Quantum Adiabatic Algorithms and Large Spin Tunnelling

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We provide a theoretical study of the quantum adiabatic evolution algorithm with different evolution paths proposed in [1]. The algorithm is applied to a random binary optimization problem (a version of the 3-Satisfiability problem) where the *n*-bit cost function is symmetric with respect to the permutation of individual bits. The evolution paths are produced, using the generic control Hamiltonians $H(\tau)$ that preserve the bit symmetry of the underlying optimization problem. In the case where the ground state of H(0) coincides with the totally-symmetric state of an *n*-qubit system the algorithm dynamics is completely described in terms of the motion of a spin-n/2. We show that different control Hamiltonians can be parameterized by a set of independent parameters that are expansion coefficients of $H(\tau)$ in a certain universal set of operators. Only one of these operators can be responsible for avoiding the tunnelling in the spin-n/2 system during the quantum adiabatic algorithm. We show that it is possible to select a coefficient for this operator that guarantees a polynomial complexity of the algorithm for all problem instances. We show that a successful evolution path of the algorithm always corresponds to the trajectory of a *classical* spin-n/2and provide a complete characterization of such paths.

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I. INTRODUCTION.

Recently a novel paradigm was suggested for the design of quantum algorithms for solving combinatorial search and optimization problems based on quantum adiabatic evolution [2]. In the quantum adiabatic evolution algorithm (QAA) a quantum state is closely following a ground state of a specially designed slowly time-varying control Hamiltonian $H(\tau)$. At the beginning of the

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algorithm the control Hamiltonian $H(0) = H_B$ has a simple form with a known ground state that is easy to prepare, and at the final moment of time it coincides with the "problem" Hamiltonian H_P which ground state encodes the solution of the classical optimization problem in question

$$H_P = \sum E_{\mathbf{z}} |\mathbf{z}\rangle \langle \mathbf{z}| \tag{1}$$

$$|\mathbf{z}\rangle = |z_1\rangle_1 \otimes |z_2\rangle_2 \otimes \cdots \otimes |z_n\rangle_n.$$
 (2)

Here E_z is a cost function defined on a set of 2^n binary strings $z = \{z_1, \ldots, z_n\} z_k = 0, 1$, each containing *n* bits. The summation in (1) is over the 2^n states $|z\rangle$ forming the computational basis of a quantum computer with *n* qubits. State $|z_k\rangle_k$ of the *k*-th qubit is an eigenstate of the Pauli matrix $\hat{\sigma}_z$ with eigenvalue $1 - 2z_k \pm 1$. If at the end of the QAA the quantum state is sufficiently close to the ground state of H_P then the solution to the optimization problem can be retrieved by the measurement.

It has been shown recently [7] that the query complexity argument that lead to the exponential lower bound for the unstructured search [8] cannot be used to rule out the polynomial time solution of NP-complete Satisfiability problem by the quantum adiabatic evolution algorithm (QAA).

A set of examples of the 3-Satisfiability problem has been recently constructed [4, 7] to test analytically the power of QAA. In these examples the cost function E_z depends on a bit-string z with n bits, $z = \{z_1, z_2, ..., z_n\}$, only via a Hamming weight of the string, $w_z = z_1 + z_2 + ... + z_n$, so that $E_z = f(w_z)$ where the function f(w) is in general non-monotonic and defines a particular instance of this "Hamming Weight Problem" (HWP). In [4, 7] the original version of QAA [2] was applied to the HWP where the control Hamiltonian is a linear interpolation in time between the initial and final Hamiltonians.

In this case, it was shown [4, 7] that the system can be trapped during the QAA in a local minimum of the cost function for a time that grows exponentially in the problem size n. It was also shown [4] that an exponential delay time in the quantum adiabatic algorithm can be interpreted in terms of the quantum-mechanical tunnelling of an auxiliary large spin between the two intermediate states.

The above example has a significance greater than just being a particular simplified case of a binary optimization problem with symmetrized cost. Indeed, one can argue that it shows a generic mechanism for setting "locality traps" in the 3-Satisfiability problem [10]. But most importantly, this example demonstrates that exponential complexity of QAA can result from a *collective phe*-

nomenon in which transitions between the configurations with low-lying energies can only occur by simultaneous flipping of large clusters containing order-n bits. In spin glasses, there is typically an exponential number of such configurations, the so-called local ground states. A similar picture may be applicable to random Satisfiability problems [15]. In some cases, these transitions can be understood and described in terms of macroscopic quantum tunnelling. A tunnelling of magnetization was observed in large-spin molecular nanomagnets [11] and in disordered ferromagnets [12].

