Quantum Monte Carlo applied to ultracold atomic gases

Jordi Boronat

Departament de Física
Universitat Politècnica de Catalunya
E-08034 Barcelona, Spain
jordi.boronat@upc.edu

Workshop and School on "Frontiers in ultracold quantum gases", Maó, June 2026

Outline

- N-body quantum systems: ground issues
- Basics on the Monte Carlo method
- Variational and Diffusion Monte Carlo
- The sign problem: Fermi systems
- Application of DMC to Fermi systems: BEC-BCS crossover
- Finite temperatures: PIMC
- Application of PIMC to dipolar gases: BKT phase transition
- Remarks

N-body Problem

- Always difficult $\ldots 3N$ degrees of freedom

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+ Quantum Mechanics

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N-body Problem
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- Classical: Molecular Dynamics, Monte Carlo
- Much more difficult: Schrödinger equation
- Quantum Monte Carlo:

  $\Longrightarrow$ Variational Monte Carlo (VMC)

  $\Longrightarrow$ Green's Function Monte Carlo (GFMC)

  $\Longrightarrow$ Diffusion Monte Carlo (DMC)

  $\Longrightarrow$ Path Integral Monte Carlo (PIMC)
- Focus only at zero temperature: VMC, DMC, PIGS

J. B., in *Microscopic Approaches to Quantum Liquids in Confined Geometries*, ed. by E. Krotscheck and J. Navarro (World Scientific, Singapore, 2002)

Variational Approach

- As we cannot solve the quantum N-body problem we have to rely on approximate methods

- Usual perturbative approach is problematic and normally unuseful due to strong atomic repulsion at short distances

- Variational theory has been more successful because it is better for hard-core-like interactions

- A perturbative approach based on correlated basis (CBF) was developed many years ago to deal with strongly correlated systems (Feenberg, Clark, Campbell, Krotscheck,...)

Variational Approach

- Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_{i}^{N} \boldsymbol{\nabla}_i^2 + \sum_{i<j}^{N} V(r_{ij})$$

- Variational Principle

$$E_{\rm v} = \frac{\langle \psi_{\rm T}(\boldsymbol{R})|H|\psi_{\rm T}(\boldsymbol{R})\rangle}{\langle \psi_{\rm T}(\boldsymbol{R})|\psi_{\rm T}(\boldsymbol{R})\rangle} \geq E_0$$

- Trial wave function of Jastrow-Slater type

$$\boxed{\psi_{\rm T}(\boldsymbol{R}) = F(\boldsymbol{R})\,\Phi(\boldsymbol{R})}$$

- Correlation factor

$$F(\boldsymbol{R}) = \prod_i \phi(\boldsymbol{r}_i) \prod_{i<j} f^{(2)}(r_{ij}) \prod_{i<j<k} f^{(3)}(r_{ij}, r_{ik}, r_{jk})$$

Variational Approach

- Free-system wave function

$$\text{Bosons} \Longrightarrow \Phi(\boldsymbol{R}) = 1$$

$$\text{Fermions} \Longrightarrow \Phi(\boldsymbol{R}) = \text{Det}|\varphi_i(r_j)|$$

- It is useful to introduce the n-particle distribution functions

$$P^{(n)}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) = \frac{N!}{(N-n)!} \frac{\int d\boldsymbol{r}_{n+1} \ldots \boldsymbol{r}_N |\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)|^2}{\int d\boldsymbol{r}_1 \ldots \boldsymbol{r}_N |\Psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)|^2}$$

- Cluster property: if particles $1, \ldots, i$ are far from the rest, $i+1, \ldots, n$ then

$$P^{(n)}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_n) \longrightarrow P^{(i)}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_i) P^{(n-i)}(\boldsymbol{r}_{i+1}, \ldots, \boldsymbol{r}_n)$$

Variational Approach

- There are not exact methods to estimate the variational energy for N particles

- Alternative: to perform the multidimensional integral in a stochastic form

$$E_{\mathrm{v}} = \int d\boldsymbol{R}\; E_{\mathrm{L}}(\boldsymbol{R}) p(\boldsymbol{R})$$

with a local energy

$$E_{\mathrm{L}}(\boldsymbol{R}) = \frac{1}{\psi_{\mathrm{T}}(\boldsymbol{R})} H\, \psi_{\mathrm{T}}(\boldsymbol{R})$$

and probability density distribution

$$p(\boldsymbol{R}) = \frac{|\psi_{\mathrm{T}}(\boldsymbol{R})|^2}{\int d\boldsymbol{R} |\psi_{\mathrm{T}}(\boldsymbol{R})|^2}$$

VMC . . .

A schematic algorithm for a Metropolis move in a continuous system is the following:

→ Initial state 0: $\mathbf{R}_i^0 \;\; (i = 1, \ldots, N)$

→ Proposed movement: $\mathbf{R}_i^{\rm f} = \mathbf{R}_i^0 + (2. * {\rm ran}() - 1.) * \boldsymbol{\Delta}$

→ Metropolis: if $(|\psi(\mathbf{R}_i^{\rm f})|^2 / |\psi(\mathbf{R}_i^0)|^2) > {\rm ran}()$ then $\mathbf{R}_i^0 = \mathbf{R}_i^{\rm f}$

→ Sampling properties: energy, distribution functions, etc.

→ Next step

Diffusion Monte Carlo (DMC)

Starting point: Schrödinger equation for N particles in imaginary time

$$-\frac{\partial\Psi(\boldsymbol{R},t)}{\partial t} = (H-E)\Psi(\boldsymbol{R},t)$$

WALKER $\longrightarrow \boldsymbol{R} = (\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$

Expanding $\Psi(\boldsymbol{R},t)$,

$$\Psi(\boldsymbol{R},t) = \sum_n c_n \exp[-(E_n - E)t]\,\Phi_n(\boldsymbol{R})$$

with

$$H\,\Phi_n(\boldsymbol{R}) = E_n\,\Phi_n(\boldsymbol{R})$$

When $t \to \infty \Longrightarrow \Phi_0(\boldsymbol{R})$: GROUND STATE

DMC . . .

To decrease the variance: Importance Sampling

$$f(\boldsymbol{R},t) = \psi_{\mathrm{T}}(\boldsymbol{R})\Psi(\boldsymbol{R},t)$$

DMC . . .

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$$f(\boldsymbol{R},t) = \psi_{\mathrm{T}}(\boldsymbol{R})\Psi(\boldsymbol{R},t)$$

Schrödinger equation for $f(\mathbf{R},t)$

$$-\frac{\partial f(\boldsymbol{R},t)}{\partial t} = -D\boldsymbol{\nabla}^2_R f(\boldsymbol{R},t) + D\boldsymbol{\nabla}_R(\boldsymbol{F}(\boldsymbol{R})f(\boldsymbol{R},t))$$

$$+ (E_{\mathrm{L}}(\boldsymbol{R}) - E)f(\boldsymbol{R},t)$$

DMC . . .

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$$+ (E_{\rm L}(\boldsymbol{R}) - E)f(\boldsymbol{R},t)$$

A_1: Free term: isotropic diffusion with constant

$$D = \frac{\hbar^2}{2m}$$

DMC ...

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Schrödinger equation for $f(\mathbf{R},t)$

$$-\frac{\partial f(\boldsymbol{R},t)}{\partial t} = -D\boldsymbol{\nabla}^2_R f(\boldsymbol{R},t) + \boxed{D\boldsymbol{\nabla}_R(\boldsymbol{F}(\boldsymbol{R})f(\boldsymbol{R},t))} + (E_{\mathrm{L}}(\boldsymbol{R}) - E)f(\boldsymbol{R},t)$$

A_2: Drift term under the drift or quantum force (*velocity*)

$$\boldsymbol{F}(\boldsymbol{R}) = 2\,\psi_{\mathrm{T}}(\boldsymbol{R})^{-1}\boldsymbol{\nabla}_R\psi_{\mathrm{T}}(\boldsymbol{R})$$

DMC . . .

To decrease the variance: Importance Sampling

$$f(\boldsymbol{R},t) = \psi_{\mathrm{T}}(\boldsymbol{R})\Psi(\boldsymbol{R},t)$$

Schrödinger equation for $f(\mathbf{R},t)$

$$\begin{aligned} -\frac{\partial f(\boldsymbol{R},t)}{\partial t} \quad = \quad & -D\boldsymbol{\nabla}^2_R f(\boldsymbol{R},t) \;+\; D\boldsymbol{\nabla}_R(\boldsymbol{F}(\boldsymbol{R})f(\boldsymbol{R},t)) \\ & + \boxed{(E_{\mathrm{L}}(\boldsymbol{R}) - E)f(\boldsymbol{R},t)} \end{aligned}$$

A_3: Branching term according to the local energy

$$E_{\mathrm{L}}(\boldsymbol{R}) = \psi_{\mathrm{T}}(\boldsymbol{R})^{-1}\, H\, \psi_{\mathrm{T}}(\boldsymbol{R})$$

DMC . . .

