# Quantum Monte Carlo Simulation

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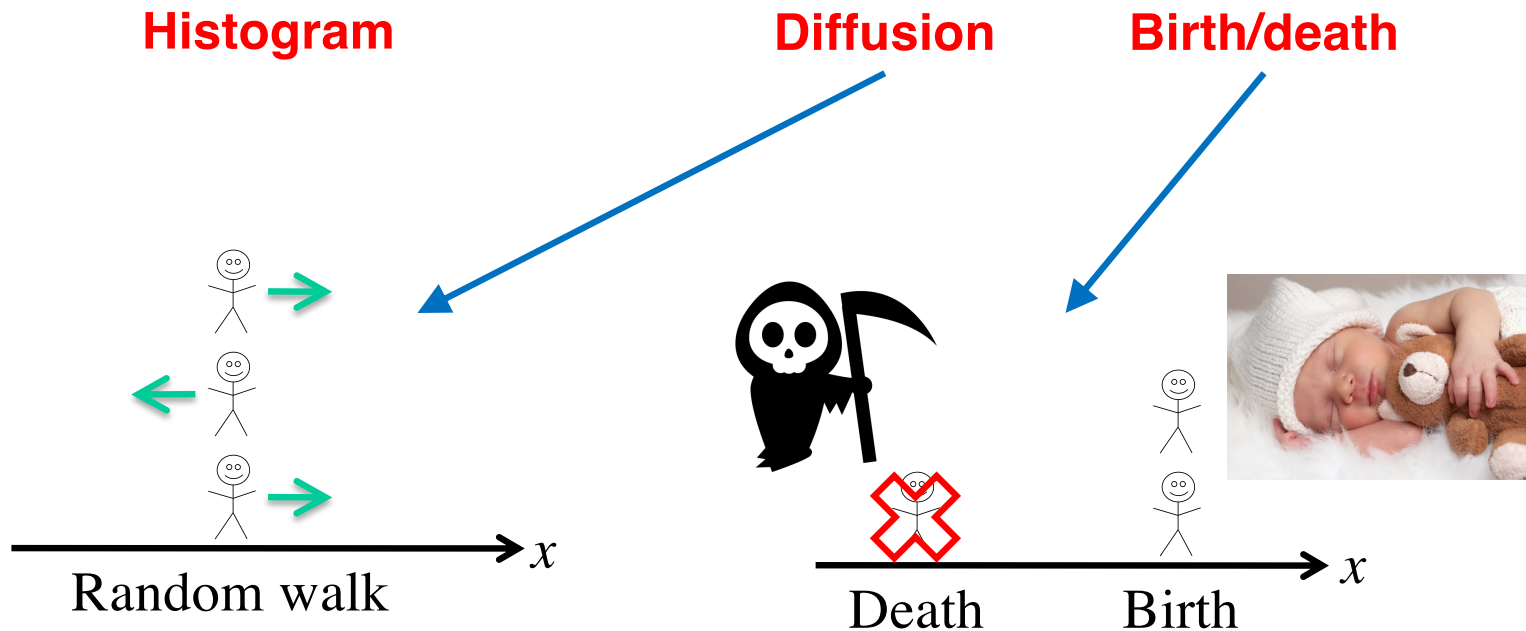
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Random walk to solve quantum eigenvalue problem
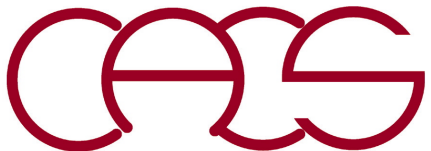
Imaginary-time Schrödinger Equation

- $\tau = it$

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

Histogram **Diffusion** **Birth/death**

Random walk

Death Birth

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

Ground-State Filter

$$\psi(x,\tau) = \exp(-H\tau/\hbar)\psi(x,0) = \sum_n c_n \phi_n(x)\exp(-E_n\,\tau/\hbar)$$

