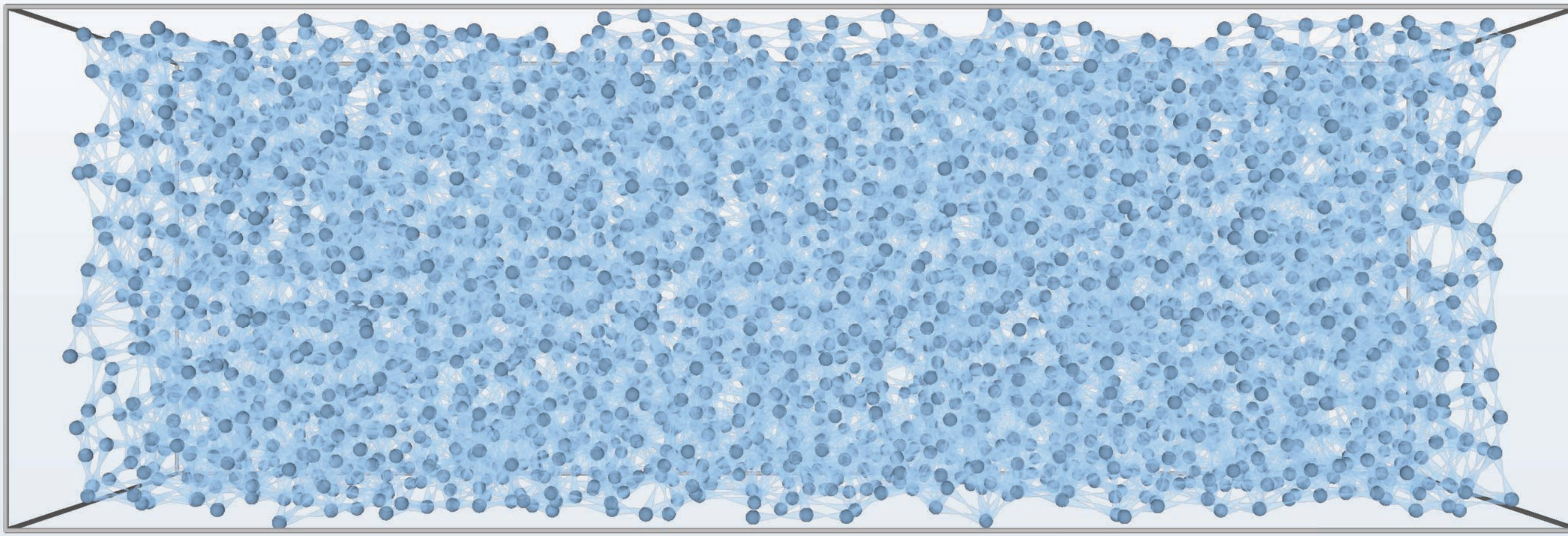
Monte Carlo Methods for Quantum Liquids

Simulating Itinerant Quantum Particles in the Spatial Continuum

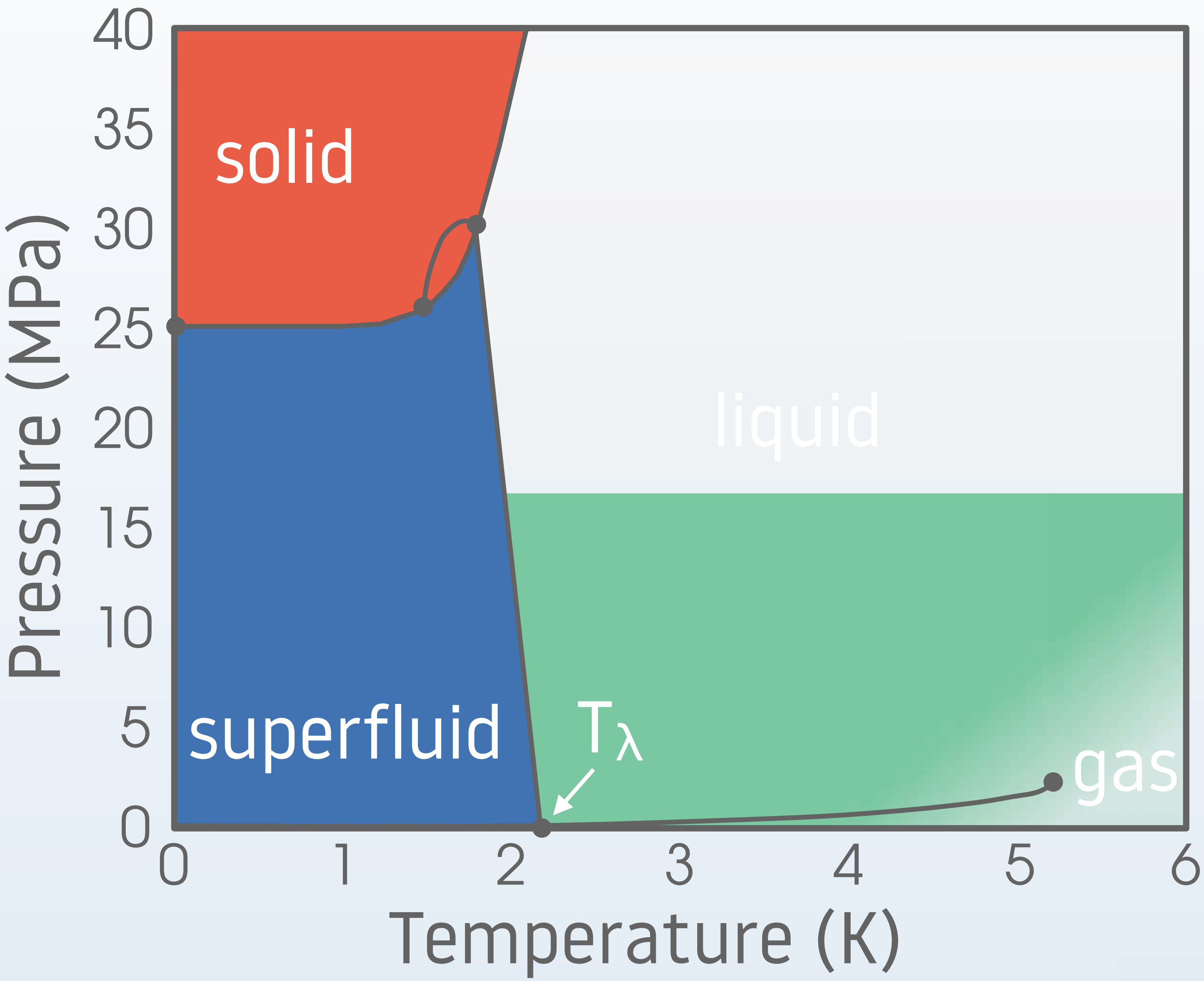


Quantum Information meets Many-body Physics: Entanglement, Thermalization and Chaos

Adrian **Del Maestro**
University of Vermont
https://github.com/agdelma

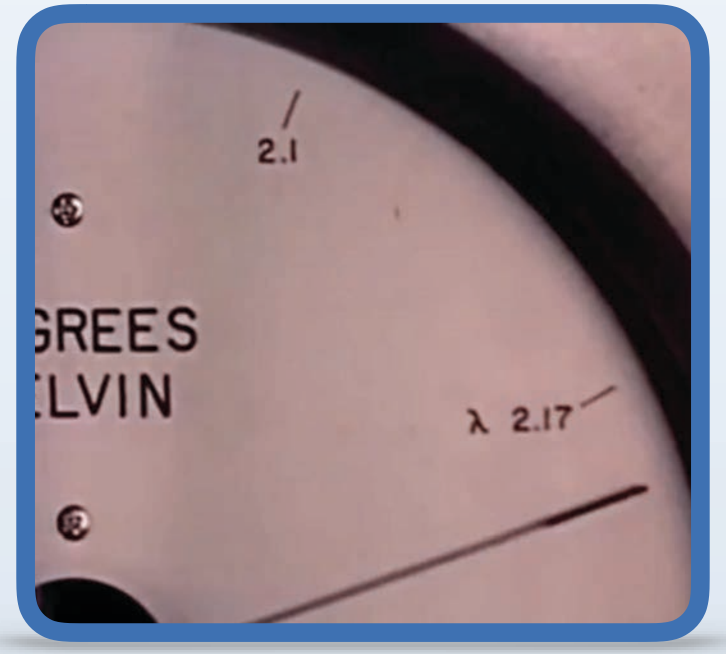

He

Helium-4 is a Quantum Liquid



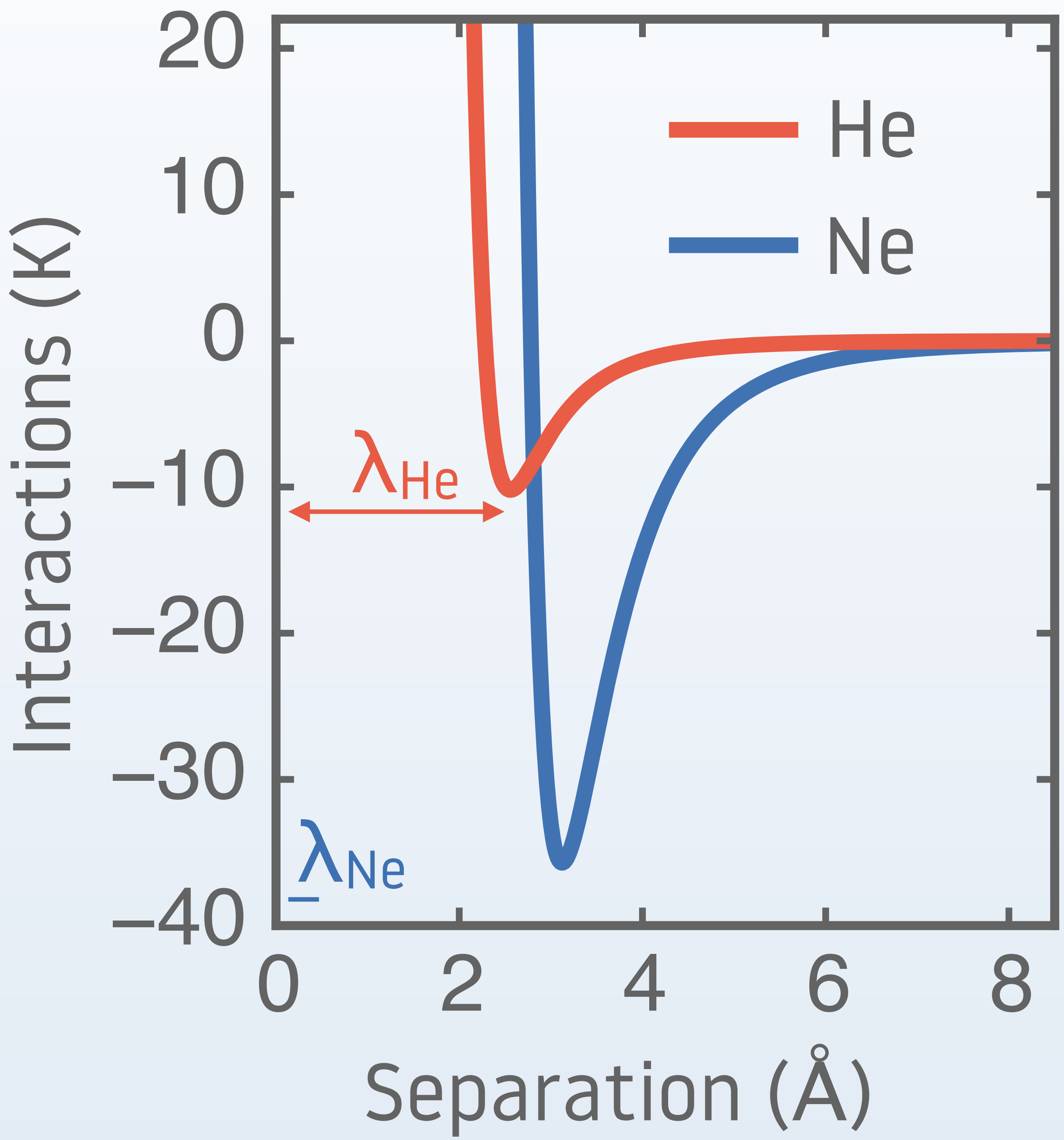
Superfluid is a fundamentally quantum state of matter

- dissipationless flow
- quantized vortices
- non-entropic flow



P. Kapitsa; J. Allen and A.D. Misener (1938)

What Makes ^{4}He so Quantum?



$$\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}}$$

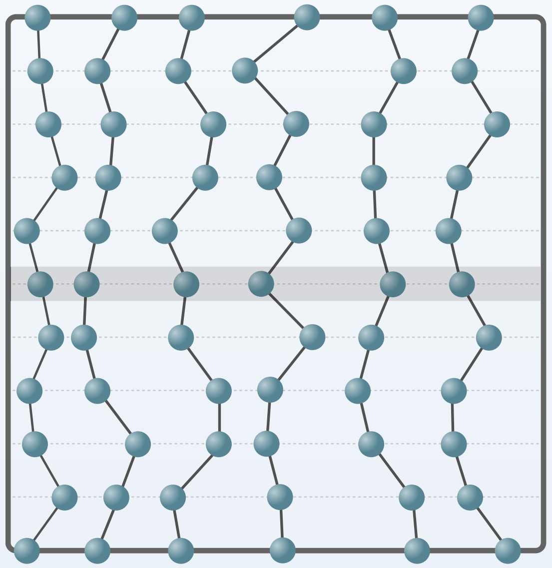
Helium-4 is the only atomic bosonic system with $\lambda_{dB} \sim r_s$ at T ~ O(1 K)

Superfluid ^4He is a macroscopic quantum phase of matter!

Can we simulate it efficiently on a classical computer?

