

# Quantum Monte Carlo Simulation

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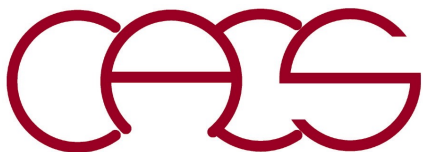
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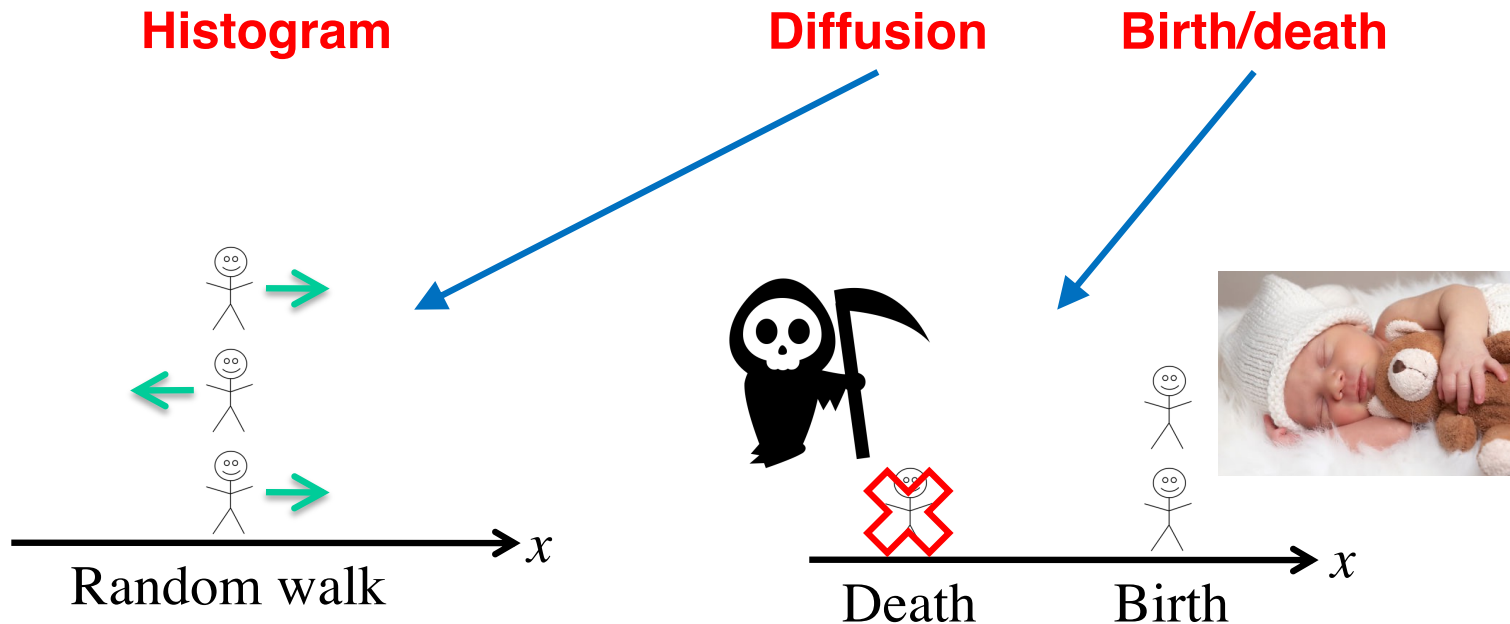
**Random walk to solve quantum  
eigenvalue problem**



# Imaginary-time Schrödinger Equation

- $\tau = it$

$$\frac{\partial}{\partial \tau} \psi(x, \tau) = -\frac{H}{\hbar} \psi(x, \tau) = \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} \psi(x, \tau) - \frac{V(x)}{\hbar} \psi(x, \tau)$$



$$D_{\text{QMC}} = \frac{\hbar}{2m} = 58 \text{ m}^2/\text{s} \gg D_{\text{water}} = 10^{-9} \text{ m}^2/\text{s}$$

# Ground-State Filter

$$\psi(x, \tau) = \exp(-H\tau/\hbar)\psi(x, 0) = \sum_n c_n \phi_n(x) \exp(-E_n \tau/\hbar) \stackrel{=1}{\text{Completeness: } |\psi\rangle = \sum_n |n\rangle\langle n| \psi\rangle}$$