The paper [1] suggests that large tunnelling barriers can be avoided in QAA by using multiple runs of QAA with realizations of the control Hamiltonians $H(\tau)$ sampled from a random ensemble. This ensemble is chosen in a sufficiently simple and general form that does not depend on the specific instance of the optimization problem. Different Hamiltonians $H(\tau)$ correspond to different paths of the unitary evolution that begin and end in the same initial and final states (modulus phase factors). The complexity of QAA with different paths for the HWP was tested numerically in [1] using an ensemble of random 8×8 matrices. The results indicate that the HWP may be solved in polynomial time with finite probability.

In case when the random paths $H(\tau)$ preserve the bit-permutation symmetry of the problem it is natural to describe the random ensemble of $H(\tau)$ in terms of the dynamics of a spin-n/2system. This approach allows for a general theoretical analysis of the algorithm. In the present paper, we perform this analysis for the random version of HWP (over-constrained 3-Satisfiability problem) by mapping the dynamics of QAA onto the motion of a quantum particle in a 1D effective potential. This allows us to compute the statistical weight of the successful evolution paths in the ensemble and provide a complete characterization of such paths.

II. QUANTUM ADIABATIC EVOLUTION ALGORITHM WITH DIFFERENT PATHS

In a QAA with different paths [1], one specifies the time-dependent control Hamiltonian $\tilde{H}(t) \equiv H(\tau)$

$$H(\tau) = (1 - \tau) H_B + \tau (1 - \tau) H_E + \tau H_P,$$
(3)

$$\tau = \frac{t}{T} \in (0, 1).$$

where the control parameter τ plays the role of dimensionless time. This Hamiltonian guides the quantum evolution of the state vector $|\psi(t)\rangle$ according to the Schrödinger equation $i\hbar \partial |\psi(t)\rangle \partial t =$

 $H(\tau)|\psi(t)\rangle$ from t = 0 to t = T, the *run time* of the algorithm. H_P is the "problem" Hamiltonian given in (1). H_B and H_E are 'driver" Hamiltonians designed to cause the transitions between the eigenstates of H_P .

An initial state of the system $|\psi(0)\rangle$ is prepared as a ground state of the initial Hamiltonian $H(0) = H_B$. It is typically constructed assuming *no* knowledge of the solution of the classical optimization problem and related ground state of H_P . In the simplest case

$$H_B = -C \sum_{j=1}^{n} \sigma_x^j, \quad |\psi(0)\rangle = 2^{-n/2} \sum_{\mathbf{z}} |\mathbf{z}\rangle, \tag{4}$$

where σ_x^j is a Pauli matrix for *j*-th qubit and C > 0 is some scaling constant. The ground state of H_B has equal projections on any of the 2^n basis states $|z\rangle$ (2).

Consider instantaneous eigenstates $|\phi_k(\tau)\rangle$ of $H(\tau)$ with corresponding eigenvalues $E_k(\tau)$ arranged in non-decreasing order at any value of $\tau \in (0, 1)$

$$H(\tau)|\phi_k(\tau)\rangle = \lambda_k(\tau)|\phi_k(\tau)\rangle, \quad k = 0, 1, \dots, 2^n - 1.$$
(5)

Provided the value of T is large enough and there is a finite gap for all $t \in (0, T)$ between the ground and exited state energies, $\Delta\lambda(\tau) = \lambda_1(\tau) - \lambda_0(\tau) > 0$, quantum evolution is adiabatic and the state of the system $|\psi(t)\rangle$ stays close to an instantaneous ground state, $|\phi_0(t/T)\rangle$ (up to a phase factor). Because $H(\tau) = H_P$ the final state $|\psi(T)\rangle$ is close to the ground state $|\phi_0(\tau = 1)\rangle$ of the problem Hamiltonian. Therefore a measurement performed on the quantum computer at t = T will find one of the solutions of combinatorial optimization problem with large probability. Quantum transition away from the adiabatic ground state occurs most likely in the vicinity of the probability of the transition is small provided that [17]

$$T \gg \hbar \dot{H}_{\rm max} \Delta \lambda_{\rm min}^{-2},$$
 (6)

where

$$\dot{H}_{\max} = \max_{\tau \in (0,1)} |\langle \phi_1(\tau) | \frac{d\dot{H}}{d\tau} | \phi_0(\tau) \rangle|,$$

$$\Delta \lambda_{\min} = \min_{\tau \in (0,1)} [\lambda_1(\tau) - \lambda_0(\tau)],$$
(7)

