Computational power of Collective Tunneling in a Quantum Annealer

Vadim Smelyanskiy
Google, Los Angeles

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Collaborators

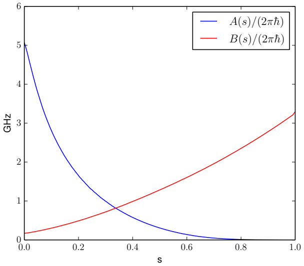
- Sergei V. Isakov (Google, LA)
- Sergio Boixo (Google, LA)
- Hartmut Neven (Google, LA)
- John Martinis (Google, LA)
- Zhang Jiang (NASA Ames, Mountain View)
- Guglielmo Mazzola (ETH, Zurich)
- Matthias Troyer (ETH, Zurich)
- Mohammad Amin (DWave)
- Anatoly Smirnov (DWave)
- Mark Dykman (Michigan State University)

Optimization via Quantum annealing

Objective: Finding global minimum of a function of N binary variables

"Problem Hamiltonian" encodes the optimization problem

$$\hat{H}_{\mathrm{P}} = -\sum_{k=1}^{K} \sum_{j_1,\ldots,j_k=1}^{N} J_{j_1,\cdots,j_k} \sigma_{j_1}^z \cdots \sigma_{j_k}^z$$



"Driver Hamiltonian" $-\sum_{j=1}^{N} \sigma_j^x$ corresponds to the spin coupling to transverse field. It gives rise to quantum dynamics. Control functions $A(s)$,$B(s)$ slow vary in time $s \in (0,1)$. Total Hamiltonian

$$\hat{H}(s) = -A(s) \sum_{j=1}^{N} \sigma_j^x + B(s) H_{\mathrm{P}}$$

Tunelling during Quantum Annealing

Basis of coherent spin states

$$|\Psi\rangle = \bigotimes_j \left[\cos\frac{\theta_j}{2}|0\rangle + e^{-i\phi_j}\sin\frac{\theta_j}{2}|1\rangle\right]$$

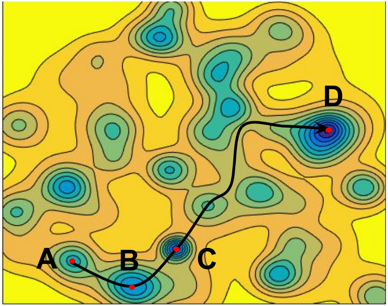
Each qubit is represented by a unit vector (point on Bloch sphere)

$$\mathbf{n}_j = (\sin\theta_j\cos\phi_j, \sin\theta_j\sin\phi_j, \cos\theta_j)$$

Effective potential

$$\langle\Psi|\hat{H}(s)|\Psi\rangle = H(s, \mathbf{n}_1, \ldots, \mathbf{n}_N)$$

Mean-field time-dependent energy landscape



D-Wave tunnelling experiments

Weak-strong cluster pair: ferromagnetic Ising spin model with local fields in z-direction

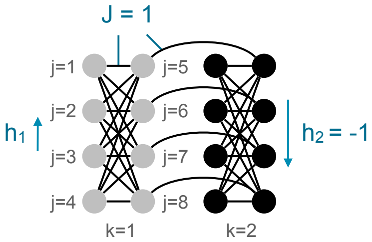
$$\hat{H}(s) = -A(s)\sum_j \sigma_j^x - B(s)\sum_{i<j} J_{ij}\,\sigma_i^z\sigma_j^z - B(s)\sum_j h_j\sigma_j^z$$

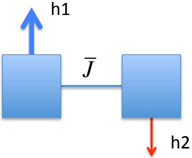
Global bifurcation mechanism:

Boixo, Smelyanskiy, et al, Nature Communications (2015)

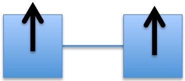
Initial stage of quantum annealing $A \gg B$ corresponds to all spins nearly pointing in x-direction

$$\langle\sigma_j^z\rangle \sim B/A, \quad \langle\sigma_i^z\sigma_j^z\rangle \propto (B/A)^2\ h_j$$





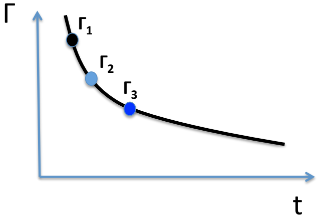
$$h_1 - h_2 < J/2$$

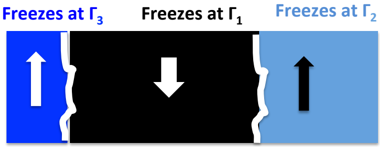


Ferromagnetic ground state

Spins aligned in the same direction

If the system dimensionality is not very high the interconnects between the parts of the system are not strong and the system parts go through the spontaneous symmetry breaking transitions at different times. This drives the system to a metastable minimum





Harris criterion:

correlation-length exponent ν of a d-dimensional uniform system satisfies $\nu < 2/d$, then the critical behavior of the corresponding disordered system (with random couplings) differs from that of its uniform analog.