Quantum Liquids

- General formulation of itinerant particles with strong interactions
- Trial wavefunctions
- Variational Monte Carlo

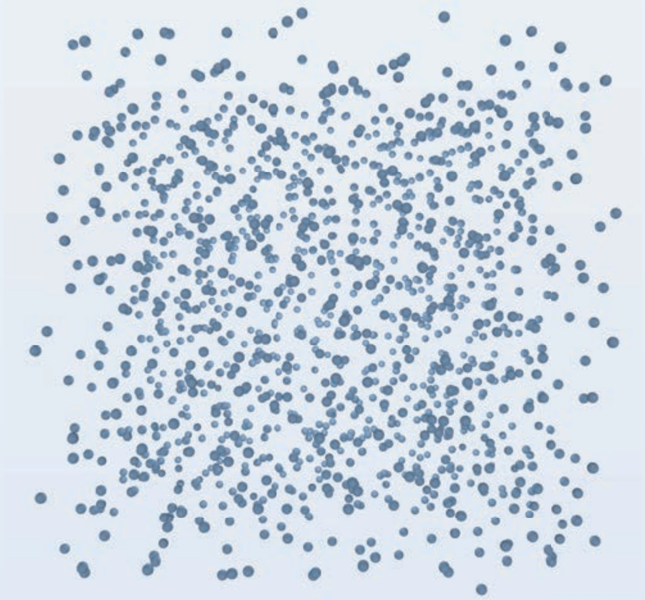


Ground State Quantum Monte Carlo

- Introduction to projector methods
- Elimination of systematic bias from a trial wavefunction
- Imaginary time propagator in the position representation
- Estimators

Some results for helium

- PIGS for the energy and structural properties



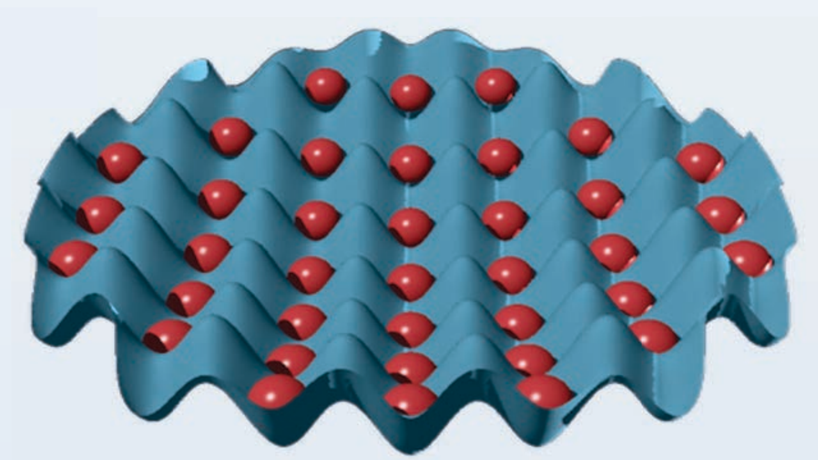
A General Description

N interacting particles in the spatial continuum

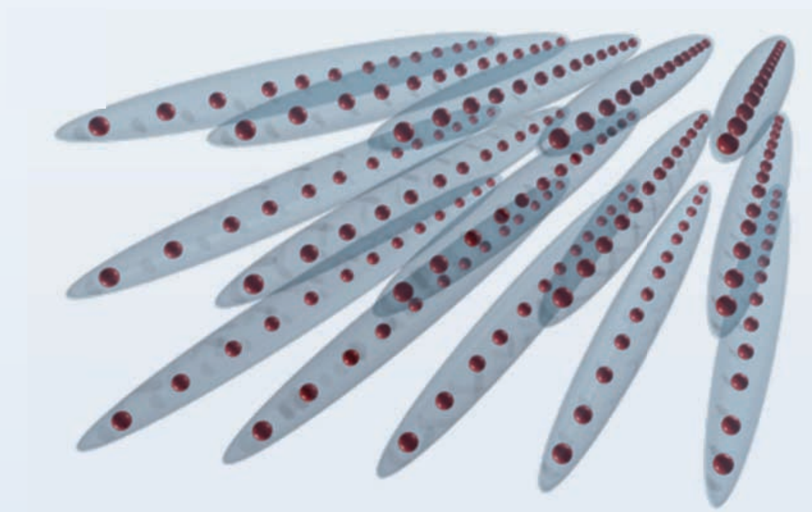
$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \hat{\nabla}_i^2 + \sum_{i=1}^{N} \hat{\mathcal{V}}_i + \sum_{i<j} \hat{\mathcal{U}}_{ij}$$

external potential

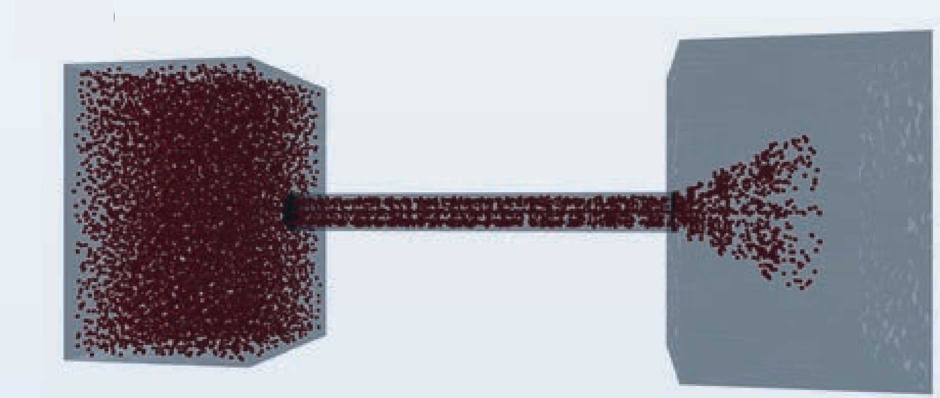
interaction potential



trapped neutral atoms in a periodic lattice



quasi-1d Bose gases



confined high-density superfluids

Measurement of Observables

We are interested in measuring the expectation value of some operator corresponding to an observable

Ground State: $$\langle \hat{O} \rangle = \frac{\langle \Psi_0 | \hat{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \qquad \hat{H} \, |\Psi_0\rangle = E_0 \, |\Psi_0\rangle$$

Finite Temperature: $$\langle \hat{O} \rangle = \frac{\mathrm{Tr} \, \hat{O} \, e^{-\beta \hat{H}}}{\mathrm{Tr} \, e^{-\beta \hat{H}}} \qquad \beta = \frac{1}{k_B T}$$

Z partition function

Variational Monte Carlo I

Can get an upper bound on the ground state energy by guessing a trial wavefunction with non-zero overlap with Ψ_0

1. Construct a trial N-particle wavefunction which depends on Q variational parameters

$$\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R}) \qquad \boldsymbol{\alpha} = \{\alpha_1, \ldots \alpha_Q\} \qquad \boldsymbol{R} = \{\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N\}$$

2. Evaluate the expectation value of the energy

$$E = \frac{\left\langle \Psi_T^{\boldsymbol{\alpha}} \middle| \hat{H} \middle| \Psi_T^{\boldsymbol{\alpha}} \right\rangle}{\left\langle \Psi_T^{\boldsymbol{\alpha}} \middle| \Psi_T^{\boldsymbol{\alpha}} \right\rangle} \geq E_0$$

high dimensional integrals

3. Vary the parameters **α** until a minimum is identified

Variational Monte Carlo II

The trial wavefunction is usually small in large regions of configuration space. Can use Metropolis method to efficiently sample only those regions where the wavefunction is large.

Local Energy: $$E_L^{\boldsymbol{\alpha}}(\boldsymbol{R}) = \frac{\hat{H}\,\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})}{\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})}$$

only need to know the action of H on the trial wavefunction (assume real)

$$E = \frac{\int \mathcal{D}\boldsymbol{R}\,\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})\,\hat{H}\,\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})}{\int \mathcal{D}\boldsymbol{R}\,[\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})]^2}$$

$$\int \mathcal{D}\boldsymbol{R} \equiv \prod_{i=1}^{N} \int \mathrm{d}^d r_i$$

$$= \frac{\int \mathcal{D}\boldsymbol{R}\left[\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})\right]^2 E_L^{\boldsymbol{\alpha}}(\boldsymbol{R})}{\int \mathcal{D}\boldsymbol{R}\,[\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})]^2} = \int \mathcal{D}\boldsymbol{R}\,\pi^{\boldsymbol{\alpha}}(\boldsymbol{R}) E_L^{\boldsymbol{\alpha}}(\boldsymbol{R})$$

stationary distribution: $$\pi^{\boldsymbol{\alpha}}(\boldsymbol{R}) = \frac{\left[\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})\right]^2}{\int \mathcal{D}\boldsymbol{R}\left[\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R})\right]^2}$$

Variational Monte Carlo III

Example: 1d simple harmonic oscillator $\hat{H} = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}x^2$

exact: $\Psi_0(x) = \mathrm{e}^{-x^2/2}$ $E_0 = \frac{1}{2}$

trial: $\Psi_T^\alpha(x) = \mathrm{e}^{-\alpha x^2}$

$$E_L^\alpha(x) = \frac{\hat{H}\,\Psi_T^\alpha(x)}{\Psi_T^\alpha(x)}$$

← local energy

$$= \alpha\left(\mathrm{e}^{-\alpha x^2} - 2\alpha x^2 \mathrm{e}^{-\alpha x^2}\right) + \frac{x^2}{2}\mathrm{e}^{-\alpha x^2}$$

$$= \alpha + x^2\left(\frac{1}{2} - 2\alpha^2\right)$$

distribution

$$\frac{\pi(x')}{\pi(x)} = \mathrm{e}^{-2\alpha(x'^2 - x^2)}$$

Variational Monte Carlo IV

Trivial to code but efficiency strongly depends on the choice of trial wavefunction

```
initialize walkers at random positions
for 1…number_MC_steps
    for 1…number_walkers
        select walker and update position R → R'
        compute p = [Ψ_T^α(R')/Ψ_T^α(R)]^2
        accept new walker with probability min(1,p)
    measure observables
```

where $p = \left[\Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R}') / \Psi_T^{\boldsymbol{\alpha}}(\boldsymbol{R}) \right]^2$

https://github.com/agdelma/qmc_ho

Variational Monte Carlo V

Systematic errors due to the choice of trial wavefunction

suppose $|\Psi_T\rangle = \gamma\,|\Psi_0\rangle + |\delta\Psi\rangle$ with $\langle\Psi_0|\delta\Psi\rangle = 0$

$$O_v = \frac{\langle\Psi_T|\hat{O}|\Psi_T\rangle}{\langle\Psi_T|\Psi_T\rangle}$$ (dropping α dependence)

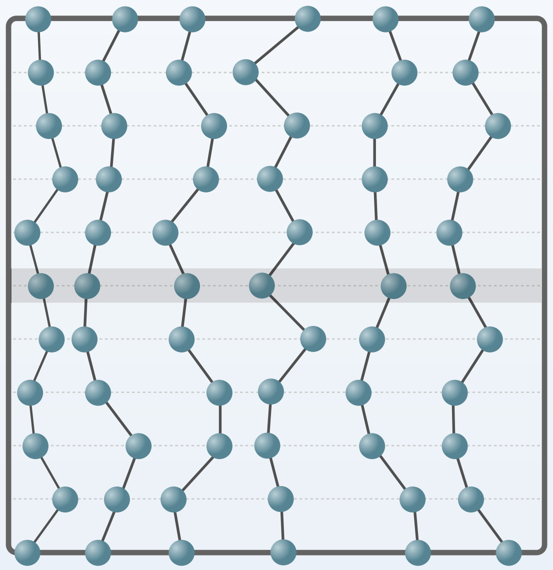
$$= \frac{(\gamma^*\,\langle\Psi_0| + \langle\delta\Psi|)\hat{O}(\gamma\,|\Psi_0\rangle + |\delta\Psi\rangle)}{|\gamma|^2 + \langle\delta\Psi|\delta\Psi\rangle}$$

$$= \frac{|\gamma|^2 O_0 + \gamma^*\,\langle\delta\Psi|\hat{O}|\Psi_0\rangle + \text{h.c.}}{|\gamma|^2 + \langle\delta\Psi|\delta\Psi\rangle}$$

$$\approx O_0 + \frac{2}{\gamma}\,\langle\delta\Psi|\hat{O}|\Psi_0\rangle$$ ⟵ dominates when $[\hat{O},\hat{H}] \neq 0$

Quantum Liquids

- General formulation of itinerant particles with strong interactions
- Trial wavefunctions
- Variational Monte Carlo

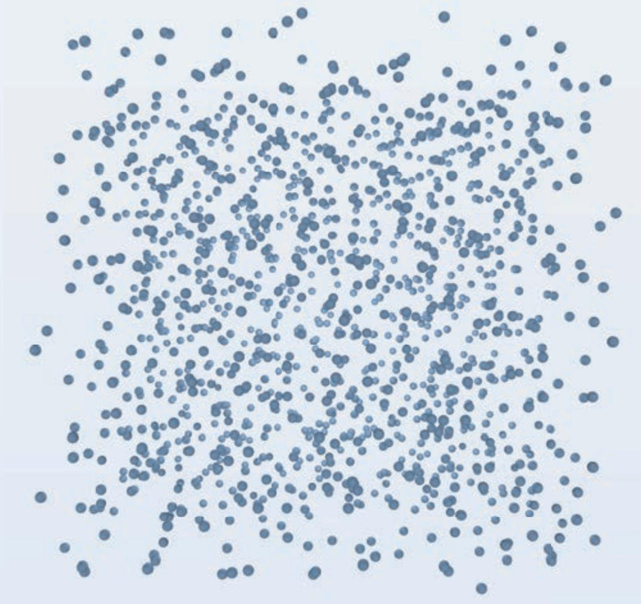


Ground State Quantum Monte Carlo

- Introduction to projector methods
- Elimination of systematic bias from a trial wavefunction
- Imaginary time propagator in the position representation
- Estimators

Some results for helium

- PIGS for the energy and structural properties



General Monte Carlo Formalism

Any Monte Carlo method, classical or quantum, can be constructed by answering 4 basic questions:

1. **Description:** What are the degrees of freedom and energetics that control them?
2. **Configurations:** How can these degrees of freedom be encoded efficiently on a computer?
3. **Observables:** How can the expectation value of operators be measured for the configurations?
4. **Updates:** How can we sample all possible configurations and what is their likelihood?

Path Integral Ground State QMC

Description

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\hat{\nabla}_i^2 + \sum_{i=1}^{N} \hat{\mathcal{V}}_i + \sum_{i<j} \hat{\mathcal{U}}_{ij}$$

N interacting particles in d-dimensions

Configurations

Projecting out the Ground State

Expand the trial wavefunction in the energy eigenstate basis

$$|\Psi_T\rangle = \sum_{j=0}^{\infty} c_j \left|\Psi_j\right\rangle \qquad \text{where} \qquad \hat{H}\left|\Psi_j\right\rangle = E_j \left|\Psi_j\right\rangle$$

apply the imaginary time evolution operator for time τ

$$|\Psi_\tau\rangle \equiv e^{-\tau\hat{H}}|\Psi_T\rangle = \sum_{n=0}^{\infty} \frac{\left(-\tau\hat{H}\right)^n}{n!} \sum_{j=0}^{\infty} c_j \left|\Psi_j\right\rangle = \sum_{n=0}^{\infty}\sum_{j=0}^{\infty} \frac{\left(-\tau E_j\right)^n}{n!} c_j \left|\Psi_j\right\rangle$$

$$= \sum_{j=0}^{\infty} e^{-\tau E_j} c_j \left|\Psi_j\right\rangle$$

exponentially damped for $E_j > E_0$

$$= e^{-\tau E_0}\left[c_0|\Psi_0\rangle + \sum_{j=1}^{\infty} e^{-\tau(E_j - E_0)} c_j \left|\Psi_j\right\rangle\right]$$

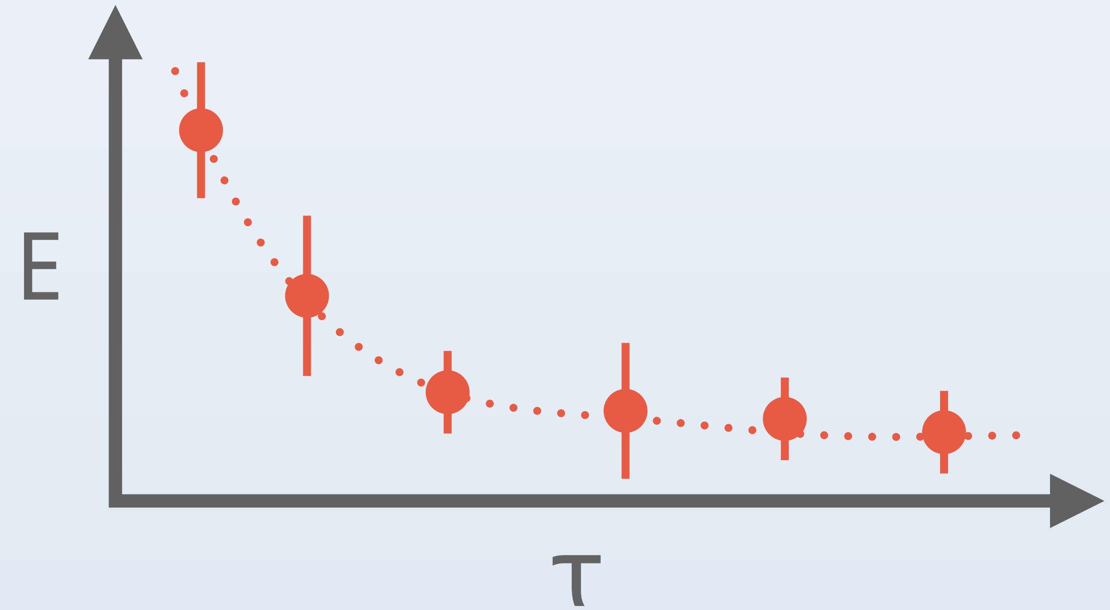
$$\lim_{\tau\to\infty} |\Psi_\tau\rangle \propto |\Psi_0\rangle$$

Elimination of Systematic Bias

For large enough τ we can reduce any systematic bias originating from the trial wavefunction

$$O_\tau = \frac{\langle \Psi_\tau | \hat{O} | \Psi_\tau \rangle}{\langle \Psi_\tau | \Psi_\tau \rangle} \simeq \frac{\langle \Psi_0 | \hat{O} | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle} \qquad \text{for } \tau \gg 1$$

practically we can perform a calculation for different values of τ and try to extrapolate the result. Expect exponential convergence for the energy.



