

Classical and Quantum MC

- In a classical system, the momenta \mathbf{p}_i and the coordinates \mathbf{x}_i are independent (commuting) variables. They can be sampled simultaneously.
- In a quantum system, the momenta and coordinates have non-trivial commutation relations. The partition function \mathcal{Z} is still defined as the sum over all states of the system weighted by the inverse temperature β .

$$\mathcal{Z} = \sum_i \exp -\beta E_i \langle \Psi_i | \Psi_i \rangle \quad (1)$$

Path Integrals

Expectation values are defined as:

$$\langle O \rangle = \sum_i \exp -\beta E_i \langle \Psi_i | O | \Psi_i \rangle.$$

where for the moment we are assuming Boltzmann (distinguishable) particles.

This expression is not very useful unless we know all the states $|\Psi_i\rangle$.

It can be converted to a path integral, though (see Feynman's thesis).

Path Integrals

The quantum partition function can be rewritten as:

$$\mathcal{Z} = \int d\mathbf{x}_1 \dots d\mathbf{x}_n \langle \mathbf{x}_0 | \exp[-H\beta/N] | \mathbf{x}_1 \rangle \dots \langle \mathbf{x}_1 | \exp[-H\beta/N] | \mathbf{x}_0 \rangle,$$

where the \mathbf{x}_i are the positions of all the particles in the system.

- Here we do not need all the states, only the high-T expansion
- $\langle \mathbf{x} | \exp[-H\tau] | \langle \mathbf{x}' \rangle \approx \exp[-V(\mathbf{x})\tau/2] \langle \mathbf{x} | \exp[-T\tau] | \mathbf{x}' \rangle \exp[-V(\mathbf{x}')\tau/2]$
- $\langle \mathbf{x} | \exp[-T\tau] | \mathbf{x}' \rangle = \mathcal{N} \exp(-(\mathbf{x} - \mathbf{x}')^2/[4\frac{\hbar^2}{2m}\tau])$
- The number of steps on the path N must be 'large enough'..
- It is possible to use exact two-body propagators and fewer steps N .

Quantum Monte
Carlo:
Zero/Finite T
and
Bosons/Fermions

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Quantum versus
Classical Monte
Carlo

Path Integrals

Zero
Temperature:
Path Integral
Ground State

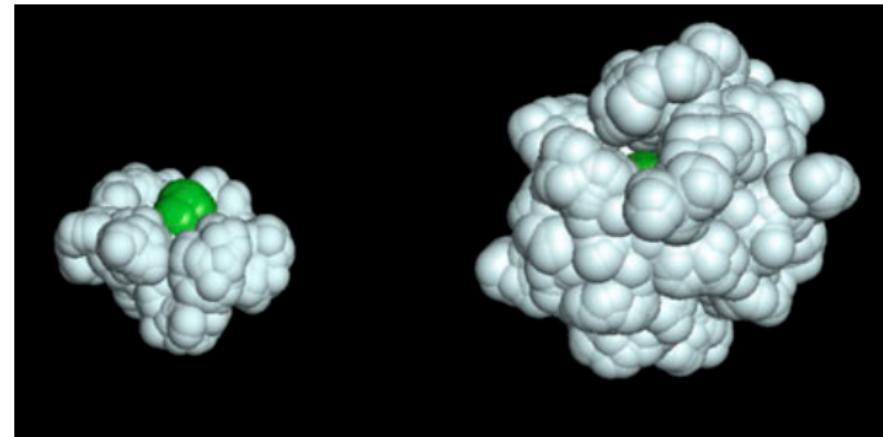
Diffusion Monte
Carlo: Bosons

Fermions

Fixed Node

Path Integrals

Examples:



10 (left) and 40 (right) He atoms around a Calcium atom.

from Rocio Rodriguez-Cantano, et. al.,
Path Integral investigations on doped helium clusters,
International Reviews in Physical Chemistry 35, 37 (2016).