Implementation on D-Wave device

(Denchev et al. PRX, 2016)

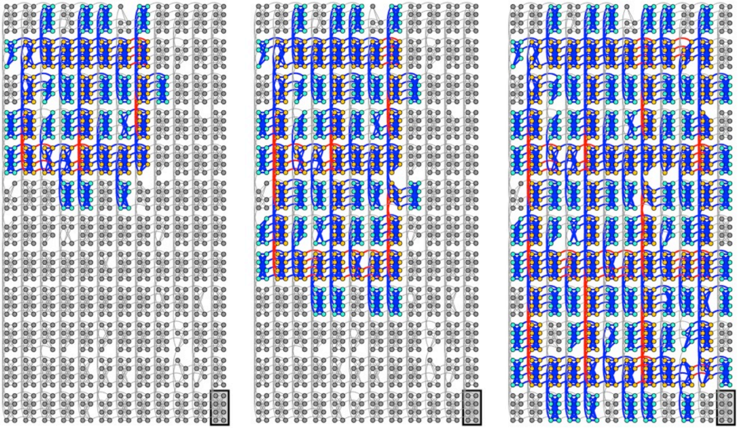
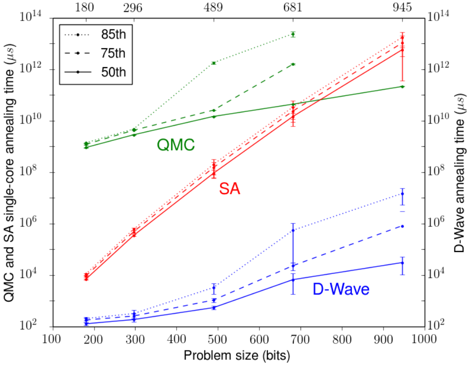


FIG. 3. Layout of the weak-strong cluster networks on the D-Wave 2X processor. Shown are three different sizes with 295, 490 and 945 qubits. Each cluster coincides with a Chimera cell with 8 qubits. Orange dots depict qubits subject to a strong local field $h_R = -1$ while the cyan dots represent the qubits with the weak field $h_L = 0.44$. Blue lines correspond to -1 connections and red lines to connections with a strength $+1$. Note that the graphs are somewhat irregular due to the fact that not all 1152 qubits are operational.

Relative performance of D-Wave and classical algorithms



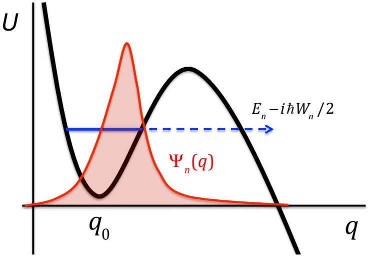
- D-Wave 2X quantum annealer achieves significant runtime advantages relative to Simulated Annealing (SA) and Quantum Monte Carlo (QMC) algorithms (up to $O(10^8)$ times faster than an optimized implementations on a single core).
- **No scaling advantage was observed for QMC**

- Quantum Monte Carlo (QMC) is a CLASSICAL algorithm providing reliable solutions to quantum many-body problems with applications ranging from materials science to complex biological systems.
- Can QMC simulate tunneling in Quantum Annealing (QA) efficiently?
- Results [Santoro et al., Science **295**, 2427 (2002); Heim et al. Science **348**, 215 (2015)] showed that QMC are useful for solving spin glass problems.
- Recent results by S. Issakov et al (arXiv:1510.08057) and Z. Jiang et al (arXiv:1603.01293), provided numerical and analytical evidence, respectively, that there is NO asymptotic speed up in quantum spin tunneling as compared to QMC simulations in certain models.
- A recent result from Google (Denchev et al. PRX 2016) showed that there is a substantial constant enhancement factor of QA compared to QMC in case of multi-qubit cotunellign

Incoherent tunneling decay of the metastable state
Particle in the potential

$$\mathbb{H} = \frac{p^2}{2m} + U(q)$$

- $\Delta \sim |\Psi_n(q_{\text{barrier exit point}})|$ is tunneling matrix element
- γ is dephasing rate
- **Incoherent tunneling conditon** $\gamma \gg \Delta$
- Incoherent tunnelling rate $W \sim \Delta^2/\gamma$



$$E_n \Longrightarrow E_n - \frac{i\hbar W_n}{2}$$

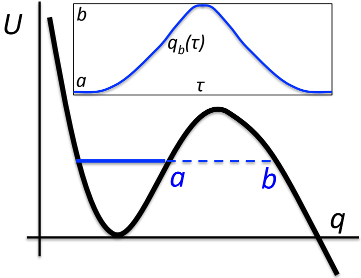
$$Z = Z_0 + \frac{i\hbar}{2k_BT}\sum_n W_n e^{-E_n/k_BT}$$

$$\frac{2\mathrm{Im}[F]}{\hbar} = W = \frac{1}{Z_0}\sum_n W_n e^{-E_n/k_BT}$$

Tunneling decay rate via instanton calculus

$$Z = \int_{q(0)=q(\beta)} \mathcal{D}q(\tau) e^{-\frac{1}{\hbar} S[q(\tau)]}$$

$$S = \int_0^\beta d\tau \left(\frac{m\dot{q}^2}{2} + U(q) \right) d\tau, \quad \beta = \frac{\hbar}{k_B T}$$



