Higher-order actions for path integral Monte Carlo simulations

QMC in the Apuan Alps IV, 2008

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Quantum many-body theory at 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,

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

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

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

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

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

since they can be computed separately

Primitive Approximation

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

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

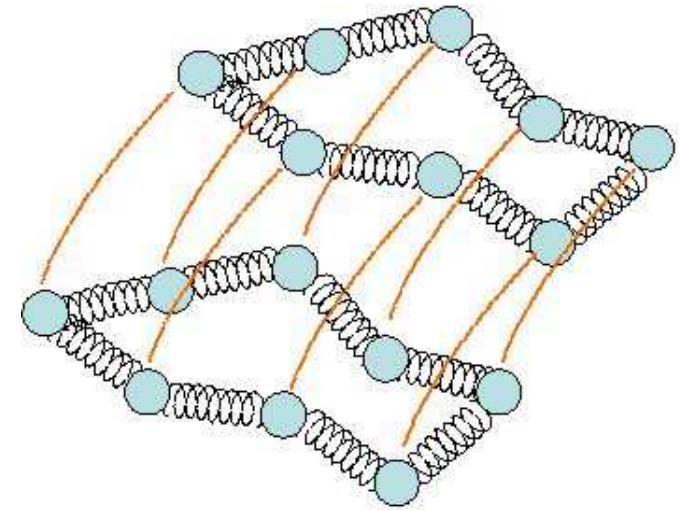
- Introducing explicitly the kinetic and potential terms

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

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

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

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

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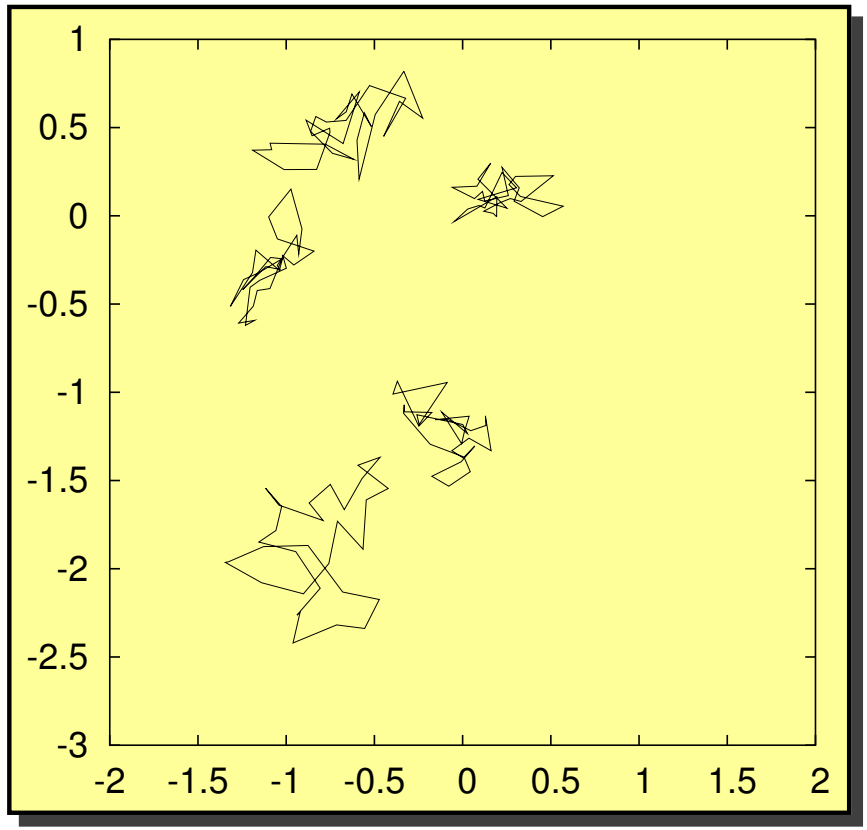
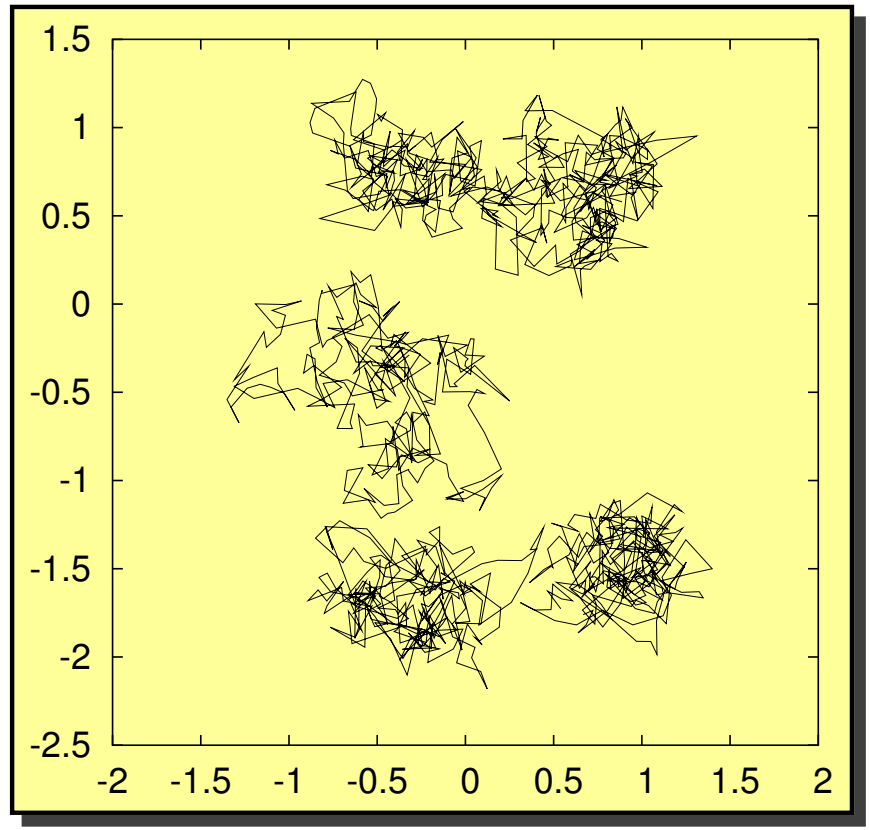


5 H_2 molecules

with 32 beads at $T = 6$ K



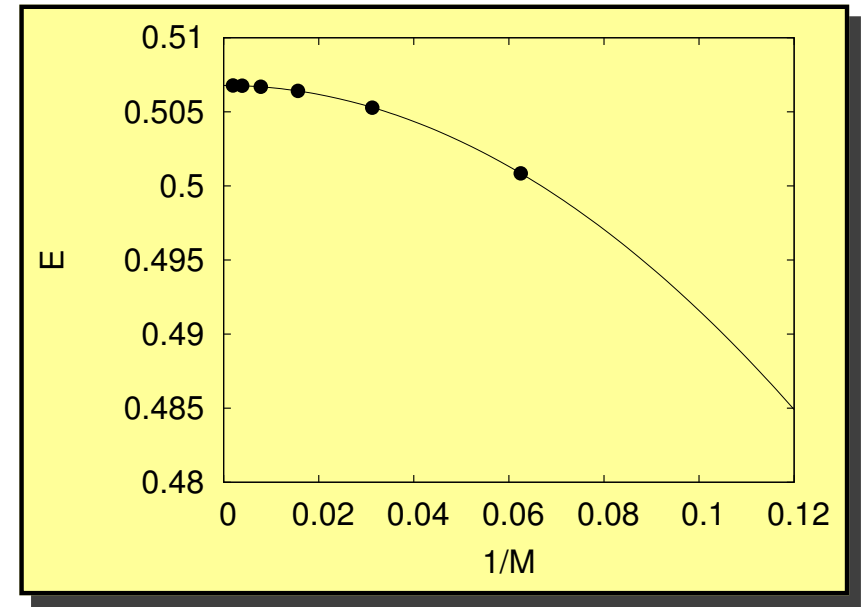
5 H_2 molecules

with 256 beads at $T = 1$ K

Convergence of PA

- The primitive approximation is accurate to second order in ϵ^2

1D Harmonic oscillator at $T = 0.2$



- Reasonable accuracy for semiclassical problems
- Not enough for quantum liquids, especially for their superfluid phases; in liquid ^{4}He ($\sim$ 3000 beads $\Longrightarrow$ *slowing down*)

First correction to PA: Takahashi-Imada

- Takahashi & Imada (1984), and independently Li & Broughton (1987), proposed a new action with a trace accurate to order ϵ^4
- The double commutator $[[V,T],V] = \hbar^2/m(\nabla V)^2$ is introduced, and the bare potential $\hat{V} = \sum_{i<j} V(r_{\alpha,ij})$ is substituted by

$$\hat{W} = \sum_{i<j}^{N} V(r_{ij}) + \frac{1}{24}\frac{\hbar^2}{m}\left(\frac{\beta}{M}\right)^2 \sum_{i=1}^{N} |\mathbf{F}_i|^2$$