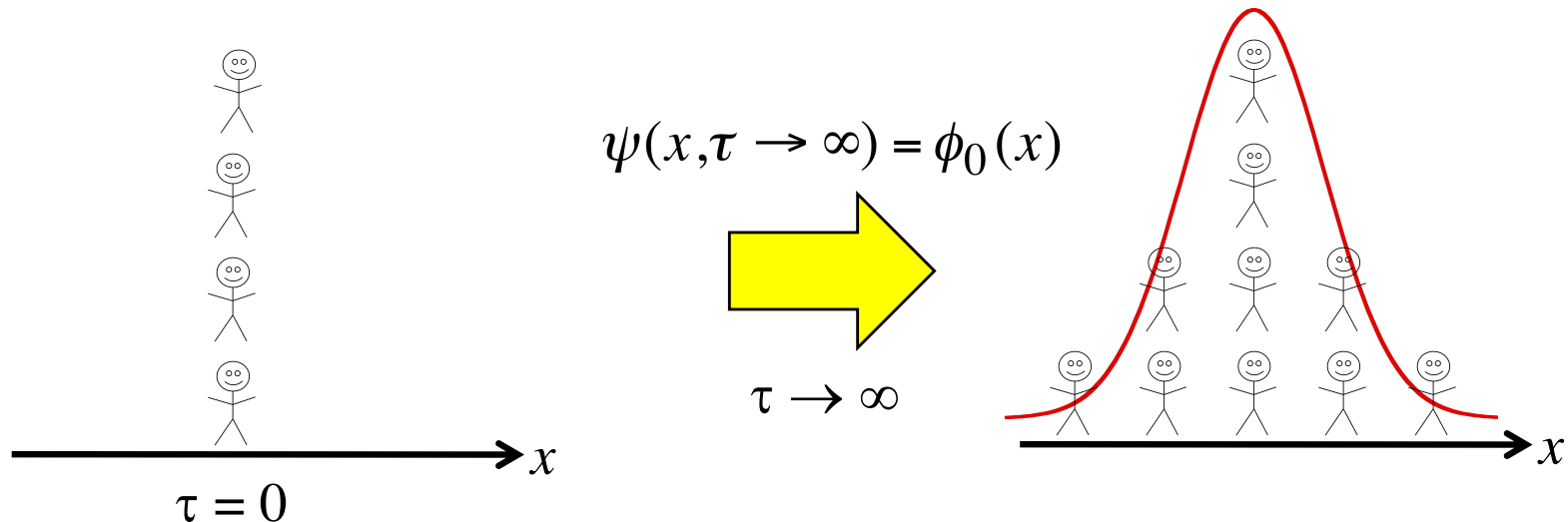Completeness: $|\psi\rangle = \overset{1}{\overbrace{\sum_n |n\rangle\langle n|}}\psi\rangle$

$$c_n = \int dx\,\phi_n(x)\psi(x,0)$$

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

- **Energy estimate**

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

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

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

$$\tau \to \infty$$

$$\tau = 0$$

Reference Energy

- **Energy measured relative to reference energy to achieve stationary population**

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

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

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

$$\int_{-\infty}^{\infty} \frac{\partial^2}{\partial x^2} \psi(x) = \left[\frac{\partial}{\partial x} \psi(x) \right]_{-\infty}^{\infty} = 0$$

- **For $\tau \to \infty$,**

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

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

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

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

Choice of Reference Energy

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

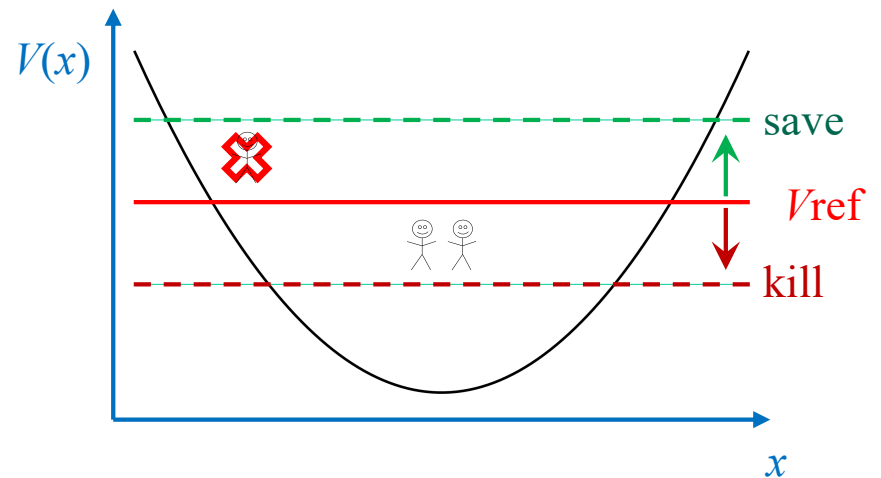$$\frac{d}{d\tau}N = \frac{V_{\text{ref}} - \langle V \rangle}{\hbar} N(\tau)$$