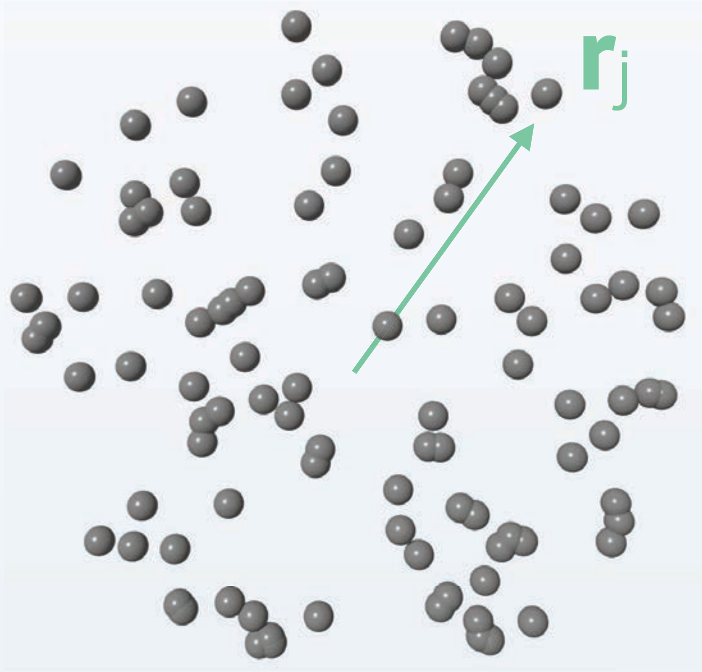
Position Basis

Evaluation of expectation values will employ first quantization in the position representation.

$$|\boldsymbol{R}\rangle = |\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N\rangle$$

$$\Psi_T(\boldsymbol{R}) = \langle \boldsymbol{R}|\Psi_T\rangle$$

$$\int \mathcal{D}\boldsymbol{R} \equiv \prod_{i=1}^{N} \int \mathrm{d}^d r_i$$



$$\Psi(\boldsymbol{R};\tau) = \langle \boldsymbol{R}|\mathrm{e}^{-\tau\hat{H}}|\Psi_T\rangle$$

$$= \int \mathcal{D}\boldsymbol{R}' \, \langle \boldsymbol{R}|\mathrm{e}^{-\tau\hat{H}}|\boldsymbol{R}'\rangle\langle \boldsymbol{R}'|\Psi_T\rangle$$

$$= \int \mathcal{D}\boldsymbol{R}' \, G(\boldsymbol{R},\boldsymbol{R}';\tau)\Psi_T(\boldsymbol{R}')$$

$$\int \mathcal{D}\boldsymbol{R} \, |\boldsymbol{R}\rangle\langle \boldsymbol{R}| = \hat{\mathbb{1}}$$

completeness

propagator / Green function

Expectation Values I

Use the completeness relation to write expectation values in the position basis

$$O_\tau = \frac{\langle \Psi_\tau | \hat{O} | \Psi_\tau \rangle}{\langle \Psi_\tau | \Psi_\tau \rangle}$$

define: $Z(\tau) \equiv \langle \Psi_\tau | \Psi_\tau \rangle$

$$\int \mathcal{D}\boldsymbol{R} \, |\boldsymbol{R}\rangle \langle \boldsymbol{R}| = \hat{\mathbb{1}}$$

$$Z(\tau) = \langle \Psi_T | e^{-\tau \hat{H}} e^{-\tau \hat{H}} | \Psi_T \rangle$$

$$= \int \mathcal{D}\boldsymbol{R} \int \mathcal{D}\boldsymbol{R}' \int \mathcal{D}\boldsymbol{R}'' \langle \Psi_T | \boldsymbol{R} \rangle \left\langle \boldsymbol{R} \middle| e^{-\tau \hat{H}} \middle| \boldsymbol{R}' \right\rangle \left\langle \boldsymbol{R}' \middle| e^{-\tau \hat{H}} \middle| \boldsymbol{R}'' \right\rangle \left\langle \boldsymbol{R}'' \middle| \Psi_T \right\rangle$$

$$= \int \mathcal{D}\boldsymbol{R} \int \mathcal{D}\boldsymbol{R}' \int \mathcal{D}\boldsymbol{R}'' \Psi_T(\boldsymbol{R}) G(\boldsymbol{R}, \boldsymbol{R}'; \tau) G(\boldsymbol{R}', \boldsymbol{R}''; \tau) \Psi_T(\boldsymbol{R}'')$$

The Propagator I

Let's investigate the imaginary time propagator

propagator: $G(\boldsymbol{R}, \boldsymbol{R}'; \tau) = \langle \boldsymbol{R} | e^{-\tau \hat{H}} | \boldsymbol{R}' \rangle$

Hamiltonian: $$\hat{H} = \underbrace{-\sum_{i=1}^{N} \frac{\hbar^2}{2m_i} \hat{\nabla}_i^2}_{\hat{T}} + \underbrace{\sum_{i=1}^{N} \hat{\mathcal{V}}_i + \sum_{i<j} \hat{\mathcal{U}}_{ij}}_{\hat{V}}$$

commutator: $[\hat{T}, \hat{V}] \neq 0 \quad \Rightarrow \quad \boxed{e^{-\tau \hat{H}} \neq e^{-\tau \hat{T}} e^{-\tau \hat{V}}}$

The Propagator II

The imaginary time propagator can be factored using the Campbell-Baker-Hausdorff formula

commutator: $[\hat{T}, \hat{V}] \neq 0 \quad \Rightarrow \quad e^{-\tau \hat{H}} \neq e^{-\tau \hat{T}} e^{-\tau \hat{V}}$

$$e^{-\tau(\hat{T}+\hat{V})} = e^{-\tau \hat{T}} e^{-\tau \hat{V}} e^{\frac{\tau^2}{2}[\hat{T},\hat{V}]+\cdots} \qquad \text{CBH}$$

$$= e^{-\tau \hat{T}} e^{-\tau \hat{V}} + O(\tau^2)$$

problems:

1. we only recover an exact representation of the wavefunction when $\tau \gg 1$
2. the correction term could diverge for some interesting potentials, e.g. δ-interactions

The Propagator III

The Hamiltonian commutes with itself $[\hat{H}, \hat{H}] = 0$

$$e^{-\tau\hat{H}} = e^{-\frac{\tau}{2}\hat{H}} e^{-\frac{\tau}{2}\hat{H}}$$

in the position representation

$$G(\boldsymbol{R}, \boldsymbol{R}'; \tau) = \left\langle \boldsymbol{R} \middle| e^{-\tau\hat{H}} \middle| \boldsymbol{R}' \right\rangle = \left\langle \boldsymbol{R} \middle| e^{-\frac{\tau}{2}\hat{H}} e^{-\frac{\tau}{2}\hat{H}} \middle| \boldsymbol{R}' \right\rangle$$

$$= \int \mathcal{D}\boldsymbol{R}'' \left\langle \boldsymbol{R} \middle| e^{-\frac{\tau}{2}\hat{H}} \middle| \boldsymbol{R}'' \right\rangle \left\langle \boldsymbol{R}'' \middle| e^{-\frac{\tau}{2}\hat{H}} \middle| \boldsymbol{R}' \right\rangle$$

$$= \int \mathcal{D}\boldsymbol{R}'' G\left(\boldsymbol{R}, \boldsymbol{R}''; \frac{\tau}{2}\right) G\left(\boldsymbol{R}'', \boldsymbol{R}'; \frac{\tau}{2}\right)$$

$\tau/2 < \tau$

The Propagator IV

Repeat this procedure M times where $M \in \mathbb{Z}$ and $M \gg 1$

$$e^{\tau \hat{H}} = \left(e^{-\frac{\tau}{M}\hat{H}}\right)^M = \left(e^{-\Delta\tau \hat{H}}\right)^M$$

$$\Delta\tau \equiv \frac{\tau}{M}$$

$\Delta\tau$ can be made arbitrarily small

using this in our propagator:

$$G(\boldsymbol{R}_0, \boldsymbol{R}_M; \tau) = \int \mathcal{D}\boldsymbol{R}_1 \cdots \int \mathcal{D}\boldsymbol{R}_{M-1} G(\boldsymbol{R}_0, \boldsymbol{R}_1; \Delta\tau) \cdots G(\boldsymbol{R}_{M-1}, \boldsymbol{R}_M; \Delta\tau)$$

$$|\boldsymbol{R}_\alpha\rangle \equiv |\boldsymbol{r}_{1\alpha}, \ldots, \boldsymbol{r}_{N\alpha}\rangle$$

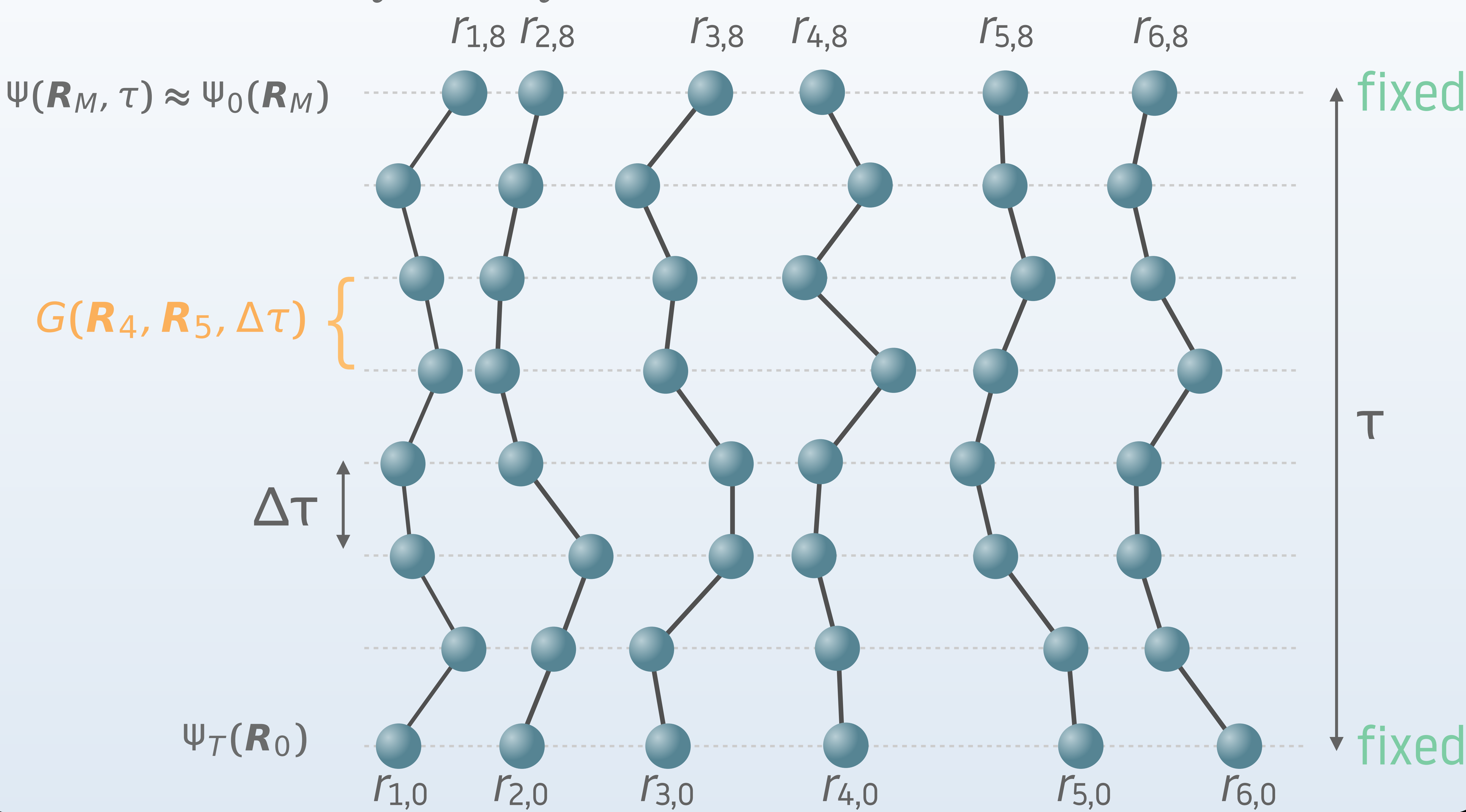
particle positions on an imaginary time slice

G can be written as a path integral describing imaginary time propagation over M discrete time slices between fixed initial and final states

The Propagator V

Visualizing for N = 6, M = 8 in one spatial dimension:

$$G(\boldsymbol{R}_0, \boldsymbol{R}_M; \tau) = \int \mathcal{D}\boldsymbol{R}_1 \cdots \int \mathcal{D}\boldsymbol{R}_{M-1} G(\boldsymbol{R}_0, \boldsymbol{R}_1; \Delta\tau) \cdots G(\boldsymbol{R}_{M-1}, \boldsymbol{R}_M; \Delta\tau)$$



Expectation Values II

Using this expression in our expectation value:

$$O_\tau = \frac{\langle \Psi_\tau | \hat{O} | \Psi_\tau \rangle}{\langle \Psi_\tau | \Psi_\tau \rangle} \qquad Z(\tau) \equiv \langle \Psi_\tau | \Psi_\tau \rangle$$

$$Z(\tau) = \langle \Psi_T | e^{-\tau \hat{H}} e^{-\tau \hat{H}} | \Psi_T \rangle$$

$$G(\boldsymbol{R}_M, \boldsymbol{R}_{2M}; \tau) = \int \mathcal{D}\boldsymbol{R}_1 \cdots \int \mathcal{D}\boldsymbol{R}_{M-1} G(\boldsymbol{R}_M, \boldsymbol{R}_{M+1}; \Delta\tau) \cdots G(\boldsymbol{R}_{2M-1}, \boldsymbol{R}_{2M}; \Delta\tau)$$

$$= \int \mathcal{D}\boldsymbol{R}_0 \int \mathcal{D}\boldsymbol{R}_M \int \mathcal{D}\boldsymbol{R}_{2M}\, \Psi_T(\boldsymbol{R}_0) G(\boldsymbol{R}_0, \boldsymbol{R}_M; \tau) G(\boldsymbol{R}_M, \boldsymbol{R}_{2M}; \tau) \Psi_T(\boldsymbol{R}_{2M})$$