In a compact form,

$$-\frac{\partial f(\boldsymbol{R},t)}{\partial t} \equiv (A_1 + A_2 + A_3) f(\boldsymbol{R},t) \equiv A f(\boldsymbol{R},t)$$

Formal solution,

$$\boxed{f(\boldsymbol{R}',t+\Delta t) = \int d\boldsymbol{R}\, G(\boldsymbol{R}',\boldsymbol{R},\Delta t)\, f(\boldsymbol{R},t)}$$

with the Green's function

$$G(\boldsymbol{R}',\boldsymbol{R},\Delta t) = \langle \boldsymbol{R}' \,|\, \exp(-A\Delta t) \,|\, \boldsymbol{R} \rangle$$

DMC relies on

- A short–time approximation for $G(\boldsymbol{R}',\boldsymbol{R},\Delta t)$
- Iteration of the integral equation to obtain $f(\boldsymbol{R},t \to \infty)$

DMC . . .

- The total Green function G is split into the product of individual Green functions G_i, each one associated to the single operator A_i.
- G_1 is the Green function corresponding to the free diffusion term (A_1),

$$G_1(\mathbf{R}', \mathbf{R}, t) = (4\pi D t)^{-\frac{3N}{2}} \exp\left[-\frac{(\mathbf{R}' - \mathbf{R})^2}{4Dt}\right] \ .$$

- In the MC simulation, the evolution given by G_1 corresponds to an isotropic gaussian movement of size proportional to $\sqrt{Dt}$.
- The sampling of Gaussian variables can be made with the Box-Muller method.

DMC . . .

- The Green function G_2 describes the movement due to the drift force appearing in A_2; its form is given by

$$G_2(\mathbf{R}',\mathbf{R},t) = \delta\left(\mathbf{R}' - \mathbf{R}(t)\right), \quad \text{where} \begin{cases} \mathbf{R}(0) = \mathbf{R} \\ \dfrac{d\mathbf{R}(t)}{dt} = D\,\mathbf{F}(\mathbf{R}(t)), \end{cases} .$$

- Under the action of G_2, the walkers evolve in a deterministic way according to the drift force $\mathbf{F}(\mathbf{R}(t))$.
- To preserve the second-order accuracy in the time step, the differential equation must also be solved with a second-order integration method.

DMC . . .

- G_3 has an exponential form, with an argument that depends on the difference between the local energy of a given walker and the prefixed value E,

$$G_3(\mathbf{R}', \mathbf{R}, t) = \exp\left[-(E_L(\mathbf{R}) - E)\, t\right]\, \delta(\mathbf{R}' - \mathbf{R}).$$

- This third term, which is called the branching factor, assigns a weight to each walker according to its local energy.
- Depending on the value of this weight the walker is replicated or eliminated in the population list.
- The branching mechanism is a key ingredient in DMC. If it is eliminated, one recovers VMC.

Fermions & DMC: . . . harder

The famous sign problem in MC has not been solved for a many-fermion system yet. However, one can somehow overcome the problem using the methods developed so far . . .

FIXED NODE (FN)

◆ The wave function can be considered a probability density only if

$$f(\boldsymbol{R},t) = \psi(\boldsymbol{R})\ \Psi(\boldsymbol{R},t) \geq 0$$

Then

$$f(\boldsymbol{R},t \to \infty) = \psi(\boldsymbol{R})\ \Phi^{\rm FN}(\boldsymbol{R})$$

◆ Nodal restriction $\Longrightarrow$ Variational upper bound to the exact eigenvalue (quality $\rightsquigarrow$ ψ)

◆ The quality of the nodal surface can be improved by changing the orbitals in the Slater determinant (backflow correlations)

Dilute Fermi gases: BEC-BCS crossover

- Easy manipulation of the interaction strength (two-body scattering amplitude) in dilute Fermi gases allows for crossing a Feshbach resonance.
- When a is negative (no bound state) the system is in the BCS side.
- In the resonance, $|a| \to \infty$. One enters a new strongly correlated regime known as unitary limit.
- In the unitary limit, the relevant energy scale is the one of the free Fermi gas

$$\frac{E}{N} = \xi \frac{3}{10} \frac{\hbar^2 k_F^2}{m}$$

- When $a > 0$, one deals with the BEC side where stable molecules (bosons) are formed.

Dilute Fermi gases: BEC-BCS crossover

- Hamiltonian

$$H = -\frac{\hbar^2}{2m}\left(\sum_{i=1}^{N_\uparrow}\nabla_i^2 + \sum_{i'=1}^{N_\downarrow}\nabla_{i'}^2\right) + \sum_{i,i'} V(r_{ii'})$$

with $V(r)$ an attractive square-well potential of depth $-V_0$ and range $nR_0^3 = 10^{-6}$ much smaller than interparticle distance.

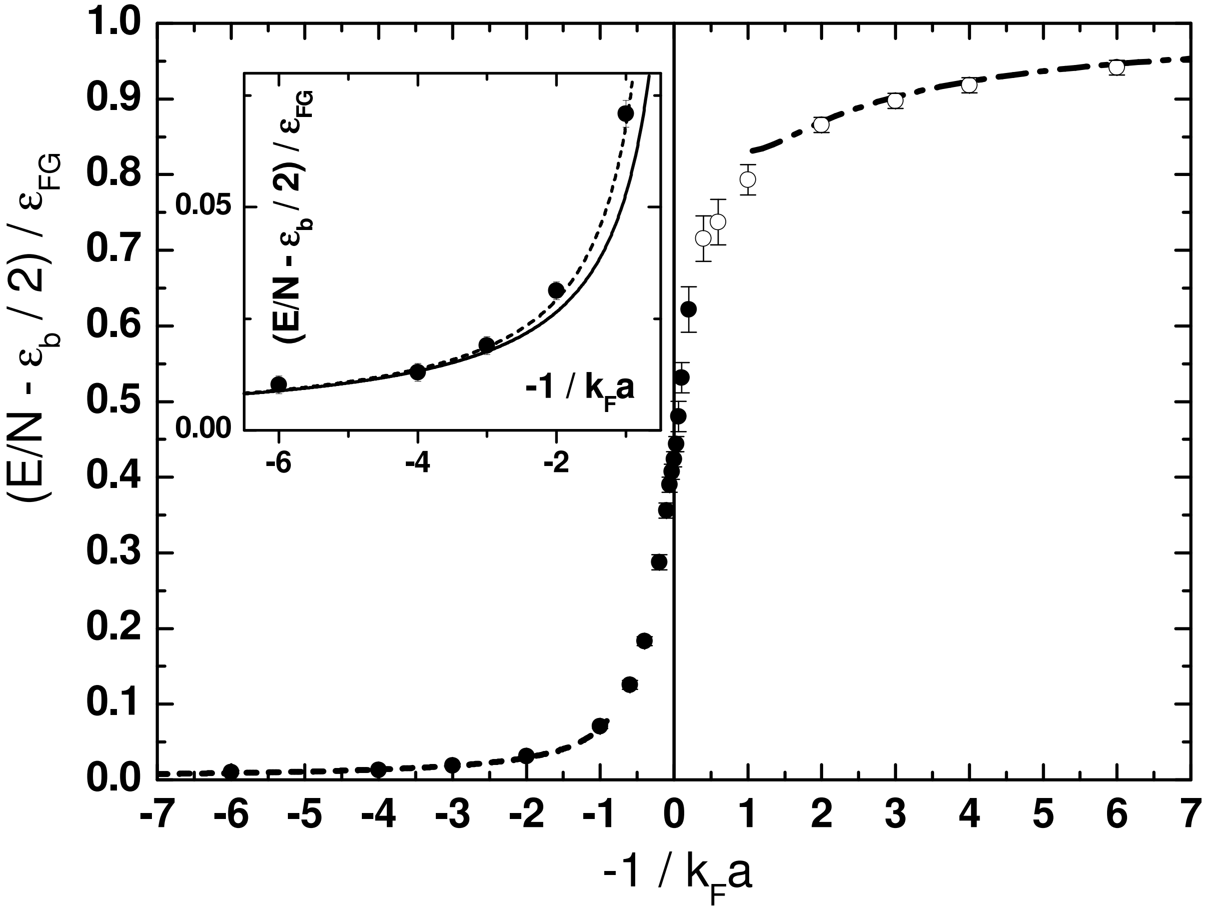
- Two models for the wave functions:

$$\psi_{JS}(\mathbf{R}) = \prod_{i,i'} \varphi(r_{ii'}) \left[\mathcal{A}\prod_{i,\alpha} e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_i}\right]\left[\mathcal{A}\prod_{i',\alpha} e^{i\mathbf{k}_\alpha\cdot\mathbf{r}_{i'}}\right]$$

$$\psi_{BCS}(\mathbf{R}) = \mathcal{A}\left(\phi(r_{11'})\phi(r_{22'})\ldots\phi(r_{N_\uparrow N_\downarrow})\right)$$

with $\phi(r)$ the two-body zero-energy wave function.