"Bounce solution":

$$\frac{\delta S}{\delta q(\tau)} = -m \frac{d^2}{d\tau^2} q_b(\tau) + U'(q_n(\tau)) = 0, \quad q_b(0) = q_b(\beta) = 0$$

$$W = \left(\frac{1}{2\pi\hbar} \int_0^\beta \dot{q}_b^2(\tau) d\tau \right)^{1/2} \left(\frac{\det[-m\frac{d^2}{d\tau^2} + U''(q_{\min})]}{\det'[-m\frac{d^2}{d\tau^2} + U''(q_b(\tau))]} \right)^{1/2} e^{-\frac{S[q_b(\tau)]}{\hbar} + \beta U(q_{\min})}$$

QMC simulations of tunneling decay

$$Z = \int_{q(0)=q(\beta)} \mathcal{D}q(\tau) e^{-\frac{\mathcal{H}[q(\tau)]}{k_B T}}$$

$$\mathcal{H}[q(\tau)] = \frac{1}{\beta} \int_0^\beta d\tau \left(\frac{m\dot{q}^2}{2} + U(q) \right) d\tau$$

QMC samples random periodic paths $q(\tau)$ with $q(0) = q(\beta)$ whose stochastic evolution in *real time t* is determined by the Metropolis algorithm for the Gibbs probability measure $P = Z^{-1} \exp[-\mathcal{H}[q(\tau)]/k_B T]$

Langevin equations (Model A of non-equilibrium dynamics)

$$\frac{\partial q(\tau,t)}{\partial t} = -\mu \frac{\partial \mathcal{H}[q(\tau,t)]}{\partial q(\tau,t)} + (2k_B T \mu)^{1/2} \eta(\tau,t)$$

$$q(0,t) = q(\beta,t), \quad \eta(0,t) = \eta(\beta,t), \quad \beta = \frac{\hbar}{k_B T}$$

Analog version of QMC

Consider *analog* device: a chain of tightly coupled over-damped nonlinear oscillators coupled to thermal reservoir

$$\Gamma = \beta/(\mu m) \quad - \quad \text{damping coefficient}, \qquad [\mu^{-1}] = [m\omega^2]$$

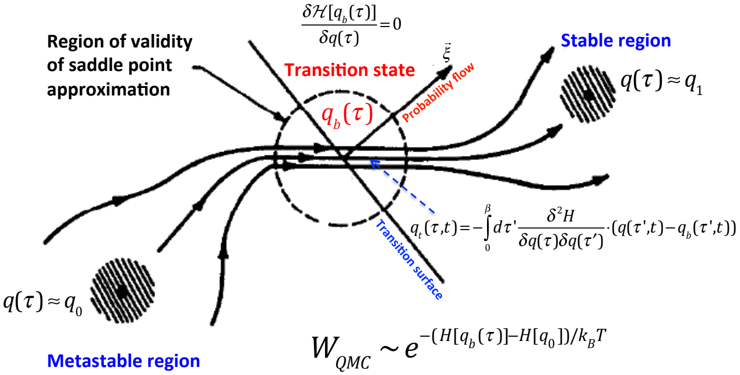
$$\Gamma \frac{\partial q(\tau,t)}{\partial t} = -\frac{1}{m} U'(q(\tau,t)) + \frac{\partial^2}{\partial \tau^2} q(\tau,t) + \left(\frac{2\,\hbar\,\Gamma}{m}\right)^{1/2} \eta(\tau,t)$$

$$q(0,t) = q(\beta,t)$$

There exists an analogy between the problem of tunneling decay of quantum systems and classical Kramers escape problem from a metastable state

- 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).
- Sidney Coleman, *Fate of the false vacuum: Semiclassical theory*, Phys. Rev. D **15**, 2929 (1977).

Tunneling decay as a Kramers escape problem



The system reaches the transition state via thermal fluctuation. Then with probability $\sim 1/2$ it moves toward the global minimum. Dynamical matrix $\delta^2\mathcal{H}/\delta q^2$ has one negative eigenvalue $\lambda_0 < 0$ related to departure from $q_b(\tau)$ corresponding to a saddle point.