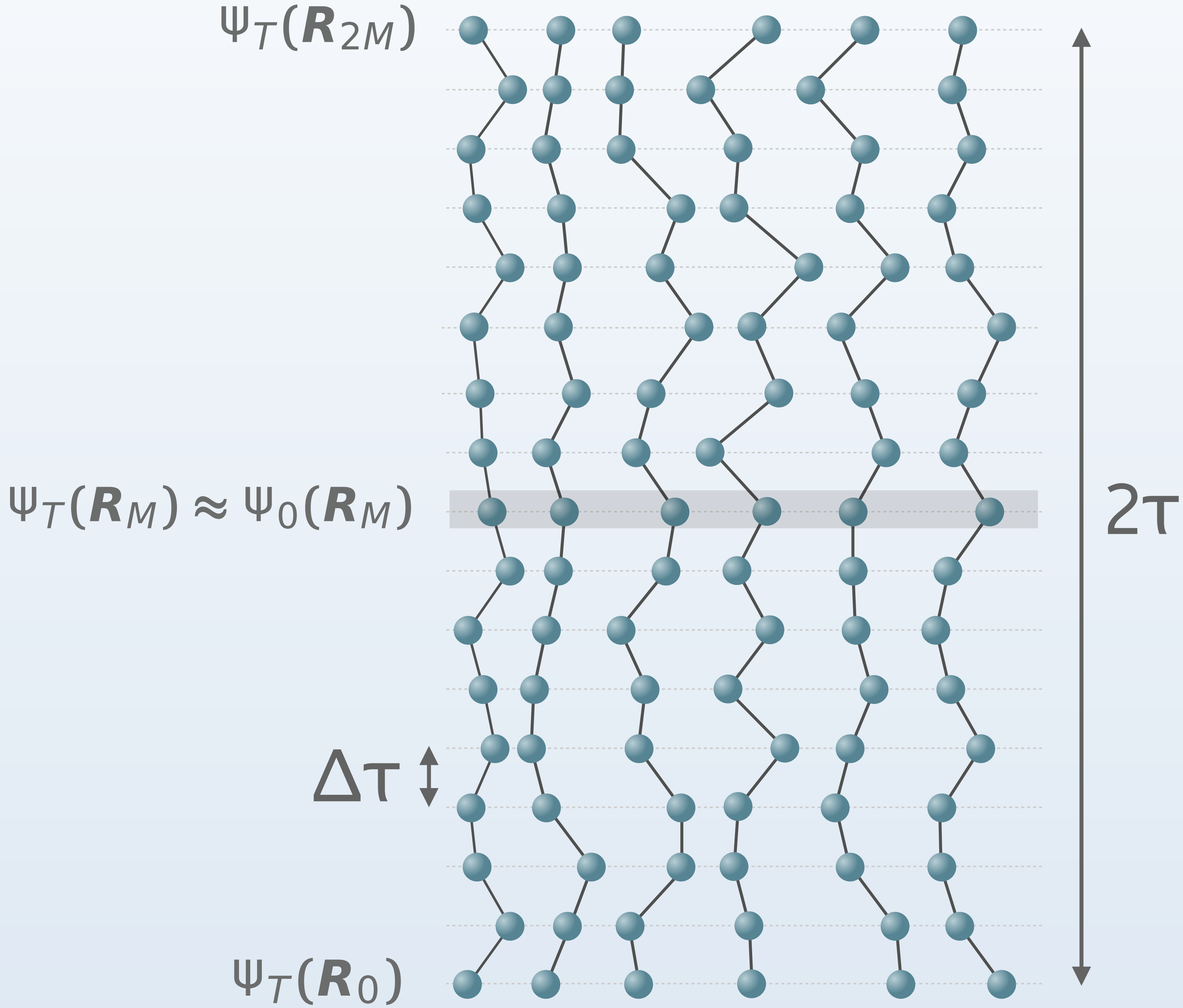
$$G(\boldsymbol{R}_0, \boldsymbol{R}_M; \tau) = \int \mathcal{D}\boldsymbol{R}_1 \cdots \int \mathcal{D}\boldsymbol{R}_{M-1} G(\boldsymbol{R}_0, \boldsymbol{R}_1; \Delta\tau) \cdots G(\boldsymbol{R}_{M-1}, \boldsymbol{R}_M; \Delta\tau)$$

$$= \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha \Psi_T(\boldsymbol{R}_0) \left[\prod_{\alpha=0}^{2M-1} G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) \right] \Psi_T(\boldsymbol{R}_{2M})$$

Expectation Values III

Visualizing the normalization inner product for N = 6, M = 8:

$$Z(\tau) = \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha \Psi_T(\boldsymbol{R}_0) \left[\prod_{\alpha=0}^{2M-1} G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) \right] \Psi_T(\boldsymbol{R}_{2M})$$



2M + 1 total imaginary time slices

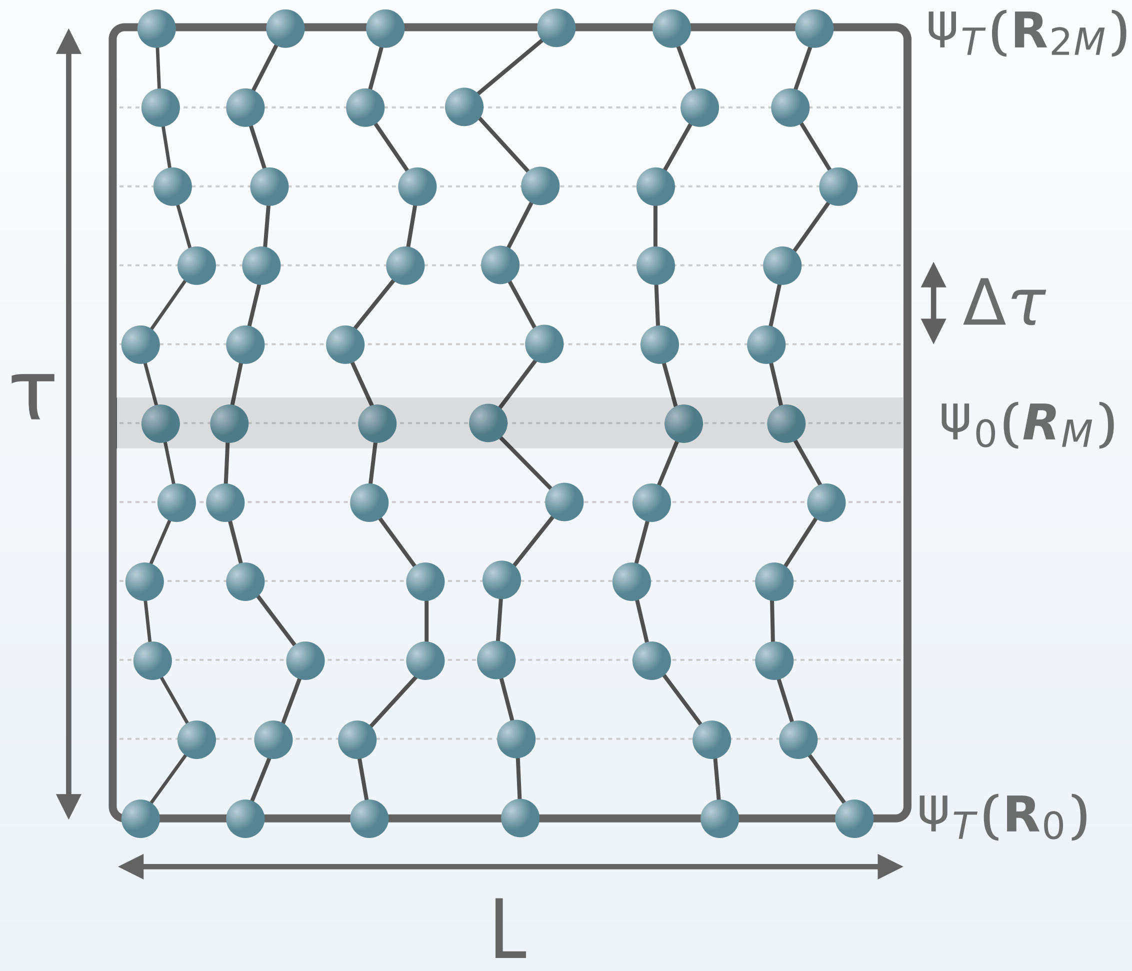
central slice is a representation of the ground state wavefunction

Path Integral Ground State QMC

Description

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\hat{\nabla}_i^2 + \sum_{i=1}^{N} \hat{\mathcal{V}}_i + \sum_{i<j} \hat{\mathcal{U}}_{ij}$$

N interacting particles in d-dimensions



Configurations

projecting a trial wavefunction to the ground state $|\Psi_0\rangle = \lim_{\tau\to\infty} e^{-\tau\hat{H}}|\Psi_T\rangle$

gives discrete imaginary time worldlines constructed from products of the short time propagator $G(\boldsymbol{R},\boldsymbol{R}';\Delta\tau) = \langle \boldsymbol{R}|e^{-\Delta\tau\hat{H}}|\boldsymbol{R}'\rangle$

Expectation Values IV

Can perform a similar procedure for the numerator:

$$O_\tau = \frac{\langle \Psi_\tau | \hat{O} | \Psi_\tau \rangle}{\langle \Psi_\tau | \Psi_\tau \rangle} \qquad Z(\tau) \equiv \langle \Psi_\tau | \Psi_\tau \rangle$$

$$\langle \Psi_\tau | \hat{O} | \Psi_\tau \rangle = \langle \Psi_T | e^{-\tau \hat{H}} \hat{O} e^{-\tau \hat{H}} | \Psi_T \rangle$$

$$\int \mathcal{D}\boldsymbol{R}\, |\boldsymbol{R}\rangle \langle \boldsymbol{R}| = \hat{\mathbb{1}}$$

estimator in position representation

$O(\boldsymbol{R}_M, \boldsymbol{R}_{M'})$

$$= \int \mathcal{D}\boldsymbol{R}_0 \int \mathcal{D}\boldsymbol{R}_M \int \mathcal{D}\boldsymbol{R}_{M'} \int \mathcal{D}\boldsymbol{R}_{2M'} \Psi_T(\boldsymbol{R}_0) G(\boldsymbol{R}_0, \boldsymbol{R}_M; \tau) \langle \boldsymbol{R}_M | \hat{O} | \boldsymbol{R}_{M'} \rangle G(\boldsymbol{R}_{M'}, \boldsymbol{R}_{2M}; \tau) \Psi_T(\boldsymbol{R}_{2M'})$$

$$= \prod_{\alpha=0}^{M} \int \mathcal{D}\boldsymbol{R}_\alpha\, \Psi_T(\boldsymbol{R}_0) \left[\prod_{\alpha=0}^{2M-1} G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) \right]$$

$$\times \prod_{\alpha=M'}^{2M'} \int \mathcal{D}\boldsymbol{R}_\alpha\, O(\boldsymbol{R}_M, \boldsymbol{R}_{M'}) \left[\prod_{\alpha=M'}^{2M'-1} G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) \right] \Psi_T(\boldsymbol{R}_{2M'})$$

Expectation Values V

Things simplify for any operator that is diagonal in the position representation

$$O_\tau = \frac{\langle \Psi_\tau | \hat{O} | \Psi_\tau \rangle}{\langle \Psi_\tau | \Psi_\tau \rangle}$$

$$\langle \boldsymbol{R} | \hat{O} | \boldsymbol{R}' \rangle = O(\boldsymbol{R}) \delta(\boldsymbol{R} - \boldsymbol{R}')$$

$$O_\tau = \frac{1}{Z(\tau)} \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha \, O(R_M) \, \Psi_T(\boldsymbol{R}_0) \left[\prod_{\alpha=0}^{2M-1} G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) \right] \Psi_T(\boldsymbol{R}_{2M})$$

a high dimensional integral that can be sampled with Metropolis Monte Carlo

Energy Expectation Value

For off-diagonal estimators (e.g. Energy) we can utilize operator relations

$$E_\tau = \frac{\langle \Psi_\tau | \hat{H} | \Psi_\tau \rangle}{\langle \Psi_\tau | \Psi_\tau \rangle} = \frac{1}{Z(\tau)} \langle \Psi_T | e^{-\tau \hat{H}} \hat{H} e^{-\tau \hat{H}} | \Psi_T \rangle$$

$$Z(\tau) = \langle \Psi_T | e^{-2\tau \hat{H}} | \Psi_T \rangle$$

consider the derivative

$$\frac{\partial Z(\tau)}{\partial (2\tau)} = - \langle \Psi_T | \hat{H} e^{-2\tau \hat{H}} | \Psi_T \rangle = - \langle \Psi_T | e^{-\tau \hat{H}} \hat{H} e^{-\tau \hat{H}} | \Psi_T \rangle$$

$$\Rightarrow \quad \boxed{E_\tau = - \frac{1}{Z(\tau)} \frac{\partial Z(\tau)}{\partial (2\tau)}}$$

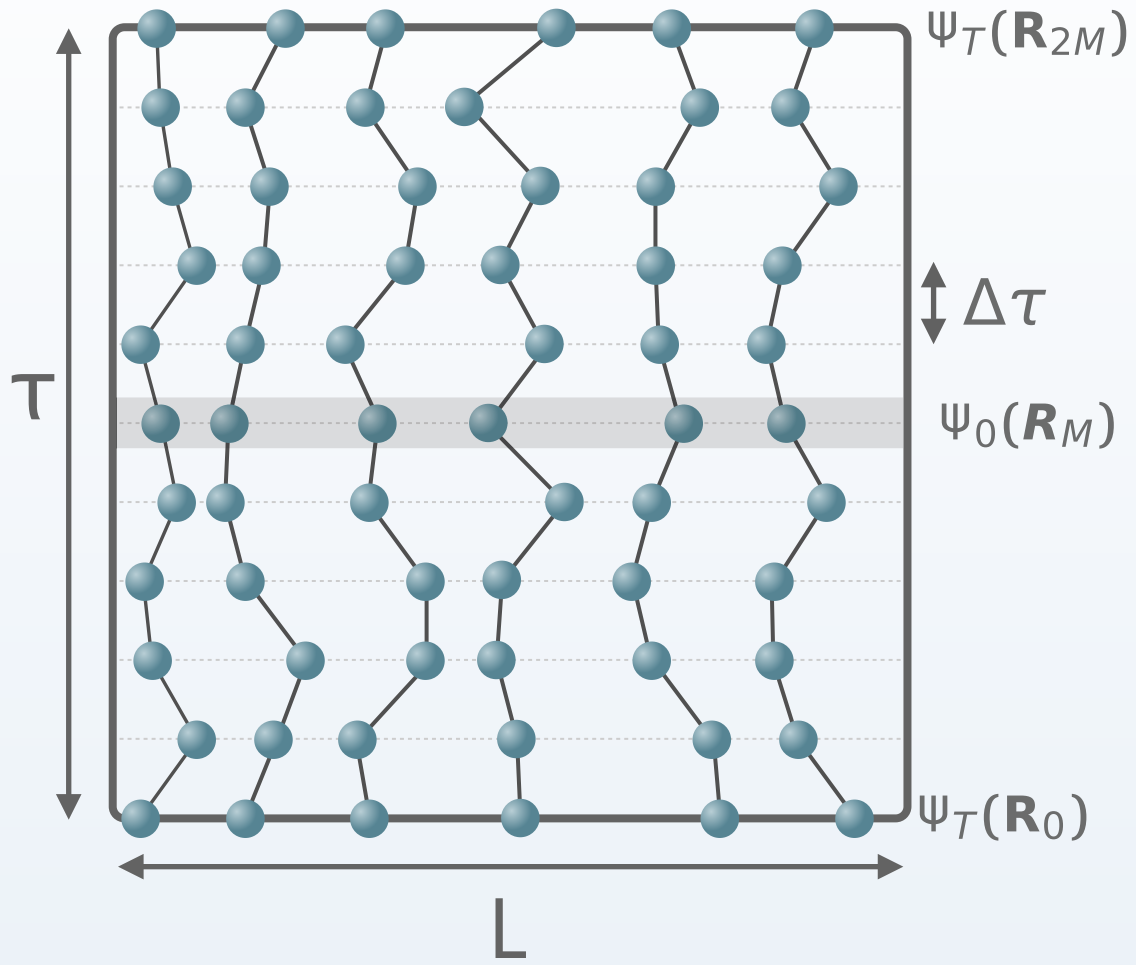
we will return to an explicit expression for this later

Path Integral Ground State QMC

Description

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\hat{\nabla}_i^2 + \sum_{i=1}^{N}\hat{\mathcal{V}}_i + \sum_{i<j}\hat{\mathcal{U}}_{ij}$$

N interacting particles in d-dimensions



Configurations

projecting a trial wavefunction to the ground state $|\Psi_0\rangle = \lim_{\tau\to\infty} e^{-\tau\hat{H}}|\Psi_T\rangle$

gives discrete imaginary time worldlines constructed from products of the short time propagator $G(\boldsymbol{R},\boldsymbol{R}';\Delta\tau) = \langle\boldsymbol{R}|e^{-\Delta\tau\hat{H}}|\boldsymbol{R}'\rangle$

Updates

Observables

exact method for computing ground state expectation values

$$O_\tau = \frac{\langle\Psi_T|e^{-\tau\hat{H}}\hat{O}e^{-\tau\hat{H}}|\Psi_T\rangle}{\langle\Psi_T|e^{-2\tau\hat{H}}|\Psi_T\rangle}$$

Short Time Propagator I

To determine the statistical weights of our configurations we need to derive a useful expression for the short time propagator

$$G(\boldsymbol{R},\boldsymbol{R}';\Delta\tau) = \left\langle \boldsymbol{R} \middle| e^{-\Delta\tau\hat{H}} \middle| \boldsymbol{R}' \right\rangle$$

returning to the Campbell-Baker-Hausdorff formula

$$e^{-\Delta\tau\hat{H}} = e^{-\Delta\tau\hat{T}} e^{-\Delta\tau\hat{V}} + O\left(\Delta\tau^2\right)$$

can make this error arbitrarily small at the cost of more time slices

we can do slightly better for free by splitting the Hamiltonian into two pieces and reversing the operator order:

$$e^{-\Delta\tau\hat{H}} = e^{-\frac{\Delta\tau}{2}\hat{V}} e^{-\Delta\tau\hat{T}} e^{-\frac{\Delta\tau}{2}\hat{V}} + O\left(\Delta\tau^3\right)$$

Short Time Propagator II

Primitive Approximation: $e^{-\Delta\tau\hat{H}} = e^{-\frac{\Delta\tau}{2}\hat{V}} e^{-\Delta\tau\hat{T}} e^{-\frac{\Delta\tau}{2}\hat{V}} + O(\Delta\tau^3)$

There are many clever Trotter decompositions that allow us to get to higher order, see, eg:

- S. A. Chin, Phys. Lett. A **226**, 344 (1997)
- S. A. Chin, Phys. Rev. A **42**, 6991 (1990)
- S. Jang, S. Jang, and G. A. Voth, J. Chem. Phys. **115**, 7832 (2001)
- R. E. Zillich, J. M. Mayrhofer, and S. A. Chin, J. Chem. Phys. **132**, 044103 (2010)

but there is no free lunch. Correction terms can be difficult to calculate and involve high order derivatives of the potential, which might not be smooth!