Dilute Fermi gases: BEC-BCS crossover



G. E. Astrakharchik, J. B., J. Casulleras, S. Giorgini, Phys. Rev. Lett **93**, 200404 (2004)

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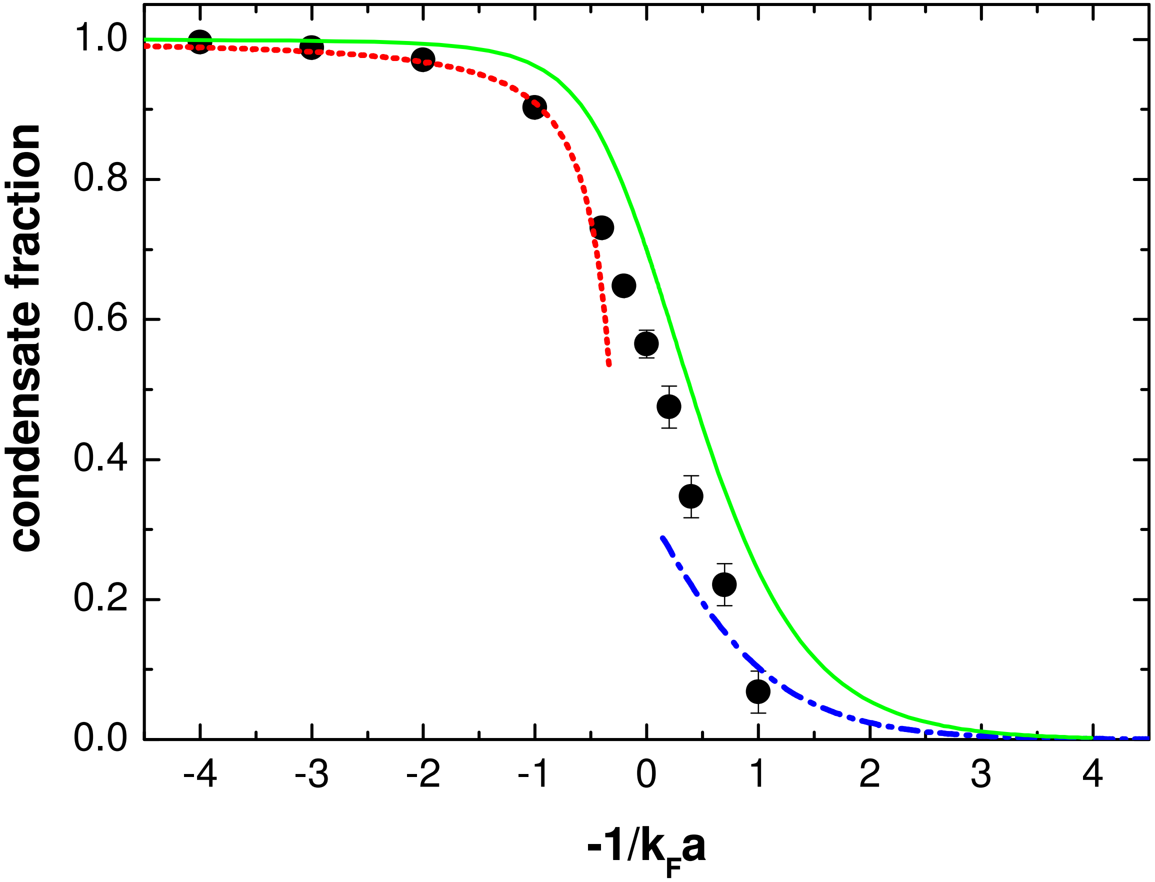

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Quantum many-body theory at $\mathrm{T} > 0$

- At $T = 0$, several options: perturbative series, variational method, integral equations (HNC), . . .
- Also Monte Carlo: VMC; GFMC and DMC $\Longrightarrow$ Exact results for bosons and probably the best ones for fermions
- For $T > 0$, the problem becomes more difficult and the number of possible approaches reduces
- Monte Carlo + Path Integral (Feynman) (PIMC) has proven to be one of the best options . . . if not the only reliable one for correlated systems

Density matrix in Statistical Mechanics

- Thermal density matrix: $\hat{\rho} = e^{-\beta \hat{H}}$, with $\hat{H}$ the Hamiltonian of the system and $\beta = 1/T$
- The expectation value of any operator $\mathcal{O}$ is

$$\langle \mathcal{O} \rangle = Z^{-1} \sum_i \langle \phi_i | \mathcal{O} | \phi_i \rangle e^{-\beta E_i}$$

with $Z = \sum_i e^{-\beta E_i}$ the partition function

- Projecting to the coordinate space,

$$\langle \mathcal{O} \rangle = Z^{-1} \int d\mathbf{R} d\mathbf{R}' \; \rho(\mathbf{R}, \mathbf{R}'; \beta) \langle \mathbf{R} | \mathcal{O} | \mathbf{R}' \rangle$$

with

$$\rho(\mathbf{R}, \mathbf{R}'; \beta) = \sum_i e^{-\beta E_i} \phi_i^\star(\mathbf{R}) \phi_i(\mathbf{R}')$$

Convolution property of the density matrix

- The density matrix can always be decomposed as

$$\rho(\mathbf{R}_1, \mathbf{R}_2; \beta) = \int d\mathbf{R}_3 \; \rho(\mathbf{R}_1, \mathbf{R}_3; \beta/2)\rho(\mathbf{R}_3, \mathbf{R}_2; \beta/2)$$

Important: We get information at a temperature $T = 1/\beta$ from knowledge at a temperature twice larger $T = 2/\beta$.

- By iterating M times,

$$\boxed{\rho(\mathbf{R}_0, \mathbf{R}_M; \beta) = \int d\mathbf{R}_1 \ldots d\mathbf{R}_{M-1} \; \rho(\mathbf{R}_0, \mathbf{R}_1; \epsilon) \ldots \rho(\mathbf{R}_{M-1}, \mathbf{R}_M; \epsilon)}$$

with $\epsilon = \beta/M$

Trotter formula

- Exact result for $\rho(\mathbf{R},\mathbf{R}';\beta)$ would require to know the full spectrum of H: impossible in practice

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- Consider $\hat{H}=\hat{K}+\hat{V}$. Using the Baker-Campbell-Hausdorff formula,

$$e^{-\epsilon\hat{K}}e^{-\epsilon\hat{V}}=e^{-\epsilon(\hat{K}+\hat{V})}e^{\epsilon^2 C_2-\epsilon^3 C_3+\ldots}$$

with $C_2=\frac{1}{2}[\hat{K},\hat{V}]$ and $C_3=\frac{1}{12}[\hat{K}-\hat{V},[\hat{K},\hat{V}]]$

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- When $M\to\infty$, $\epsilon=\beta/M\to 0$, the linear term dominates $\Longrightarrow$ Trotter Formula

$$\boxed{e^{-\beta\hat{H}}=\lim_{M\to\infty}\left(e^{-\beta\hat{K}/M}e^{-\beta\hat{V}/M}\right)^M}$$

Primitive Approximation

◆ In a first approximation (Primitive Approximation (PA)), terms of order ϵ^2 and higher are neglected

$$e^{-\epsilon(\hat{K}+\hat{V})} = e^{-\epsilon\hat{K}} e^{-\epsilon\hat{V}}$$

◆ Kinetic and potential terms are easily evaluated

$$\langle \mathbf{R} | e^{-\epsilon(\hat{K}+\hat{V})} | \mathbf{R}' \rangle = \int d\mathbf{R}'' \langle \mathbf{R} | e^{-\epsilon\hat{K}} | \mathbf{R}'' \rangle \langle \mathbf{R}'' | e^{-\epsilon\hat{V}} | \mathbf{R}' \rangle$$

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Primitive Approximation

- The partition function is ($\mathbf{R} \equiv \{\mathbf{r}_1, \ldots, \mathbf{r}_N\}$)