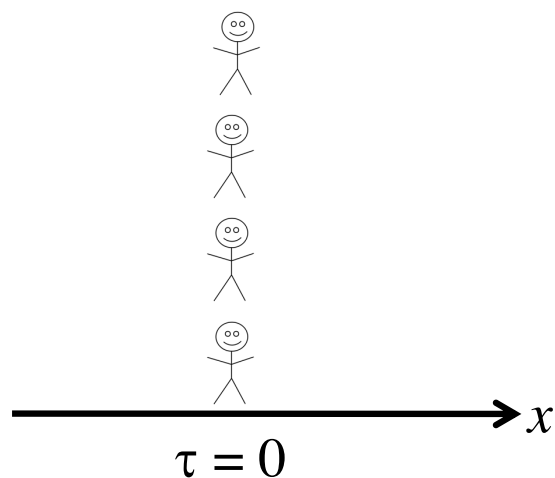
$$c_n = \int dx \phi_n(x) \psi(x, 0) \quad \langle 0|H|0\rangle = E_0 < E_1 < \dots$$

$$\lim_{\tau \rightarrow \infty} \psi(x, \tau) = c_0 \phi_0(x) \exp(-E_0 \tau/\hbar)$$

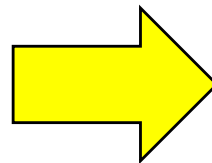
- **Energy estimate**

$$E_0 = \langle V \rangle = \frac{\int_{-\infty}^{\infty} V(x) \psi(x, \tau) dx}{\int_{-\infty}^{\infty} \psi(x, \tau) dx} \cong \frac{1}{N} \sum_{i=1}^N V(x_i)$$

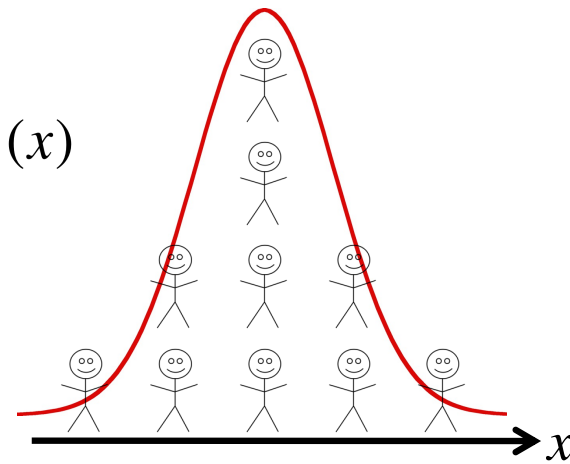
It's not  $\psi^*(x, \tau) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x, \tau)$



$$\psi(x, \tau \rightarrow \infty) = \phi_0(x)$$



$$\tau \rightarrow \infty$$



# Reference Energy

- Energy measured relative to reference energy to achieve stationary population

$$\frac{\partial}{\partial \tau} \psi(x, \tau) = \frac{\hbar}{2m} \frac{\partial^2}{\partial x^2} \psi(x, \tau) - \frac{V(x) - V_{\text{ref}}}{\hbar} \psi(x, \tau)$$

$$\begin{aligned} \int_{-\infty}^{\infty} \frac{\partial}{\partial \tau} \psi(x, \tau) dx &= \left[ \frac{\hbar}{2m} \frac{\partial}{\partial x} \psi(x, \tau) \right]_{-\infty}^{\infty} - \int \frac{V(x)}{\hbar} \psi(x, \tau) dx + \frac{V_{\text{ref}}}{\hbar} \int \psi(x, \tau) dx \\ &= - \int \frac{V(x)}{\hbar} \psi(x, \tau) dx + \frac{V_{\text{ref}}}{\hbar} \int \psi(x, \tau) dx \\ &\quad \int_{-\infty}^{\infty} dx \frac{\partial^2}{\partial x^2} \psi(x) = \left[ \frac{\partial}{\partial x} \psi(x) \right]_{-\infty}^{\infty} = 0 \end{aligned}$$