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

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

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

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

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

$V(x)$

save

V_{ref}

kill

x

Quantum Monte Carlo Algorithm

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

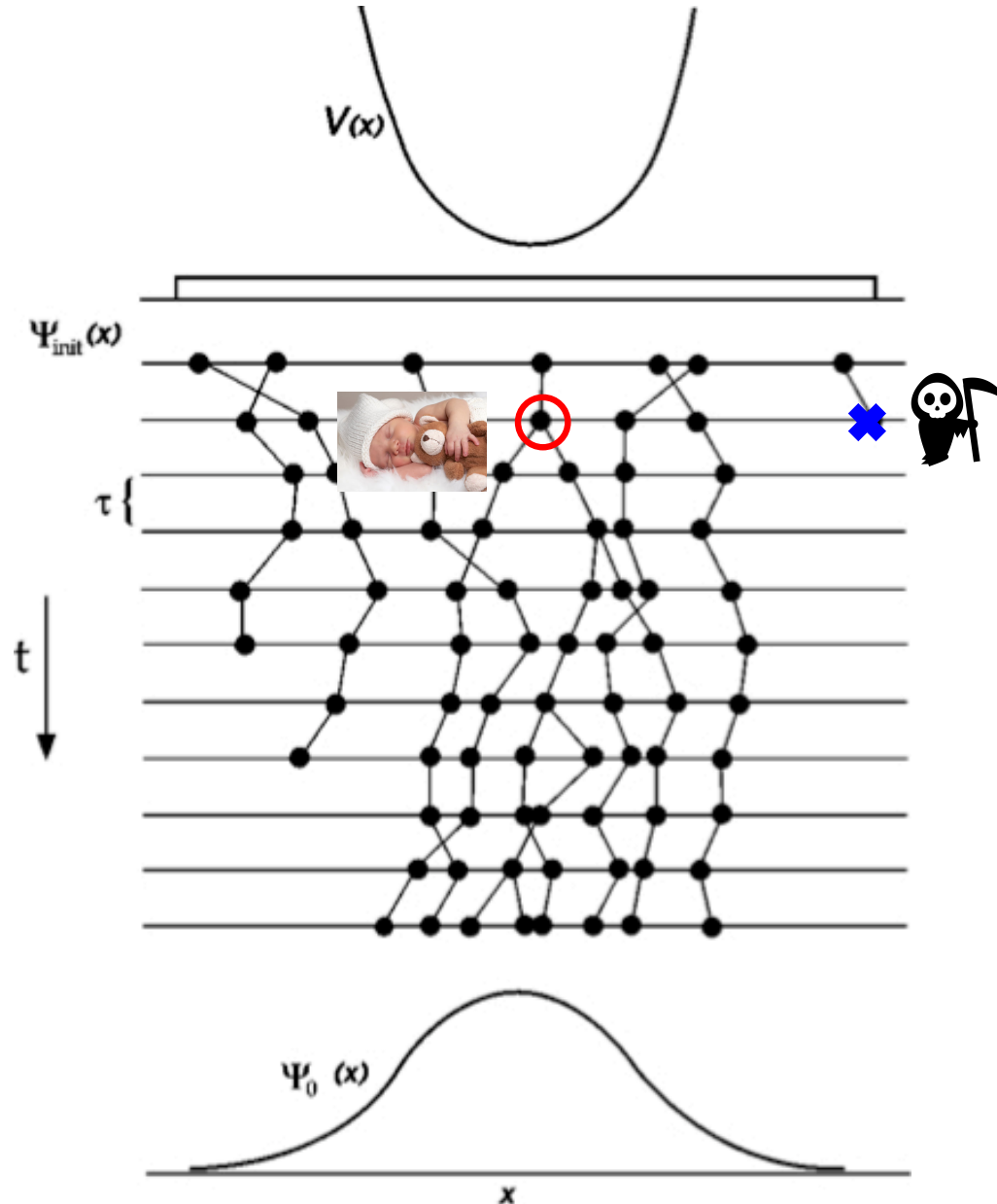2. Compute the reference energy, $V_{\text{ref}} = \Sigma_i\, V(x_i)/N_0$.