with $\mathbf{F}_i = \sum_{j\neq i}^{N} \boldsymbol{\nabla}_i V(r_{ij})$

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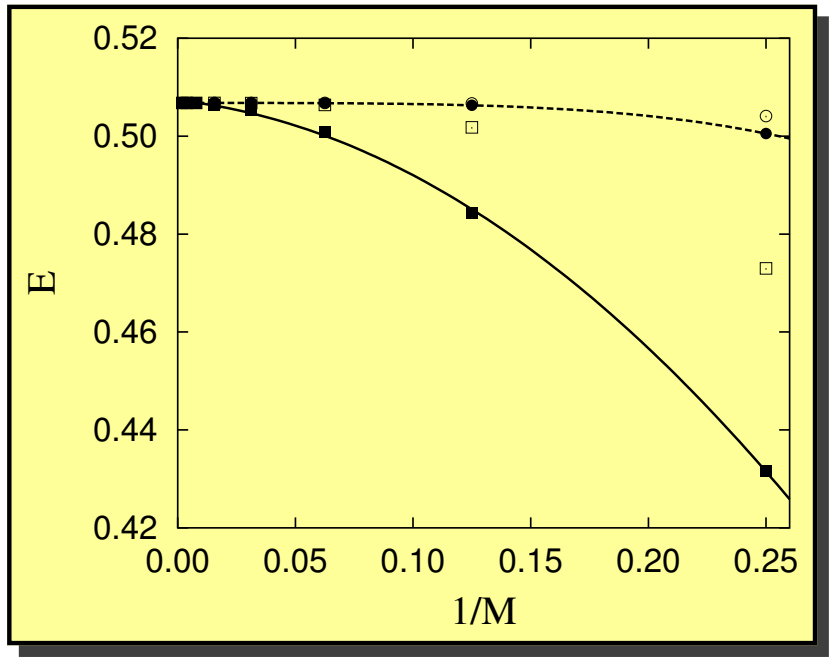
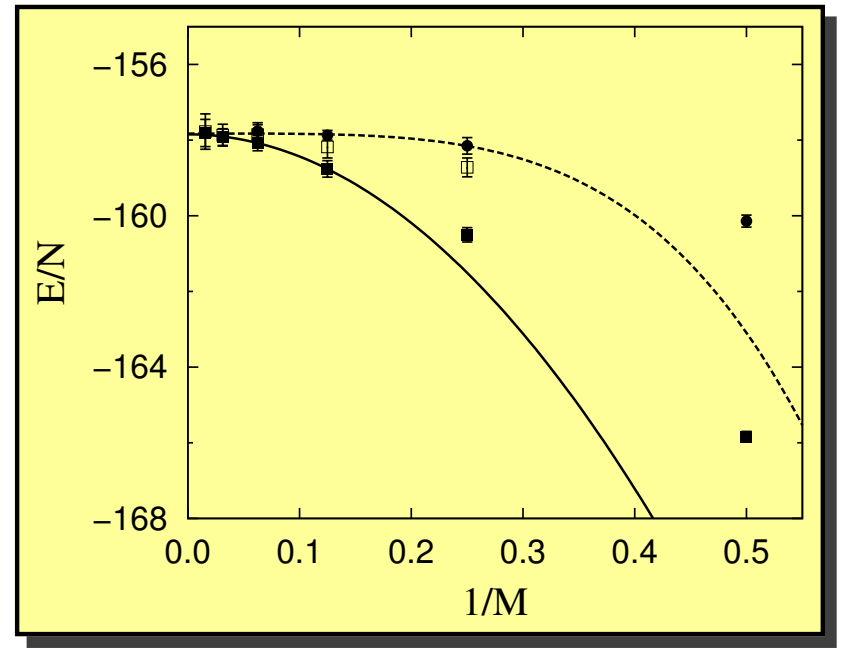


1D Harmonic oscillator

$T = 0.2$



Liquid Ne, $\rho = 0.0363$ Å^{-3}

$T = 25.8$ K

L. Brualla, K. Sakkos, J. B., and J. Casulleras, J. Chem. Phys. **121**, 636 (2004)

Possible paths for improvement

- Takahashi-Imada (TIA) behaves as ϵ^4; not enough for reaching efficiently superfluid regimes

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$$\rho(\mathbf{R},\mathbf{R}';\epsilon) = \prod_{i=1}^{N} \rho(\mathbf{r}_i,\mathbf{r}'_i;\epsilon) \prod_{i<j}^{N} \exp\left[-U(\mathbf{r}_{ij},\mathbf{r}'_{ij};\epsilon)\right]$$

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- PDM is accurate, but not easy to use and restricted in practice to radial potentials
- In our group we have followed a different way: to achieve higher orders in the expansion of $e^{-\epsilon\hat{H}}$ following recent proposals of Siu Chin

Chin Action (t_0, a_1) (I)

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

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

with

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

and parameters

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

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

Chin Action (t_0, a_1) (II)

Explicitly,

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

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

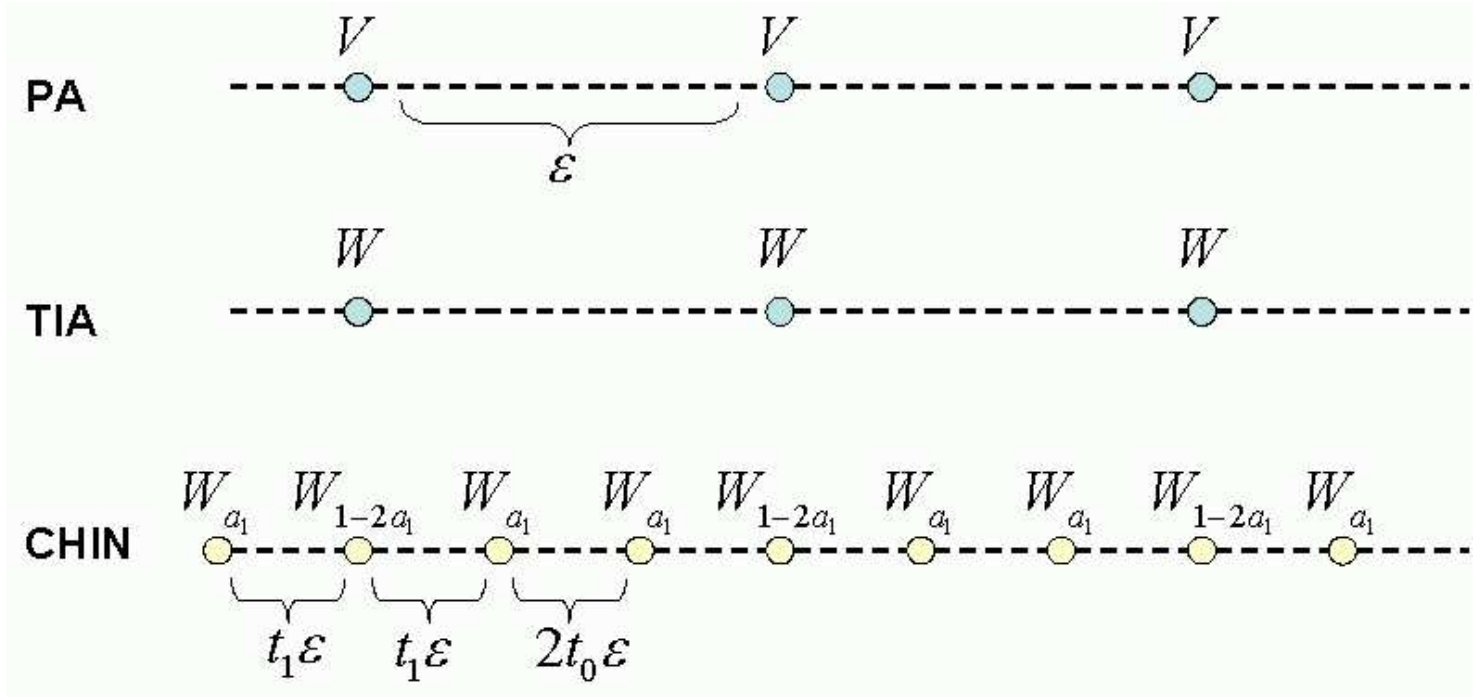
$$\times \sum_{i=1}^{N} \left[\frac{1}{t_1}(\mathbf{r}_{\alpha,i} - \mathbf{r}_{\alpha A,i})^2 + \frac{1}{t_1}(\mathbf{r}_{\alpha A,i} - \mathbf{r}_{\alpha B,i})^2 + \frac{1}{2t_0}(\mathbf{r}_{\alpha B,i} - \mathbf{r}_{\alpha+1,i})^2 \right]$$

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

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

Chin Action (t_0, a_1) (II)

Schematically,



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

PIMC Estimators

Properties of the system are calculated using statistical estimators which use the stochastic variables of the p.d.f. generated by the Metropolis method

$$\langle O \rangle = \frac{1}{N_s} \sum_{i=1}^{N_s} O(\mathbf{R}_i)$$

- Total energy (thermodynamic): $E/N = -(1/NZ)\partial Z/\partial \beta$
- Kinetic energy (thermodynamic): $K/N = (m/N\beta Z)\partial Z/\partial m$
- Potential energy: $V/N = E/N - K/N$
- In general, for any operator $O(\mathbf{R})$,

$$O(\mathbf{R}) = -\frac{1}{\beta}\frac{1}{Z(V)}\left.\frac{dZ(V+\lambda O)}{d\lambda}\right|_{\lambda=0}$$

Sampling in PIMC

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- 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)

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

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

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

Chin Action: optimization

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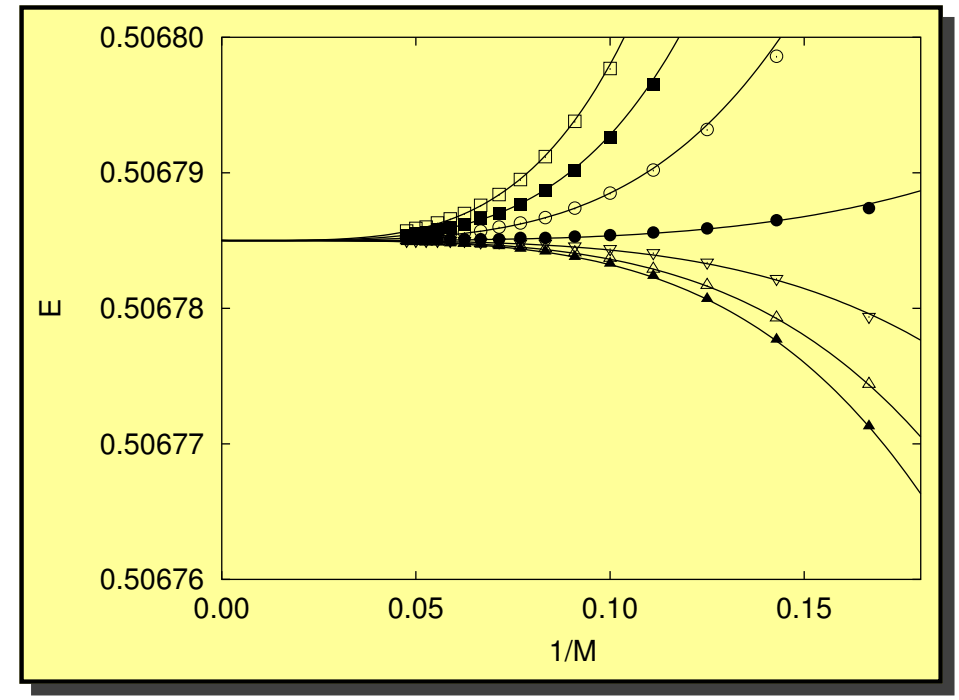
1D Harmonic Oscillator

