Higher-order actions for path integral Monte Carlo simulations

*QMC in the Apuan Alps IV, 2008*

Jordi Boronat

Departament de Física i Enginyeria Nuclear
Universitat Politècnica de Catalunya
Barcelona, Spain

In collaboration with: Joaquim Casulleras, Konstantinos Sakkos and Riccardo Rota
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
- 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

\[
\rho(\mathbf{R}, \mathbf{R}'; \beta) = \sum_i e^{-\beta E_i} \phi_i^*(\mathbf{R}) \phi_i(\mathbf{R}')
\]
Convolution property of the density matrix

- The density matrix can always be decomposed as

\[ \rho(R_1, R_2; \beta) = \int dR_3 \rho(R_1, R_3; \beta/2) \rho(R_3, R_2; \beta/2) \]

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

- By iterating \( M \) times,

\[ \rho(R_0, R_M; \beta) = \int dR_1 \ldots dR_{M-1} \rho(R_0, R_1; \epsilon) \ldots \rho(R_{M-1}, R_M; \epsilon) \]

with \( \epsilon = \beta/M \)
Trotter formula

Exact result for $\rho(R, R'; \beta)$ 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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with $C_2 = \frac{1}{2} [\hat{K}, \hat{V}]$ and $C_3 = \frac{1}{12} [\hat{K} - \hat{V}, [\hat{K}, \hat{V}]]$
- When $M \to \infty$, $\epsilon = \beta / M \to 0$, the linear term dominates $\implies$ **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 $\epsilon^2$ 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

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

since they can be computed separately
Primitive Approximation

♦ The partition function is \( \{ \mathbf{r}_1, \ldots, \mathbf{r}_N \} \)

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

♦ Introducing explicitly the kinetic and potential terms

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

$$
\exp \left[ -\frac{Mm}{2\beta\hbar^2} (r_{\alpha,i} - r_{\alpha+1,i})^2 \right]
$$
Mapping the quantum problem to a classical one

5 H₂ molecules
with 32 beads at $T = 6$ K

5 H₂ molecules
with 256 beads at $T = 1$ K
Convergence of PA

- The primitive approximation is accurate to second order in $\epsilon^2$

  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 $\Rightarrow$ 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 $\epsilon^4$

- The double commutator $[[[V, T], V], V] = \hbar^2/m(\nabla V)^2$ is introduced, and the bare potential $\hat{V} = \sum_{i<j} V(r_{\alpha,ij})$ is substituted by

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

with $F_i = \sum_{j \neq i}^N \nabla_i V(r_{ij})$
First correction to PA: Takahashi-Imada

1D Harmonic oscillator

$T = 0.2$

Liquid Ne, $\rho = 0.0363 \text{ Å}^{-3}$

$T = 25.8 \text{ K}$

Possible paths for improvement

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- Ceperley & Pollock introduced the pair action (PDM)

$$\rho(R, R'; \epsilon) = \prod_{i=1}^{N} \rho(r_i, r'_i; \epsilon) \prod_{i<j}^{N} \exp \left[ -U(r_{ij}, r'_{ij}; \epsilon) \right]$$
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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 \(\epsilon^6\) order for the harmonic oscillator

\[
e^{-\epsilon \hat{H}} \approx e^{-v_1 \epsilon \hat{W}_{a_1}} e^{-t_1 \epsilon \hat{T}} e^{-v_2 \epsilon \hat{W}_{1-2a_1}} e^{-t_1 \epsilon \hat{T}} e^{-v_1 \epsilon \hat{W}_{a_1}} e^{-2t_0 \epsilon \hat{T}}
\]

with

\[
\hat{W}_{a_1} = \hat{V} + (u_0/v_1)a_1 \epsilon^2 \hat{W} \quad (0 \leq a_1 \leq 1)
\]
\[
\hat{W}_{1-2a_1} = \hat{V} + (u_0/v_2)(1 - 2a_1) \epsilon^2 \hat{W}
\]

and parameters

\[
v_1 = \frac{1}{6(1-2t_0)^2}
\]
\[
v_2 = 1 - 2v_1
\]
\[
t_1 = \frac{1}{2} - t_0 \quad (0 \leq t_0 \leq \frac{1}{2}(1 - \sqrt{3}))
\]
\[
u_0 = \frac{1}{12} \left[ 1 - \frac{1}{1-2t_0} + \frac{1}{6(1-2t_0)^3} \right]
\]
Chin Action \((t_0, a_1)\) (II)