In this case use the pair product approximation

D. M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995)

Short Time Propagator III

$$G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = \langle \boldsymbol{R}_\alpha | e^{-\Delta\tau \hat{H}} | \boldsymbol{R}_{\alpha+1} \rangle$$

$$= \langle \boldsymbol{R}_\alpha | e^{-\frac{\Delta\tau}{2}\hat{V}} e^{-\Delta\tau \hat{T}} e^{-\frac{\Delta\tau}{2}\hat{V}} | \boldsymbol{R}_{\alpha+1} \rangle + O(\Delta\tau^3)$$

$$\simeq \int \mathcal{D}\boldsymbol{R} \int \mathcal{D}\boldsymbol{R}' \, \langle \boldsymbol{R}_\alpha | e^{-\frac{\Delta\tau}{2}\hat{V}} | \boldsymbol{R} \rangle \, \langle \boldsymbol{R} | e^{-\Delta\tau \hat{T}} | \boldsymbol{R}' \rangle \, \langle \boldsymbol{R}' | e^{-\frac{\Delta\tau}{2}\hat{V}} | \boldsymbol{R}_{\alpha+1} \rangle$$

$$V(\boldsymbol{R}_\alpha) \equiv \sum_{i=1}^{N} \mathcal{V}(\boldsymbol{r}_{i,\alpha}) + \frac{1}{2} \sum_{i,j} \mathcal{U}(\boldsymbol{r}_{i,\alpha} - \boldsymbol{r}_{j,\alpha})$$

diagonal in position basis

$$\simeq \int \mathcal{D}\boldsymbol{R} \int \mathcal{D}\boldsymbol{R}' e^{-\frac{\Delta\tau}{2} V(\boldsymbol{R}_\alpha)} \delta(\boldsymbol{R}_\alpha - \boldsymbol{R}) \langle \boldsymbol{R} | e^{-\Delta\tau \hat{T}} | \boldsymbol{R}' \rangle e^{-\frac{\Delta\tau}{2} V(\boldsymbol{R}_{\alpha+1})} \delta(\boldsymbol{R}' - \boldsymbol{R}_{\alpha+1})$$

$$\simeq e^{-\frac{\Delta\tau}{2} V(\boldsymbol{R}_\alpha)} \, \langle \boldsymbol{R}_\alpha | e^{-\Delta\tau \hat{T}} | \boldsymbol{R}_{\alpha+1} \rangle \, e^{-\frac{\Delta\tau}{2} V(\boldsymbol{R}_{\alpha+1})}$$

$G_0(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau)$ free / bare propagator

$$G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = e^{-\frac{\Delta\tau}{2} V(\boldsymbol{R}_\alpha)} e^{-\frac{\Delta\tau}{2} V(\boldsymbol{R}_{\alpha+1})} G_0(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) + O(\Delta\tau^3)$$

Free Propagator I

$$G_0(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = \langle \boldsymbol{R}_\alpha | e^{-\Delta\tau \hat{T}} | \boldsymbol{R}_{\alpha+1} \rangle$$

Write the position state in terms of plane waves:

$$|\boldsymbol{R}\rangle = |\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N\rangle$$
$$= \prod_{i=1}^{N} \int \frac{\mathrm{d}^d k_i}{(2\pi)^d} e^{i\boldsymbol{k}_i \cdot \boldsymbol{r}_i} |\boldsymbol{k}_1, \ldots, \boldsymbol{k}_N\rangle \,.$$

To simplify notation, it is conventional to define: $\lambda_i = \dfrac{\hbar^2}{2m_i}$

$$\hat{T} = -\sum_{i=1}^{N} \lambda_i \hat{\nabla}_i^2$$

Free Propagator II

$$G_0(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = \langle \boldsymbol{R}_\alpha | e^{-\Delta\tau \hat{T}} | \boldsymbol{R}_{\alpha+1} \rangle$$

$$\left\langle \boldsymbol{R} \middle| e^{-\Delta\tau\hat{T}} \middle| \boldsymbol{R}' \right\rangle = \prod_{i=1}^{N} \int \frac{\mathrm{d}^d k_i}{(2\pi)^d} \int \frac{\mathrm{d}^d k_i'}{(2\pi)^d} e^{-i\boldsymbol{k}_i\cdot\boldsymbol{r}_i} e^{i\boldsymbol{k}_i'\cdot\boldsymbol{r}_i'} \left\langle \boldsymbol{k}_1, \ldots, \boldsymbol{k}_N \middle| e^{-\Delta\tau \sum_{j=1}^{N} \lambda_j \hat{\nabla}_j^2} \middle| \boldsymbol{k}_1', \ldots, \boldsymbol{k}_N' \right\rangle$$

$$= \prod_{i=1}^{N} \int \frac{\mathrm{d}^d k_i}{(2\pi)^d} \int \frac{\mathrm{d}^d k_i'}{(2\pi)^d} \exp\left(-\lambda_i \Delta\tau \left| \boldsymbol{k}_i' \right|^2 - i\boldsymbol{k}_i \cdot \boldsymbol{r}_i + i\boldsymbol{k}_i' \cdot \boldsymbol{r}_i' \right) \left\langle \boldsymbol{k}_1, \ldots, \boldsymbol{k}_N \middle| \boldsymbol{k}_1', \ldots, \boldsymbol{k}_N' \right\rangle$$

$$= \prod_{i=1}^{N} \int \frac{\mathrm{d}^d k_i}{(2\pi)^d} \int \frac{\mathrm{d}^d k_i'}{(2\pi)^d} \exp\left(-\lambda_i \Delta\tau \left| \boldsymbol{k}_i' \right|^2 - i\boldsymbol{k}_i \cdot \boldsymbol{r}_i + i\boldsymbol{k}_i' \cdot \boldsymbol{r}_i' \right) (2\pi)^d \delta\left(\boldsymbol{k}_i - \boldsymbol{k}_i' \right)$$

$$= \prod_{i=1}^{N} \int \frac{\mathrm{d}^d k_i}{(2\pi)^d} \exp\left[-\lambda_i \Delta\tau |\boldsymbol{k}_i|^2 + i\boldsymbol{k}_i \cdot (\boldsymbol{r}_i' - \boldsymbol{r}_i) \right]$$

$$= \prod_{i=1}^{N} (4\pi\lambda_i\Delta\tau)^{-d/2} \exp\left[-\sum_{i=1}^{N} \frac{\left| \boldsymbol{r}_i - \boldsymbol{r}_i' \right|^2}{4\lambda_i \Delta\tau} \right]$$

product of Gaussians ⇒ can be exactly sampled!

Short Time Propagator IV

Putting everything together:

$$G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = e^{-\frac{\Delta\tau}{2}V(\boldsymbol{R}_\alpha)} e^{-\frac{\Delta\tau}{2}V(\boldsymbol{R}_{\alpha+1})} G_0(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) + O(\Delta\tau^3)$$

0

work at fixed error

simplify to identical particles: $\lambda_i \to \lambda = \hbar^2/2m$

$$|\boldsymbol{R}_\alpha - \boldsymbol{R}_{\alpha+1}|^2 \equiv \sum_{i=1}^{N} |\boldsymbol{r}_{i,\alpha} - \boldsymbol{r}_{i,\alpha+1}|^2$$

$$G_0(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = (4\pi\lambda\Delta\tau)^{-dN/2} e^{-\frac{1}{4\lambda\Delta\tau}|\boldsymbol{R}_\alpha - \boldsymbol{R}_{\alpha+1}|^2}$$

$$G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = (4\pi\lambda\Delta\tau)^{-dN/2} e^{-\frac{1}{4\lambda\Delta\tau}|\boldsymbol{R}_\alpha - \boldsymbol{R}_{\alpha+1}|^2 - \frac{\Delta\tau}{2}[V(\boldsymbol{R}_\alpha) + V(\boldsymbol{R}_{\alpha+1})]}$$

can define a link action: $S(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = -\ln[G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau)]$

Configuration Weights

Recall the normalization factor:

$$Z(\tau) = \langle \Psi_T | e^{-\tau \hat{H}} e^{-\tau \hat{H}} | \Psi_T \rangle$$

$$G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) = \frac{e^{-\frac{1}{4\lambda\Delta\tau}|\boldsymbol{R}_\alpha - \boldsymbol{R}_{\alpha+1}|^2 - \frac{\Delta\tau}{2}[V(\boldsymbol{R}_\alpha) + V(\boldsymbol{R}_{\alpha+1})]}}{(4\pi\lambda\Delta\tau)^{-dN/2}}$$

$$= \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha \Psi_T(\boldsymbol{R}_0) \left[\prod_{\alpha=0}^{2M-1} G(\boldsymbol{R}_\alpha, \boldsymbol{R}_{\alpha+1}; \Delta\tau) \right] \Psi_T(\boldsymbol{R}_{2M})$$

$$= (4\lambda\Delta\tau)^{-NMd} \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha \Psi_T(\boldsymbol{R}_0) e^{-\sum_{\alpha=0}^{2M-1} \frac{|\boldsymbol{R}_{\alpha+1} - \boldsymbol{R}_\alpha|}{4\lambda\Delta\tau} - \Delta\tau\left[\frac{1}{2}V(\boldsymbol{R}_0) + \frac{1}{2}V(\boldsymbol{R}_{2M}) + \sum_{\alpha=1}^{2M-1} V(\boldsymbol{R}_\alpha)\right]} \Psi_T(\boldsymbol{R}_{2M})$$

$$= (4\lambda\Delta\tau)^{-NMd} \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha \, e^{-\tilde{S}}$$

$$\tilde{S} = \sum_{\alpha=0}^{2M-1} \frac{|\boldsymbol{R}_{\alpha+1} - \boldsymbol{R}_\alpha|}{4\lambda\Delta\tau} + \Delta\tau \left[\frac{1}{2}V(\boldsymbol{R}_0) + \frac{1}{2}V(\boldsymbol{R}_{2M}) + \sum_{\alpha=1}^{2M-1} V(\boldsymbol{R}_\alpha) \right] - \ln[\Psi_T(\boldsymbol{R}_0)] - \ln[\Psi_T(\boldsymbol{R}_{2M})]$$

Importance Sampling

Z(τ) is a high ($N \bullet M \bullet d$) dimensional integral that can be sampled with Monte Carlo

configuration: $\boldsymbol{X} = \{\boldsymbol{R}_\alpha, \ldots \boldsymbol{R}_{2M}\}$ $\quad \int \mathrm{d}\boldsymbol{X} = \prod_{\alpha=0}^{2M} \int \mathcal{D}\boldsymbol{R}_\alpha$

probability distribution: $\pi(\boldsymbol{X}) = e^{-\tilde{S}(\boldsymbol{x}) - NMd \ln(4\pi\lambda\Delta\tau)}$

probability density: $p(\boldsymbol{X}) = \dfrac{\pi(\boldsymbol{X})}{\int \mathrm{d}\boldsymbol{X}' \, \pi(\boldsymbol{X}')}$

operator dependent weight function

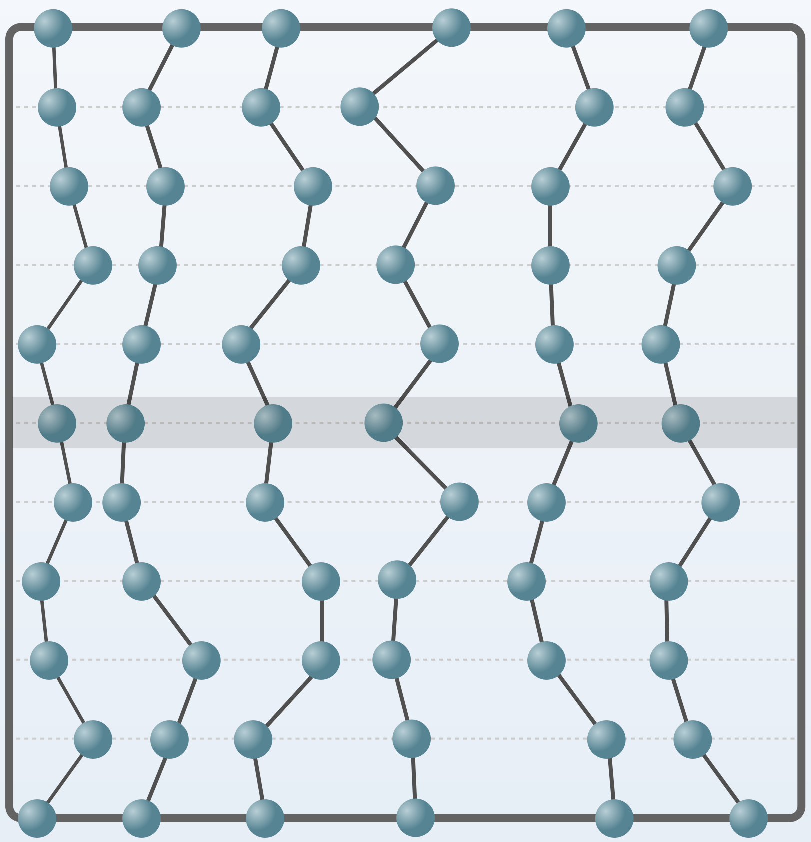
expectation value: $\langle \hat{O} \rangle = \int \mathrm{d}\boldsymbol{X} \, w_{\hat{O}}(\boldsymbol{X}) p(\boldsymbol{X})$

Configurations are not uniformly likely but are instead given by the probability $p(\mathbf{X})$

The path integral ground state (PIGS) algorithm will allow us to generate configurations $\mathbf{X}$ according to $p(\mathbf{X})$ and to use these configurations to accumulate the weight functions $w_O(\mathbf{X})$ for any observable.