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

3. For each walker,

   a. Randomly move the walker to the right or left by a fixed step length Δs.

   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 $\langle V \rangle = \Sigma_i\, V(x_i)/N$ & the actual number of random walkers N. The new reference potential is given by

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

   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.
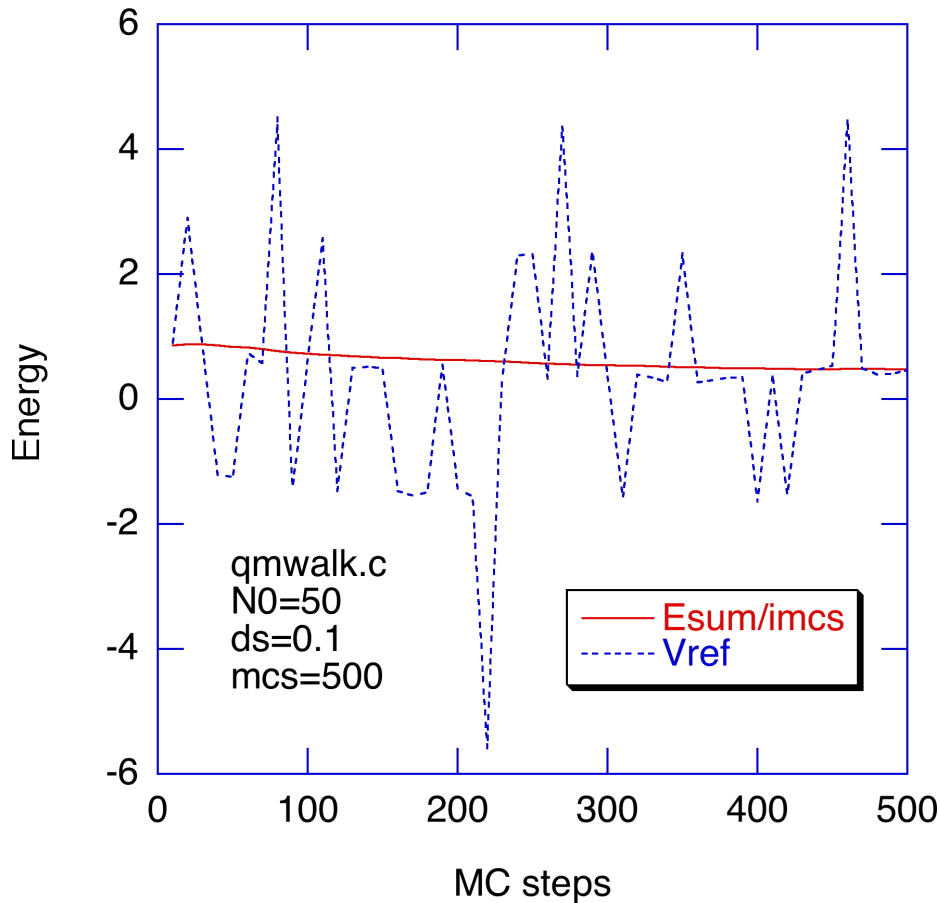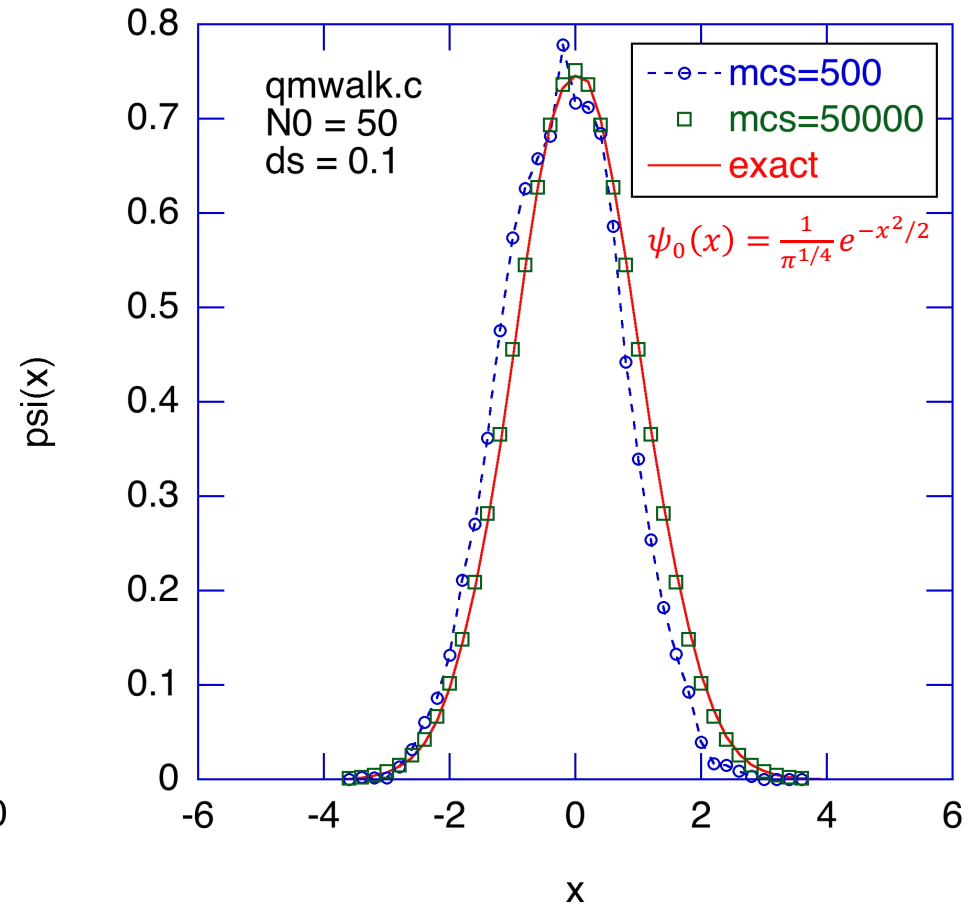
Random Walk + Birth/Death