Kramers escape rate

$$W_{QMC} = B_{QMC} \exp\left(-\frac{\mathcal{H}[q_b(\tau)]}{k_B T}\right) = B_{QMC} \exp\left(-\frac{S[q_b(\tau)]}{\hbar}\right)$$

$$\frac{W_{\mathrm{QMC}}}{W_{\mathrm{QT}}} = \frac{\mu|\lambda_0|}{2\pi}$$

λ_0 is a single negative eigenvalue of the operator $-m\frac{d^2}{d\tau^2} + U''(q_b(\tau))$

$$V[q] = \epsilon q^2 - \alpha q^4 \Longrightarrow \lambda_0 = -3\epsilon, \qquad [\epsilon] = [m\omega^2]$$

$$\frac{W_{\mathrm{QMC}}}{W_{\mathrm{QT}}} = \frac{3\mu\epsilon}{2\pi}$$

- Classical quantities μ,ϵ, no quantum enchancement if analogue device is used.
- In digital implementation $W_{\mathrm{QMC}}/W_{\mathrm{QT}} \propto \beta$ (imaginary time)

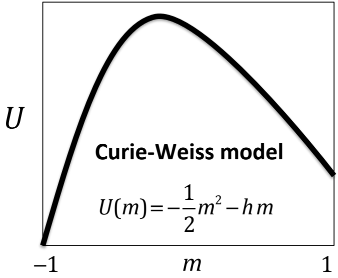
Tunneling in spin systems

Natural model to study incoherent tunneling in multi-qubit systems is mean-field spin$-1/2$ model in which system Hamiltonian is symmetric with respect to permutation of individual qubit operators.

Lipkin, Meshkov and Glick model (nuclear physics, quantum spin systems, Bose-Einstein, condensates, circuit QED)

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

$$\hat{m}_\alpha = \frac{1}{N}\sum_{i=1}^{N}\sigma_i^\alpha \equiv \frac{2\hat{S}_\alpha}{N}, \quad \alpha = x, y, z$$



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

WKB approach for multi-qubit thermally-assisted tunneling

A. Garg, J. Math. Phys. (1998), Bapst and Semerjian, JSP (2012), Kechedzhi, Smelyanskiy, PRX (2016)

Total spin of the system S conserves. We work in the basis of total spin and total spin projection on z axis $\hat{S}_z|M,S\rangle = M|M,S\rangle$

$$\Psi = \sum_{S=0}^{N/2} \sum_{\gamma=1}^{\mathcal{N}(N,S)} \sum_{M=-S}^{S} C_M^{S,\gamma} |M,S,\gamma\rangle, \quad \Omega(N,S) = \binom{N}{\frac{N}{2}-S} - \binom{N}{\frac{N}{2}-S-1}$$

Wave-function amplitudes $C_m^{S,\gamma}$ obey the stationary Schrödinger equation

$$-\Gamma \sum_{\alpha=\pm} \sqrt{(S+\alpha\,M)(S-\alpha\,M+1)}C_{m-\alpha} - NU(2M/N)C_m = EC_m$$

WKB solution has usual form $C_m = \frac{1}{\sqrt{v(M,E)}} \exp\left(i \int_{M_1}^{M} dM'\, p(M',E)\right)$. Here p is classical momentum of the system with Hamiltonian

$$H(M,p) = -2\Gamma\sqrt{S^2 - M^2}\cos p - NU(2M/N) = E$$

WKB approach for multi-qubit tunneling (cont.)

2 integrals of motion: energy $e = \frac{E}{N/2}$ and total spin $\ell = \frac{S}{N/2} \in (0,1)$.

Rescaled coordinate $m = \frac{M}{N/2} \in (-\ell, \ell)$

$$e_\ell(m,p) = -2\Gamma\sqrt{\ell^2 - m^2}\cos p - U(m),$$
$$u_{\rm eff}(m) = e(m,0)$$

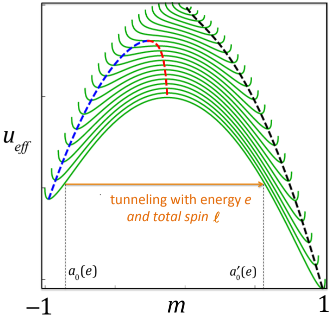
Action and momentum under the barrier

$$p(e,\ell) = i\,\mathrm{arcsinh}\frac{v(e,\ell,q)}{\Gamma\sqrt{\ell^2 - q^2}}$$

$$A(e,\ell) = \oint_{a_0(e,\ell)} \mathrm{Im}\, p(m,e,\ell)|dm$$

Number of states with a given total spin

$$\Omega(N,S) \sim \exp[NQ(\ell)]$$



Tunneling decay of metastable state: Partition function approach

$$E_n \Longrightarrow E_n - i\hbar W_n/2$$
$$W = -\frac{2}{\beta}\frac{\mathrm{Im}(Z_0)}{\mathrm{Re}(Z_0)} = \frac{\sum_n W_n e^{-\beta E_n/\hbar}}{\sum_n e^{-\beta E_n/\hbar}}$$