Updates

Need to construct a series of updates that efficiently sample configuration space



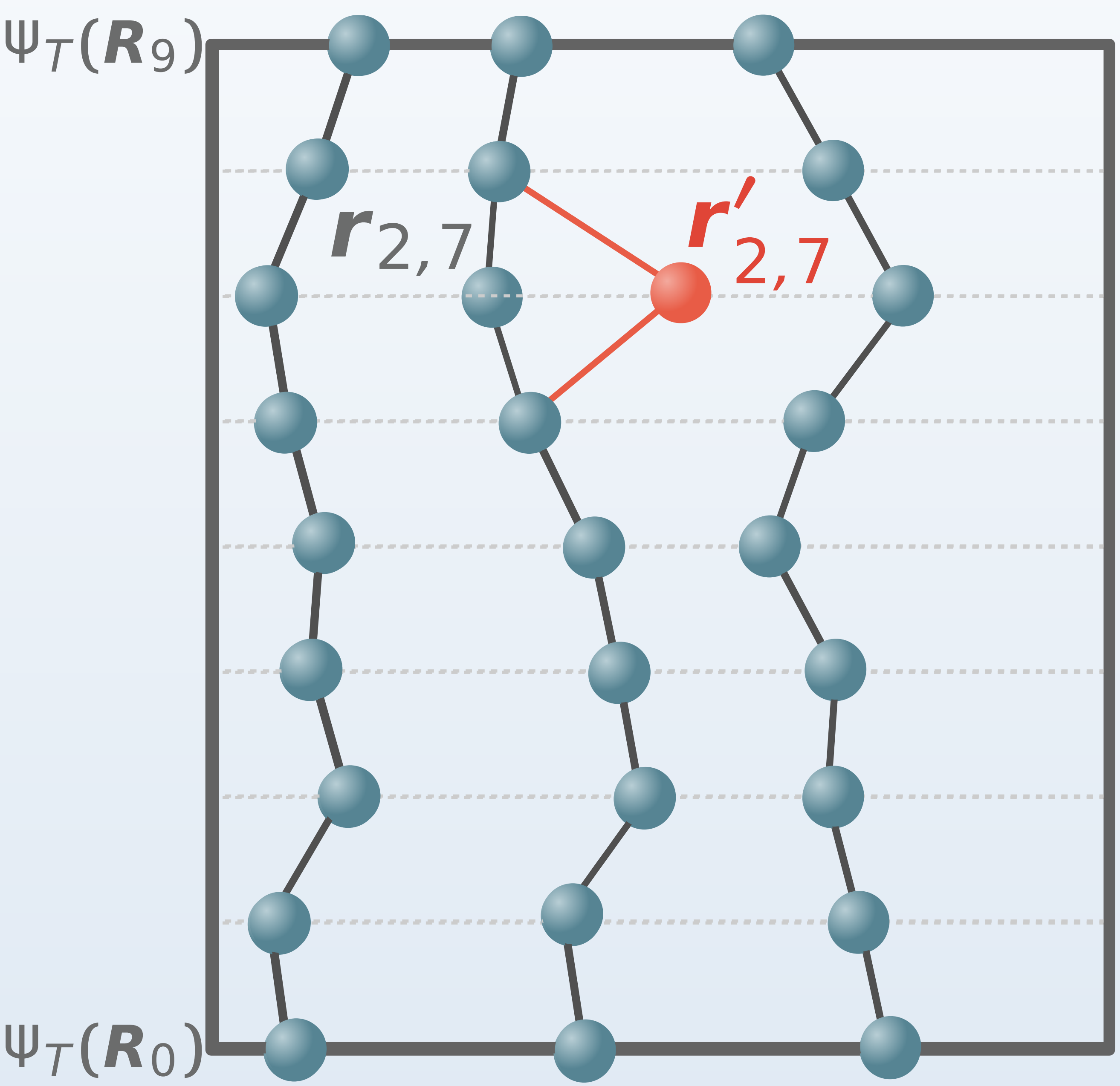
single-bead (local) updates: Metropolis sampling of both the kinetic and potential action

multiple-bead (non-local) updates: can sample the free propagator exactly and use Metropolis sampling for the potential action.

Single Bead Displace

Select a bead at random and shift its position by δ

$j = 2, \gamma = 7$



accept with probability

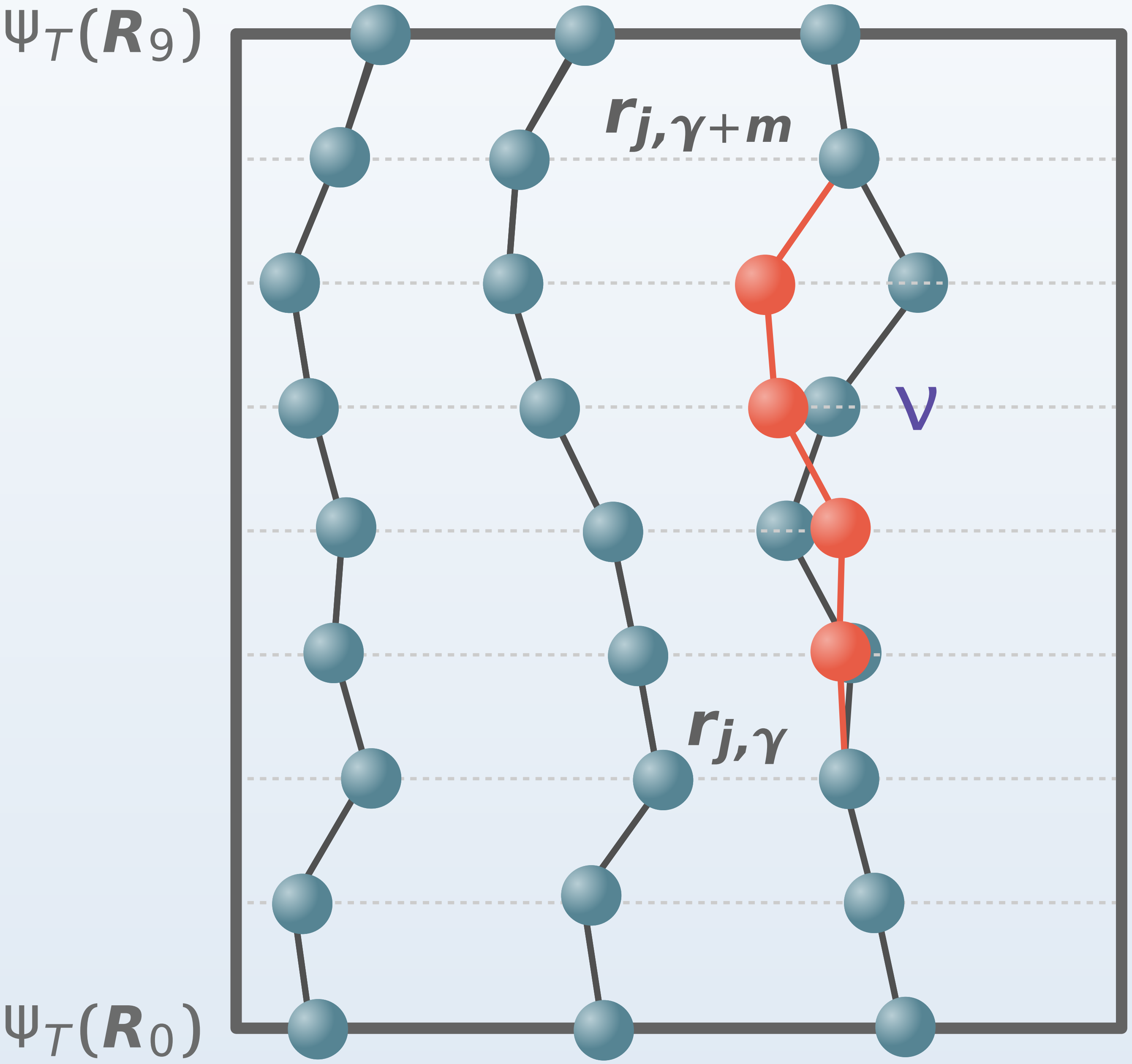
$$P_{\text{displace}} = \min\left[1, e^{-\Delta\tilde{S}_{j,\gamma}}\right]$$

$$\Delta\tilde{S}_{j,\gamma} = \frac{1}{4\pi\lambda\Delta\tau}\left[\left|\boldsymbol{r}_{j,\gamma+1} - \boldsymbol{r}'_{j,\gamma}\right|^2 + \left|\boldsymbol{r}'_{j,\gamma} - \boldsymbol{r}_{j,\gamma-1}\right|^2 - \left|\boldsymbol{r}_{j,\gamma+1} - \boldsymbol{r}_{j,\gamma}\right|^2 - \left|\boldsymbol{r}_{j,\gamma} - \boldsymbol{r}_{j,\gamma} - 1\right|^2\right] + \Delta\tau\left\{\mathcal{V}(\boldsymbol{r}'_{j,\gamma}) - \mathcal{V}(\boldsymbol{r}_{j,\gamma}) + \sum_{i\neq j}\left[\mathcal{U}(\boldsymbol{r}'_{j,\gamma} - \boldsymbol{r}_{i,\gamma}) - \mathcal{U}(\boldsymbol{r}_{j,\gamma} - \boldsymbol{r}_{i,\gamma})\right]\right\}$$

Multi Bead Staging I

Select a worldline j and slice γ at random and generate a new section of path of length *m*

$j = 3, \gamma = 2, m = 5$



want to sample the product of *m* free particle density matrices

$$G_0(\boldsymbol{r}_{j,\gamma}, \boldsymbol{r}_{j,\gamma+1}; \Delta\tau) \cdots G_0(\boldsymbol{r}_{j,\gamma+m-1}, \boldsymbol{r}_{j,\gamma+m}; \Delta\tau)$$

choose a single slice, ν, in this product and construct the probability distribution for propagation to that position, constrained by the fixed endpoints

$$\begin{aligned}\pi_0(\boldsymbol{r}_\nu|\boldsymbol{r}_\gamma, \boldsymbol{r}_{\gamma+m}) &= G(\boldsymbol{r}_\gamma, \boldsymbol{r}_\nu; (\nu-\gamma)\Delta\tau)G(\boldsymbol{r}_\nu, \boldsymbol{r}_{\gamma+m}; (\gamma+m-\nu)\Delta\tau) \\ &\propto \exp\left[-\frac{|\boldsymbol{r}_\nu - \boldsymbol{r}_\gamma|^2}{4\lambda(\nu-\gamma)\Delta\tau}\right]\exp\left[-\frac{|\boldsymbol{r}_{\gamma+m} - \boldsymbol{r}_\nu|^2}{4\lambda(\gamma+m-\nu)\Delta\tau}\right] \\ &\propto \exp\left[-\frac{|\boldsymbol{r}_\nu - \bar{\boldsymbol{r}}_\nu|^2}{2\sigma^2}\right]\end{aligned}$$

$$\bar{\boldsymbol{r}}_\nu = \frac{1}{m}\left[(\gamma+m-\nu)\boldsymbol{r}_\gamma + (\nu-\gamma)\boldsymbol{r}_{\gamma+m}\right]$$

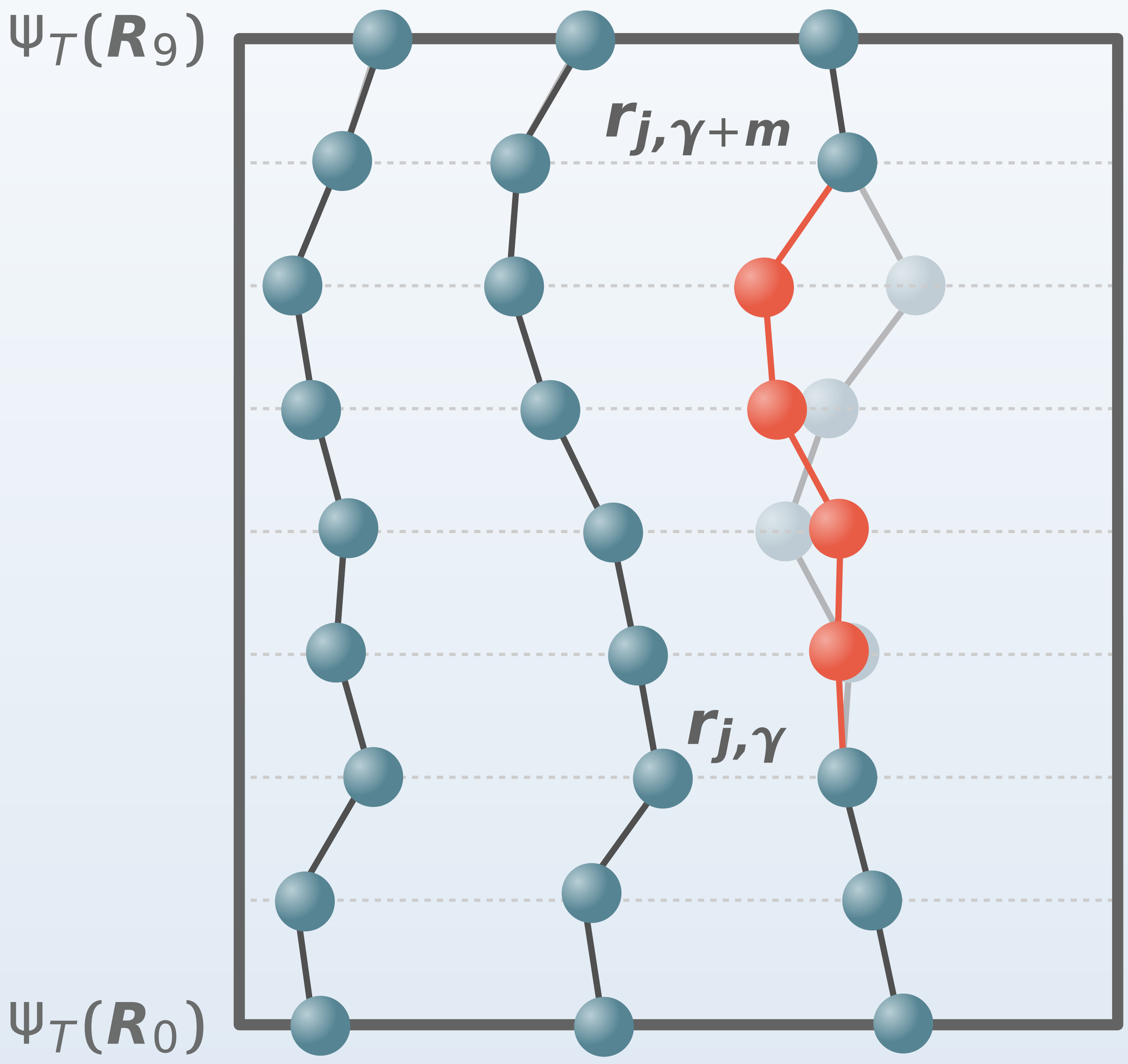
$$\sigma^2 = \frac{2\lambda}{\frac{1}{(\gamma+m-\nu)\Delta\tau} + \frac{1}{(\nu-\gamma)\Delta\tau}}$$

Gaussian random numbers!