- For  $\tau \rightarrow \infty$ ,

$$\psi(x, \tau) \approx c_0 \phi_0(x) \exp(-(E_0 - V_{\text{ref}}) \tau / \hbar)$$

$$\therefore \frac{\partial}{\partial \tau} \psi(x, \tau) \approx \frac{V_{\text{ref}} - E_0}{\hbar} \psi(x, \tau)$$

$$\int \frac{V_{\text{ref}} - E_0}{\hbar} \psi(x, \tau) dx = - \int \frac{V(x)}{\hbar} \psi(x, \tau) dx + \frac{V_{\text{ref}}}{\hbar} \int \psi(x, \tau) dx$$

$$\therefore \frac{E_0}{\hbar} \int \psi(x, \tau) dx = \int \frac{V(x)}{\hbar} \psi(x, \tau) dx \quad \Rightarrow \quad E_0 = \frac{\int V(x) \psi(x, \tau) dx}{\int \psi(x, \tau) dx} = \langle V \rangle$$

# Choice of Reference Energy

- **Number of random walkers:**  $N(\tau) = \int_{-\infty}^{\infty} \psi(x, \tau) dx$

$$\frac{d}{d\tau} N = \frac{V_{\text{ref}} - \langle V \rangle}{\hbar} N(\tau)$$

$$\therefore \int_{-\infty}^{\infty} \frac{\partial}{\partial \tau} \psi(x, \tau) dx = - \int \frac{V(x)}{\hbar} \psi(x, \tau) dx + \frac{V_{\text{ref}}}{\hbar} \int_{-\infty}^{\infty} \psi(x, \tau) dx$$

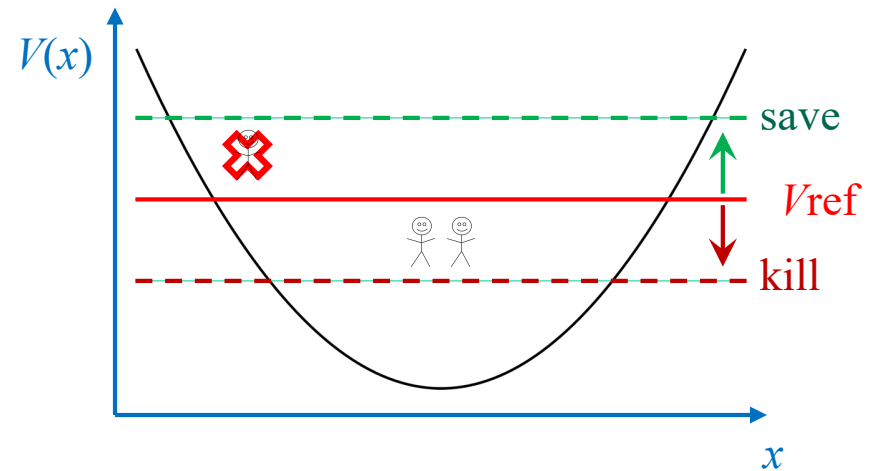
- **Choose new  $V_{\text{ref}}$  to counter-balance the current population growth**

$$-\frac{d}{d\tau} N|_{\text{current}} = \frac{V_{\text{ref}}^{\text{new}} - \langle V \rangle}{\hbar} N(\tau)$$

$$\frac{V_{\text{ref}}^{\text{new}}}{\hbar} = \frac{\langle V \rangle}{\hbar} - \frac{dN/d\tau}{N(\tau)}$$

$$\therefore V_{\text{ref}} = \langle V \rangle - \frac{N_0}{N(\tau) \Delta \tau} (N(\tau + \Delta \tau) - N(\tau))$$

$\hbar = 1$  (atomic unit)



For numerical stability, replace  $N$  by  $N(\tau = 0) = N_0$

# Quantum Monte Carlo Algorithm

1. Place  $N_0$  walkers at the initial set of positions  $x_i$ .

2. Compute the reference energy,  $V_{\text{ref}} = \sum_i V(x_i)/N_0$ .

3. For each walker,  $D = \frac{\hbar}{2m} = \frac{1}{2} \text{(a. u.)} = \frac{(\Delta s)^2}{2\Delta\tau}$

a. Randomly move the walker to the right or left by a fixed step length  $\Delta s$ .

b. Compute  $\Delta V = V(x) - V_{\text{ref}}$  & a random number  $r \in [0, 1]$ . If  $\Delta V > 0$  &  $r < \Delta V \Delta\tau$  ( $\Delta\tau = \Delta s^2$ ), then remove the walker. If  $\Delta V < 0$  &  $r < -\Delta V \Delta\tau$ , then add another walker at  $x$ . Otherwise, just leave the walker at  $x$ .