$T = 0.1$

$a_1 = 0.33$

$t_0 = 0.09, 0.10, \ldots, 0.15$

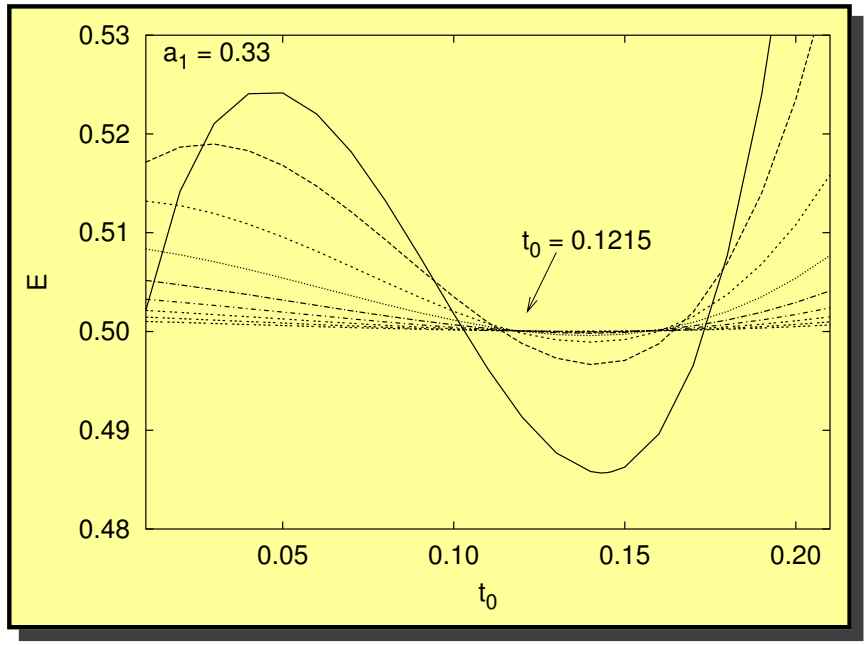
(from top to bottom)

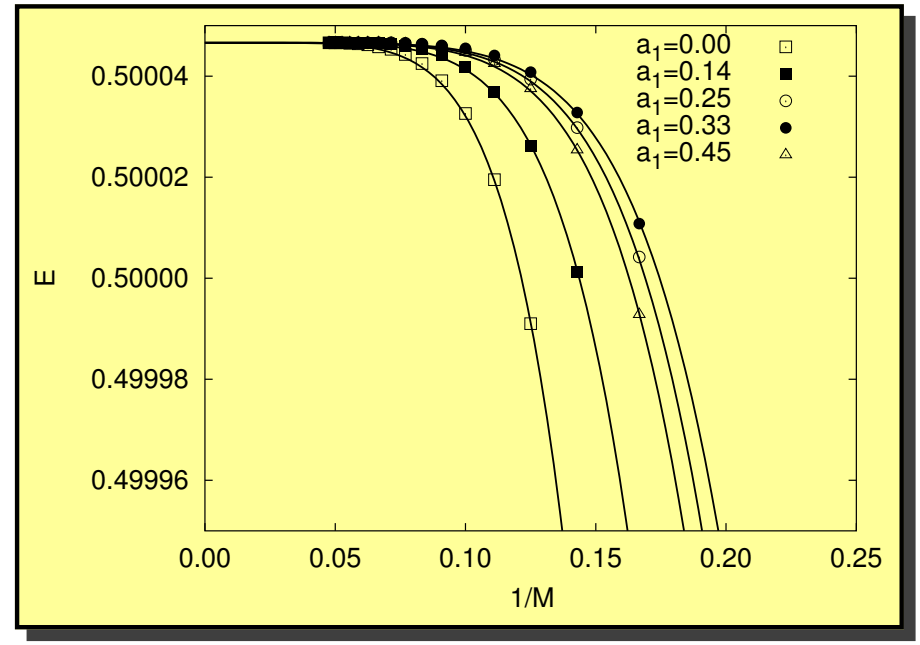


THE ZERO-SLOPE CURVE IS CROSSED !

Optimization (II)

Harmonic oscillator ($T = 0.1$)





Isotime curves (= number of beads)

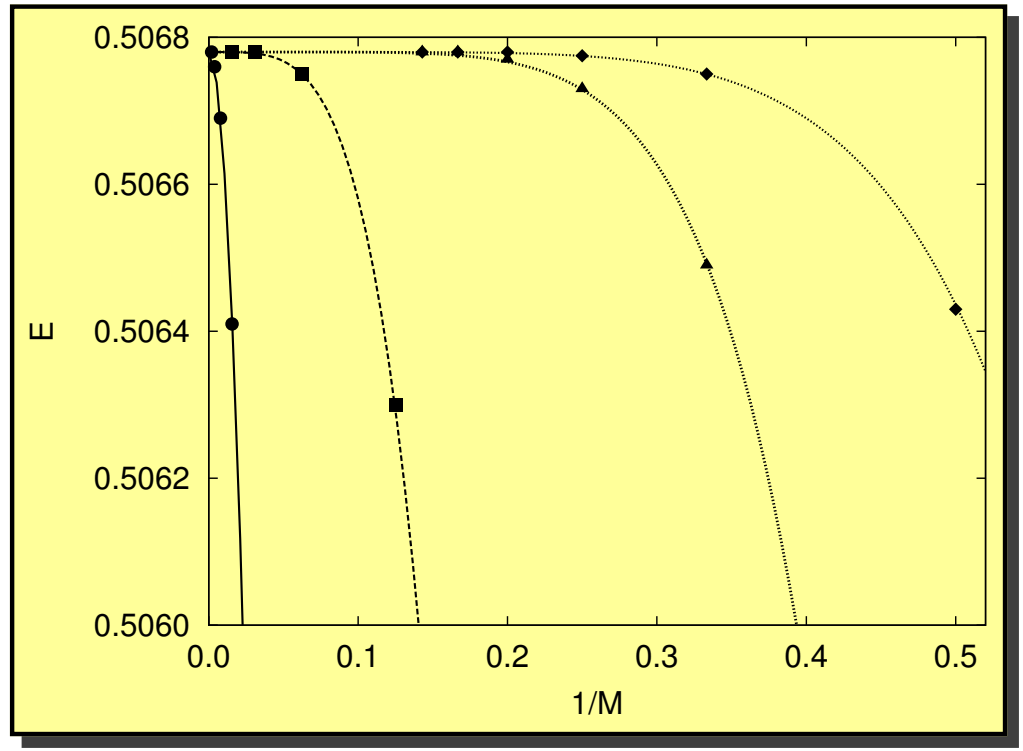
$a_1 = 0.33$

Optimal values:

$a1 = 0.00 \quad t_0 = 0.1430$
$a1 = 0.14 \quad t_0 = 0.0724$
$a1 = 0.25 \quad t_0 = 0.1094$
$a1 = 0.33 \quad t_0 = 0.1215$
$a1 = 0.45 \quad t_0 = 0.1298$

Results for different actions

Harmonic oscillator ($T = 0.2$)

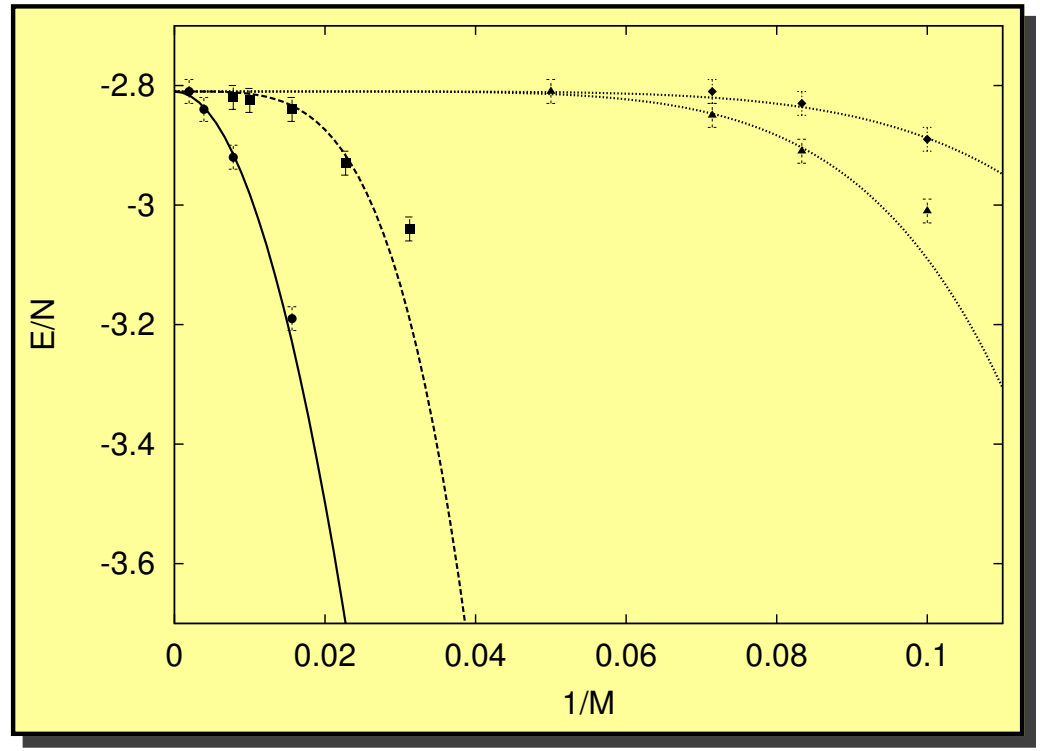


● → PA ($M = 512$) ■ → TIA ($M = 128$)

▲ → Chin-t_0 ($M = 6$) ♦ → Chin-(t_0,a_1) ($M = 4$)

Results for different actions

LIQUID ^{4}HE ($T = 5.1$ K)