The r.h.s. in Eq. (6) gives an upper bound estimate for the required runtime of the algorithm and the task is to find its asymptotic behavior in the limit of large $n \gg 1$. The numerator in (6) is of

the order of the largest eigenvalue of $dH/d\tau = H_P - H_B + (1 - 2\tau)H_E$, which typically scales polynomially with n. However, ΔE_{\min} can scale down exponentially with n and in such cases the required runtime of the quantum adiabatic algorithm to find a solution grows exponentially fast with the size of the input.

One should note that the second term in the r.h.s. of (3) is zero at $\tau = 0$ and $\tau = 1$. Therefore, by using different driver Hamiltonians H_E one can design a family of (possibly random) adiabatic evolution paths that start at $\tau = 0$ in the same generically chosen initial state and arrive at the ground state of H_P at $\tau = 1$. In general, different paths will correspond to different minimum gaps g_{\min} and one can introduce the distribution of minimum gaps. This distribution can be used to compute the fraction of the adiabatic evolution paths f that arrive at the ground state of H_P within polynomial time,

$$T \le c n^{-\alpha}, \quad \alpha > 0, \quad c = \mathcal{O}(1). \tag{8}$$

For a successfully designed family of paths the fraction f is bounded from below by a polynomial in 1/n which leads to the average polynomial complexity of QAA.

III. BINARY OPTIMIZATION PROBLEM WITH SYMMETRIC COST FUNCTION

Consider a binary optimization problem defined on a set of *n*-bit strings z with the cost function E_z in the following form:

$$E_{\mathbf{z}} = f_{\mathbf{z}}(w_{\mathbf{z}}), \quad w_{\mathbf{z}} = \sum_{j=1}^{n} z_{j}.$$
 (9)

This cost is symmetric with respect to the permutation of bits, it depends on a string z only through the number of unit bits in the string w_z (the Hamming weight). In this paper we consider the cost function (9) in the following form which is generalization of the cost introduced in [4, 7, 9]

$$E_{\mathbf{z}} = \sum_{i_1 < i_2 < i_3} c(z_{i_1} + z_{i_2} + z_{i_3}),$$

$$c(m) = p_0 \delta_{m,0} + p_1 \delta_{m,1} + p_2 \delta_{m,2} + p_3 \delta_{m,3}.$$
(10)

Here the sum is over all possible 3-bit subsets of the *n*-bit string z. A subset $z_{i_1} + z_{i_2} + z_{i_3}$ contributes to the total cost a weight factor p_k where k is a number of units bits in the subset. A set of weights $\{p_k\}$ defines an instance of this generalized Hamming Weight Problem (HWP). One can formulate a random version of HWP, e.g., by drawing numbers $\{p_k\}$ independently from a uniform distribution defined over a certain range.

In the limit of large $n \gg 1$ the cost function (10) takes the following form:

$$E_{\mathbf{z}} = l^3 G_P\left(1 - \frac{w_{\mathbf{z}}}{l}\right), \qquad G_P(q) = \sum_{k=0}^3 \beta_k q^k, \tag{11}$$

here l = n/2 and we only keep the terms of the leading order in n. The coefficients β_k in (11) are linear combinations of p_k

$$\beta_k = \frac{\xi_k}{2} \left[p_1 + (-1)^k p_2 \right] + \frac{1}{6} \binom{3}{k} \left[p_0 + (-1)^k p_3 \right].$$
(12)

here $\xi_k = 1$ for k = 0, 1 and $\xi_k = -1$ for k = 2, 3.

The function $G_P(q)$ in (11) is a third degree polynomial in q, and the form of the function depends on the coefficients $\beta_k(p_k)$. It is easy to show that there is a finite size region in the parameter space $\{p_k\}$ where $G_P(q)$ is a non-monotonic function of q that has global and local minima on the interval $q \in (-1, 1)$. Those minima are separated by a finite barrier with width $\delta q = \mathcal{O}(1)$. The barrier separates strings that have close values of the cost E_z but are at large Hamming distance from each other: they have $\mathcal{O}(n)$ distinct bits. This property can lead to exponentially small minimum gaps in QAA due to the onset of low-amplitude quantum tunnelling [4].

