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

Zhang Jiang

QuAIL, NASA Ames Research Center, Moffett Field, CA
SGT Inc., Greenbelt, MD

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Vadim N. Smelyanskiy, Sergio Boixo, Sergei V. Isakov, Hartmut Neven
Google, Venice, CA

Guglielmo Mazzola, Matthias Troyer
Institute for Theoretical Physics, ETH Zurich, Zurich, Switzerland
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

\[ Z = e^{-\beta \hat{H}_q} \approx \prod_{j=1}^{P} e^{-\beta \Gamma \hat{\mathcal{K}} / P} e^{-\beta \hat{U} / P} = e^{-\beta H_c(\beta) / P}. \]
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 \( m \equiv m_z \in (-\ell, \ell) \).
QMC probability functional

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

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

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

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 $B(\tau)$. 
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 $\sigma(\tau, t)$. 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

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

$$\mathcal{H}_0[m] = -\Gamma m_x(\tau) - U[m_z(\tau)]$$
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.
\[ H = \frac{-2\Gamma m_x - m_z^2 - hm_z}{N} \]

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

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

Logarithm of escape rate ($\alpha$)

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

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

Optimal value of total spin ($\ell$)

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

$\Gamma = 0.3$, $h = 0.1$
Future work

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