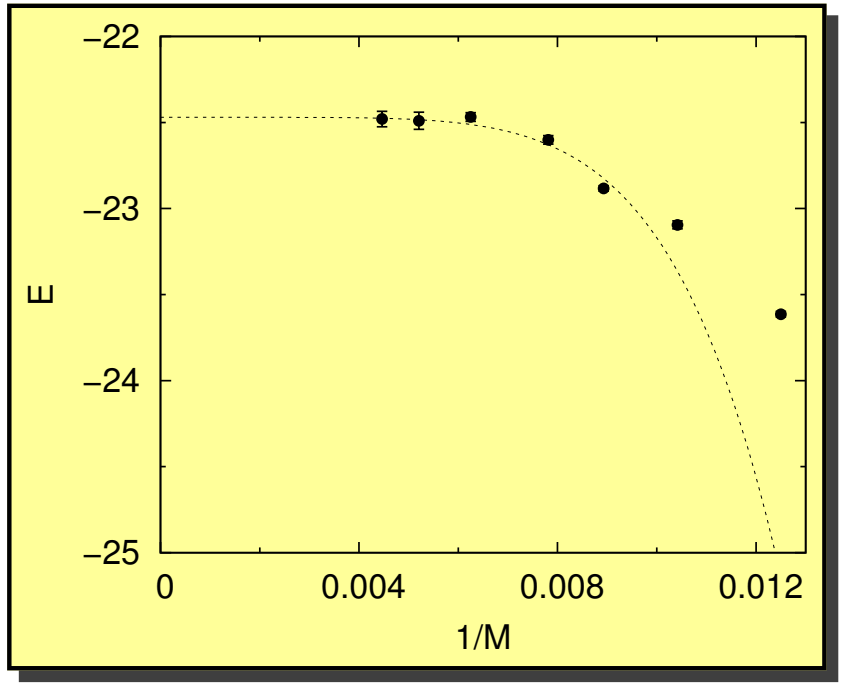


● → PA ($M = 512$) ■ → TIA ($M = 128$)

▲ → Chin-t_0 ($M = 20$) ♦ → Chin-(t_0,a_1) ($M = 14$)

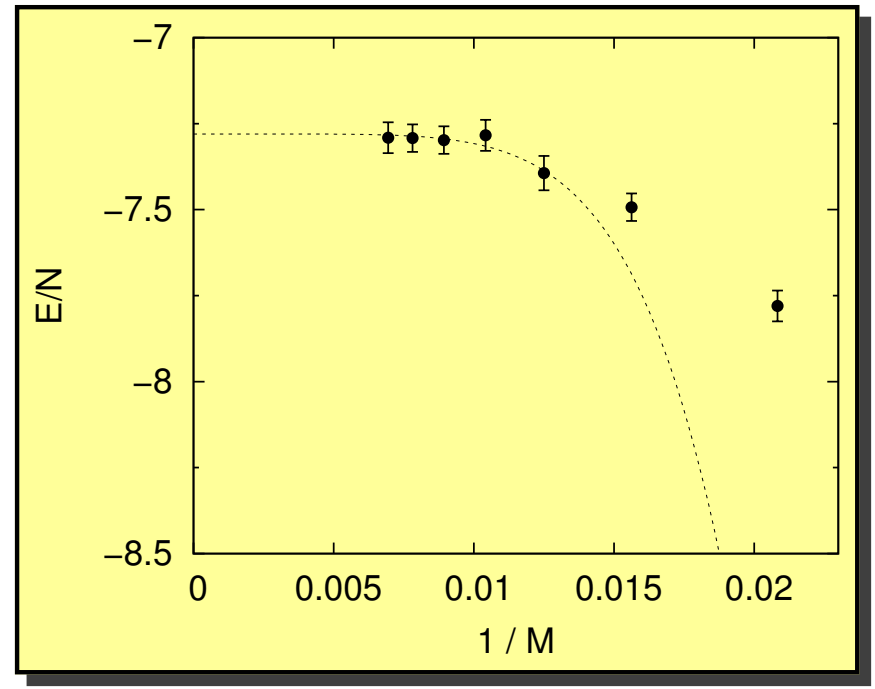
Results for more exigent problems

. . .



H_2 drop with 22 molecules

$T = 1.0$ K



Liquid ^{4}He

$T = 0.8$ K

The lines correspond to 6th order fits:

$$E/N = (E/N)_0 + A(1/M)^6$$

Computational efficiency

	Cost per bead	Reduction # beads	Performance factor
PA	1.0	1	1.0
TIA	2.9	4	1.4
Chin-t_0	4.8	38	7.9
Chin-(t_0, a_1)	7.2	58	8.0

The computational cost per bead increases appreciably, but this increase is largely compensated for the sizeable decrease of the number of beads required to reach the asymptote $\epsilon \to 0$

Symmetrization: sampling of permutations

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

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- For bosons the action must be symmetric

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

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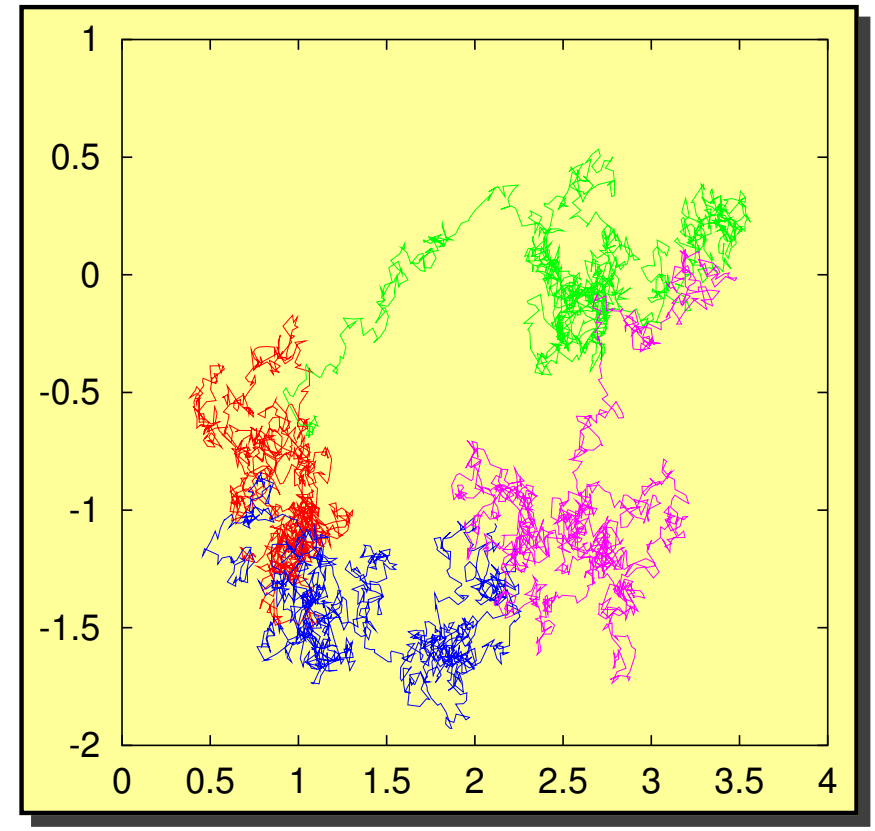
$$\rho_{\rm B}(\mathbf{R}_0, \mathbf{R}_1; \beta) = \frac{1}{N!} \sum_P \rho(\mathbf{R}_0, P\mathbf{R}_1; \beta)$$

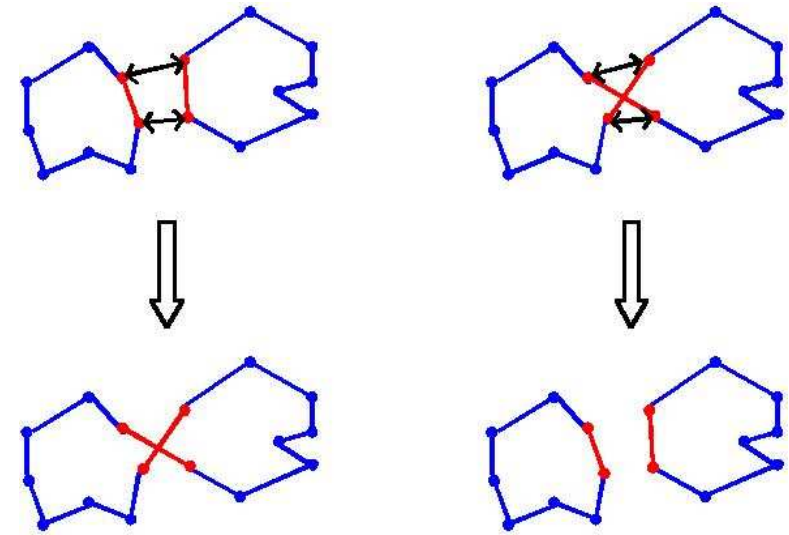
- Sampling the permutation space produces longer polymeric chains which are formed by more than one particle:

SUPERFLUIDITY



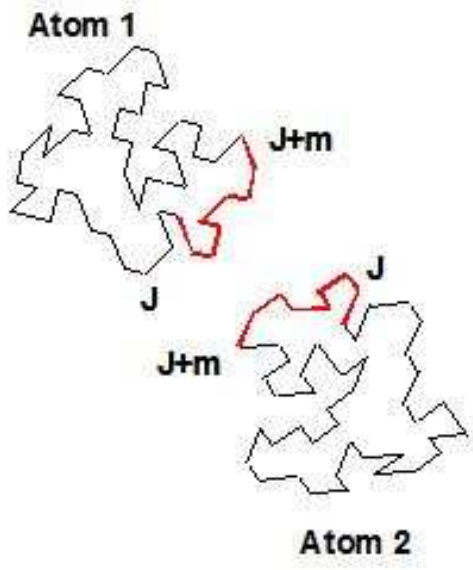
Permutations

- Sampling over all the possible paths and connections
- Care has to be taken to ensure the achievement of equilibrium during the time of a simulation (many atoms involved)
- To take into account correctly the periodic boundary conditions to have always continuous paths