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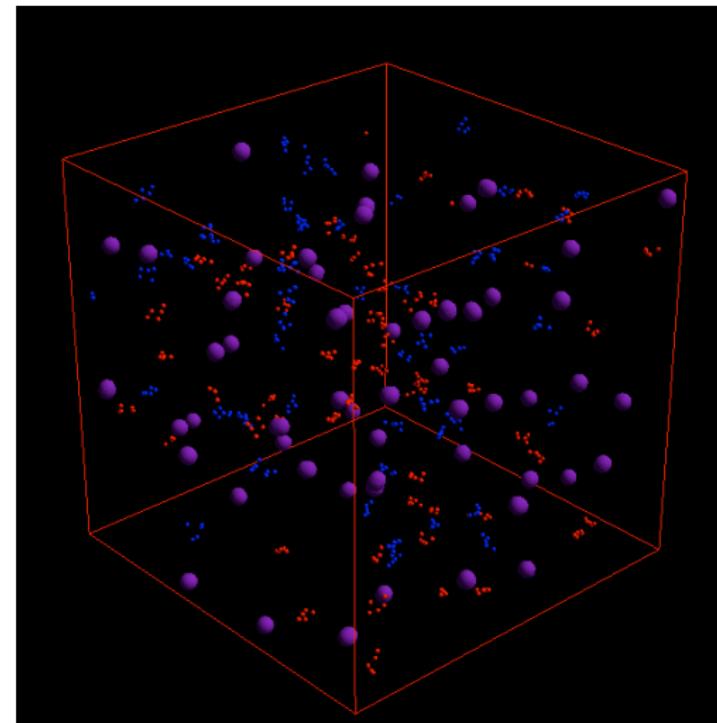
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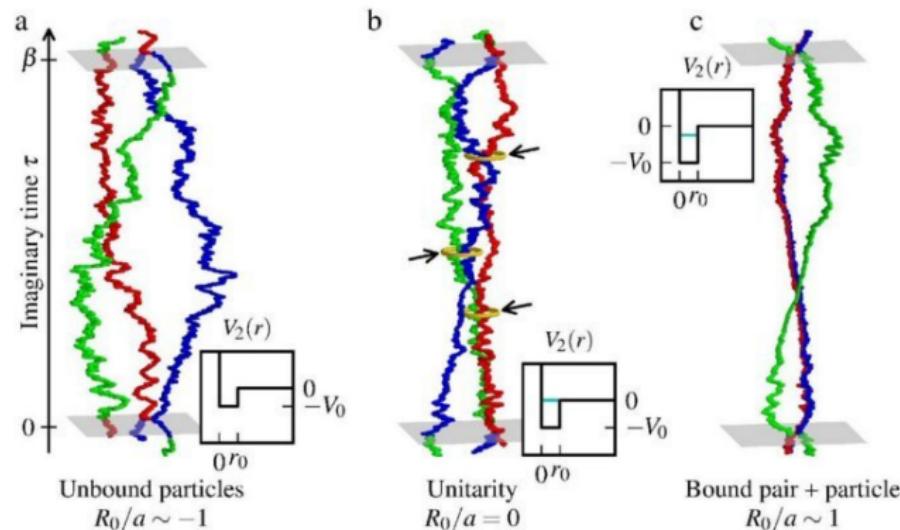


from code used to for OCP in neutron star crust:
Abbar, Carlson, Duan, and Reddy, PRC 2015.

Zero Temperature: Path Integral Ground State

- In the limit $T \rightarrow 0$, the paths become infinitely long.
- We are interested in stationary states with good quantum numbers.
- These will have no dependence on the 'time' in the simulation.
- Add a 'trial' wave function on both ends and construct a path
- For 'large enough' τ_1 and τ_2 , we get the ground state expectation value
- This is called 'path-integral ground state', can sample with Metropolis.
- The trial wave function Ψ_T encodes the symmetries (boson/fermions), etc.) and the quantum numbers of the state.

Three bosons



from S. Piatecki and W. Krauth Efimov-driven phase transitions of the unitary Bose gas Nature Communications 5, 3503 (2014)

Path Integral Ground State

- The paths can be sampled with Metropolis Monte Carlo using a weight:
- $W(\mathbf{x}_i) = \langle \Psi^\dagger(\mathbf{x}_0) | \prod_{i=0}^N [G(\mathbf{x}_i, \mathbf{x}_{i+1}; \delta\tau)] | \Psi(\mathbf{x}_N) \rangle$
- For general expectation values, we can insert operators anywhere as long as τ_1 and τ_2 are 'large enough'.
- 'Large enough' is related to the size of the gap in the spectrum
- For the Hamiltonian (or if we have accurate $|\Psi_T\rangle$), we can move the expectation value to one end of the path.

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Diffusion Monte Carlo for Many Bosons

- For bosons the wave function should be symmetric with respect to interchange
- The ground state for distinguishable particles is the same as that for Bosons in general (assuming the same interaction).
- Diffusion Monte Carlo is a Markov Chain Monte Carlo algorithm (no history)
- The Diffusion Monte Carlo algorithm described on Tuesday carries over for many-particle systems.