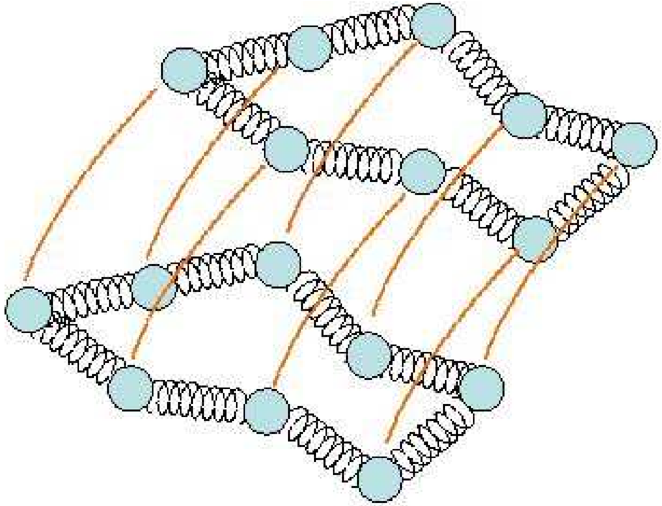
$$Z = \int d\mathbf{R}_1 \ldots d\mathbf{R}_M \prod_{\alpha=1}^{M} \rho_{\mathsf{PA}}(\mathbf{R}_\alpha, \mathbf{R}_{\alpha+1}) \quad \text{with} \quad \mathbf{R}_{M+1} = \mathbf{R}_1$$

- Introducing explicitly the kinetic and potential terms

$$\rho_{\mathsf{PA}}(\mathbf{R}_\alpha, \mathbf{R}_{\alpha+1}) =$$

$$\left(\frac{Mm}{2\pi\beta\hbar^2}\right)^{3N/2} \exp\left\{ -\sum_{i=1}^{N} \frac{Mm}{2\beta\hbar^2} (\mathbf{r}_{\alpha,i} - \mathbf{r}_{\alpha+1,i})^2 - \frac{\beta}{M} \sum_{i<j}^{N} V(r_{\alpha,ij}) \right\}$$

Mapping the quantum problem to a classical one

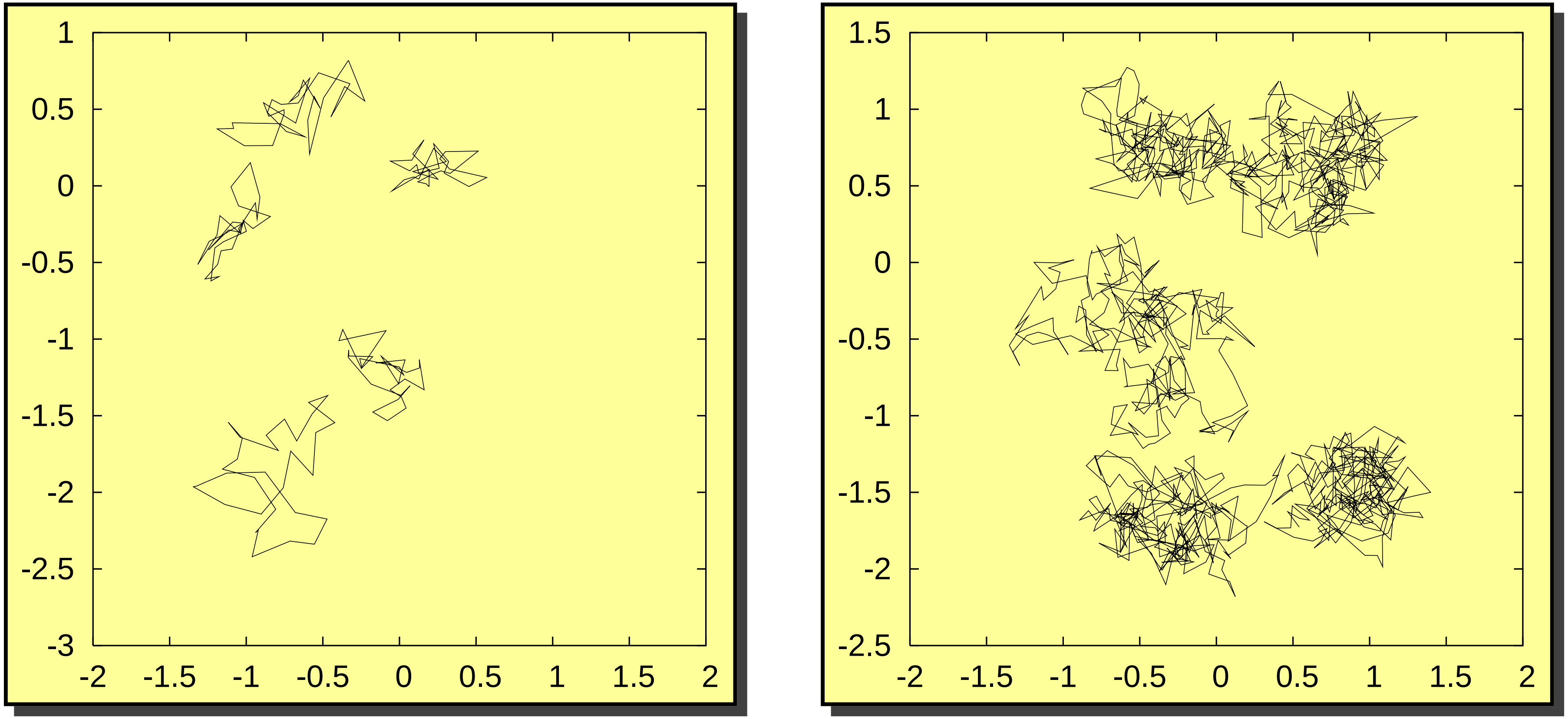


The quantum problem can be mapped to a classical problem of polymers (Chandler & Wolynes (1981))

- Every *quantum* particle is described as a polymer with a number of beads which increases when the temperature T decreases
- Every bead interacts with all the beads having the same index through $V(r)$; harmonic coupling between successive beads of a given particle

$$\exp\left[-\frac{Mm}{2\beta\hbar^2}(\mathbf{r}_{\alpha,i}-\mathbf{r}_{\alpha+1,i})^2\right]$$

Mapping the quantum problem to a classical one



5 H_2 molecules

with 32 beads at $T = 6$ K

5 H_2 molecules

with 256 beads at $T = 1$ K

Sampling in PIMC

- Simplest method: bead a bead + movement of the center of mass of the polymer
- But . . . slowing down problems for long chains
- Smart collective movements are necessary to eliminate the slowing down in the sampling
- We use the *staging* method, which allows for an exact sampling of the free action (harmonic bead-bead couplings)

$$\rho_0(x_i, x_{i+1}; \epsilon) \ldots \rho_0(x_{i+j-1}, x_{i+j}; \epsilon) =$$

$$\left(\frac{m}{2\pi\hbar^2 j\epsilon}\right)^{1/2} \exp\left[-\frac{m}{2\hbar^2 j\epsilon}(x_i - x_{i+j})^2\right]$$

$$\times \prod_{k=0}^{j-2} \left(\frac{m_k}{2\pi\hbar^2\epsilon}\right)^{1/2} \exp\left[-\frac{m_k}{2\hbar^2\epsilon}(x_{i+k+1} - x^\star_{i+k+1})^2\right]$$

Symmetrization: sampling of permutations

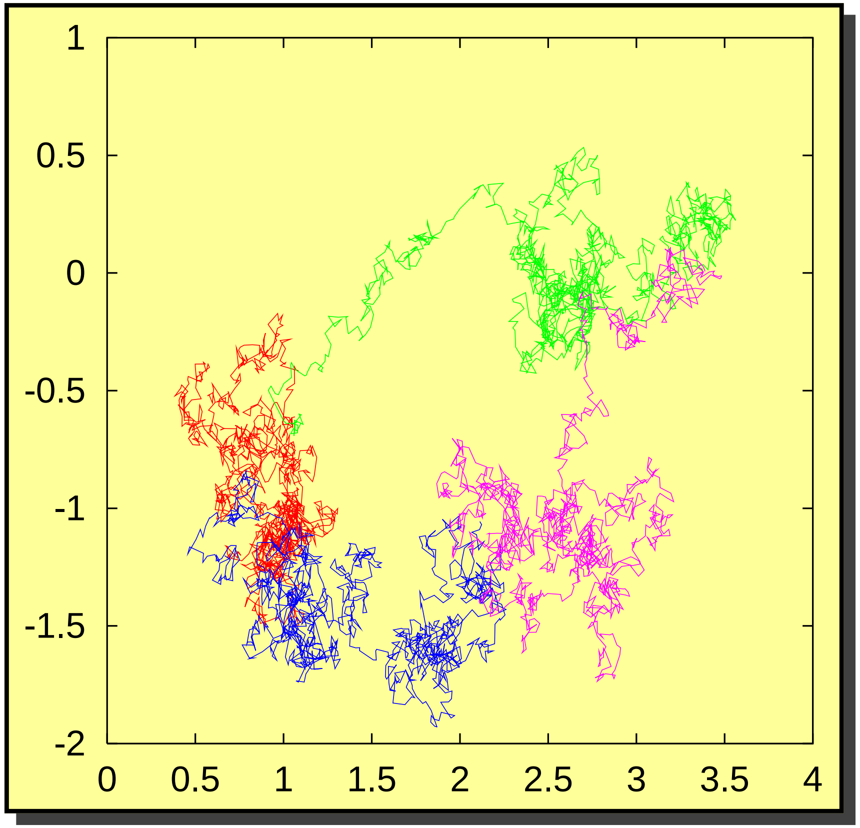
- At very low temperatures $T \simeq T_c$ it is necessary to introduce the correct quantum statistics

