Instantons in quantum annealing: thermally assisted tunneling vs quantum Monte Carlo simulations

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Quantum Monte Carlo (QMC)

- Quantum Monte Carlo provides reliable solutions to quantum many-body problems.
- It can also be used in classical optimization problems as an alternative to simulated annealing.
- Whether quantum tunneling can be simulated efficiently by quantum Monte Carlo?

Why QMC?

- Recent Google result (arXiv:1512.02206) showed that there is no asymptotic speed up when the D-Wave quantum annealer is compared to QMC, although a constant factor 10^8 is observed.
- There exists an analogy between the tunneling decay of quantum systems and classical escape-over-a-barrier problem.

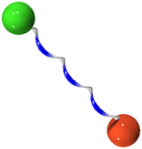
  J.S. Langer, *Theory of Condensation point*, Annals of Physics **41**, 108 (1967).

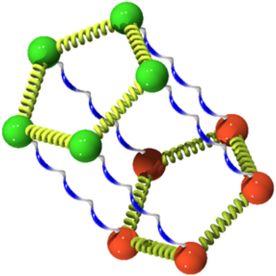
  M.Buttiker and R.Landauer, *Nucleation theory of overdamped soliton motion*, Phys. Rev. Lett. **43**, 1457 (1979).

What is QMC?

Path-integral Monte Carlo works by Trotterizing the partition function in imaginary time

$$Z = e^{-\beta \hat{H}_q} \approx \prod_{j=1}^{P} e^{-\beta \Gamma \hat{K}/P} e^{-\beta \hat{U}/P} = e^{-\beta H_c(\beta)/P} .$$





Tunneling in spin systems

We consider the mean-field model where the system Hamiltonian is symmetric with respect to permutation of individual spins

$$\hat{H} = -N\Gamma \hat{m}_x - Ng(\hat{m}_z)$$

$$\hat{m}_\alpha = \frac{1}{N}\sum_{i=1}^{N} \sigma_i^\alpha \,, \quad \alpha = x, y, z$$

Here $g(m)$ is a nonlinear term that allows for co-existing local and global minima for $m \in (-1, 1)$.

The WKB Hamiltonian is

$$H_{\mathrm{WKB}}(m, p) = -2\Gamma N \sqrt{\ell^2 - m^2} \cos p - Ng(m) \,,$$

where $\ell = 2S/N \in (0, 1)$ and $m \equiv m_z \in (-\ell, \ell)$.

QMC probability functional

We define the state vector

$$\underline{\sigma}(\tau) = \{\sigma_1(\tau), \ldots, \sigma_N(\tau)\}, \quad \underline{\sigma}(0) = \underline{\sigma}(\beta)$$

The probability of a state vector is

$$P[\underline{\sigma}(\tau)] = \mathcal{Z}^{-1} \exp\left[-\beta N E[\underline{\sigma}(\tau)]\right],$$

$$E[\underline{\sigma}(\tau)] = -\frac{1}{\beta}\int_0^\beta g[m(\tau)]d\tau - \frac{J(\beta)}{\beta}\sum_{j=1}^{N} \kappa[\sigma_j(\tau)]\,.$$

The function κ equals to the number of times $\sigma_j(\tau)$ changes its sign.
Order parameter: the total magnetization

$$m[\underline{\sigma}(\tau)] = \frac{1}{N}\sum_{i=1}^{N} \sigma_i(\tau)\,.$$

QMC probability functional in reduced space

There is a Gibbs probability measure $P[m(\tau)] = Z^{-1} e^{-N\beta F[m(\tau)]}$ for the magnetization order parameter $m(\tau)$ (*Bapst, Semerjian, 2012*)

$$F[m(\tau)] = \frac{1}{\beta}\int_0^\beta [m(\tau)g'(m(\tau)) - g(m(\tau))]d\tau - \frac{1}{\beta}\log \Lambda[g'(m(\tau))]$$

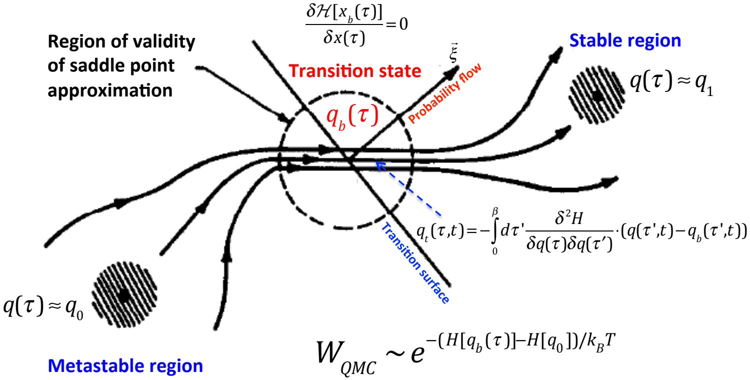
Here, the functional $\Lambda[\lambda(\tau)]$ is

$$\Lambda[\lambda(\tau)] = \mathrm{Tr} K^{\beta,0}[\mathbf{B}(\tau)], \quad K^{\tau_2,\tau_1} = \mathrm{T}_+ e^{-\int_{\tau_1}^{\tau_2} d\tau H_0(\tau)}$$

$$H_0(\tau) = -\mathbf{B}(\tau)\cdot\boldsymbol{\sigma}, \quad \mathbf{B}(\tau) = (\Gamma, 0, \lambda(\tau)) \,,$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is vector of Pauli matrices. The propagator K corresponds to a spin-1/2 evolving under the magnetic field $\mathbf{B}(\tau)$.