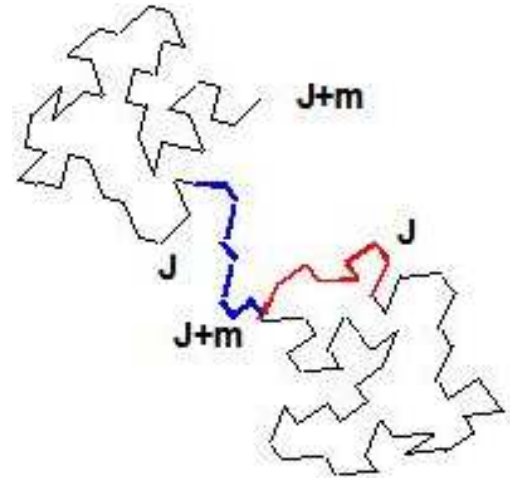


D. M. Ceperley, Rev. Mod. Phys. **67**, 271 (1995)

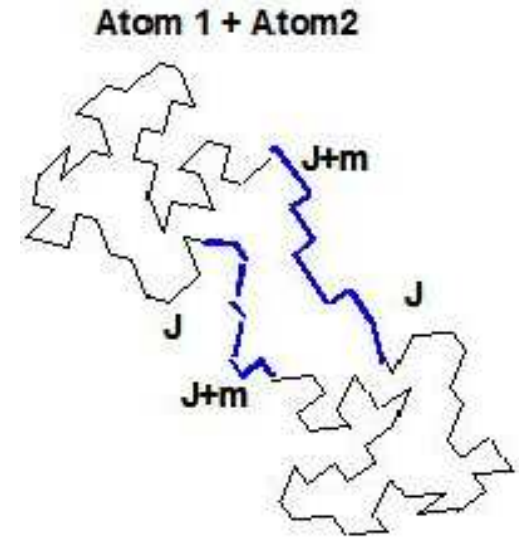
Proposing a pair permutation . . .



Initially the two atoms are separated



A staging chain is constructed connecting the bead J of atom 1 with the bead J+m of atom 2



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Searching for permutations (Ceperley)

1. Transition probabilities table
   $t_{i\alpha,j\alpha+m} = \exp(-(r_{i\alpha} - r_{j\alpha+m})^2/(4m\lambda\epsilon))$
2. Select at random atom i. Select j with probability $t_{i\alpha,j\alpha+m}/h_{i\alpha}$ with $h_{i\alpha} = \sum_k t_{i\alpha,k\alpha+m}$
3. Continue until n different atoms are selected
4. Accept the trial permutation with probability (*take* i, j, k)

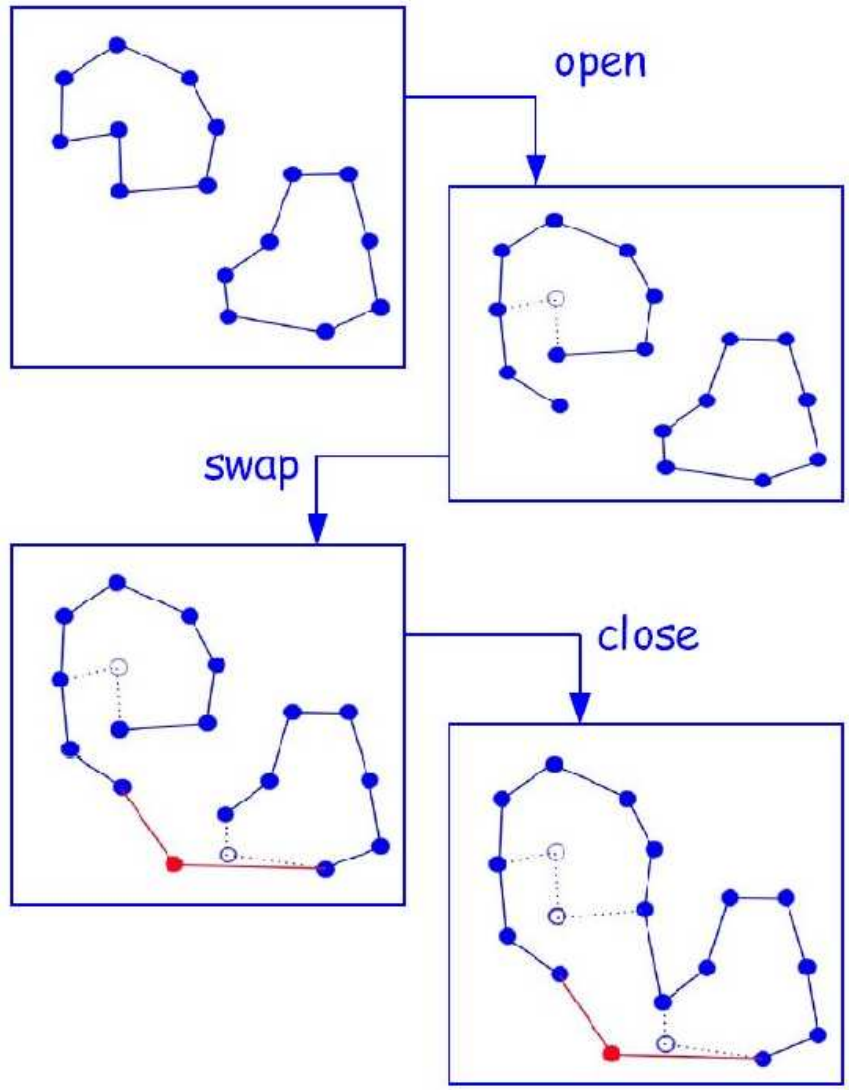
$$A = \min\left(1, \frac{h_{i\alpha}/t_{i\alpha,i\alpha+m} + h_{j\alpha}/t_{j\alpha,j\alpha+m} + h_{k\alpha}/t_{k\alpha,k\alpha+m}}{h_{i\alpha}/t_{i\alpha,j\alpha+m} + h_{j\alpha}/t_{j\alpha,k\alpha+m} + h_{k\alpha}/t_{k\alpha,i\alpha+m}}\right)$$

5. If the trial permutation is accepted go on and do Metropolis test (only potential part of the action)

Efficiency in the permutation sampling

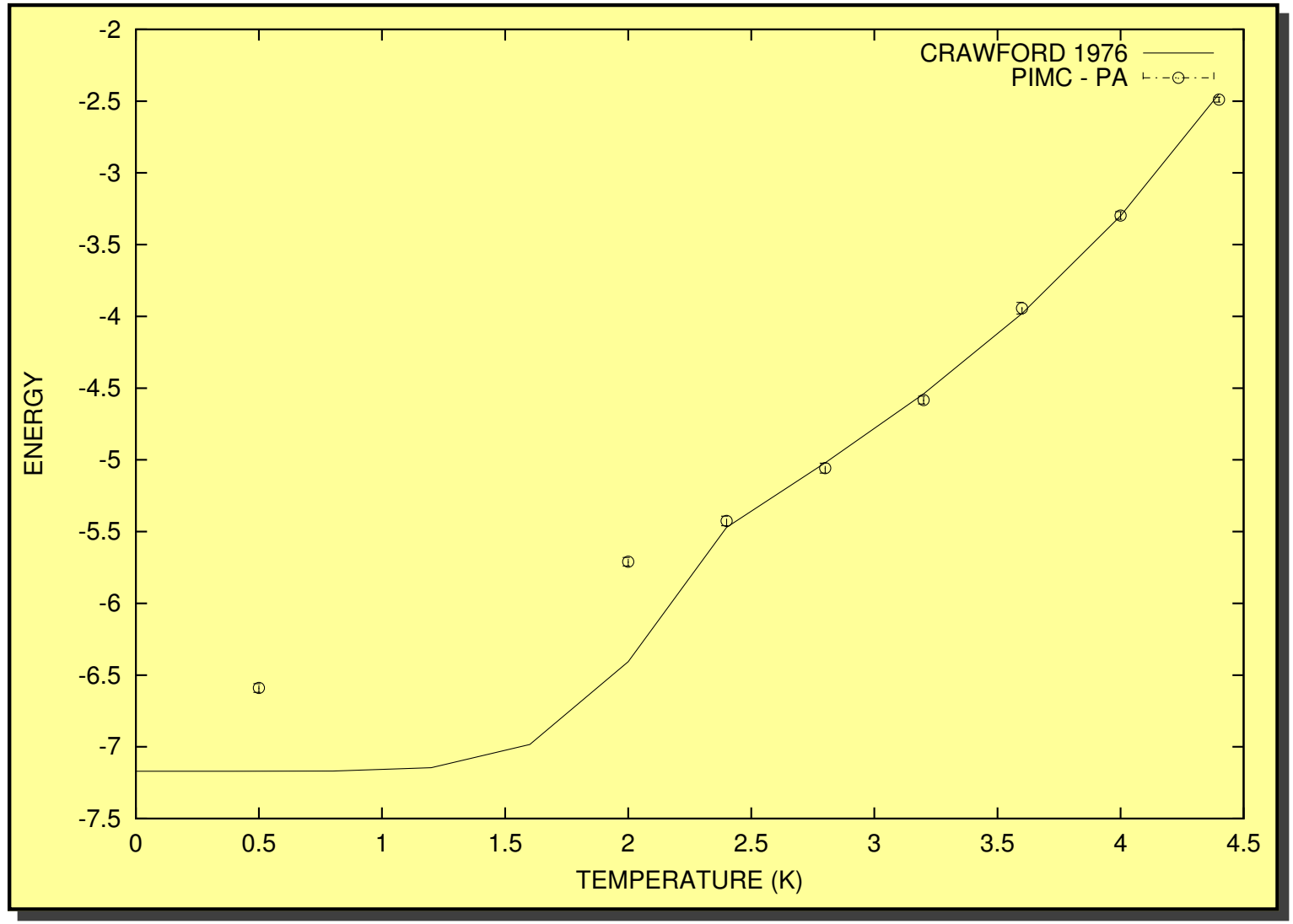
- Over all the trial permutations only 5% are accepted (free-action test) and therefore sampled
- Over all the permutations sampled only 1% are accepted by Metropolis $\Longrightarrow$ Very low efficiency
- The length of the staging chain (joining different particles) is selected for maximizing the ratio of Metropolis-accepted permutations per real time unit
- Permutations involving more than 3 or 4 polymers are extremely difficult to appear, . . . but they are important for a correct estimation of the superfluid density