- For bosons the action must be symmetric

$$\rho_{\rm B}(\mathbf{R}_0,\mathbf{R}_1;\beta) = \frac{1}{N!}\sum_P \rho(\mathbf{R}_0,P\mathbf{R}_1;\beta)$$

- Sampling permutations produces longer polymeric chains with more than one particle:

SUPERFLUIDITY



Worm Algorithm

- Proposed for Prokof'ev, Boninsegni and Svistunov for PIMC in the grand canonical ensemble.
- The WA works in an extended configuration space, with two sectors:

  ⇒ Z-sector: standard PIMC space of closed polymers (*diagonal*)

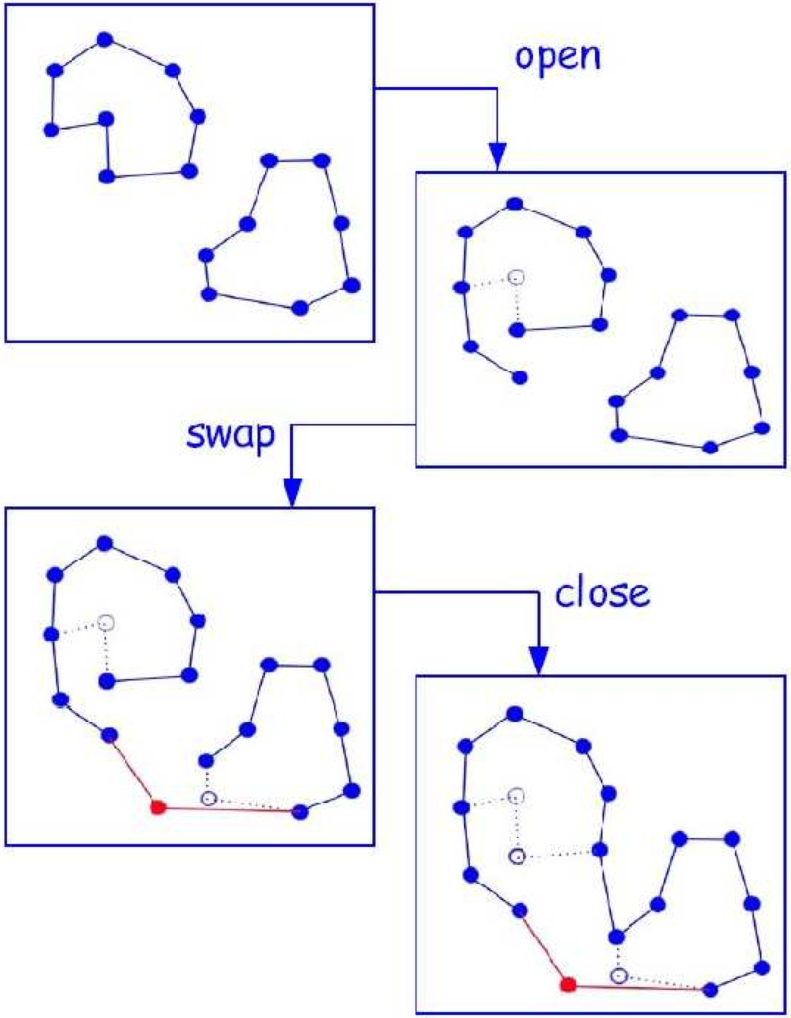
  ⇒ G-sector: All the polymers are closed except one, the worm (*non diagonal*).
- The generalized partition function is

$$Z_W = Z + C Z_G$$

with $C > 0$ a dimensionless parameter fixed for all the simulation.

- C controls the relative statistics of both sectors.

Worm Algorithm



- Key ingredient: An open chain (*worm*) is introduced in the simulation.
- By the swap operation, long permutations are achieved.
- Specially useful for the estimation of the superfluid density and the one-body density matrix.

High-order actions

We chose the $(t_0,\ a_1)$ Chin expansion due to its large flexibility (S. A. Chin and C. R. Chen, J. Chem. Phys. **117**, 1409 (2002)); exact ϵ^6 order for the harmonic oscillator

$$\boxed{e^{-\epsilon\hat{H}} \simeq e^{-v_1\epsilon\hat{W}_{a_1}} e^{-t_1\epsilon\hat{T}} e^{-v_2\epsilon\hat{W}_{1-2a_1}} e^{-t_1\epsilon\hat{T}} e^{-v_1\epsilon\hat{W}_{a_1}} e^{-2t_0\epsilon\hat{T}}}$$

with

$$\begin{aligned} \hat{W}_{a_1} &= \hat{V} + (u_0/v_1)a_1\epsilon^2\,\hat{W} \qquad (0 \le a_1 \le 1) \\ \hat{W}_{1-2a_1} &= \hat{V} + (u_0/v_2)(1-2a_1)\epsilon^2\,\hat{W} \end{aligned}$$

and parameters

$$v_1 = \frac{1}{6(1-2t_0)^2} \qquad t_1 = \frac{1}{2} - t_0 \quad \left(0 \le t_0 \le \frac{1}{2}\left(1 - \frac{1}{\sqrt{3}}\right)\right)$$

$$v_2 = 1 - 2v_1 \qquad u_0 = \frac{1}{12}\left[1 - \frac{1}{1-2t_0} + \frac{1}{6(1-2t_0)^3}\right]$$

High-order actions

Explicitly,

$$\rho_{\text{T0A1}}(\mathbf{R}_\alpha, \mathbf{R}_{\alpha+\mathbf{1}}) =$$

$$\left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{9N/2} \left(\frac{1}{2t_1^2 t_0}\right)^{3N/2} \int d\mathbf{R}_{\alpha A} d\mathbf{R}_{\alpha B} \;\; \exp\left\{ - \frac{m}{2\hbar^2\epsilon} \right.$$

$$\times \sum_{i=1}^{N} \left[\frac{1}{t_1}(\mathbf{r}_{\alpha,i} - \mathbf{r}_{\alpha A,i})^2 + \frac{1}{t_1}(\mathbf{r}_{\alpha A,i} - \mathbf{r}_{\alpha B,i})^2 + \frac{1}{2t_0}(\mathbf{r}_{\alpha B,i} - \mathbf{r}_{\alpha+1,i})^2 \right]$$