Kramers escape problem



The system reaches the transition state via thermal fluctuation. Then with probability $\sim 1/2$ it moves toward the global minimum.

Kramers escape in QMC

QMC samples paths $\underline{\sigma}(\tau, t)$. When the path $m(\tau, t)$ moves from the local minimum to the global minimum by fluctuation, it has to go through the **transition state** $m_z(\tau)$

$$W_{\mathrm{QMC}} \propto e^{-\beta N \Delta F}, \quad \Delta F = F[m_z(\tau)] - F(m_0)\,.$$

Here $m_z(\tau)$ is the saddle point of the functional F that satisfies the equation

$$\left.\frac{\delta F[m(\tau)]}{\delta m(\tau)}\right|_{m_z(\tau)} = 0, \quad m_z(0) = m_z(\beta)\,.$$

Instantons in QMC

Variational equations $\delta F = 0$ take the form

$$m_z(\tau) = \frac{\delta \log \Lambda(\lambda(\tau))}{\delta \lambda(\tau)}, \quad \lambda(\tau) = \frac{dU[m_z(\tau)]}{dm_z}.$$

We introduce vector of magnetization components

$$\mathbf{m}(\tau) = \frac{\mathrm{Tr}[K^{\beta,\tau} \boldsymbol{\sigma} K^{\tau,0}]}{\mathrm{Tr} K^{\beta,0}}$$

Optimal trajectory is a classical rotator in nonlinear potential

$$\frac{d\mathbf{m}(\tau)}{d\tau} = -2i \frac{\partial \mathcal{H}_0[\mathbf{m}(\tau)]}{\partial \mathbf{m}} \times \mathbf{m}(\tau)$$

$$\mathcal{H}_0[\mathbf{m}] = -\Gamma m_x(\tau) - U[m_z(\tau)]$$

Instantons in QMC II

Two integrals of motion

$$\mathcal{H}_0[\mathbf{m}] = e, \quad \mathbf{m}(\tau) \cdot \mathbf{m}(\tau) = \ell^2$$

Then the solution can be written in the following form:

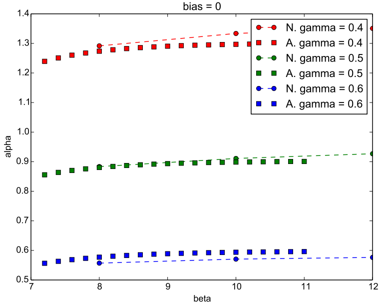
$$\begin{aligned} m_x &= \sqrt{\ell^2 - m_z^2} \cosh p(m_z, e) \\ m_y &= -i\sqrt{\ell^2 - m_z^2} \sinh p(m_z, e) \\ e(m_z, p) &= -2\Gamma\sqrt{\ell^2 - m_z^2} \cos p - g(m_z), \end{aligned}$$

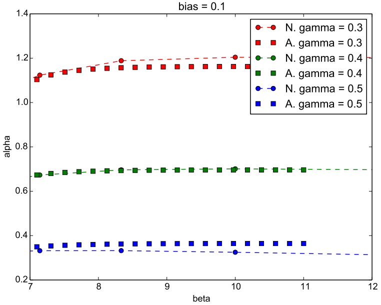
The equation for $m_z(\tau)$ is identical to that of the WKB instanton trajectory.

QMC for Curie Weiss model

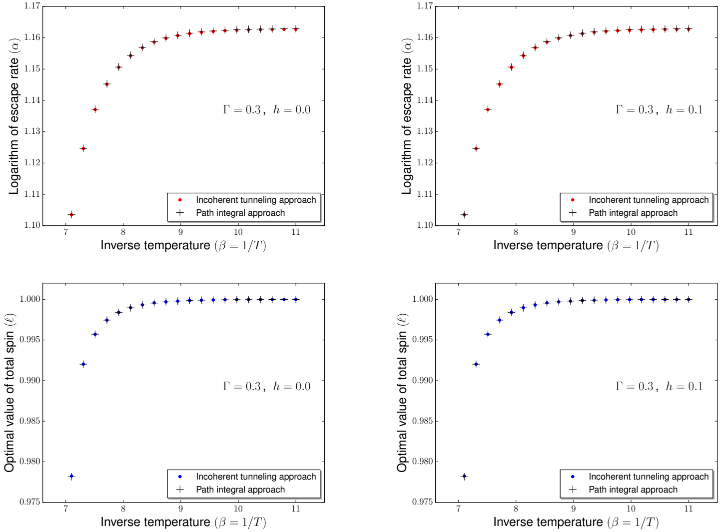
$$\frac{H}{N} = -2\Gamma m_x - m_z^2 - hm_z$$

$$W_{\mathrm{QMC}} = B_{\mathrm{QMC}} e^{-\alpha N}, \quad \alpha = \alpha(\beta, \Gamma, h)$$





Comparison of QMC and thermally assisted tunneling



Future work

- Quantum Monte Carlo with open boundary condition
- Calculate the prefactor for QMC and quantum annealing
- More general spin coupling