4. Compute the mean potential energy  $\langle V \rangle = \sum_i V(x_i)/N$  & the actual number of random walkers  $N$ . The new reference potential is given by

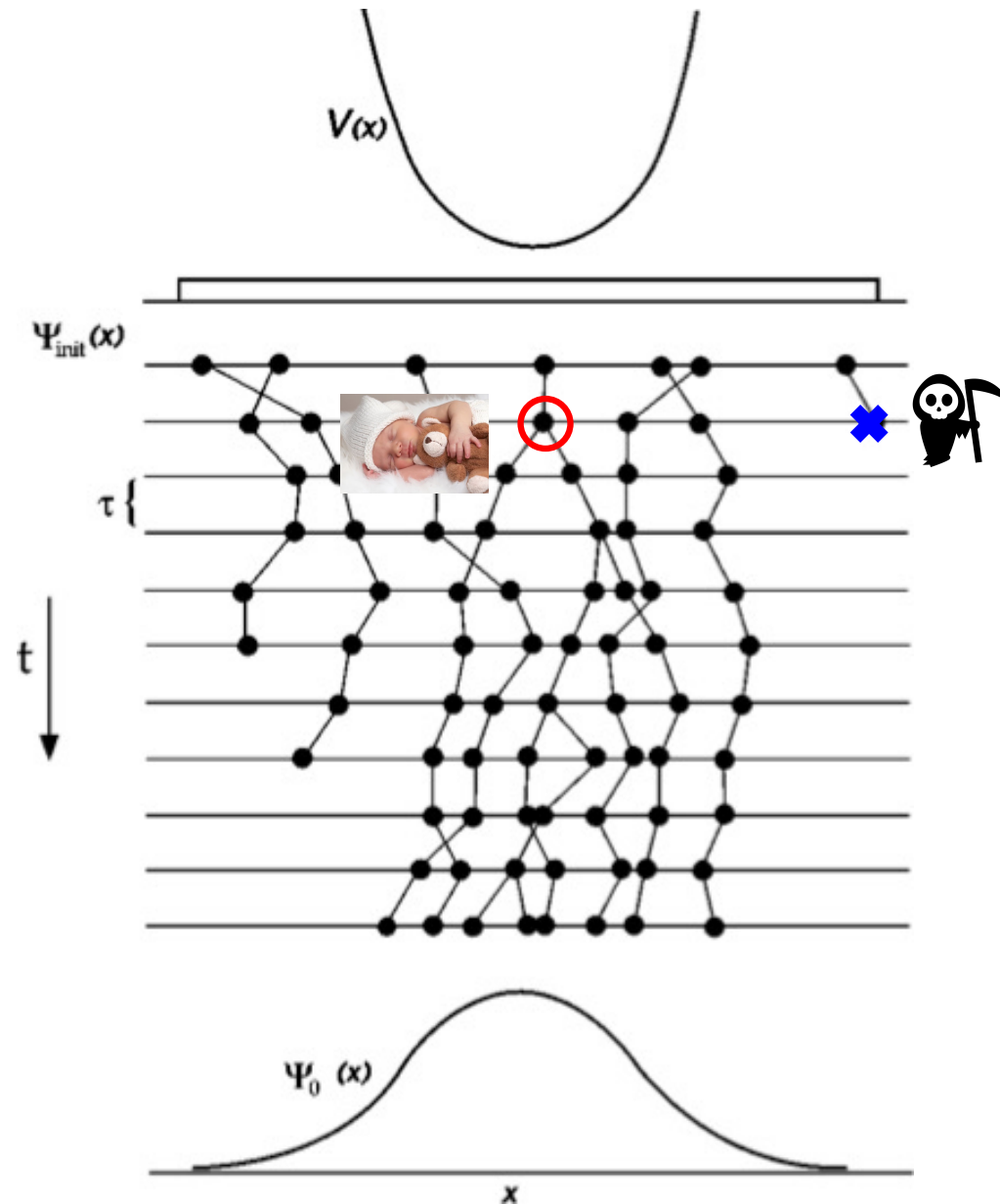
$$V_{\text{ref}} = \langle V \rangle - \frac{N(\tau + \Delta\tau) - N(\tau)}{N(\tau)\Delta\tau} N_0$$

$$\Delta\psi(x, \tau) = -\frac{\Delta V(x)}{\hbar} \Delta\tau \cdot \psi(x, \tau)$$

The average  $\langle V \rangle$  is an estimate of the ground state energy.