IV. CONSTRUCTION OF THE CONTROL HAMILTONIAN

A. Representation in terms of operator components of the total spin

It is natural to consider the control Hamiltonians (3) for solving the HWPs that are symmetric with respect to permutation of individual bits (2). In what follows, we use the normalized components of the total spin operator \hat{S} for the system of *n* individual spins- $\frac{1}{2}$

$$\hat{n}_j = \frac{1}{l}\hat{S}_j, \qquad \hat{S}_j = \frac{1}{2}\sum_{i=1}^n \hat{\sigma}_j^i, \qquad l = \frac{n}{2}.$$
 (13)

Here \hat{S}_j are the projections of the total spin operator on the *j*-th axis (j = x, y, z) and $\hat{\sigma}_j^i$ are Pauli matrices for the *i*-th spin. For the sake of bookkeeping, in (13) and also throughout the paper we use "hats" for the spin operators, such as \hat{S}_j , \hat{n}_j , and some others, in order to distinguish them from their corresponding eigenvalues $(S_j \text{ and } n_j, \text{ respectively, in the above example}).$

To obtain the problem Hamiltonian (1) we make use of the obvious connection between the values of the Hamming weight function w_z of an *n*-bit string z and corresponding eigenvalues n_z

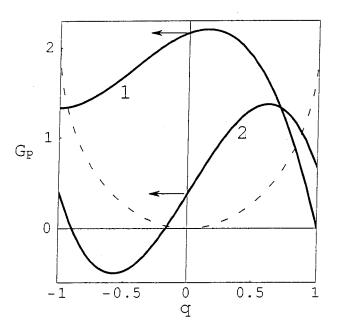


FIG. 1: Plots of the cost function (11) G_p vs q for different choices of the weights $\{p_k\}$. Curve 1 corresponds to $p_0 = 0$, $p_1 = 3$, $p_2 = 1$, $p_3 = 1$, and the cost function $G_P(q)$ has a global minimum at q = 1, corresponding to the string z with the Hamming weight zero, $z_1 = z_2 = \ldots = z_n = 0$. It also has a local minimum at q = -1 corresponding to the bit string with Hamming weight $n, z_1 = z_2 = \ldots = z_n = 1$. The curve 1 yields the particular form of the cost function $G_P(q)$ considered in [4], [1]. Curve 2 corresponds to $p_0 = 0.5, p_1 = 2.5, p_2 = -2, p_3 = 0.3$, it has a global minimum at $q = q^*$ inside of the interval (-1, 1). This minimum corresponds to approximately $\binom{n}{nw^*}$ bit strings z that all have the same Hamming weight $w_z = w^* = n(1-q^*)/2$.

of the spin projection operator \hat{n}_z

$$\hat{n}_z |\mathbf{z}\rangle = n_z |\mathbf{z}\rangle, \quad n_z = 1 - \frac{w_z}{l}.$$
 (14)

Then from Eqs. (2),(11) and (14) we obtain

$$H_P(\hat{n}_z) = l^3 G_P(\hat{n}_z) \,. \tag{15}$$

We chose the driver H_B in a bit-symmetric form that coincides with (4) (up to a constant term)

$$H_B = l^3 G_B(\hat{n}_x), \quad G_B(x) \equiv 2(1-x).$$
 (16)

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B. Bit-symmetric drivers H_E

It was proposed in [1] that H_E can be constructed using some generic ensemble of random matrices. The bit-symmetric random drivers for the cost functions of the type (10) can be constructed as follows [1]. One generates an 8×8 random Hermitian matrix A with zero diagonal elements and non-diagonal elements that are independent random numbers identically distributed in a certain interval. Matrix elements of A_{z_i, z_j, z_k} can be enumerated by all possible configurations of a 3-bit string $\{z_i, z_j, z_k\}$. Then H_E takes the form

$$H_E = \sum_{i < j < k} \sum_{\mathbf{z} \in \{0,1\}^n} A_{z_i, z_j, z_k} |\mathbf{z}\rangle \langle \mathbf{z}|, \qquad (17)$$

Here $|z\rangle$ are computational basis states Eq. (1) corresponding to bit-strings $z = \{z_1, \ldots, z_n\}$. Each randomly selected A generates H_E and therefore a random path modification of the QAA.