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

Numerical Example

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

Left plot axis labels: Energy (vertical), MC steps (horizontal)

Left plot legend and annotations:
qmwalk.c
N0=50
ds=0.1
mcs=500

Legend:
— Esum/imcs
--- Vref

(after 0.4×500 = 200 MC steps of thermalization)

Right plot axis labels: psi(x) (vertical), x (horizontal)

Right plot annotations:
qmwalk.c
N0 = 50
ds = 0.1

Legend:
--○-- mcs=500
□ mcs=50000
— exact

$$\psi_0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}$$

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

Where to Go from Here

- **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)
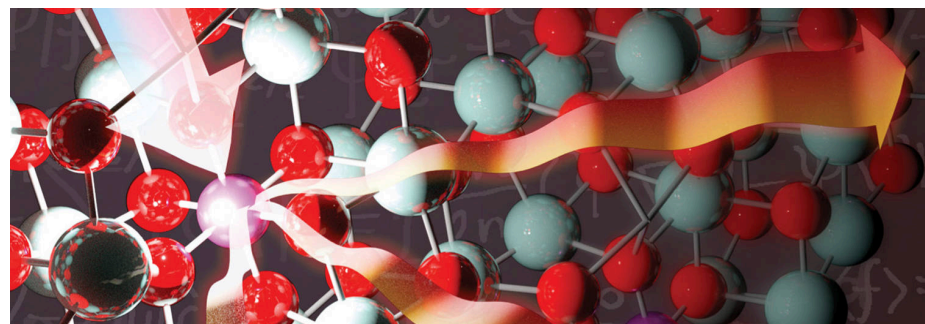
- **QMC for realistic materials**

  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**

  NetKet: https://www.netket.org