Path Integral Ground state versus Diffusion Monte Carlo

Path Integral Ground State uses Metropolis Monte Carlo to sample:

$$P(\mathbf{x}_i) = \langle \Psi_T | (\mathbf{x}_0) \rangle \prod_i \langle \mathbf{x}_i | \exp[-H\delta\tau] | \mathbf{x}_{i+1} \rangle \langle (\mathbf{x}_N | \Psi_T \rangle \quad (2)$$

Diffusion Monte Carlo uses Markov Chain Monte Carlo with branching to sample:

$$P(\mathbf{x}_i) \langle \langle \Psi_T | (\mathbf{x}_0) \rangle \rangle^2 \prod_i \langle \mathbf{x}_i | \exp[-H\delta\tau] | \mathbf{x}_{i+1} \rangle \frac{\langle (\mathbf{x}_{i+1} | \Psi_T \rangle}{\langle \mathbf{x}_i | \Psi_T \rangle} \quad (3)$$

- These are the same paths, only the sampling algorithm is different.
- DMC can calculate 'true' expectation values by remembering the history of each path for a 'long enough' time.
- Metropolis Monte Carlo is free from biases of branching (finite population).
- Diffusion Monte Carlo may be able to more efficiently sample the space.

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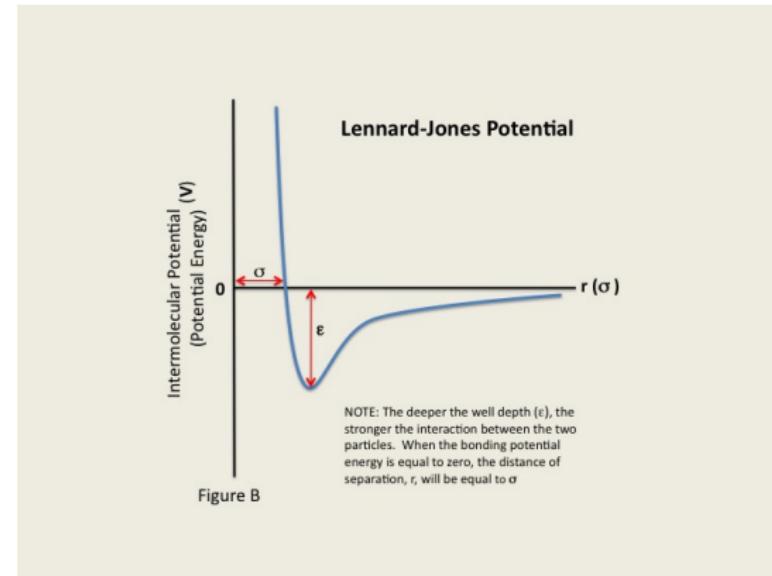
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Example: Bose Liquid w/ Lennard Jones potential



- Consider a system with a Lennard-Jones potential:
- $V(r) = 4c[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^6]$
- Simple model potential used to simulate quantum liquids

Bose Liquid

A reasonable trial wave function for the liquid state is:

$$|\Psi_T\rangle = \prod_{i < j} f^c(r_{ij}) |\Phi\rangle,$$

where $|\Phi\rangle = 1$ for this simple case. Typically $|\Phi\rangle$ is a mean-field solution (e.g. Gross-Pitaevski). The 'Jastrow' correlation $f^c(r_{ij})$ depends only upon the distance between the two particles. It keeps two particles from overlapping.

- The ground state wave function is positive definite (no sign problem).
- This wave function supports a finite condensate fraction (particles with zero momenta).
- In liquid 4He the condensate fraction at equilibrium density is a bit below 10%.
- Cold Bose Atomic gases typically have weakly repulsive interactions and a condensate fraction near 100%.

Momentum Distribution and Condensate Fraction

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- The momentum distribution of particles is given by
- $n(\mathbf{k}) = \langle \Psi(x'_1, x_2, \dots) \exp[i\mathbf{k} \cdot (x'_1 - x_1)] | \Psi(x_1, x_2, \dots) \rangle$
- This is a simple average of the off-diagonal one-body density matrix
- The momentum distribution is normalized $\int d\mathbf{k} n(\mathbf{k}) = 1$
- The second moment is the kinetic energy.
- The condensate fraction is $n(\mathbf{k}) = 0$.

How can one obtain information about the momentum distribution?
What would be a good wave function in the solid regime? What
would be the condensate fraction in the solid?

VMC and DMC for Many Fermions

- For Fermions a reasonable trial function for a system with a similar interaction (liquid 3He) is:
- $|\Psi_T\rangle = \prod_{i < j} f^c(r_{ij}) |\Phi\rangle$,
- where now $|\Phi\rangle$ is a Slater determinant or a sum of Slater determinants.
- A Slater determinant is an anti-symmetrized product of single particle states:
- $|\Phi\rangle = \mathcal{A} \prod_i [\phi_i(\mathbf{x}_i)]$
- The square of the wave function is positive definite, so VMC works just like for bosons.
- DMC is different, though (see below).