New proposal: Worm Algorithm

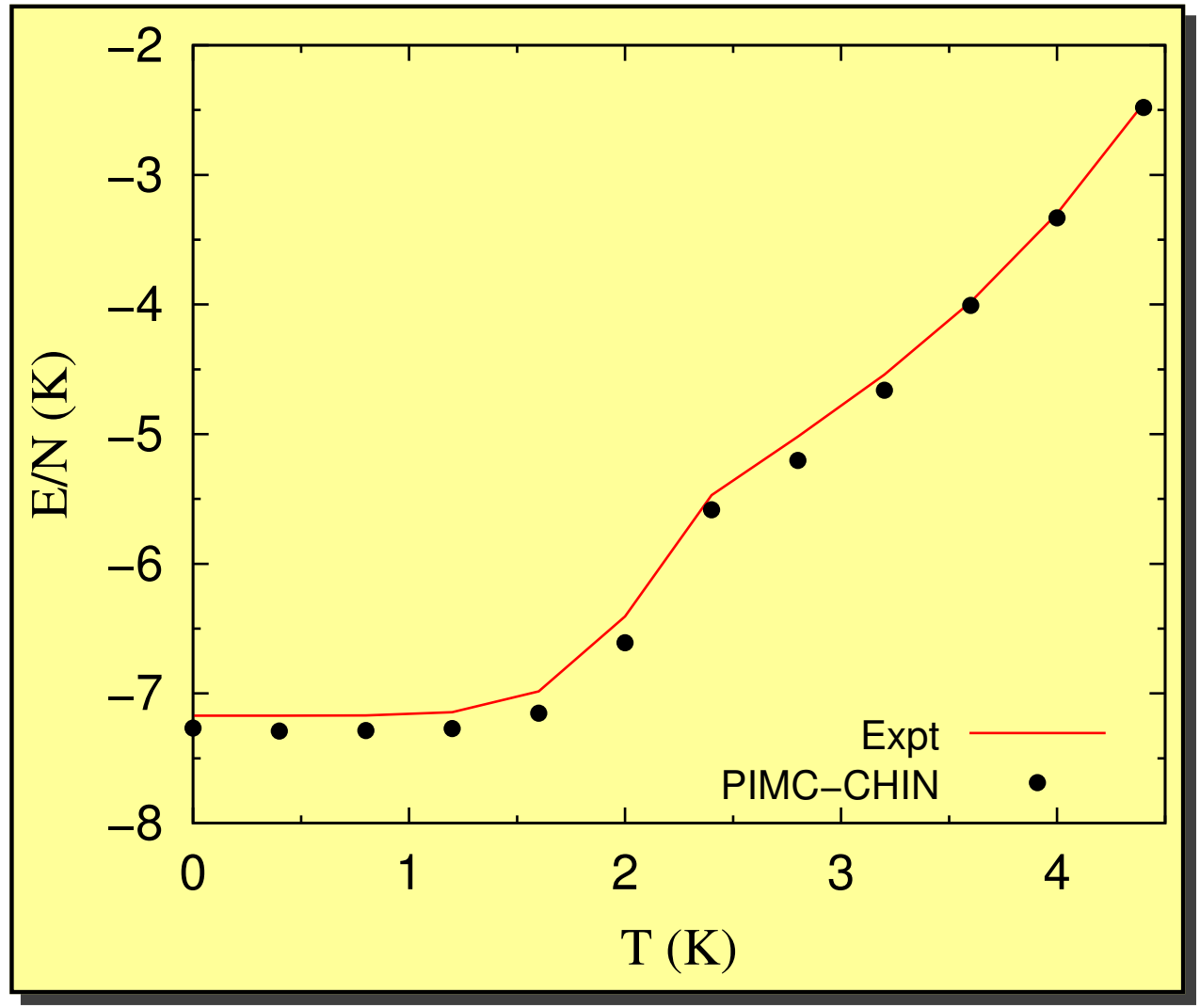


- Proposed for Prokof'ev, Boninsegni and Svistunov for PIMC in the grand canonical ensemble.
- Key ingredient: An open chain (*worm*) is introduced in the simulation.
- By the swap operation, long permutations are in practice achieved.
- Specially useful for the estimation of the superfluid density and the one-body density matrix.