Multi Bead Staging II

Select a worldline j and slice γ at random and generate a new section of path of length *m*

$j = 3, \gamma = 2, m = 5$



accept with probability

$$P_{\text{staging}} = \min\left[1, e^{-\Delta\tilde{S}_{j,\gamma,m}}\right]$$

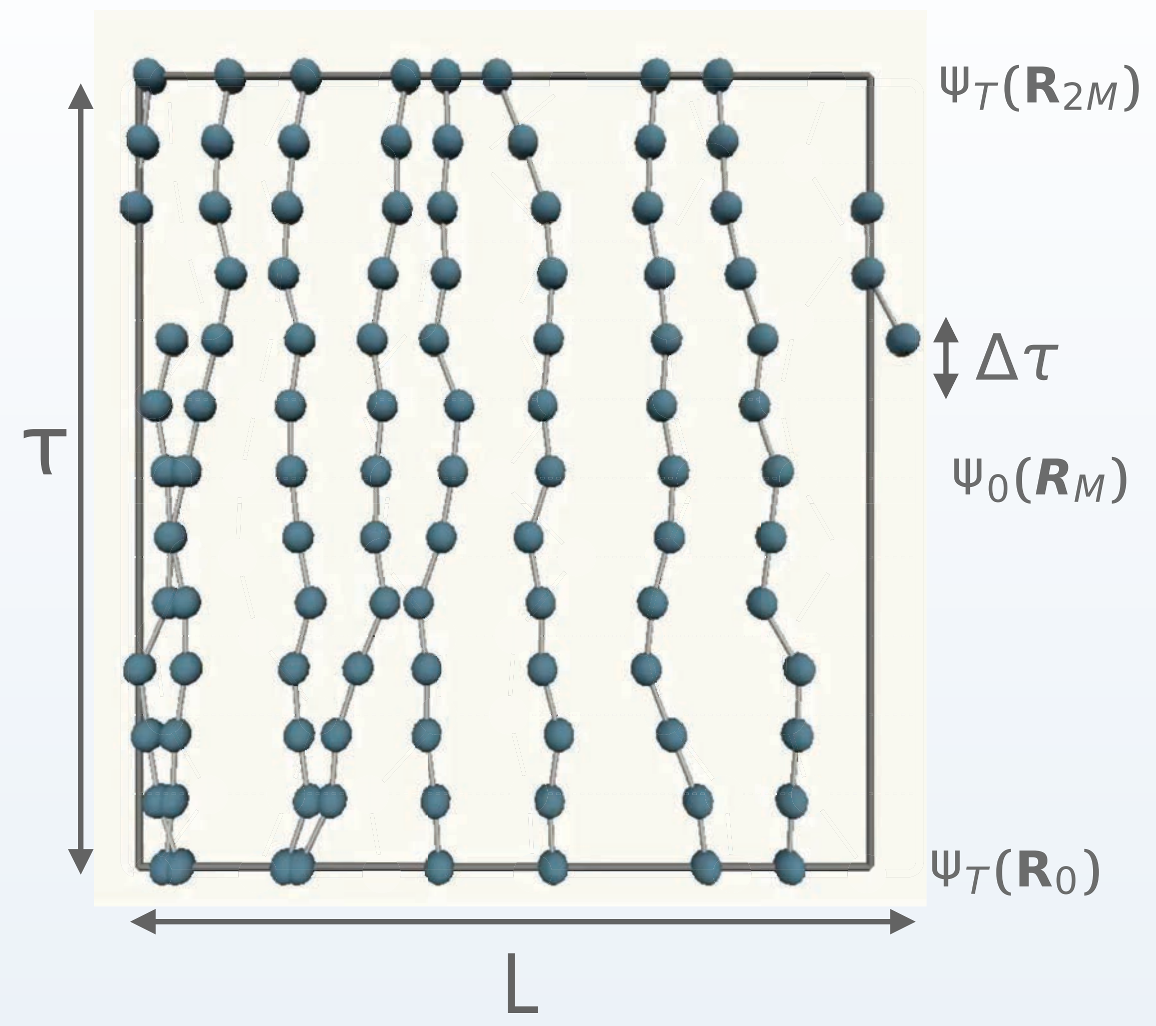
$$\Delta\tilde{S}_{j,\gamma,m} = \Delta\tau \sum_{\alpha=\gamma+1}^{\gamma+m-1} \Big\{ \mathcal{V}(\boldsymbol{r}'_{j,\alpha}) - \mathcal{V}(\boldsymbol{r}_{j,\alpha}) + \sum_{i\neq j} \left[\mathcal{U}(\boldsymbol{r}'_{j,\alpha} - \boldsymbol{r}_{i,\alpha}) - \mathcal{U}(\boldsymbol{r}_{j,\gamma} - \boldsymbol{r}_{i,\alpha}) \right] \Big\}$$

Path Integral Ground State QMC

Description

$$\hat{H} = -\sum_{i=1}^{N} \frac{\hbar^2}{2m_i}\hat{\nabla}_i^2 + \sum_{i=1}^{N} \hat{\mathcal{V}}_i + \sum_{i<j} \hat{\mathcal{U}}_{ij}$$

N interacting particles in d-dimensions



Configurations

projecting a trial wavefunction to the ground state $|\Psi_0\rangle = \lim_{\tau\to\infty} e^{-\tau\hat{H}}|\Psi_T\rangle$

gives discrete imaginary time worldlines constructed from products of the short time propagator $G(\mathbf{R},\mathbf{R}';\Delta\tau) = \langle \mathbf{R}|e^{-\Delta\tau\hat{H}}|\mathbf{R}'\rangle$

Observables

exact method for computing ground state expectation values

$$O_\tau = \frac{\langle\Psi_T|e^{-\tau\hat{H}}\hat{O}e^{-\tau\hat{H}}|\Psi_T\rangle}{\langle\Psi_T|e^{-2\tau\hat{H}}|\Psi_T\rangle}$$

Updates

Local and non-local bead updates with weights given by $\pi(\mathbf{X})$

Energy Estimator

Now that we have a closed expression for $Z(\tau)$ we can directly compute an estimator for the energy

$$\langle E_T \rangle = -\frac{1}{Z(\tau)} \frac{\partial Z(\tau)}{\partial (2\tau)} = \frac{1}{Z(\tau)} \int \mathrm{d}\boldsymbol{X}\, \pi(\boldsymbol{X}) w_{\hat{H}}(\boldsymbol{X})$$

$$w_{\hat{H}}(\boldsymbol{X}) = \frac{1}{2M} \left\{ \sum_{\alpha=0}^{2M-1} \left[\frac{dN}{2\Delta\tau} - \frac{|\boldsymbol{R}_{\alpha+1} - \boldsymbol{R}_\alpha|^2}{4\lambda\Delta\tau^2} \right] + \frac{1}{2} V(\boldsymbol{R}_0) + \frac{1}{2} V(\boldsymbol{R}_{2M}) + \sum_{\alpha=1}^{2M-1} V(\boldsymbol{R}_\alpha) \right\}$$

Path Integral Ground State QMC

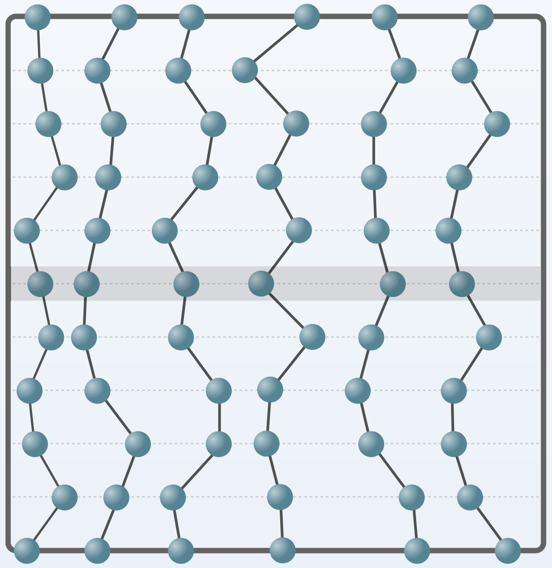
We are ready to code it up!

```
initialize all beads at random positions
for 1…number_MC_steps
    for 1…N
        for 0…2M
            perform a single slice displacement
        for 0..2M/m
            perform a staging update
    measure observables
```

https://github.com/agdelma/qmc_ho

Quantum Liquids

- General formulation of itinerant particles with strong interactions
- Trial wavefunctions
- Variational Monte Carlo

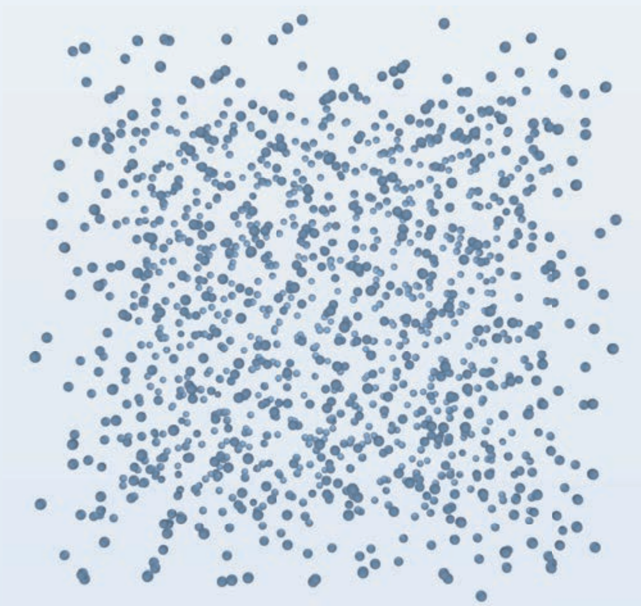


Ground State Quantum Monte Carlo

- Introduction to projector methods
- Elimination of systematic bias from a trial wavefunction
- Imaginary time propagator in the position representation
- Estimators

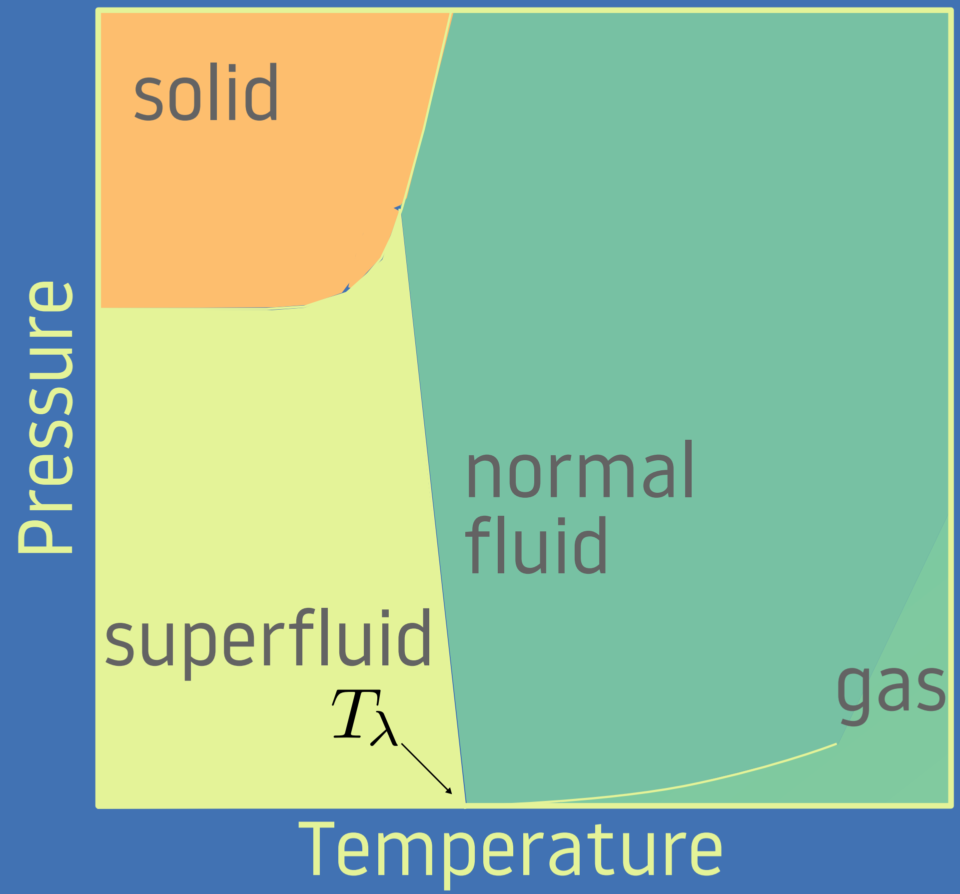
Some results for helium

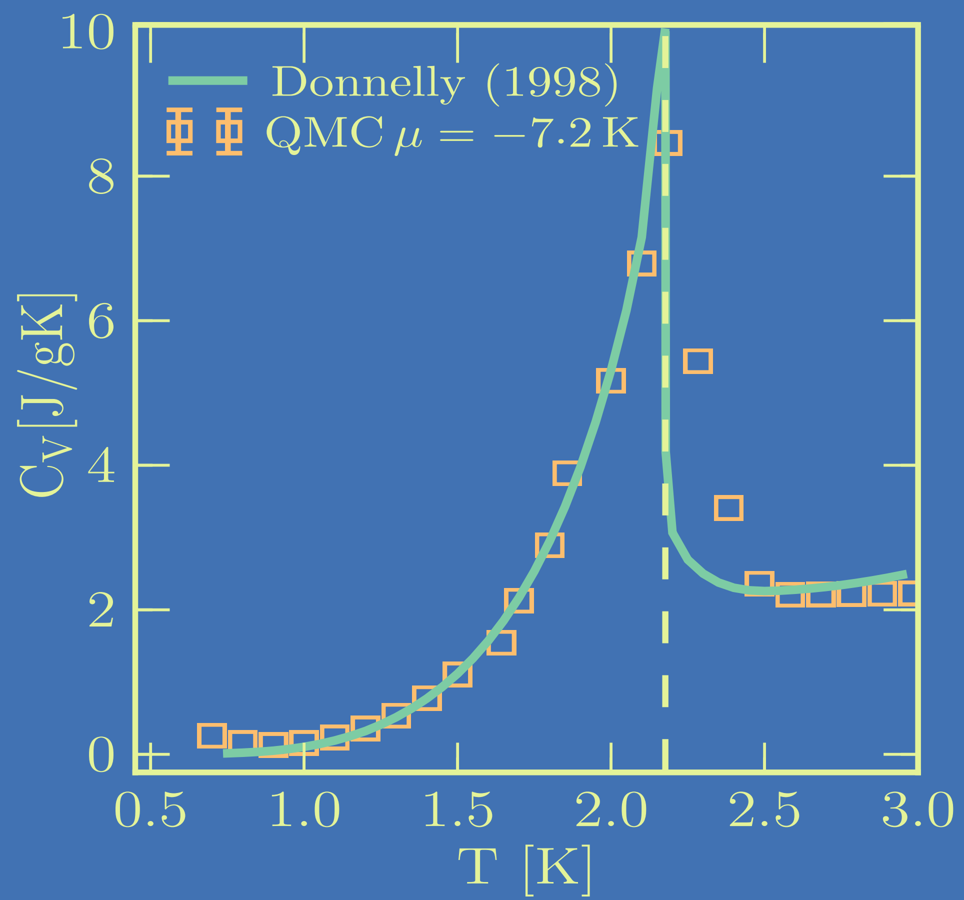
- PIGS for the energy and structural properties