From the above discussion, it follows that the matrix of the operator H_E (17) is symmetric with respect to the bit permutations and therefore it commutes with the operator of a total spin \hat{S}^2 of a system of *n* spins $\frac{1}{2}$. This means that H_E acts independently in each of the sub-spaces corresponding to certain values of the total spin $0 \le l \le \frac{n}{2}$ [22]. It follows from (15) and (16) that the same is true for the total control Hamiltonian (3)

$$\left[H(\tau), \hat{\mathbf{S}}^2\right] = 0, \quad \tau \in (0, 1).$$
(18)

Since in our case the initial state (4) is a totally symmetric combination of all states and therefore corresponds to the maximal spin $l = \frac{n}{2}$, our system always stays in this sub-space during the algorithm. Therefore in the analysis of the complexity of QAA one can reduce the $2^n \times 2^n$ matrix of $H(\tau)$ to the $(2n+1) \times (2n+1)$ matrix that only involves the states with different spin projections of the *maximum* total spin $l = \frac{n}{2}$. Binary strings corresponding to the quantum states from this subspace are distinguished from each other by their Hamming weight only.

In Appendix A, we show that in the case of real-valued symmetric matrices A and in the largespin limit, the bit-symmetric driver H_E (17) can be presented as a linear combination of 6 operators expressed in terms of the large spin operator components \hat{n}_x , \hat{n}_z acting in the subspace with $l = \frac{n}{2}$. Using this fact, and also Eqs. (15) and (16) one can write a bit-symmetric control Hamiltonian (3) in the following form

$$\frac{1}{l^3}H(\tau) \equiv G(\tau, \hat{n}_x, \hat{n}_z) = (1 - \tau) G_B(\hat{n}_x) + \tau (1 - \tau) G_E(\hat{n}_x, \hat{n}_z) + \tau G_P(\hat{n}_z), \quad (19)$$

$$G_E(\hat{n}_x, \hat{n}_z) = \gamma_1 \hat{n}_x + \gamma_2 \hat{n}_x^2 + \gamma_3 \hat{n}_x^3 + \gamma_4 \hat{n}_x \hat{n}_z + \gamma_5 \hat{n}_x \hat{n}_z^2 + \gamma_6 \hat{n}_x^2 \hat{n}_z,$$
(20)

where $\{\gamma_k\}$ (k = 1, ..., 6) are independent real coefficients given in Eq. (A8). As we show in Appendix A, any random realization of the matrix A can be mapped onto combinations of drivers (20) by the appropriate choice of the coefficients γ_k . This fact allows us to analyze the minimum gap in QAA with different paths (3) using the WKB analysis of the dynamics of a spin- $\frac{n}{2}$ in the large spin limit $(n \gg 1)$.

V. ADIABATIC EVOLUTION OF A LARGE SPIN

A. WKB approximation for the large spin

Our analysis in this section is a particular application of the WKB-type approach commonly used for the description of quantum spin tunnelling in magnetics [18], [19], [20], [12]. This approach is applicable for the large spins (l >> 1), which is the case of interest for us.

We choose z as a quantization axis and following the standard procedure to obtain the effective quasi-classical Hamiltonian in polar coordinates $\{\theta, \varphi\}$ with $\theta \in [0, \pi]$ and $\varphi \in [0, 2\pi]$. We make use of the Villain transformation [23]

$$\hat{n}_x = \sqrt{1 + \epsilon - \hat{n}_z \left(\hat{n}_z + \epsilon \right)} \cos\left(\hat{\varphi} \right), \quad \epsilon = \frac{1}{l},$$
(21)

where azimuthal angle operator $\hat{\varphi}$ satisfies the commutation relation

$$[\hat{\varphi}, \hat{n}_z] = i\epsilon. \tag{22}$$

In a change of notation we introduce a coordinate q and canonically-conjugate momentum \hat{p} (cf. [23])

$$q = \hat{n}_z, \qquad \hat{p} = -i\epsilon \frac{d}{dq} \equiv -\hat{\varphi},$$
(23)

 $(-1 \le q \le 1)$. Expanding (21) in the large spin limit $\epsilon \ll 1$, we obtain

$$\hat{n}_x = (1 - q^2)^{1/2} \cos \hat{p} + \epsilon \frac{\cos \hat{p}}{2(1 + q)} + \mathcal{O}(\epsilon^2).$$
(24)