Many Fermions (VMC)

- For unpolarized systems with two spin components (liquid 3He, electrons,...) we have the product of two determinants $|\Phi\rangle$
- These can be evaluated in the simulation as determinant
- The determinants have columns labeled by the state (eg. momentum states) and rows by the particle number
- The computer time is of order N^3 for a full evaluation.

$$\Psi = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) & \cdots & \phi_1(\mathbf{r}_N) \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) & \cdots & \phi_2(\mathbf{r}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(\mathbf{r}_1) & \phi_N(\mathbf{r}_2) & \cdots & \phi_N(\mathbf{r}_N) \end{vmatrix}$$

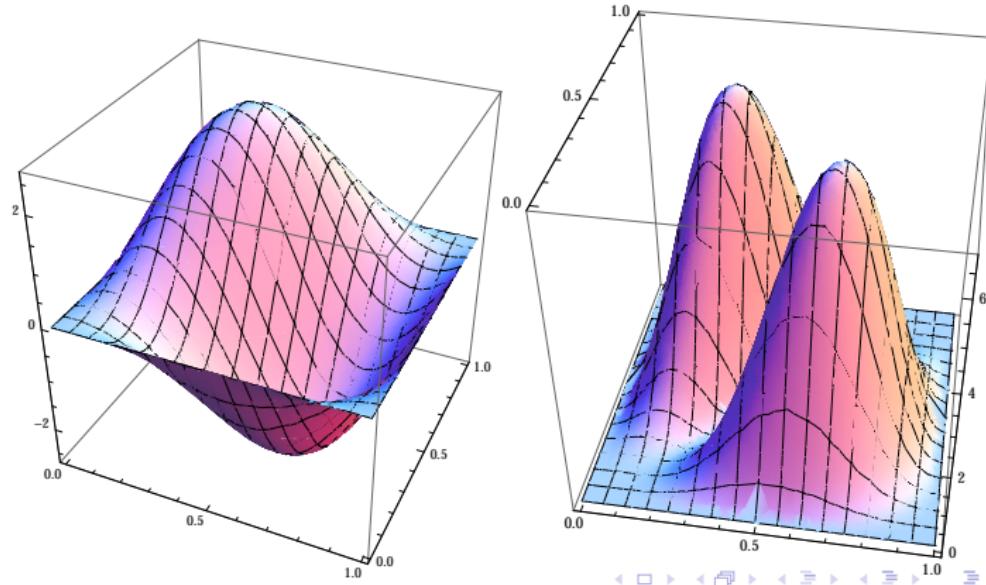
- Faster to update one column at a time (move one particle in VMC).

DMC for Fermions

- For fermions the wave function is not positive definite.
- Therefore it cannot be used as an importance function
- Simple Example: particles in a one-dimensional box
- Slater determinant over one particle momentum states (here 3 particles):
 - $\phi_1 = 1$
 - $\phi_2 = \cos(2\pi x)$
 - $\phi_2 = \sin(2\pi x)$
- All particles within $0 < x < 1$ (periodic boundary conditions).
- $|\Phi\rangle = \text{Det}|\phi_i x_j|$
- Take importance function $\Psi_G = 1$ for now.

Fermions

- This wave function has total momentum zero.
- Rearrangement of $1, \exp[ikx], \exp[-ikx]$.
- Wvfn simplifies to $\sin[\pi(x_1 - x_2)] \sin[\pi(x_1 - x_3)] \sin[\pi(x_2 - x_3)]$
- Sign of wave function determined by permutations (even or odd)
- Always true in one dimension
- Can plot vs $x_{12} = x_1 - x_2$ and $x_{13} = x_1 - x_3$



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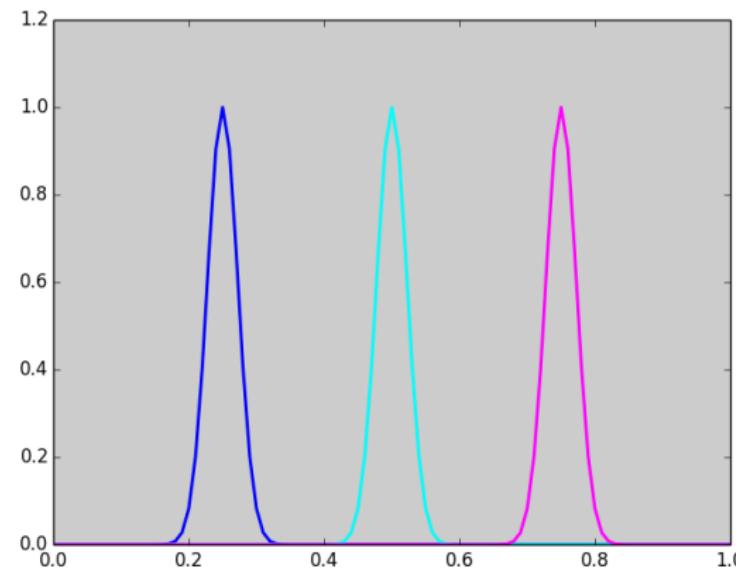
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Fixed Node