- Number of states with a given total spin $\Omega(N,S) \sim \exp[NQ(\ell)]$

$$Q(\ell) = \frac{1+\ell}{2}\log\frac{2}{1+\ell} + \frac{1-\ell}{2}\log\frac{2}{1-\ell}$$

$$W \propto \exp\left(-\frac{N}{2}\alpha\right), \quad \alpha = \mathfrak{F} - \mathfrak{F}_0$$
$$\mathfrak{F} = \min_{\ell}\min_{e\in\Omega_\ell}\left[\beta e + A(e,\ell) - Q(\ell)\right], \quad \mathfrak{F}_0 = \min_{\ell}\min_{e\in\Omega_\ell}\left[\beta e - Q(\ell)\right]$$

QA can scale better than SA (*Kechedzhi, Smelyanskiy, PRX (2016)*)

$$W \propto \exp\left(-\frac{N}{2}\alpha\right), \quad \alpha = \mathfrak{F} - \mathfrak{F}_0$$

$$\mathfrak{F} = \min_{\ell} \min_{e\in\Omega_\ell} \left[\beta e + A(e,\ell) - Q(\ell)\right], \quad \mathbb{A}_0 = \min_{\ell} \min_{e\in\Omega_\ell} \left[\beta e - Q(\ell)\right]$$

▲ Extremal conditions for $\mathfrak{F}$

$$\ell^* = \tanh\left|\frac{\partial A_{\ell^*}(e^*)}{\partial \ell}\right|, \qquad \beta = \left|\frac{\partial A_{\ell^*}(e^*)}{\partial e}\right| = \tau_0(e^*, \ell^*)$$

▲ Extremal conditions for free energy $\mathfrak{F}_0$

$$e = e_0, \quad \ell = \ell_0$$

energy and total spin that minimize mean-field free energy of the metastable state

$$\frac{\partial \alpha}{\partial \beta} = e^*(\beta) - e_0(\beta)$$

Rising temperature will increase tunneling transition rate if the optimal tunneling energy is greater then the expectation value of energy in metastable state

Path Integral formulation

Using the Suzuki-Trotter formula quantum problem is mapped onto a classical one with one additional (imaginary time) dimension $\tau \in (0, \beta)$. In the limit of infinite number of Trotter slices Z is given by an integral over the array of spin paths

$$\underline{s}(\tau) = \{s_1(\tau), \ldots, s_N(\tau)\}, \quad s_i(\tau) = \pm 1/2, \quad \underline{s}(0) = \underline{s}(\beta)$$

Each path is parametrized by the locations of points ("kinks") at the imaginary time axis where the sign of $s_j(\tau)$ changes.

$$\mathcal{Z} = \int \mathcal{D}\underline{s}(\tau) \prod_{i=1}^{N} \Gamma^{\kappa[s_j(\tau)]} e^{-N \int_0^\beta U(m(\tau)) d\tau},$$

$$m[\underline{s}(\tau)] = \frac{2}{N} \sum_{i=1}^{N} s_i(\tau)$$

- Here $\kappa[s_j(\tau)]$ equals to the number of domain walls (kinks) in $s_j(\tau)$
- $m[\underline{s}(\tau)]$ is an order parameter –z-component to total magnetization

QMC probability functional

QMC is a method to evaluate the path integrals defined above. It samples from a Gibbs distribution corresponding to Z using the Metropolis-Hastings algorithm by implementing a series of stochastic updates of the state vector of individual spin paths $\underline{s}(\tau)$.

$$\underline{s}(\tau) = \{s_1(\tau), \dots, s_N(\tau)\}, \quad \underline{s}(0) = \underline{s}(\beta), \quad s_j(\tau) = \pm 1/2$$

- each spin path is parametrized by domain walls along imaginary time axis
- new domain walls are generated via a Poisson process with decay time $1/\Gamma$
- two domains from different path components $s_i(\tau), s_j(\tau)$ are updated together with probability proportional to their overlap and coupling energy

Gibbs distribution

$$\mathcal{P}_G[\underline{\sigma}(\tau)] = \mathcal{Z}^{-1} \prod_{i=1}^{N} \Gamma^{\kappa[\sigma_j(\tau)]} e^{-N \int_0^\beta U(m(\tau)) d\tau}$$

QMC probability functional in reduced space

Because of the mean-field character of the model it is possible to obtain in a closed form a Gibbs probability measure $P[m(\tau)] = Z^{-1}e^{-N\beta F[m(\tau)]}$ for the magnetization per spin order parameter $m(\tau)$ (*Bapst, Semerjian, 2012*)

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

Here, $m(0) = m(\beta)$ and the functional $\Lambda[\lambda(\tau)]$ equals

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

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

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

Instanton trajectory

$$\delta F[m(\tau)]/\delta m(\tau) = 0, \quad m(0) = m(\beta)$$

Two types of solutions

- Static solution:

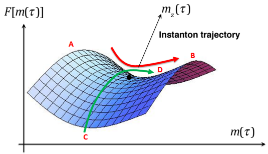
$$m(\tau) = m_i = const, \qquad \frac{dF[m_i]}{dm} = 0$$

$$m_i = m_0, m_1 \quad (\text{local and global minima of } \mathrm{F}_0(\mathrm{m})$$

Free energy of Quantum ferromagnet

$$F[m] = m\,U'(m) - U(m) - \frac{1}{\beta}\log\left(2\cosh(\beta\sqrt{(U'(m))^2 + \Gamma^2})\right)$$

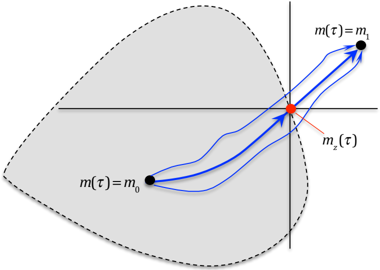
- Dynamic solution, $m_z(\tau) \neq \text{const}$. Instanton is a saddle point of $F[m(\tau)]$



Kramers escape

We study the stochastic trajectories $\underline{s}(\tau, t)$ by inspecting their projections $m(\tau, t)$. The trajectory spends a long time near the metastable state m_0. Occasionally, a large fluctuation occurs corresponding to the escape event where the path $m(\tau, t)$ moves away from m_0 and arrives at the vicinity of the global minimum m_1. The free energy $\mathcal{F}[m(\tau, t)]$ is increasing until it reaches the saddle point of the functional $\mathcal{F}$.

The quasi-stationary statistical distribution over $m(\tau)$ has the Gibbs form $P_G[m(\tau)]$ everywhere in the domain of the local minimum except in the small vicinity of the saddle point $|\mathcal{F}[m(\tau) - \mathcal{F}[m_z(\tau)| \lesssim \beta^{-1}$, where deviations from $P_G[m(\tau)]$ allow for the probability current flow away from the metastable state

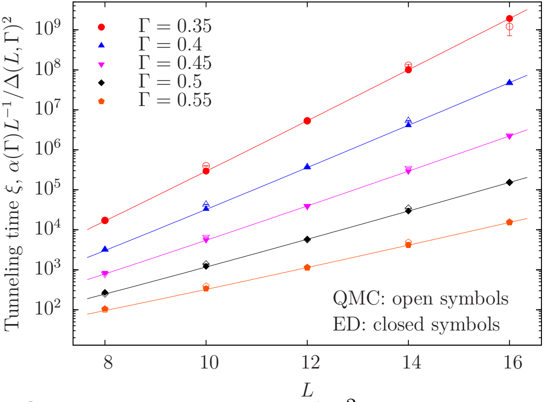


$$W \propto e^{-\beta N \Delta F}$$

$$\Delta F = F[m^*(\tau)] - F[m_0]$$

QMC tunneling rate scales like quantum rate

We obtain numerically the QMC tunneling rate for a fully connected ferromagnetic Ising model between the two orientations at low temperature. Gap Δ obtained by Exact Diagonalization (ED).



We find that QMC tunneling rate $\propto \Delta^{-2}$, which is the incoherent quantum tunneling rate.

Instantons in QMC

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

$$m_z(\tau) = \frac{\delta \log \Lambda(\lambda(\tau))}{\delta \lambda(\tau)} = \frac{\mathrm{Tr}[K^{\beta,\tau}\sigma_z K^{\tau,0}]}{\mathrm{Tr}K^{\beta,0}}$$

$$\lambda(\tau) = \frac{dU[m_z(\tau)]}{dm_z}$$

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

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

To analyze these equation we introduce vector of magnetization components

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

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

$$
\begin{aligned}
m_x &= \sqrt{\ell^2 - m_z^2}\cosh p(m_z, e)\\
m_y &= -i\sqrt{\ell^2 - m_z^2}\sinh p(m_z, e)\\
\frac{dm_z}{d\tau} &= v(e, m_z)\\
e(m_z, p) &= -2\Gamma\sqrt{\ell^2 - m_z^2}\cos p - U(m_z), \quad v = \frac{\partial e}{\partial p}
\end{aligned}
$$

- Equation for $dm_z(\tau)/d\tau$ is identical with that for the WKB instanton trajectory.
- **Self-consistent equation for ℓ**

$$
\mathbf{m}(\tau) = \frac{\mathrm{Tr}[K^{\beta,\tau}\hat{\boldsymbol{\sigma}}K^{\tau,0}]}{\mathrm{Tr}K^{\beta,0}} \quad \underset{\tau=0}{\Longrightarrow} \quad \ell^2(\mathrm{Tr}K^{\beta,0})^2 = \sum_{j=x,y,z}\left(\mathrm{Tr}(K^{\beta,0}\sigma_j)\right)^2
$$

$$
K^{\beta,0} = T_+\exp\left(\int_0^\beta(\Gamma\sigma_x + g'(m_z(\tau))\sigma_z)d\tau\right)
$$