Finally, we write the scaled Hamiltonian of the system (19) in terms of the new variables

$$G(\hat{n}_{x}, \hat{n}_{z}, \tau) \equiv \mathcal{H}(q, \hat{p}, \tau),$$

$$\mathcal{H}(q, \hat{p}, \tau) = \mathcal{H}(q, \hat{p}, \tau) + \Delta \mathcal{H}(q, \hat{p}, \tau),$$
 (25)

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where

$$H(q,\hat{p},\tau) = G\left(\sqrt{1-q^2}\cos\hat{p},q,\tau\right),$$
(26)

$$[q, \hat{p}] = i \epsilon, \tag{27}$$

and ΔH is a small correction

$$\Delta \mathbf{H}(q, \hat{p}, \tau) = \epsilon \frac{\cos \hat{p}}{2(1+q)} \frac{\partial G}{\partial n_x} + \mathcal{O}(\epsilon^2), \tag{28}$$

(here $\partial G/\partial n_x$ has the same arguments as G in (26)).

The stationary Schrődinger equation (5) in the new basis

$$\mathcal{H}(q,\hat{p},\tau)\Psi_k(q;\tau) = \lambda_k(\tau)\Psi_k(q;\tau),\tag{29}$$

can be solved in the WKB approximation with the small parameter $\epsilon \ll 1$ playing the role of a Plank constant. Then the wave function $\Psi(q)$ takes the form

$$\Psi(q) = B(q) \exp\left[\frac{iA(q)}{\epsilon}\right],\tag{30}$$

where in the leading order in ϵ the action function A(q) satisfies the following Hamilton-Jacobi equation

$$H\left(q, \frac{dA(q)}{dq}, \tau\right) = \lambda.$$
(31)

This equation describes a 1D auxiliary mechanical system with coordinate q, momentum p, energy λ , and Hamiltonian function $H(q, p, \tau)$. Classical orbits satisfy the Hamiltonian equations

$$\dot{q}(t) = \mathcal{H}_p(q(t), p(t), \tau), \quad \dot{p}(t) = -\mathcal{H}_q(q(t), p(t), \tau),$$
(32)

where H_q and H_p stand for the partial derivatives of H with respect to q and p, respectively. Stationary points of the dynamics (q_*, p_*) correspond to the elliptic and saddle points of the Hamiltonian function

$$H_q(q_*, p_*, \tau) = 0, \quad H(q_*, p_*, \tau) = 0,$$
(33)

Elliptic points are minima (or maxima) of $H(q, p, \tau)$ on the (q, p) plane. They satisfy the condition

$$\Omega_*^2 = H_{pp}(q_*, p_*, \tau) H_{qq}(q_*, p_*, \tau) - H_{qp}(q_*, p_*, \tau) > 0.$$
(34)

where H_{pp} is understood as a second derivative of H with respect to p, etc. Saddle points correspond to $\Omega_*^2 < 0$ in (34).

In the limit $\epsilon \ll 1$ the adiabatic ground state $\Psi_0(q; \tau)$ (29) is localized in the small vicinity of the fixed points (q_*, p_*) corresponding to the global minimum of $H(q, p, \tau)$ at a given value of τ . To logarithmic accuracy the WKB-asymptotic (30) of the ground-state wave function is determined by the mechanical action for the imaginary-time instanton trajectory (q(t), p(t)) emanating from the fixed point (q_*, p_*)

$$\Psi_{0}(q;\tau) \approx \overline{\Psi}_{0}(q;q_{*},p_{*},\tau) \propto \exp\left[-\frac{i}{\epsilon} \int_{-i\infty}^{0} dt \,\dot{q}(t)p(t)\right],$$

$$q(-i\infty) = q_{*}, \quad p(-i\infty) = p_{*}, \quad q(0) = q.$$
(35)

Integration in (35) is along the imaginary axis $(-i\infty, 0)$. The instanton trajectory obeys Eq. (32) with the boundary conditions given above and $t \in (-i\infty, 0)$ corresponding to the line of integration in (35). The choice of the final instant, t = 0, is arbitrary since the instanton trajectory is degenerate with respect to a shift of the time axis.