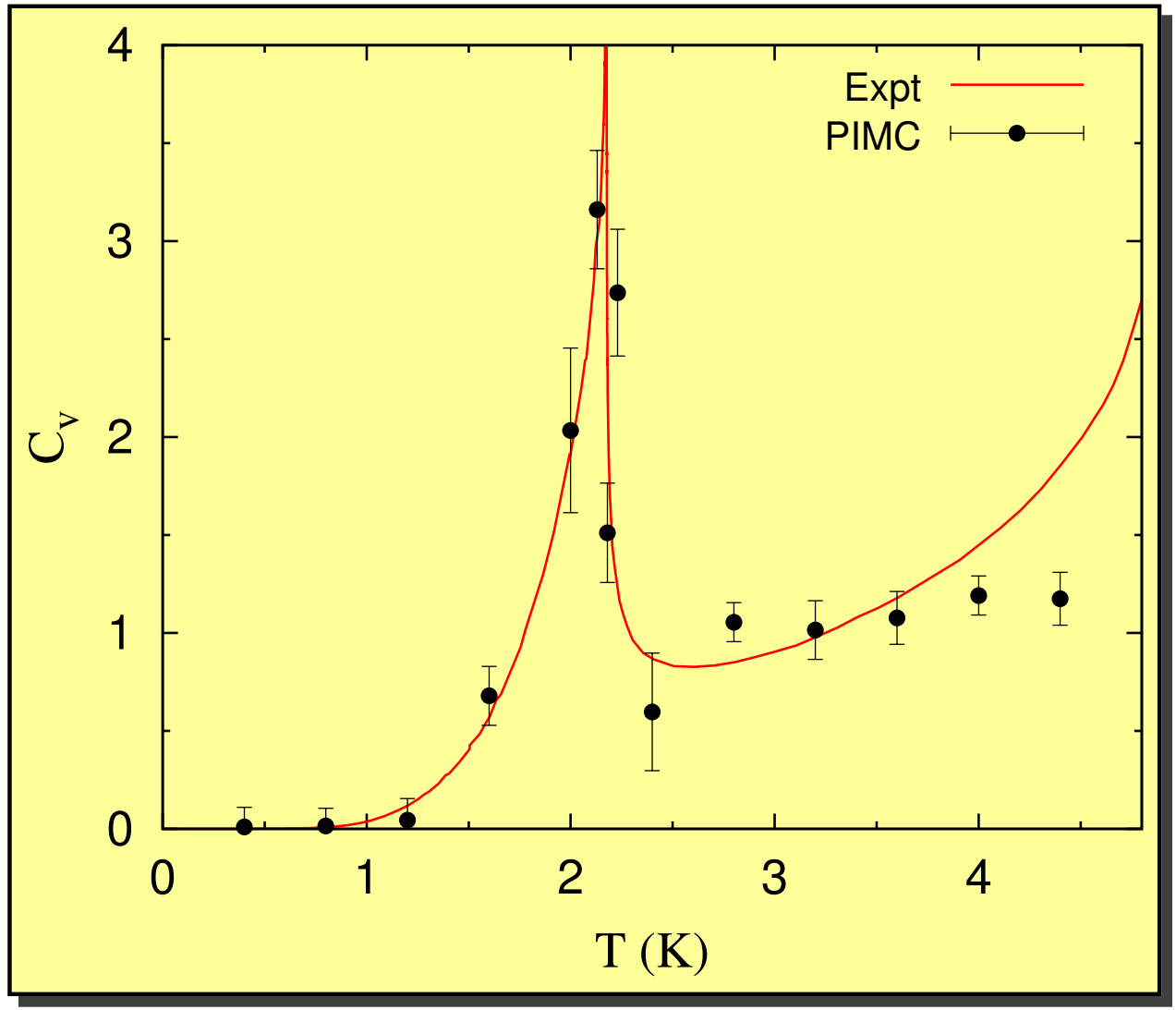
Results for bulk ^{4}He



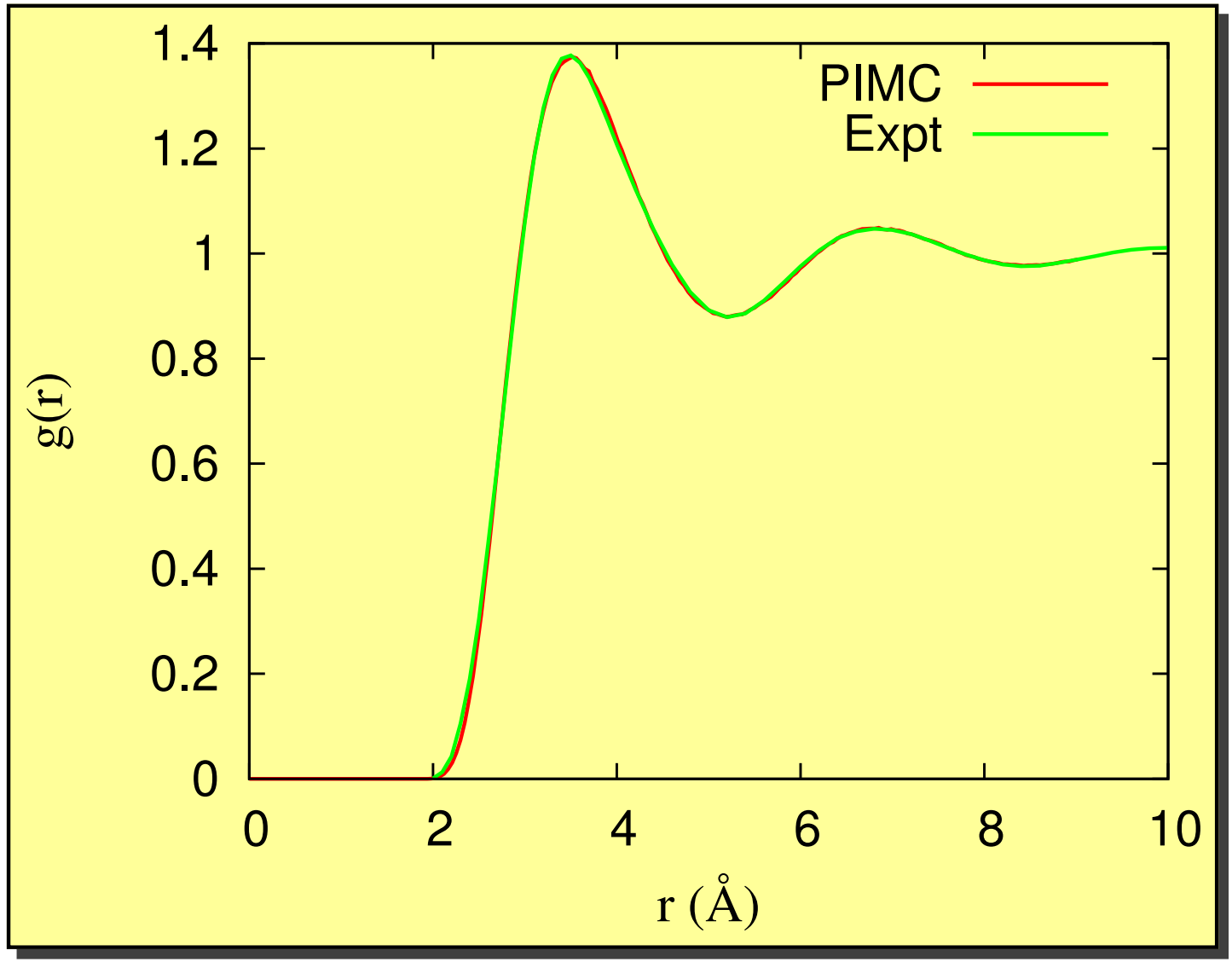
Results for bulk ^{4}He



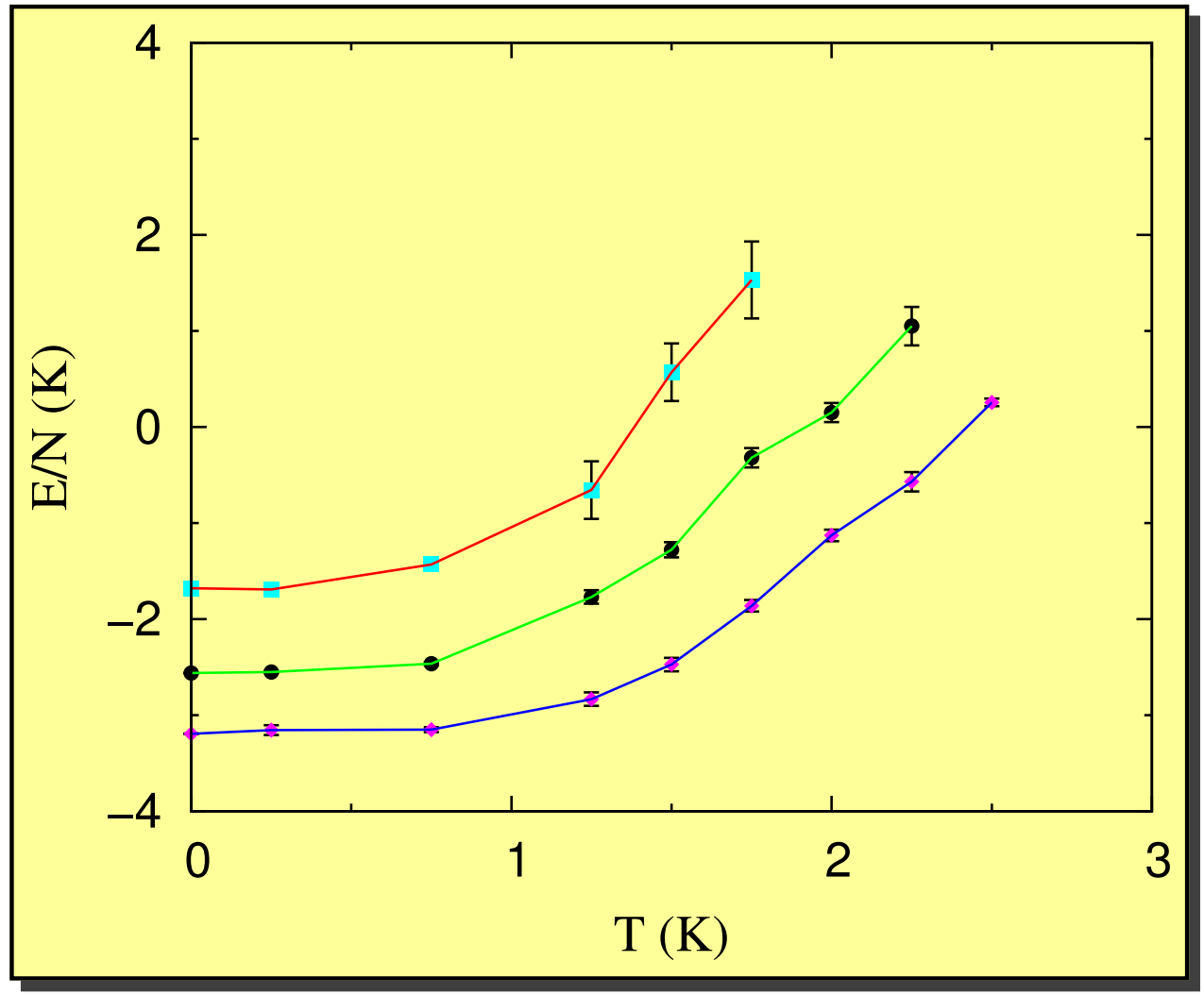
Results for bulk ^{4}He



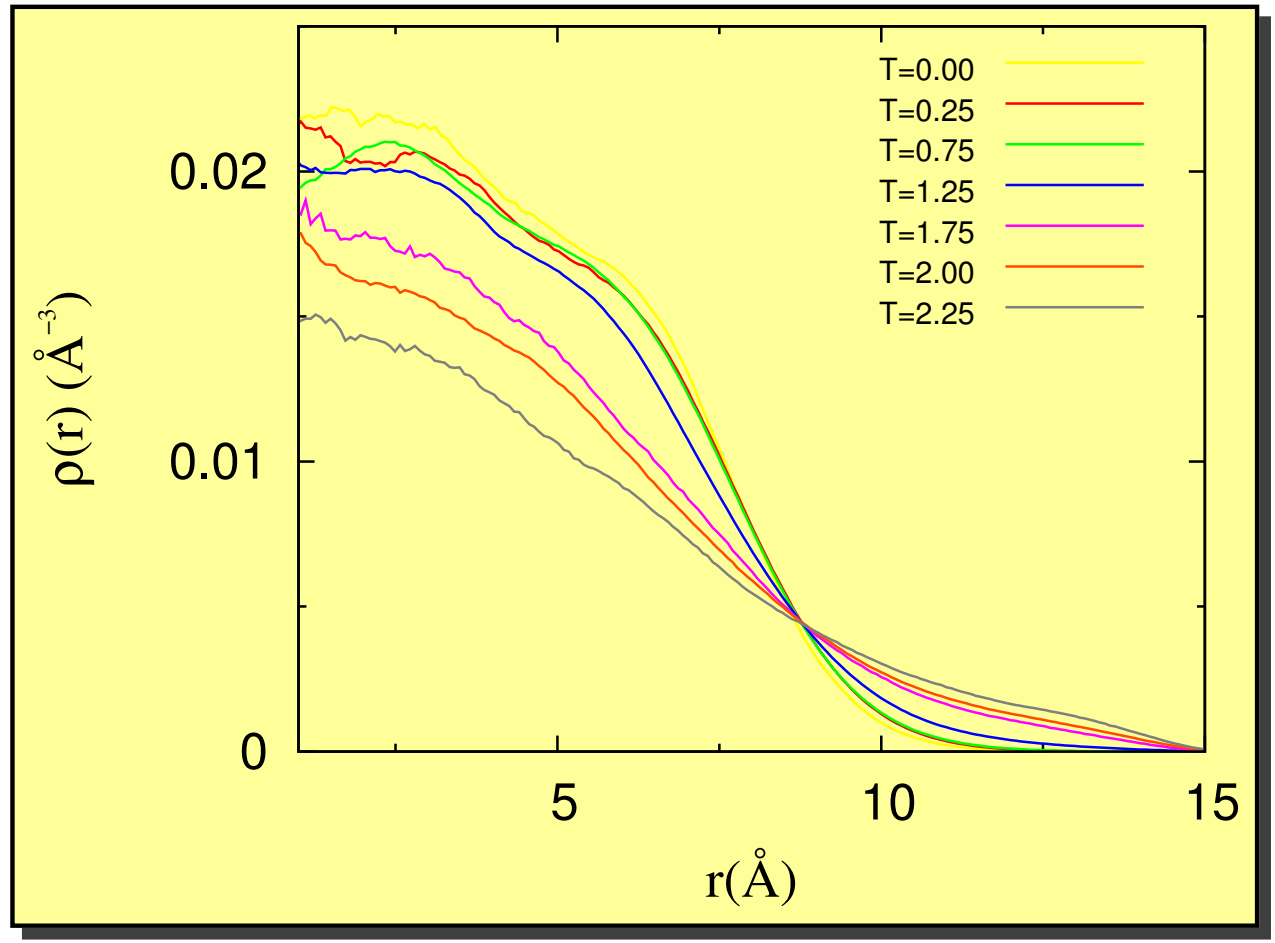
Results for bulk ^{4}He



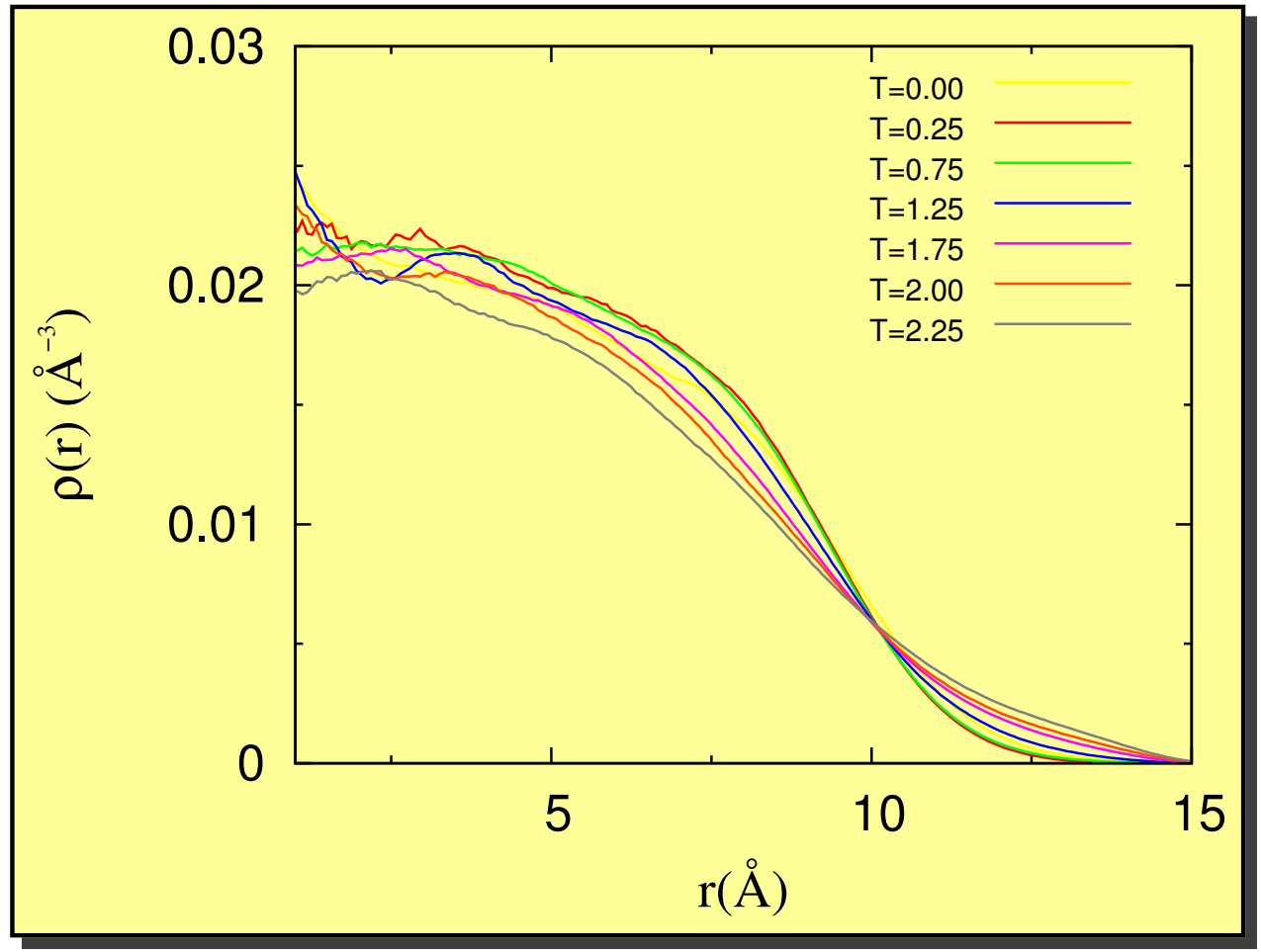
Small ^{4}He drops



Small ^{4}He drops



Small ^{4}He drops



Towards the ground state: PIGS

- The PIMC formalism can be extended to the limit $T \to 0 \Longrightarrow$ PIGS method (A. Sarsa *et al.*, J. Chem. Phys. **113**, 1366 (2000))
- The key point is to identify the Green's function (GFMC, DMC) with the thermal density matrix (PIMC)

$$G(\mathbf{R}, \mathbf{R}'; \tau) = \rho(\mathbf{R}, \mathbf{R}'; \beta)$$

and use the convolution property of ρ.

- Difference: In PIMC one forces periodic boundary conditions in imaginary time required by taking the trace of ρ (*closed chains*); in PIGS one truncates the path by inserting trial wave functions ψ_T (*open chains*).

Towards the ground state: PIGS

- Expectation values

$$\langle O \rangle = \frac{\langle \psi_T | G(\tau - \tau_0) O G(\tau_0) | \psi_T \rangle}{\langle \psi_T | G(\tau - \tau_0) G(\tau_0) | \psi_T \rangle}$$

$\Rightarrow$ For $\tau_0 = 0$, one recovers the mixed estimator of DMC

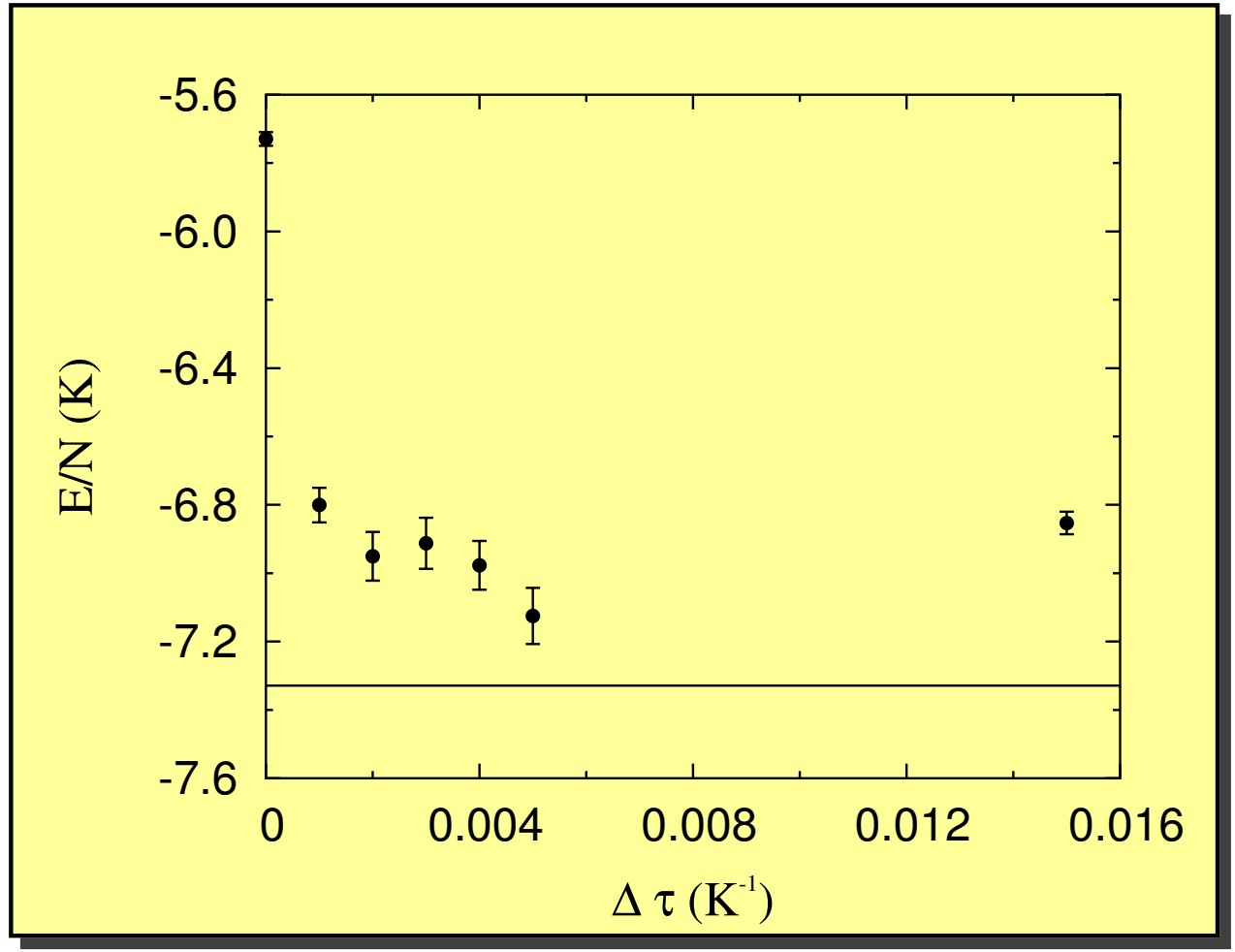
$\Rightarrow$ For $\tau_0 = \tau/2$ one gets exact estimation of O if $\tau/2$ is large enough

- How to reach long times ? To use the convolution property and a good approximation for the short-time ($\Delta\tau$) Green's function

