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.


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

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

where \( \ell = 2S/N \in (0, 1) \) and \( m \equiv m_z \in (-\ell, \ell) \).
We define the state vector

\[ \sigma(\tau) = \{\sigma_1(\tau), \ldots, \sigma_N(\tau)\}, \quad \sigma(0) = \sigma(\beta) \]

The probability of a state vector is

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

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

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

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

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

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

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

The system reaches the transition state via thermal fluctuation. Then with probability $\sim 1/2$ it moves toward the global minimum.
QMC samples paths \( \sigma(\tau, t) \). 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** \( m_z(\tau) \)

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

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

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

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

Optimal trajectory is a classical rotator in nonlinear potential

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

$$\mathcal{H}_0[m] = -\Gamma m_x(\tau) - U[m_z(\tau)]$$
Two integrals of motion

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

Then the solution can be written in the following form:

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

The equation for \( m_z(\tau) \) is identical to that of the WKB instanton trajectory.
\[
\frac{H}{N} = -2\Gamma m_x - m_z^2 - hm_z
\]

\[
W_{QMC} = B_{QMC} e^{-\alpha N}, \quad \alpha = \alpha(\beta, \Gamma, h)
\]
Comparison of QMC and thermally assisted tunneling

![Comparison of QMC and thermally assisted tunneling](image)

**Incoherent tunneling approach**

**Path integral approach**

Optimal value of total spin ($\ell$)

- $\Gamma = 0.3$, $h = 0.0$
- $\Gamma = 0.3$, $h = 0.1$

Logarithm of escape rate ($\alpha$)

- $\Gamma = 0.3$, $h = 0.0$
- $\Gamma = 0.3$, $h = 0.1$

Inverse temperature ($\beta = 1/T$)

- $0.975$
- $0.980$
- $0.985$
- $0.990$
- $0.995$
- $1.000$

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Future work

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