Solving self-consistent equation

We introduce a replica qubit and write the self-consistent condition as

$$\ell^2(\mathrm{Tr}K^{\beta,0})^2 = \mathrm{Tr}\Big(K^{\beta,0}\otimes K^{\beta,0}\sum_{j=x,y,z}\sigma_j\otimes\sigma_j\Big)$$

$$\sum_{j=x,y,z}\sigma_j\otimes\sigma_j = P_S - 3P_A$$

P_A is projector onto anti-symmetric (singlet) subspace

P_S is projector onto symmetric (triplet) subspace

We use basis of Bell states

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$$

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

To analyze the double propagator $K^\beta \otimes K^\beta$, we consider the Hamiltonian

$$H_0^{(2)} = -\Gamma(\sigma_x^1 + \sigma_x^2) - g'(m_z)(\sigma_z^1 + \sigma_z^2)$$

$$(\sigma_x^1 + \sigma_x^2)\, P_A = (\sigma_z^1 + \sigma_z^2)\, P_A = 0, \quad H_0^{(2)}\, P_A = 0$$

$$K^{\beta,0} \otimes K^{\beta,0} = T_+ \exp\left(-\int_0^\beta H_0^{(2)}(\tau)d\tau\right), \qquad K^{\beta,0} \otimes K^{\beta,0}\, P_A = 1$$

The anti-symmetric singlet state $|\Psi^-\rangle$ is a dark state, and the triplet states are closed under evolution with $H_0^{(2)}(\tau)$

$$\ell^2 = 1 - \frac{4}{\mathrm{Tr}\,(K^\beta \otimes K^\beta P_S) + 1} = 1 - \frac{4}{\kappa_0 + \kappa_+ + \kappa_- + 1}$$

▲ **Total spin ℓ is determined by the sum of eigenvalues κ_α of $K^\beta \otimes K^\beta$**

Eigenvalues of the super-operator $\boldsymbol{K}^{\beta} \otimes \boldsymbol{K}^{\beta}$

Consider the time evolution of a state $|\Xi(\tau)\rangle$ in the triplet subspace:

$$|\Xi(\tau)\rangle = K^{\tau,0} \otimes K^{\tau,0} \, |\Xi(0)\rangle = -\xi_x(\tau) \left|\Phi^-\right\rangle - i\xi_y(\tau) \left|\Phi^+\right\rangle + \xi_z(\tau) \left|\Psi^+\right\rangle$$

$$\xi_x, \xi_y, \xi_z \ \text{take real values}$$

$$\frac{d\boldsymbol{\xi}}{d\tau} = -2i \frac{\partial \mathcal{H}_0[\mathbf{m}(\tau)]}{\partial \mathbf{m}} \times \boldsymbol{\xi}, \qquad \mathcal{H}_0[\mathbf{m}(\tau)] = -\Gamma m_x(\tau) - U[m_z(\tau)], \qquad \textbf{(1)}$$

We compare this equation with the equation for instanton

$$\frac{d\mathbf{m}(\tau)}{d\tau} = -2i \frac{\partial \mathcal{H}_0[\mathbf{m}(\tau)]}{\partial \mathbf{m}} \times \mathbf{m}(\tau), \quad \mathbf{m}(0) = \mathbf{m}(\beta)$$

- ▲ **instanton trajectory $m(\tau)$ is one of the 3 independent solutions of Eq.(1)**
- ▲ **it is periodic and corresponds to the eigenvalue κ_0 =1 of $\boldsymbol{K}^{\beta,0} \otimes \boldsymbol{K}^{\beta,0}$**

Because the equation

$$\frac{d\boldsymbol{\xi}}{d\tau} = -2i\frac{\partial\mathcal{H}_0[\mathbf{m}(\tau)]}{\partial\mathbf{m}} \times \boldsymbol{\xi}, \qquad (1)$$

corresponds to the "rotation" around the time-dependent magnetic field the following bilinear form is a constant of motion

$$B\big(\boldsymbol{\xi}(\tau),\boldsymbol{\eta}(\tau)\big) = \xi_x(\tau)\eta_x(\tau) + \xi_y(\tau)\eta_y(\tau) + \xi_z(\tau)\eta_z(\tau) = const \qquad (2)$$

where $\boldsymbol{\xi}(\tau), \boldsymbol{\eta}(\tau)$ are two solutions of Eq.(1).
Using Eq.(2) and the equation for the instanton we obtain remaining two eigenvalues of $\boldsymbol{K}^{\boldsymbol{\beta},\mathbf{0}} \otimes \boldsymbol{K}^{\boldsymbol{\beta},\mathbf{0}}$

$$\boldsymbol{\xi}^{\alpha)}(\beta) = \kappa_\alpha\, \boldsymbol{\xi}^{(\alpha)}(0), \qquad \kappa_\alpha = \exp\left(2\alpha\left|\frac{\partial S_\ell(e)}{\partial\ell}\right|\right), \quad \alpha = 0, \pm 1$$

$$\ell^2 = 1 - \frac{4}{\kappa_0 + \kappa_+ + \kappa_- + 1} \quad \Longrightarrow \quad \ell = \tanh\left|\frac{\partial S_\ell(e)}{\partial\ell}\right|$$