$$\langle O \rangle = \frac{\int [\prod_{i=0}^{M} d\mathbf{R}_i] O(\mathbf{R}_{M/2}) \psi_T(\mathbf{R_0}) [\prod_{\mathbf{i=0}}^{\mathbf{M-1}} \rho(\mathbf{R_i}, \mathbf{R_{i+1}}; \mathbf{\Delta}\tau)] \psi_{\mathbf{T}}(\mathbf{R_M})}{\int [\prod_{i=0}^{M} d\mathbf{R}_i] \psi_T(\mathbf{R_0}) [\prod_{\mathbf{i=0}}^{\mathbf{M-1}} \rho(\mathbf{R_i}, \mathbf{R_{i+1}}; \mathbf{\Delta}\tau)] \psi_{\mathbf{T}}(\mathbf{R_M})}$$

Towards the ground state: PIGS

- Preliminary results on ^{4}He. Only one time step $\Delta\tau$.
- Dependence on $\Delta\tau$:



Conclusions

- The action (t_0, a_1) has been used for the first time in PIMC and has shown a 6th order efficiency, not only in model problems but in real and more exigent systems (^{4}He, H_2)
- With respect to the Takahashi-Imada approximation, the new action does not require any additional derivative of the potential
- Migrating a TIA code to a Chin one is rather easy since the basic routines are the same
- In spite of substituting a bead by three beads, the efficiency of the staging corresponds to the one of a time step ϵ

Conclusions

- Easier, general and with a more clear dependence with ϵ than the pair action approximation (Ceperley)
- This is our choice for finite-temperature simulations in quantum fluids . . .
- And very promising for the ground state using PIGS. Fermions ?

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THANKS FOR YOUR ATTENTION !