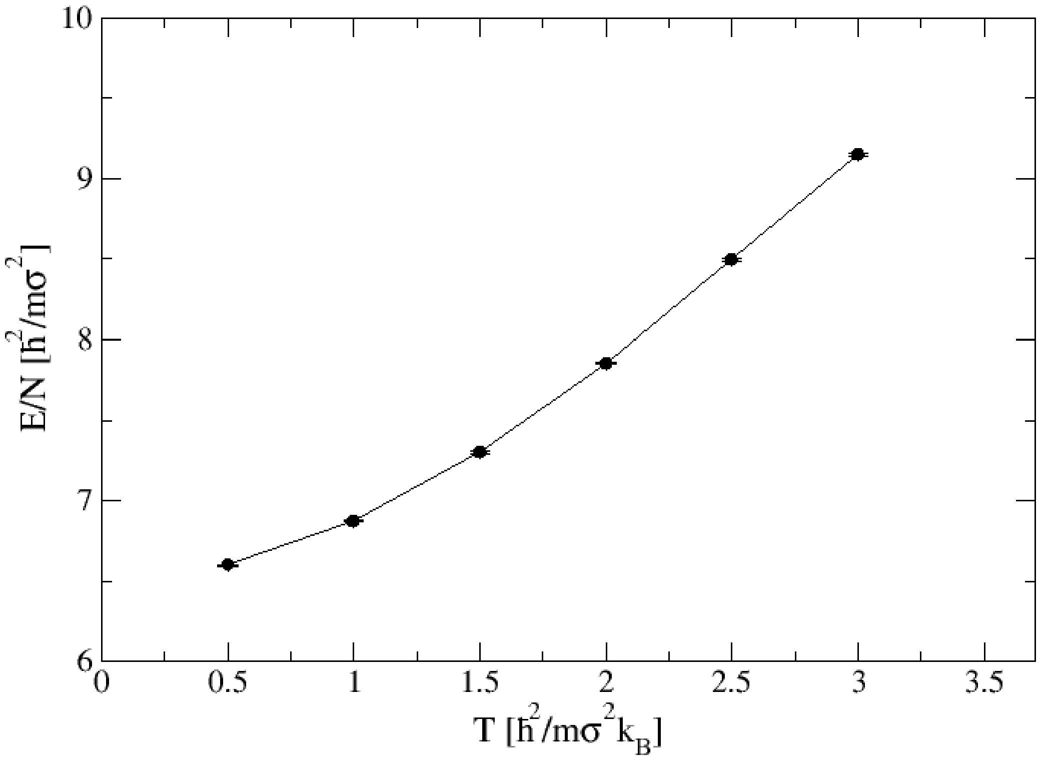
- Energy/Particle for increasing particle number at fixed temperature and density
- Cao-Berne density matrix is used
- Goal is to find thermodynamic limit for practical use



$T(\hbar^2/m\sigma^2 k_B)^{-1} = 2.0, n(\sigma^3)^{-1} = 0.2063$

Many Particle System

- Energy/Particle at converged 'M' and thermodynamic limit at varying T
- Find linear dependence at higher temperatures