Explicitly,

\[
\rho_{t_0a_1}(R_\alpha, R_{\alpha+1}) = \\
\left(\frac{m}{2\pi\hbar^2\epsilon}\right)^{9N/2} \left(\frac{1}{2t_1^2t_0}\right)^{3N/2} \int dR_{\alpha A}dR_{\alpha B} \exp \left\{ -\frac{m}{2\hbar^2\epsilon} \right\} \\
\times \sum_{i=1}^{N} \left[ \frac{1}{t_1} (r_{\alpha,i} - r_{\alpha A,i})^2 + \frac{1}{t_1} (r_{\alpha A,i} - r_{\alpha B,i})^2 + \frac{1}{2t_0} (r_{\alpha B,i} - r_{\alpha+1,i})^2 \right] \\
-\epsilon \sum_{i<j}^{N} (v_1 V(r_{\alpha,ij}) + v_2 V(r_{\alpha A,ij}) + v_1 V(r_{\alpha B,ij})) \\
-\epsilon^3 u_0 \frac{\hbar^2}{m} \sum_{i=1}^{N} \left( a_1 |F_{\alpha,i}|^2 + (1 - 2a_1) |F_{\alpha A,i}|^2 + a_1 |F_{\alpha B,i}|^2 \right) \}
\]
Chin Action \((t_0, a_1)\) (II)

Schematically,

\[
\begin{align*}
\text{PA} & \quad \includegraphics[width=\textwidth]{schematic.png} \\
\text{TIA} & \\
\text{CHIN} & \quad \includegraphics[width=\textwidth]{schematic.png}
\end{align*}
\]

\[
e^{-e \dot{H}} \approx e^{-v_1 e \tilde{W}_{a_1}} e^{-t_1 e \tilde{T}} e^{-v_2 e \tilde{W}_{1-2a_1}} e^{-t_1 e \tilde{T}} e^{-v_1 e \tilde{W}_{a_1}} e^{-2t_0 e \tilde{T}}
\]
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

\[
\langle O \rangle = \frac{1}{N_s} \sum_{i=1}^{N_s} O(R_i)
\]

- 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 \( O(R) \),

\[
O(R) = - \frac{1}{\beta Z(V)} \frac{1}{d\lambda} \frac{dZ(V + \lambda O)}{d\lambda} \bigg|_{\lambda=0}
\]
Sampling in PIMC

Simplest method: bead a bead + movement of the center of mass of the polymer
Sampling in PIMC

- Simplest method: bead a bead movement of the center of mass of the polymer
- But … slowing down problems for long chains
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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)

\[
\begin{align*}
\rho_0(x_i, x_{i+1}; \epsilon) \cdots \rho_0(x_{i+j-1}, x_{i+j}; \epsilon) = & \left( \frac{m}{2\pi \hbar^2 j \epsilon} \right)^{1/2} \exp \left[ - \frac{m}{2\hbar^2 j \epsilon} (x_i - x_{i+j})^2 \right] \\
& \times \prod_{k=0}^{j-2} \left( \frac{m_k}{2\pi \hbar^2 \epsilon} \right)^{1/2} \exp \left[ - \frac{m_k}{2\hbar^2 \epsilon} (x_{i+k+1} - x_{i+k+1}^*)^2 \right]
\end{align*}
\]
Chin Action: optimization

... Coming back to the Chin’s approximation for the action, we need to work on a previous step ➞
Optimization of the parameters $t_0$ and $a_1$
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Optimization of the parameters $t_0$ and $a_1$

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:**

- \( a_1 = 0.00 \) \( t_0 = 0.1430 \)
- \( a_1 = 0.14 \) \( t_0 = 0.0724 \)
- \( a_1 = 0.25 \) \( t_0 = 0.1094 \)
- \( a_1 = 0.33 \) \( t_0 = 0.1215 \)
- \( a_1 = 0.45 \) \( t_0 = 0.1298 \)
Results for different actions

Harmonic oscillator \((T = 0.2)\)

- \(\bullet \rightarrow \text{PA} \ (M = 512)\)
- \(\square \rightarrow \text{TIA} \ (M = 128)\)
- \(\triangle \rightarrow \text{Chin-}t_0 \ (M = 6)\)
- \(\diamond \rightarrow \text{Chin-} (t_0, a_1) \ (M = 4)\)
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

... 