Start with 3 fermions at specific locations in the box (this defines the initial sign).



After some point all interchanges are equally possible. Converging to boson (Boltzmann) solution.

Fermions

- There are some 'special' problems that can be treated with no sign problem, usually with auxiliary field techniques.
- Examples are attractive Hubbard model (cold atoms), Shell model with attractive interactions, SU(4) symmetric systems, ...
- Otherwise, we can use standard algorithm (with a positive definite importance function) for some finite imaginary time τ .
- Statistical errors will increase with τ , problem gets worse with system size.
- The exchange of one pair of fermions in a large system will change the overall sign.
- Need to understand something about the excitations of the system to judge convergence.
- We want $E(\text{gap}) \tau \gg 1$.

Fermions: Fixed Node

- The Fixed Node method provides a Hamiltonian that provides an approximate solution for Fermi systems.
- This approximate solution provides an upper bound to the true energy.
- It is possible to optimize the solution by trying different nodes
- Simple implementation: Hard-Wall Boundary condition when $\Psi_T = 0$.
- The node is a surface in $3N-1$ dimensional space, we are solving for the best (lowest energy) state with that nodal surface.
- Because the constraint is in a lower dimensional space, the solution is often quite accurate.

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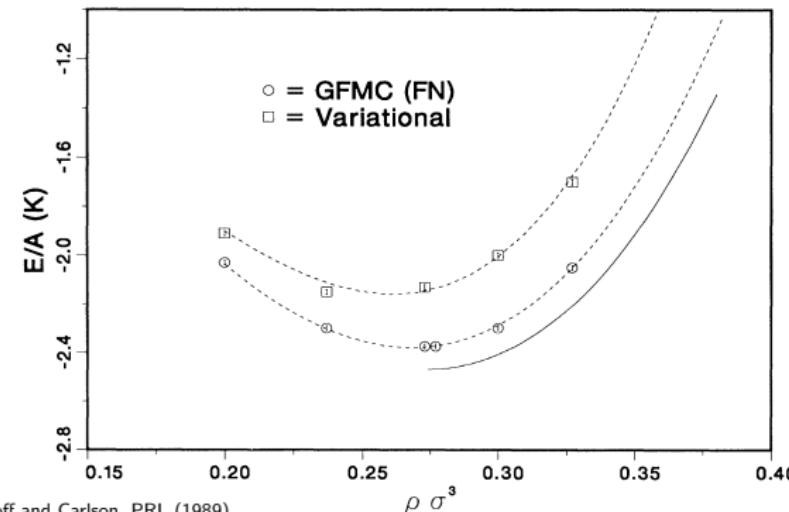
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Fixed Node

Fixed Node: Liquid 3He

- Compare Variational (upper curve), Fixed Node (middle curve), and 'Released Node' or 'Transient Estimation' (lower curve):
- The fixed-node results include "backflow" effects:
 $r_j \rightarrow r_j + \sum_{i \neq j} \eta(r_{ij}) \mathbf{r}_{ij}$
- Three-body correlations (always positive) also included in VMC
- Kinetic energy per particle is ≈ 12



from R. M. Panoff and Carlson, PRL (1989).

Fixed Node: Cold Atoms at Unitarity

- Cold Fermi Atoms have an interaction range \ll the interparticle spacing
- The strength of the interaction can be tuned to infinite scattering length (zero energy bound state in the two-body system).
- For example, $V = -\frac{2}{\mu} \frac{\mu^2}{\cosh^2(\mu r)}$, for large μ .
- The ground state energy is a constant (the Bertsch parameter ξ) times the Free Fermi Gas Energy ($= \frac{3}{5} \frac{\hbar^2}{2m} k_F^2$ for any density).
- For a free-particle Slater determinant the fixed-node result is ≈ 0.54
- Optimized BCS fixed-node results give $\xi \approx 0.38$.
- The exact result is $\xi \approx 0.370(5)$