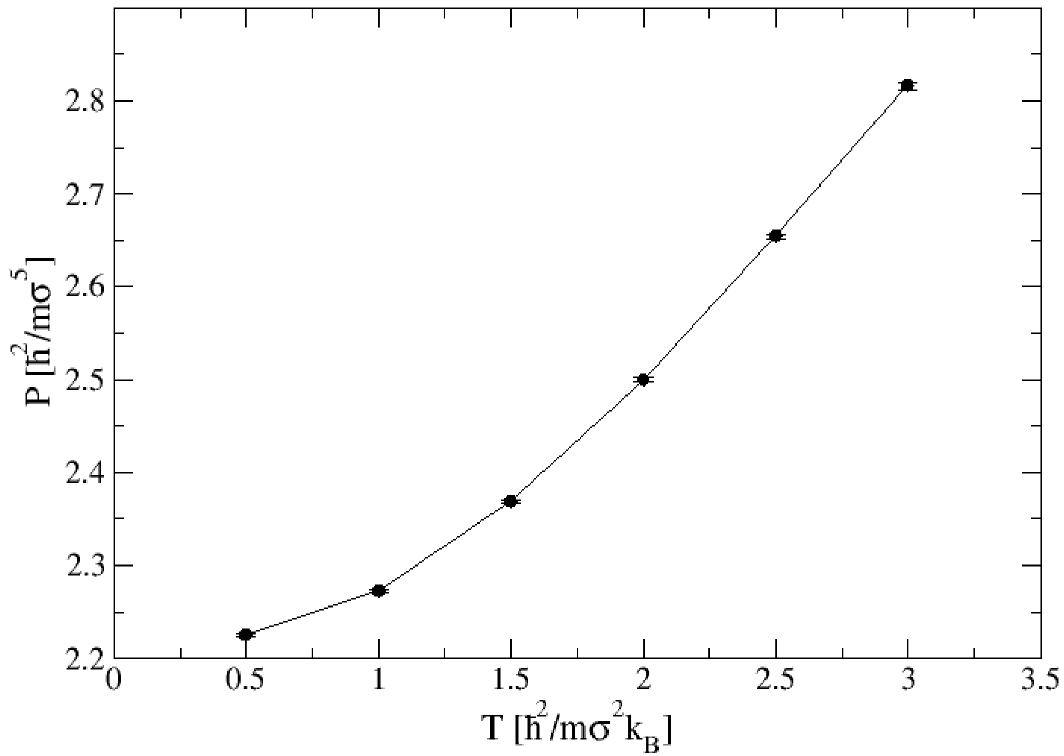


$n(\sigma^3)^{-1} = 0.2063$

Many Particle System

- Pressure at converged 'M' and thermodynamic limit at varying T

- Find linear dependence at higher temperatures

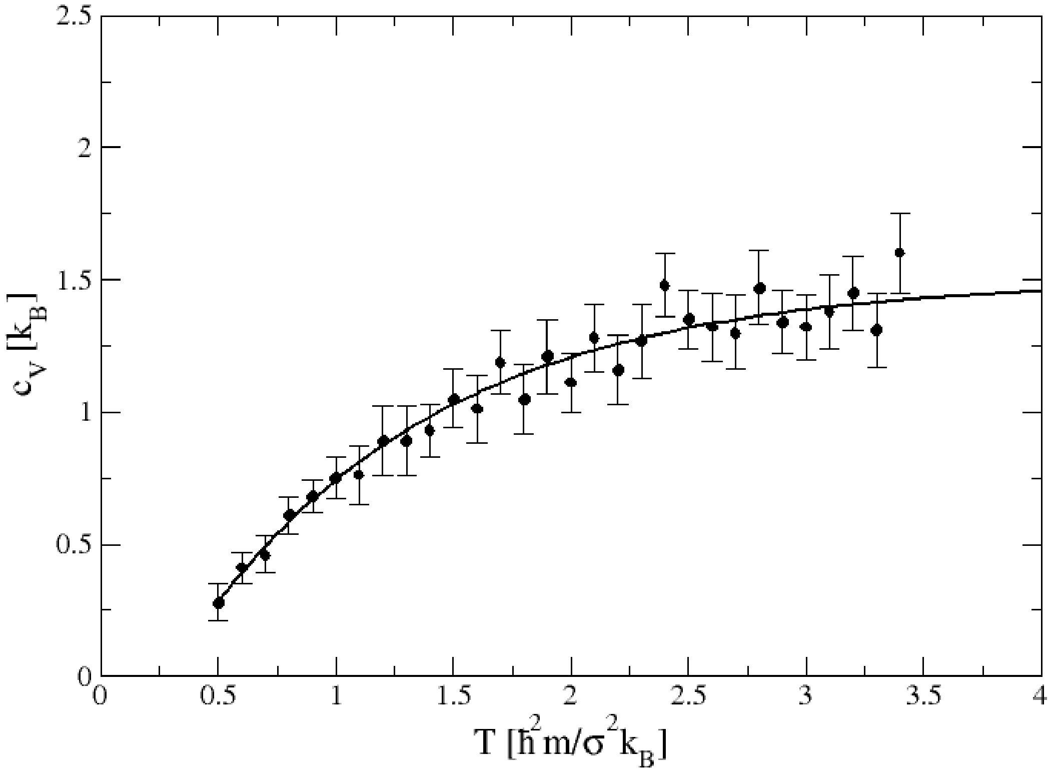


$n(\sigma^3)^{-1} = 0.2063$

Many Particle System

- Specific heat at converged 'M' and thermodynamic limit at varying T

- At higher T find expected result given by equipartition theorem



$n(\sigma^3)^{-1} = 0.2063$

Summary

- Carried out calculations for system of distinguishable hard spheres, 'Boltzmannons'
- For the two-body problem we found no difference between IA and CB density matrices
- For the larger system we found thermodynamic limit at the N=400 range
- Found expected behaviour at higher T, with quantum effects taking over at lower T

Thank-you

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