Tunneling decay of metastable state: Two-point Green function approach

Quantum imaginary time propagator : analytical continuation in metastable domain

$$\langle s|e^{-\beta H}|s'\rangle = G_\beta(s,s') = \sum_n e^{-\beta E_n}\,\Psi_n(s)\Psi_n^*(s')$$

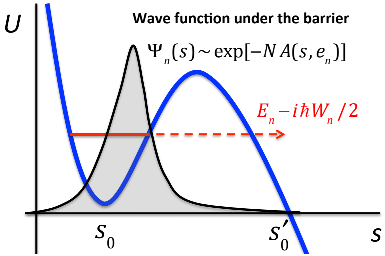
$$H|\Psi_n\rangle = E_n|\Psi_n\rangle, \quad \Psi_n(s) = \langle s|\Psi_n\rangle$$

Application to spin systems: $|s_i\rangle = \bigotimes_{k=1}^{N} |s_i^k\rangle, \quad i = 1,\ldots,N$

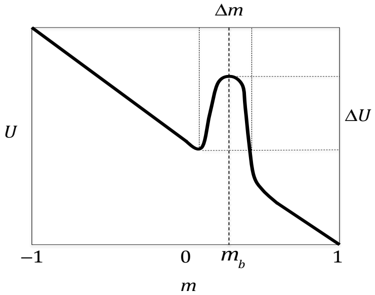
$$\lim_{\beta\to\infty} -\frac{G_\beta(s_0,s_0')}{\beta} = \Psi_0(s_0)\Psi_0(s_0')$$

$$\propto e^{-NA}$$

Only one of the wavefunction amplitudes has an exponential decay in it!!



Corollary: Spike Hamiltonian. A popular model



$$U(m) = U_0(m) + \Delta U\, f\left(\frac{m - m_b}{\Delta m}\right)$$

$$\Delta U = cN^{-\chi}, \quad \Delta m = dN^{-\delta},$$

$$0 < \chi < \delta < 1$$

$\Delta m \gg 1/N$ for WKB to work

The WKB tunneling rate for a spike cost function is:

$$W_{\text{tunn}} = B_{\text{tunn}}\, e^{-\kappa N^{1-\delta-\chi/2}}\ .$$

The time complexity is polynomial in N when $1 - \delta - \chi/2 < 0$.
From our instanton analysis: both QA and QMC (with many replicas) scale exponentially better than SA in this case.

Implications for instantons in more general systems

$$H(t) = -A(t)\sum_{j=1}^{N}\sigma_j^x + B(t)H_{\mathrm{P}}$$

$$H_{\mathrm{P}} = -\sum_{k=1}^{K}\sum_{j_1,\ldots,j_k=1}^{N} J_{j_1,\cdots,j_k}\sigma_{j_1}^z\cdots\sigma_{j_k}^z$$

$$\underline{\mathbf{m}} = (\mathbf{n}_1, \mathbf{n}_2, \ldots, \mathbf{n}_N)$$

$$\mathbf{n}_j = (\sin\theta_j\cos\phi_j, \sin\theta_j\sin\phi_j, \cos\theta_j)$$

$$|\Psi_{\underline{\mathbf{m}}}\rangle = \bigotimes_j\left[\cos\frac{\theta_j}{2}|0\rangle + e^{-i\phi_j}\sin\frac{\theta_j}{2}|1\rangle\right]$$

$$U(\underline{\mathbf{m}}, s) = \langle\Psi_{\underline{\mathbf{m}}}|H(t)|\Psi_{\underline{\mathbf{m}}}\rangle$$

Action in imaginary time

$$A = \frac{i\hbar}{2}\sum_{i=1}^{D}\omega[\mathbf{n}_j(\tau)] + \int_0^{\beta} d\tau\, V[\mathbf{n}_1(\tau),\ldots,\mathbf{n}_N(\tau)]$$

$$\omega[\mathbf{n}(\tau)] = \int_0^{\infty} d\tau(1-\cos\theta(\tau))\dot{\phi}(\tau), \quad \phi_j(\tau) \to -i\varphi_j(\tau)$$

Purely imaginary azimuthal angle

Minima of $U(\mathbf{m})$ give boundary conditions for instantons.
If Hamiltonian H contains only σ_x^j and σ_z^j.

$$Re[\phi_j^{\alpha}] = 2\pi n, \quad Im[\phi_j^{\alpha}] = 0, \quad \frac{\partial U(\cos\theta_j^{\alpha})}{\partial\theta_j} = 0$$