H₂ drop with 22 molecules

\( T = 1.0 \text{ K} \)

Liquid \(^4\)He

\( T = 0.8 \text{ K} \)

The lines correspond to 6th order fits:

\[
E/N = (E/N)_0 + A(1/M)^6
\]
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 $\epsilon \to 0$. 

<table>
<thead>
<tr>
<th></th>
<th>Cost per bead</th>
<th>Reduction # beads</th>
<th>Performance factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>PA</td>
<td>1.0</td>
<td>1</td>
<td>1.0</td>
</tr>
<tr>
<td>TIA</td>
<td>2.9</td>
<td>4</td>
<td>1.4</td>
</tr>
<tr>
<td>Chin-$t_0$</td>
<td>4.8</td>
<td>38</td>
<td>7.9</td>
</tr>
<tr>
<td>Chin-$(t_0, a_1)$</td>
<td>7.2</td>
<td>58</td>
<td>8.0</td>
</tr>
</tbody>
</table>
Symmetrization: sampling of permutations

- At very low temperatures $T \sim T_c$ it is necessary to introduce the correct quantum statistics
Symmetrization: sampling of permutations

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- For bosons the action must be symmetric

$$\rho_B(\mathbf{R}_0, \mathbf{R}_1; \beta) = \frac{1}{N!} \sum_P \rho(\mathbf{R}_0, P\mathbf{R}_1; \beta)$$
Symmetrization: sampling of permutations

- At very low temperatures $T \approx T_c$ it is necessary to introduce the correct quantum statistics
- For bosons the action must be symmetric

$$\rho_B(R_0, R_1; \beta) = \frac{1}{N!} \sum_P \rho(R_0, PR_1; \beta)$$

- 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

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

A staging chain is constructed connecting the bead J of atom 2 with the bead J+m of atom 1
Searching for permutations (Ceperley)

1. Transition probabilities table
   \[ t_{i\alpha,j\alpha+m} = \exp\left(-\left(r_{i\alpha} - r_{j\alpha+m}\right)^2/(4m\lambda\epsilon)\right) \]

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 (\textit{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 (\textit{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 \( \implies \) 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 $^4\text{He}$
Results for bulk $^4$He

![Graph showing the relationship between E/N (K) and T (K) for bulk $^4$He.]
Results for bulk $^4$He

![Graph showing results for bulk $^4$He with experimental (Expt) and PIMC data points.](image)
Results for bulk $^4$He
Small $^4$He drops
Small $^4$He drops
Small $^4$He drops

![Graph showing the density profile $\rho(r)$ as a function of the distance $r$ for different temperatures $T$. The graph includes curves for $T=0.00$, $T=0.25$, $T=0.75$, $T=1.25$, $T=1.75$, $T=2.00$, and $T=2.25$. The x-axis represents $r$ in Å, and the y-axis represents $\rho(r)$ in Å$^{-3}$. The colors correspond to different temperatures, with $T=0.00$ in yellow, $T=0.25$ in red, $T=0.75$ in green, $T=1.25$ in blue, $T=1.75$ in magenta, $T=2.00$ in orange, and $T=2.25$ in gray.]
Towards the ground state: PIGS

- The PIMC formalism can be extended to the limit $T \to 0 \implies$ 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)

  \[ G(R, R'; \tau) = \rho(R, R'; \beta) \]

and use the convolution property of $\rho$.

- **Difference**: In PIMC one forces periodic boundary conditions in imaginary time required by taking the trace of $\rho$ (*closed chains*); in PIGS one truncates the path by inserting trial wave functions $\psi_T$ (*open chains*).
Towards the ground state: PIGS

- Expectation values

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

⇒ For \(\tau_0 = 0\), one recovers the mixed estimator of DMC

⇒ 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

\[
\langle O \rangle = \frac{\int [\prod_{i=0}^{M} dR_i] O(R_{M/2}) \psi_T(R_0) [\prod_{i=0}^{M-1} \rho(R_i, R_{i+1}; \Delta \tau)] \psi_T(R_M)}{\int [\prod_{i=0}^{M} dR_i] \psi_T(R_0) [\prod_{i=0}^{M-1} \rho(R_i, R_{i+1}; \Delta \tau)] \psi_T(R_M)}
\]
Towards the ground state: PIGS

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

![Graph showing the dependence of $E/N$ 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 \((^4\text{He}, \text{H}_2)\)

- 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 \(\epsilon\)
Conclusions

- Easier, general and with a more clear dependence with $\epsilon$ 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!