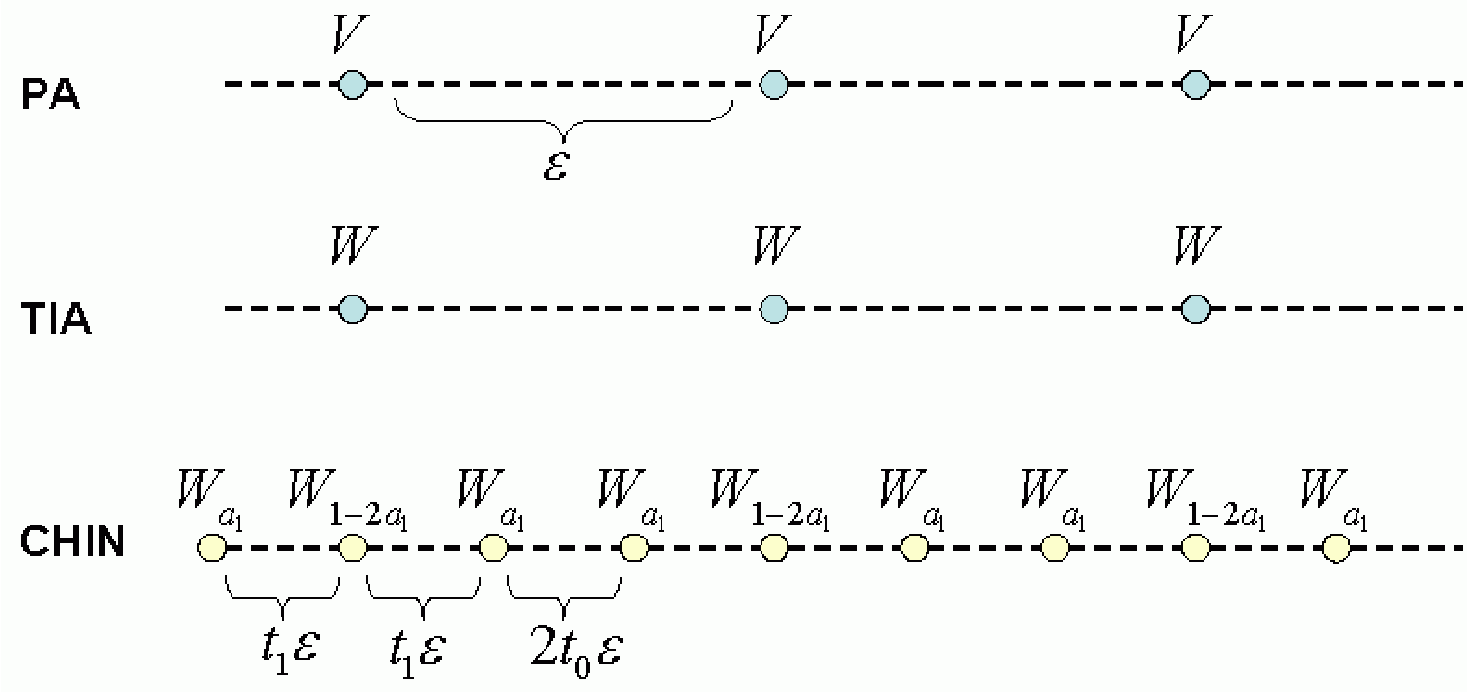
$$-\epsilon \sum_{i<j}^{N} (v_1 V(r_{\alpha,ij}) + v_2 V(r_{\alpha A,ij}) + v_1 V(r_{\alpha B,ij}))$$

$$\left. -\epsilon^3 u_0 \frac{\hbar^2}{m} \sum_{i=1}^{N} (a_1 |\mathbf{F}_{\alpha,i}|^2 + (1-2a_1)|\mathbf{F}_{\alpha A,i}|^2 + a_1 |\mathbf{F}_{\alpha B,i}|^2) \right\}$$

K. Sakkos, J. Casulleras, and J. B., JCP **130**, 204109 (2009)

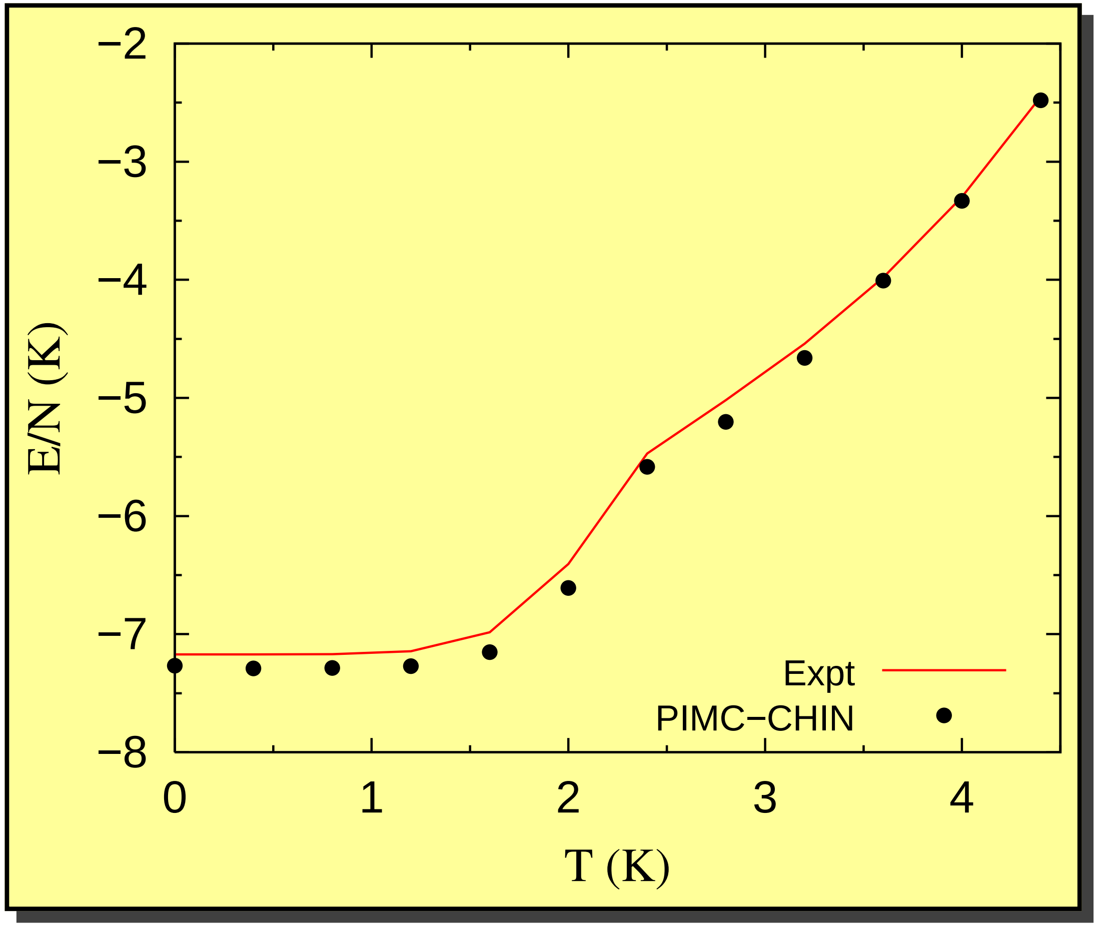
High-order actions

Schematically,



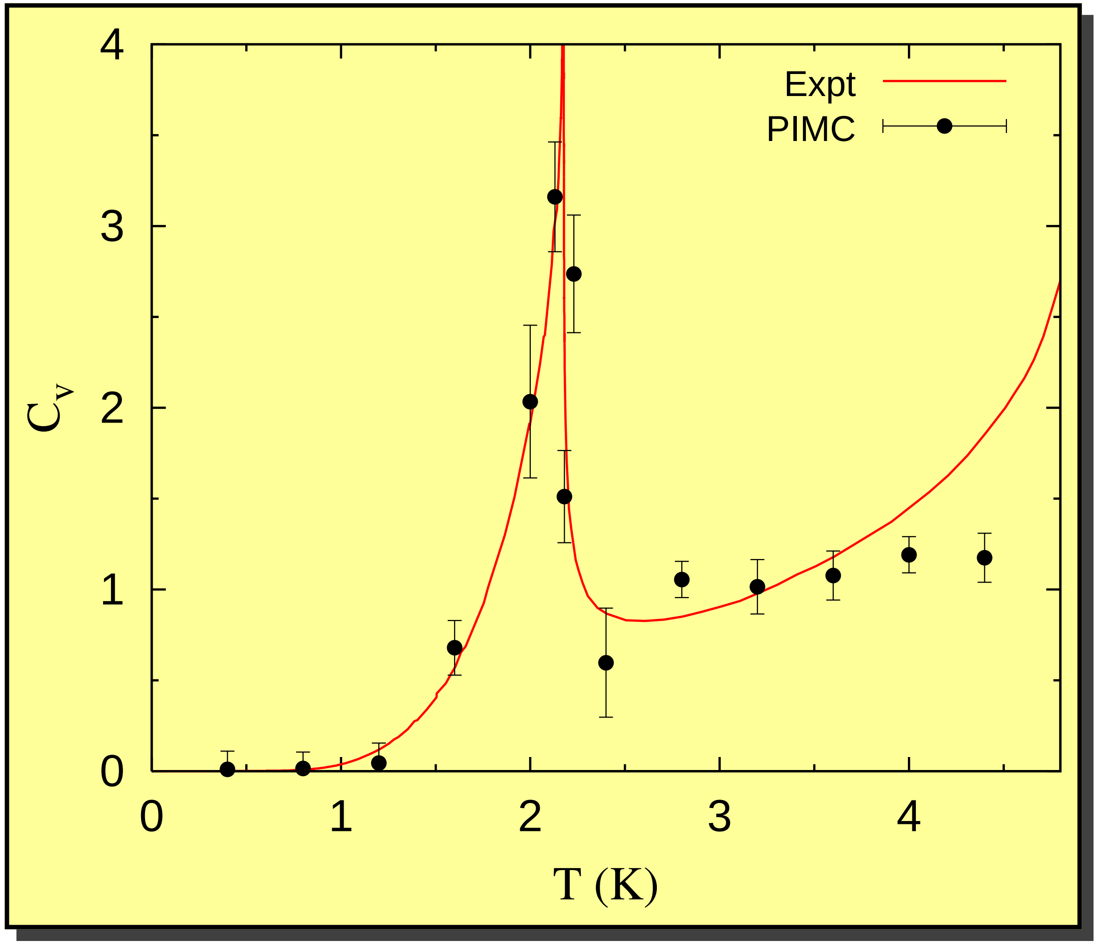
$$\boxed{e^{-\epsilon \hat{H}} \simeq e^{-v_1 \epsilon \hat{W}_{a_1}} e^{-t_1 \epsilon \hat{T}} e^{-v_2 \epsilon \hat{W}_{1-2a_1}} e^{-t_1 \epsilon \hat{T}} e^{-v_1 \epsilon \hat{W}_{a_1}} e^{-2t_0 \epsilon \hat{T}}}$$