5. Repeat steps 3–4 until the estimates of the ground state energy  $\langle V \rangle$  have reached a steady state value with only random fluctuations. Average  $\langle V \rangle$  over many Monte Carlo steps to compute the ground state energy.

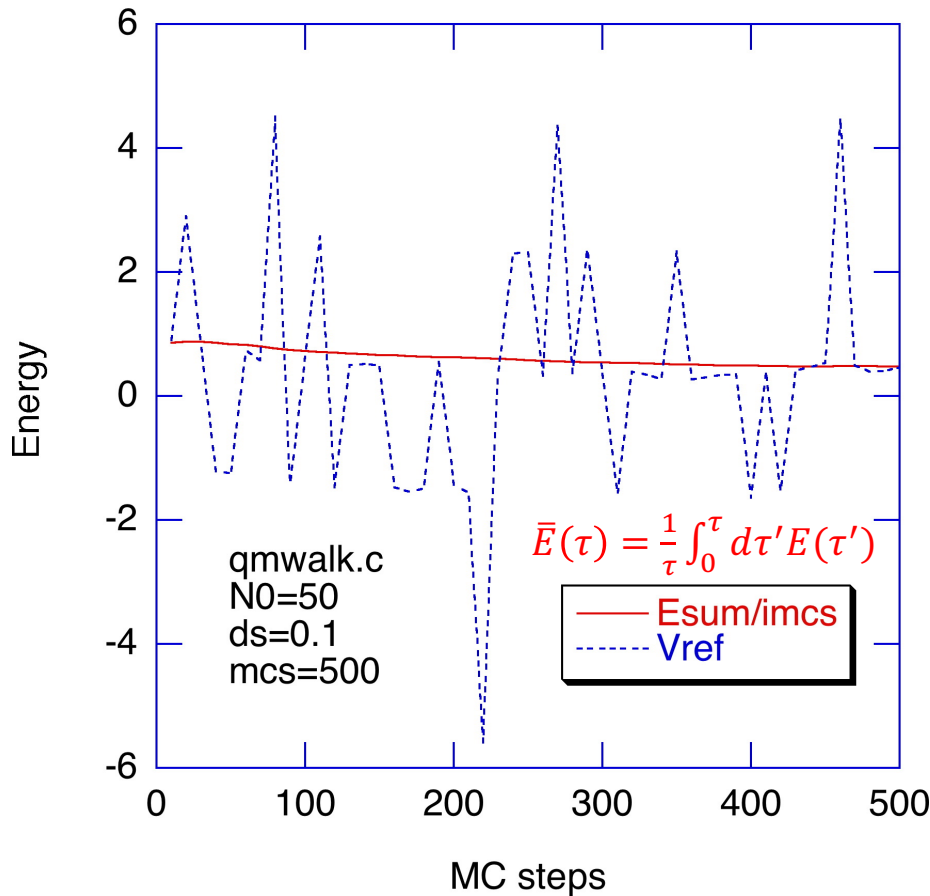
# Random Walk + Birth/Death



W. M. C. Foulkes *et al.*, *Rev. Mod. Phys.* **73**, 33 ('01)

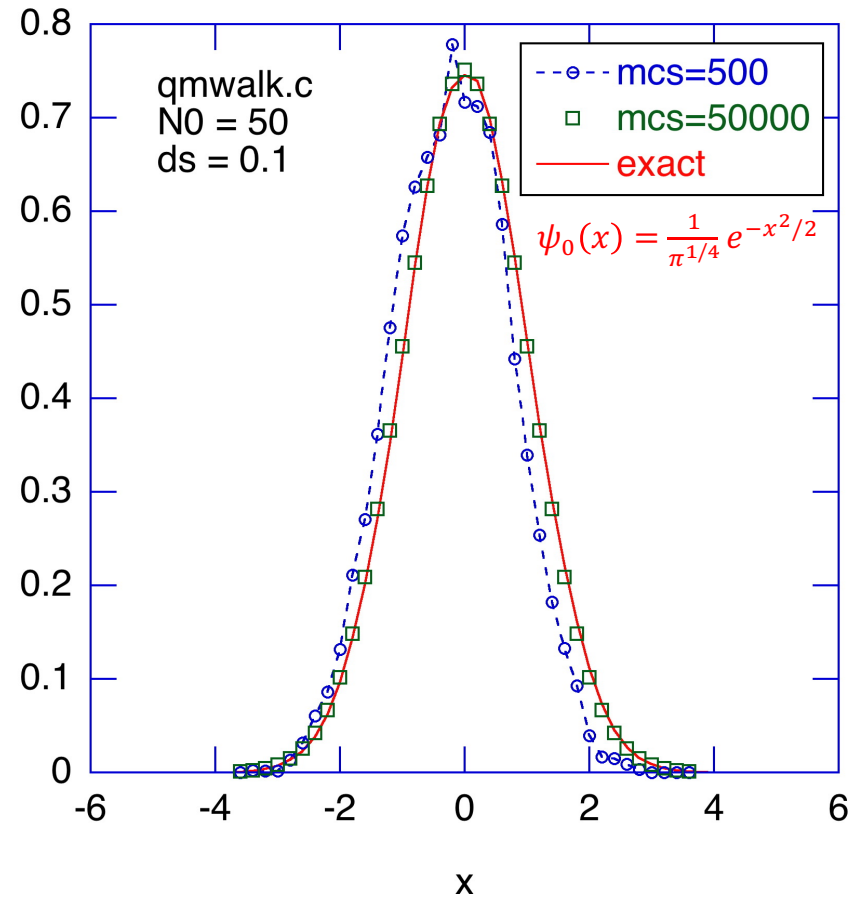
# Numerical Example

- $V(x) = x^2/2$  (in atomic unit)



(after  $0.4 \times 500 = 200$  MC steps of thermalization)

$$D = \frac{\hbar}{2m} = \frac{1}{2} \text{ (a. u. )} = \frac{(\Delta S)^2}{2\Delta\tau}$$



$$\frac{1}{\tau} \int_{-\infty}^{+\infty} \frac{\Delta^2}{2} \varphi(\Delta) d\Delta = D$$