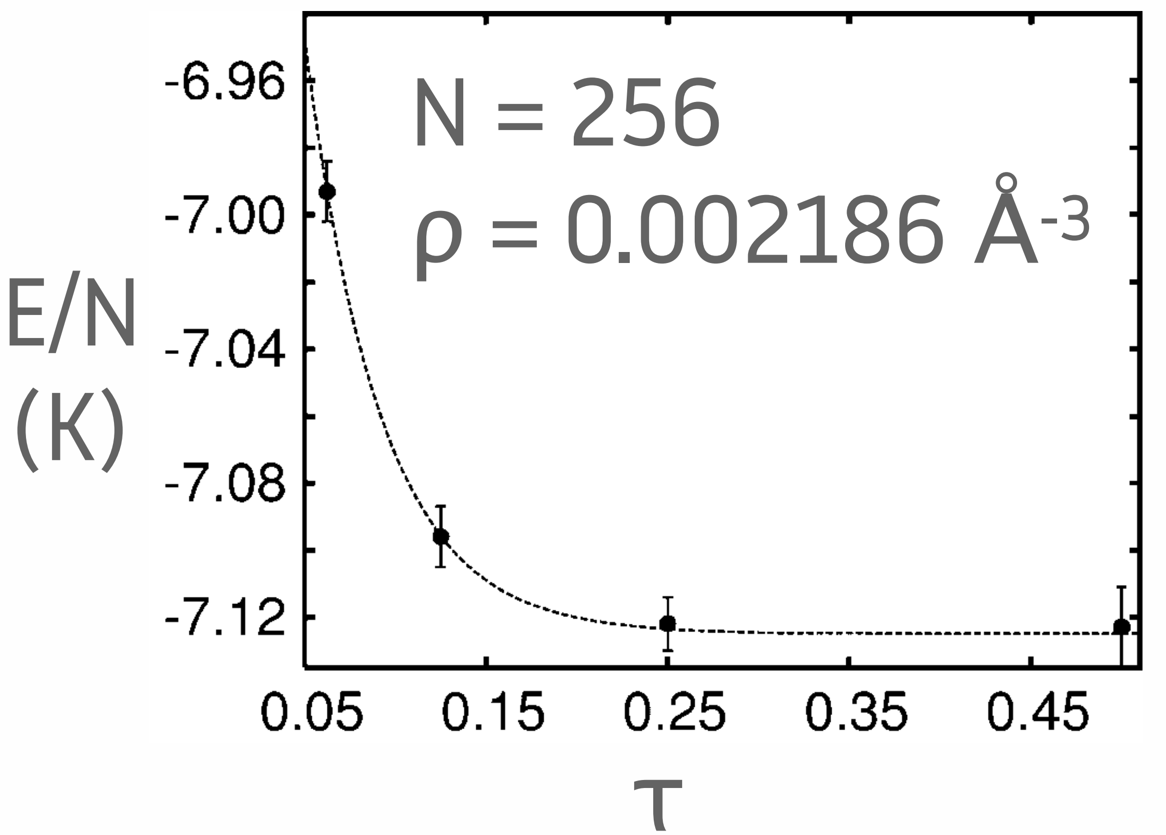
What about our real quantum liquid

helium-4



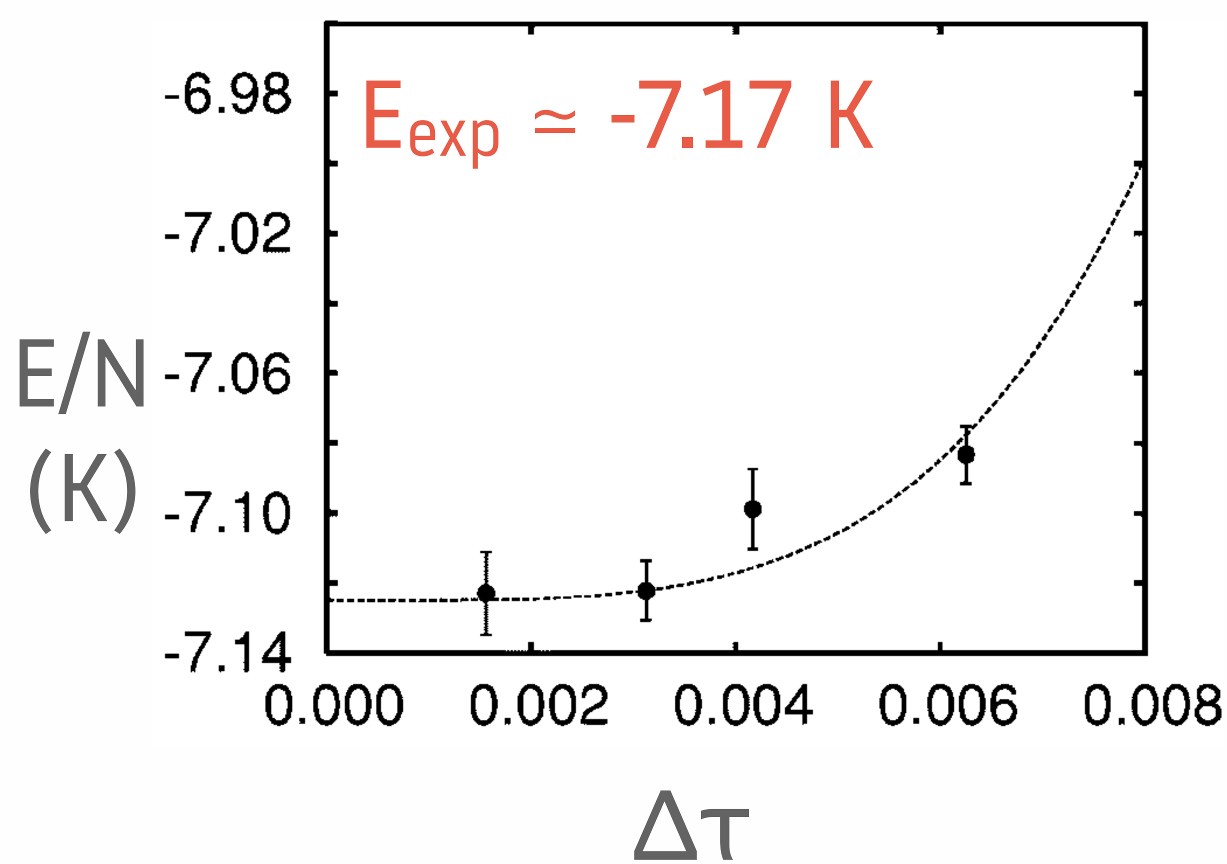


Ground State Energy of ^{4}He



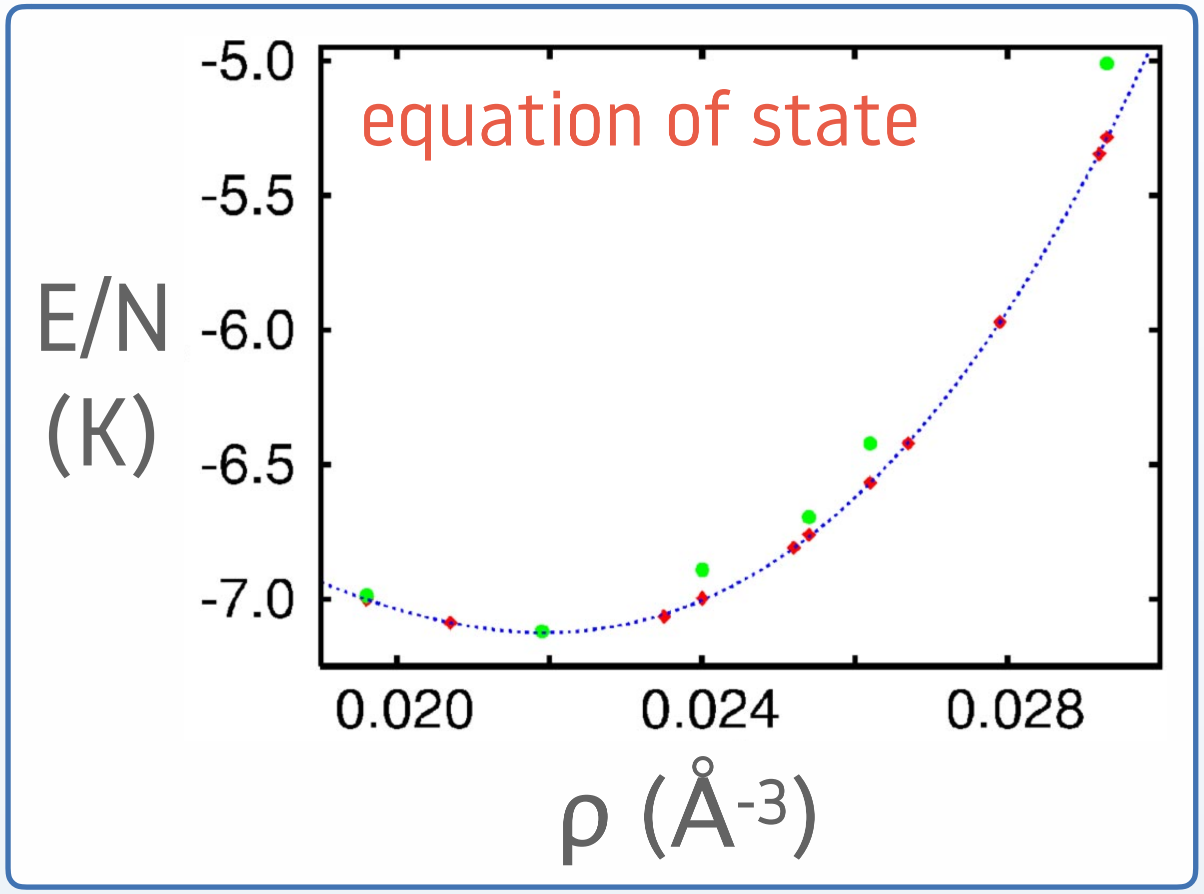
convergence in imaginary time length at fixed $\Delta\tau = 0.003125\ K^{-1}$

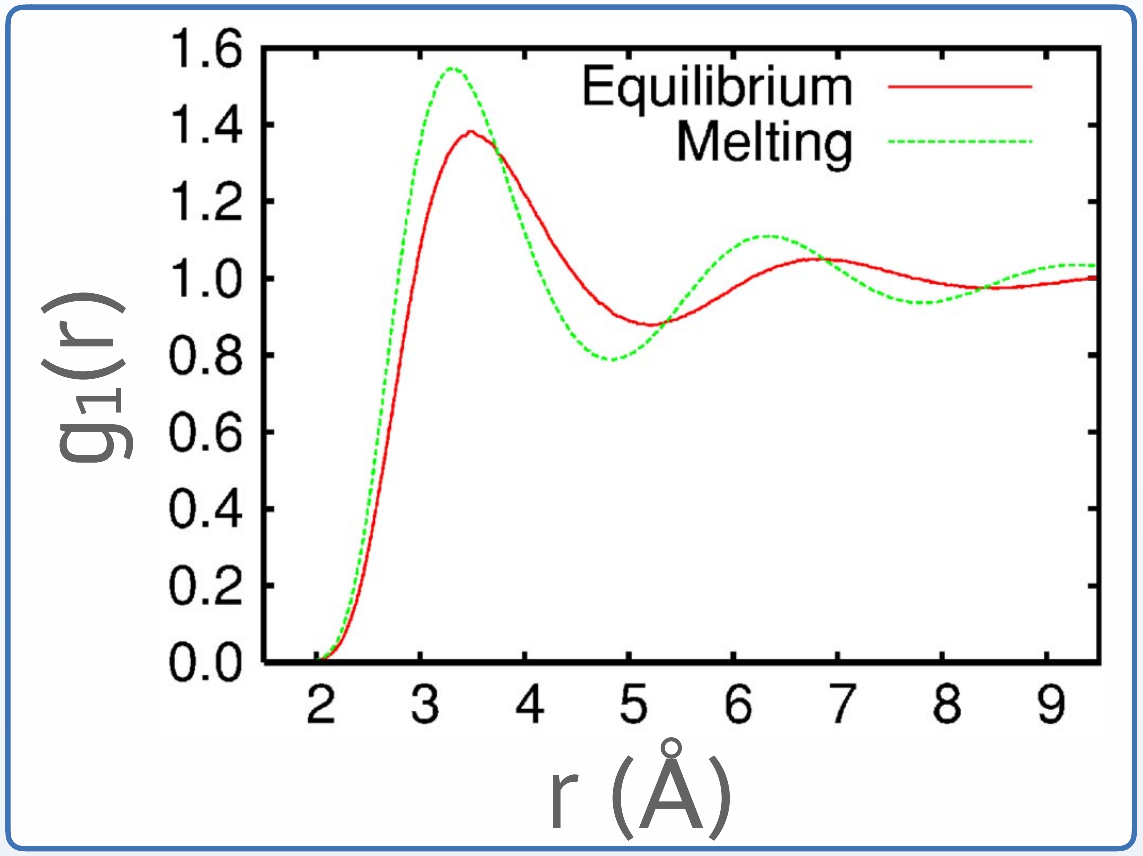
convergence in imaginary time step at fixed $\tau = 0.25\ K^{-1}$



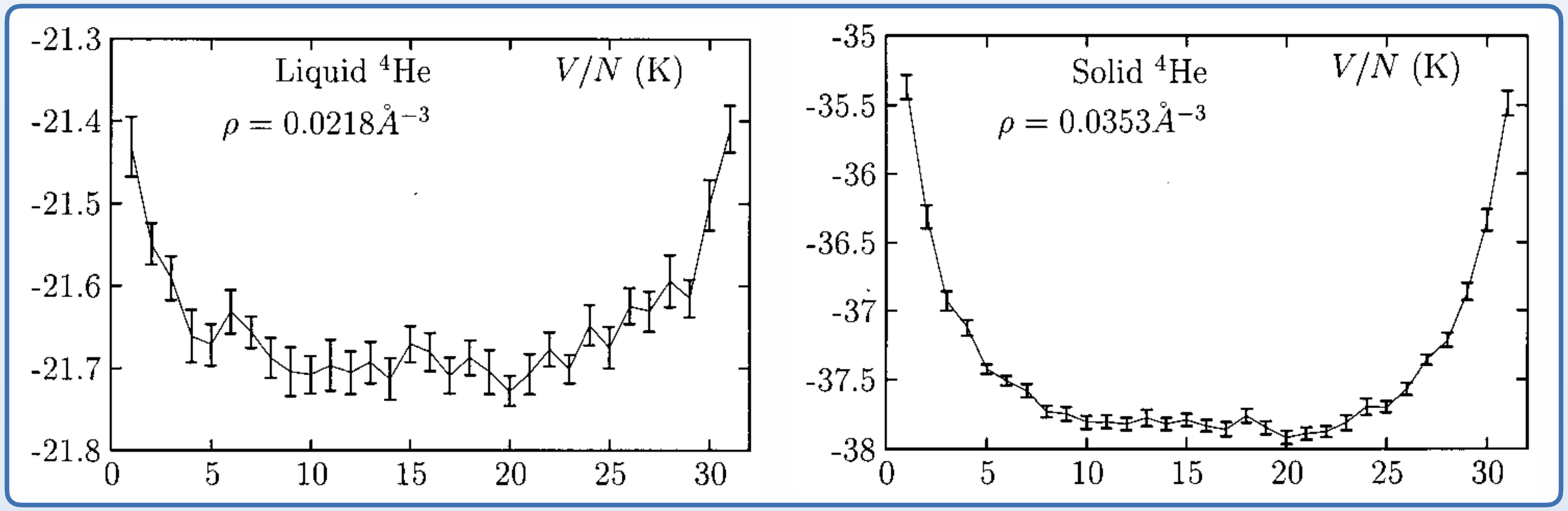
A. Sarsa, K. E. Schmidt, and W. R. Magro, J. Chem. Phys. 113, 1366 (2000)
J. E. Cuervo, P.-N. Roy, and M. Boninsegni, J. Chem. Phys. 122, 114504 (2005)

Structural Properties of ^{4}He





$$\Psi_T(\boldsymbol{R}) = \exp\left[-\frac{1}{2}\sum_{i<j} u(|\boldsymbol{r}_i - \boldsymbol{r}_j|)\right]$$



A. Sarsa, K. E. Schmidt, and W. R. Magro, J. Chem. Phys. 113, 1366 (2000)
J. E. Cuervo, P.-N. Roy, and M. Boninsegni, J. Chem. Phys. 122, 114504 (2005)

Sources & Writing Your Own Code

- M. Ceperley, *Path Integrals in the Theory of Condensed Helium*, Rev. Mod. Phys. 67, 279 (1995).
- A. Sarsa, K. E. Schmidt, and W. R. Magro, *A Path Integral Ground State Method*, J. Chem. Phys. 113, 1366 (2000).
- J. E. Cuervo, P.-N. Roy, and M. Boninsegni, *Path integral ground state with a fourth-order propagator: Application to condensed helium*. Chem. Phys. 122, 114504 (2005).
- Y. Yan and D. Blume, *Path Integral Monte Carlo Ground State Approach: Formalism, Implementation, and Applications*, J. Phys. B: Atom., Mol., and Opt. 50, 223001 (2017).

- https://github.com/agdelma/qmc_ho
- http://code.delmaestro.org
- https://github.com/DelMaestroGroup

Partners in Research & Computing

NSF

XSEDE

Extreme Science and Engineering
Discovery Environment

VACC

VERMONT ADVANCED COMPUTING CORE

UNIVERSITY OF VERMONT