Results for bulk ^{4}He



Energy as a function of temperature, crossing T_λ

Results for bulk ^{4}He



Specific heat close to T_λ

Example of ultracold gases: stripe phase

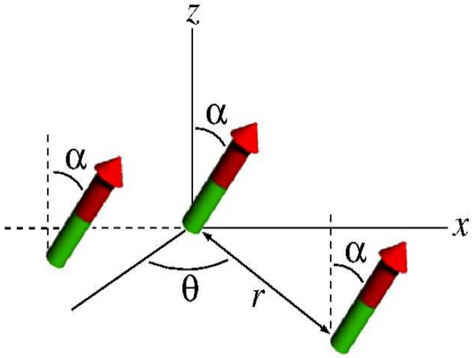
- We studied quantum dipoles in a plane with variable polarization direction
- Hamiltonian

$$H = -\frac{\hbar^2}{2m}\sum_j \nabla_j^2 + \sum_{i<j} V_{dd}(\mathbf{r}_{ij})$$

- Dipole-dipole potential

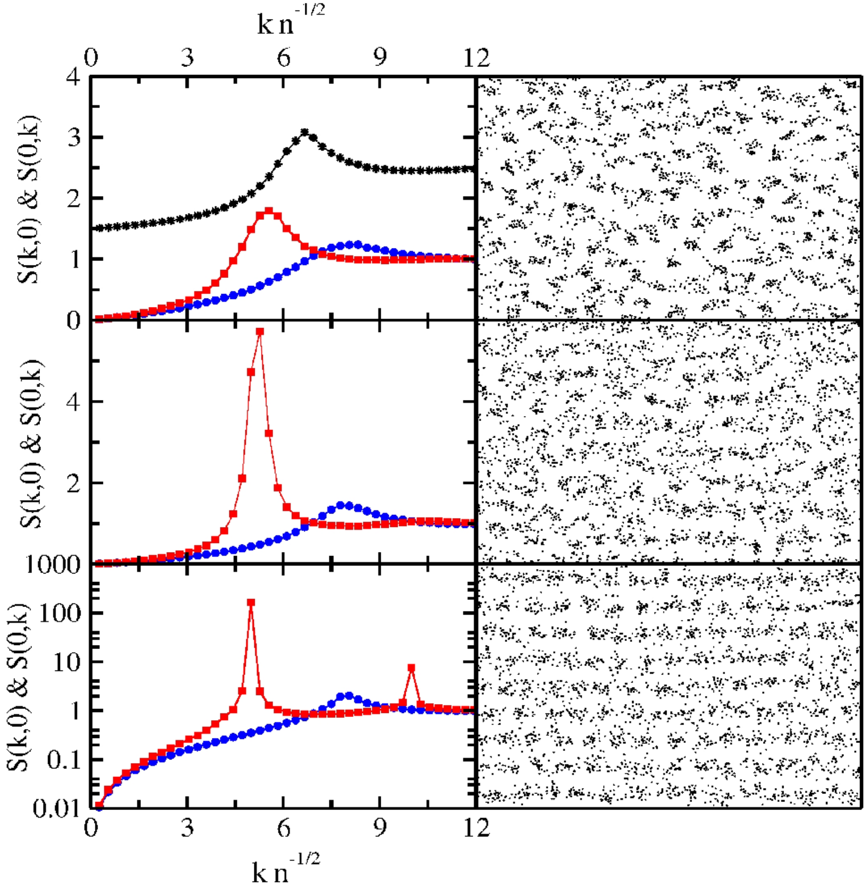
$$V_{dd}(\mathbf{r}) = \frac{C_{dd}}{4\pi}\left[\frac{\hat{\mathbf{p}}_1\cdot\hat{\mathbf{p}}_2 - 3(\hat{\mathbf{p}}_1\cdot\hat{\mathbf{r}})(\hat{\mathbf{p}}_2\cdot\hat{\mathbf{r}})}{r^3}\right] = \frac{C_{dd}}{4\pi}\frac{1-3\lambda^2\cos^2\theta}{r^3}$$

with $\lambda = \sin\alpha$



Stripe phase

When the density increases and the critical angle is approached, one observes a stripe phase due to the anisotropic interaction

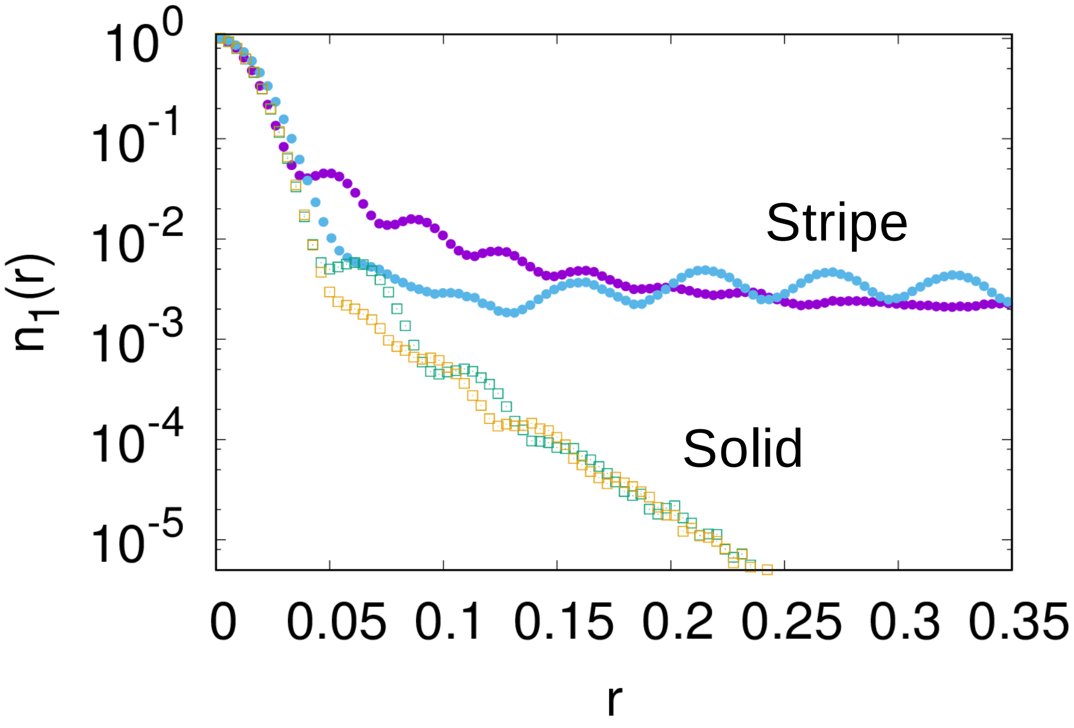


From top to bottom: $n = 64,\ \alpha = 0.58;\ n = 128,\ \alpha = 0.58;$ $n = 256,\ \alpha = 0.61$

Superstripes

One-body density matrix. Comparison between stripe and solid phases.