A. Einstein, *Ann. Phys.* **17**, 549 (1905)



# Where to Go from Here

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- **Types of QMC for many electrons: diffusion MC & variational MC (zero temperature); path-integral MC (finite temperature)**

*Interacting Electrons*, Martin, Reining & Ceperley (Cambridge Univ. Press, '16)

- **QMC for realistic materials**

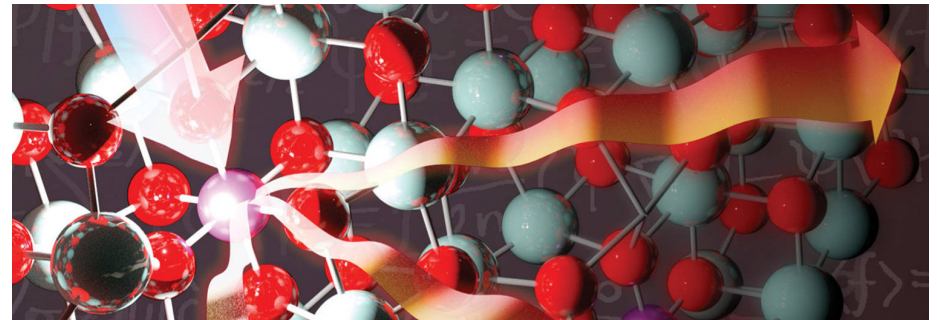
*Quantum Monte Carlo simulations of solids*, Foulkes et al., *Rev. Mod. Phys.* **73**, 33 ('01)

- **QMC software**

*QMCPACK*: <http://qmcpack.org>

*QWalk*: <http://qwalk.github.io/mainline>

*CASINO*: <https://vallico.net/casinoqmc>



- **Neural networks to represent many-electron wave functions (~ variational QMC)**

*NetKet*: <https://www.netket.org>