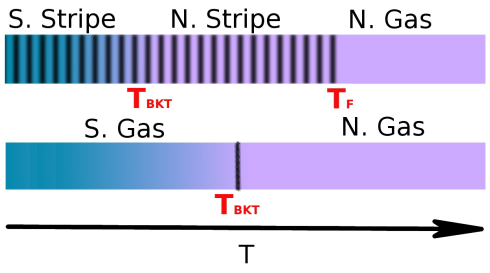
Off-diagonal long-range order is obtained for stripes $\Longrightarrow$ Superstripes

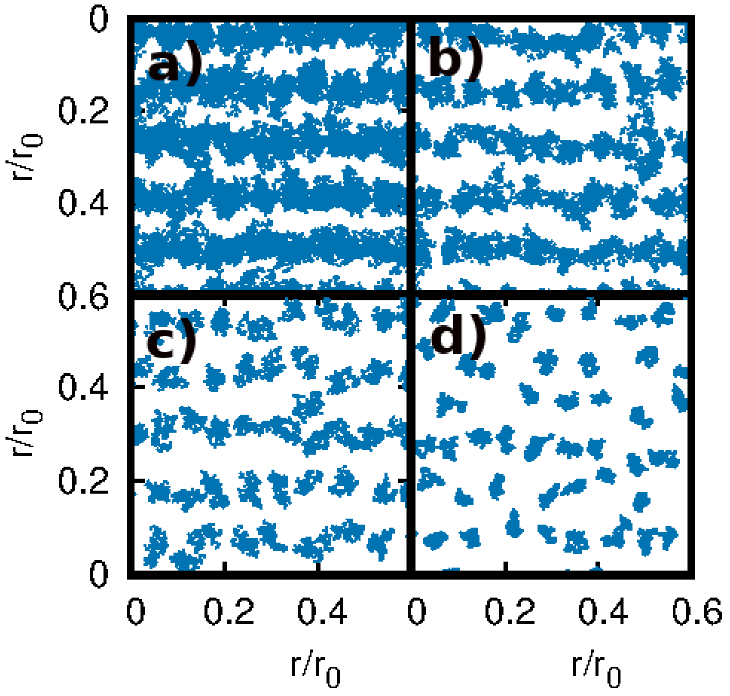


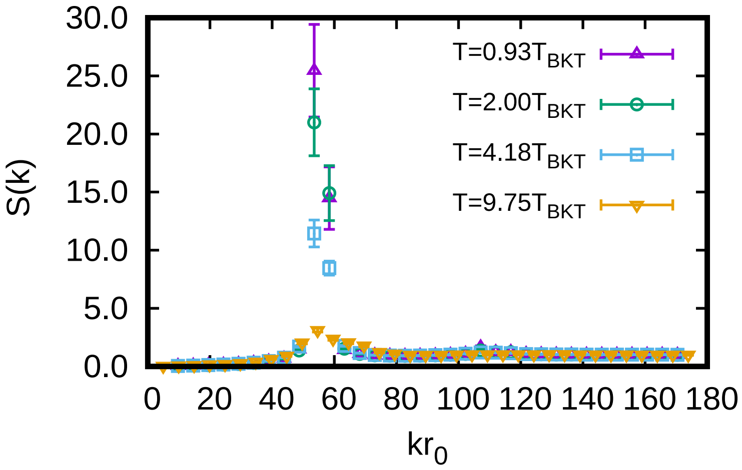
R. Bombin *et al.*, PRL **119**. 250402 (2017)

BKT phase transition

With PIMC we have studied the superfluid transition of stripes





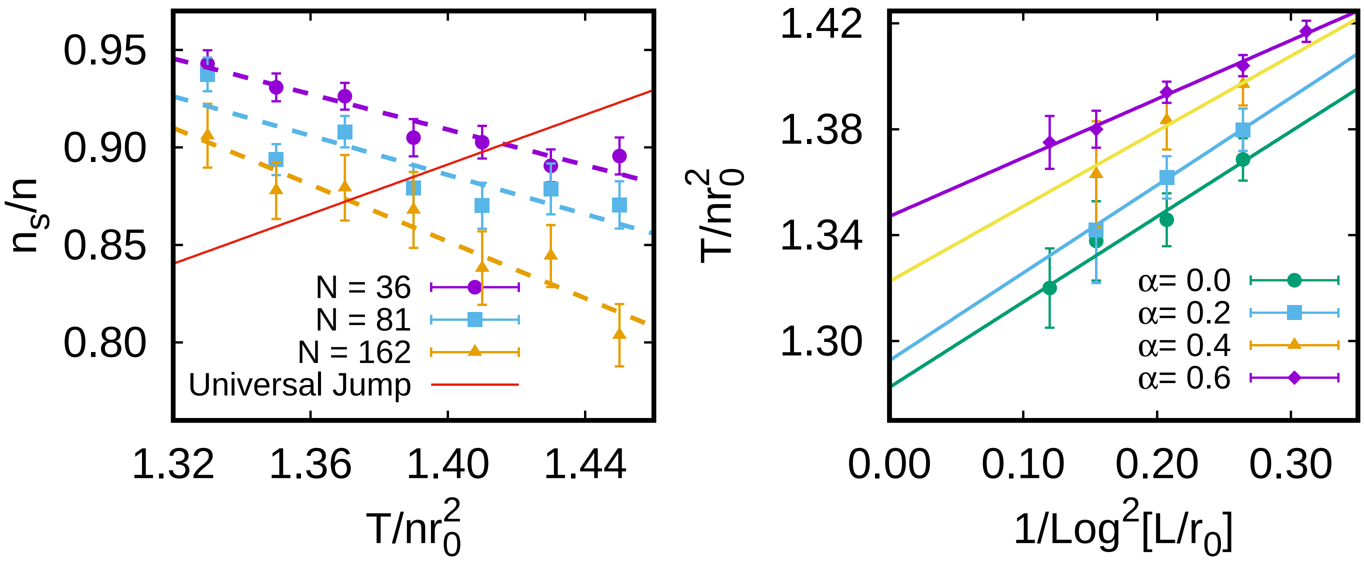


Temperature increases from a) to d)

BKT phase transition

The critical temperature is obtained using finite-size scaling (A. Filinov *et al.*, PRL **105**, 070401 (2010))

In the gas phase,



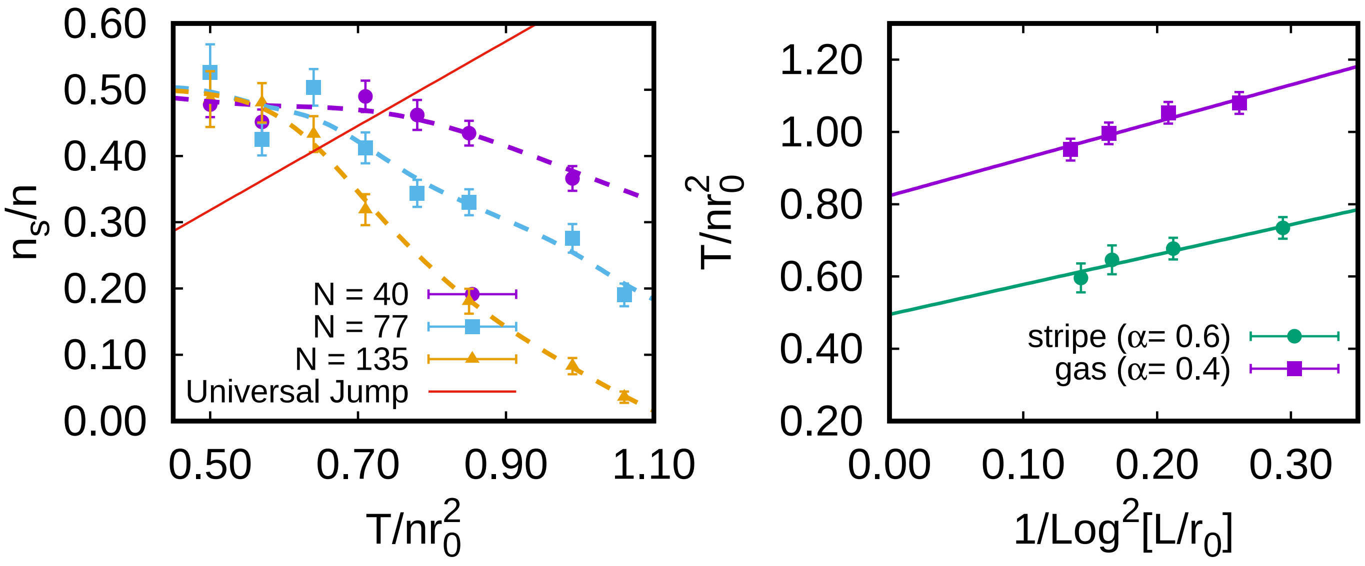
Critical temperature increases with α

Universal BKT jump: $n_s(T_c, L)/n = 2mk_B/(\pi\hbar^2)\, T_c/n$

Scaling law: $T_c(L) = T_c(\infty) + b/\log^2(L)$

BKT phase transition

Comparison between the gas and stripe phases at the same density,



Critical temperature decreases in the stripe phase

R. Bombín *et al.*, PRA **100**, 063614 (2019)

Remarks

- Quantum Monte Carlo has become a standard tool for quantum many-body problems
- Bosons: exact results
- Fermions: still difficult but one can manage . . .
- Finite temperature with PIMC allows for accurate predictions on thermal behavior and phase transitions

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THANKS FOR YOUR ATTENTION !