We note that the WKB asymptotic (35) decays exponentially fast as the coordinate q in (35) moves away from its value at the global minimum q_* into the classically inaccessible region. This corresponds to the growth of the imaginary part of the action in (35), similar to the conventional quantum tunnelling in the potential. In the vicinity of (q_*, p_*) the ground-state wave function $\Psi_0(q)$ takes the form similar to that of harmonic oscillator:

$$\Psi_{0}(q) = c \times \exp\left[\frac{i}{\epsilon} \left(p_{*} \,\delta q - \frac{H_{qp}}{2H_{pp}} \delta q^{2}\right) - \frac{m_{*} \,\Omega_{*}^{2} \delta q^{2}}{2\epsilon}\right],$$

$$m^{*} = \frac{1}{|H_{pp}(q_{*}, p_{*}, \tau)|},$$
(36)

here $\omega_* > 0$ is defined in (34). Similarly, the energy spectrum in that region corresponds to the classical elliptic orbits with oscillation frequency Ω_*

$$\lambda_k - \mathcal{H}(q_*, p_*, \tau) \sim \epsilon \,\Omega_*\left(k + \frac{1}{2}\right), \quad k = 0, 1, \dots$$
(37)

We note that the frequency Ω_* depends on τ and determines the time-varying instantaneous gap between the ground and first exited states, $\Delta \lambda = \epsilon \Omega_*(\tau)$.

VI. LOCAL AND GLOBAL BIFURCATIONS DURING THE QAA

It can be seen from Eq. (26) that the global minimum of $H(q, p, \tau)$ will correspond to $p_* = \pm k\pi$ ($k = 0, \pm 1, \ldots$) provided that the following condition holds for all n_x :

$$\omega_x \equiv -\frac{\partial G\left(n_x, q_*(\tau), \tau\right)}{\partial n_x} \neq 0, \tag{38}$$

where the positive and negative signs of ω_x correspond to even and odd values of k, respectively. The value of q_* in (38) corresponds to the global minimum of the effective potential $U(q, \tau)$

$$U(q) = G(\sqrt{1 - q^2}, q, \tau), \quad U(q) - U(q_*) > 0.$$
(39)

Under the above condition the Hamiltonian function of the system near the global minimum $(q_*, 0)$ exactly corresponds to that of the harmonic oscillator with effective frequency Ω_* (34) and mass m_* (36)

$$H(q, p, \tau) = \frac{1}{2m_{*}(\tau)}p^{2} + \frac{m_{*}\Omega_{*}^{2}(\tau)(q - q_{*}(\tau))^{2}}{2},$$

$$\frac{1}{m_{*}} = -\sqrt{1 - q_{*}^{2}} \frac{\partial G\left(\sqrt{1 - q_{*}^{2}}, q_{*}, \tau\right)}{\partial n_{x}},$$

$$m_{*}\Omega_{*}^{2} = U''(q_{*}).$$
(40)

In the WKB picture the ground state of the system correspond to the particle performing zero-level oscillations near the bottom of the slowly varying potential $U(q, \tau)$. There are two types of the bifurcations that can destroy the above adiabatic picture:

1. Local bifurcation

Assume that at some instant of time $\tau = \tau_0$ the effective mass $m_*(\tau)$ goes to infinity. In the vicinity of this point the Hamiltonian function (26) can be approximated as follows:

$$H(q, p, \tau) = \frac{a_0}{4!} p^4 - \frac{b_0}{2!} s p^2 + \frac{c}{2!} \delta q^2 + d_0 s \delta q + \mathcal{O}(s^{5/2}),$$

$$\delta q = q - q_*(\tau_0), \quad s = \tau - \tau_0,$$
(41)

where

$$a_{0} = \frac{\partial^{2}G}{\partial n_{x}^{2}} (1 - q_{*}^{2}(\tau_{0})), \quad b_{0} = \frac{\partial^{2}G}{\partial n_{x}\partial\tau} \sqrt{1 - q_{*}^{2}(\tau_{0})},$$

$$c_{0} = \frac{\partial^{2}U}{\partial q^{2}}, \quad d_{0} = \frac{\partial^{2}U}{\partial q\partial\tau},$$
(42)

in the above equations all functions are evaluated at the point $(q_*(\tau_0), p = 0)$. Equation (41) corresponds to A_3 bifurcation point [24]. It can be seen from (41) that for $\tau > \tau_0$ the single global minimum of $H(q, p, \tau)$ splits into the two minima with nonzero momenta

$$p_*^{\pm}(\tau) \approx \pm \left(\frac{6b_0(\tau - \tau_0)}{a_0}\right)^{1/2}, \quad \tau - \tau_0 > 0.$$
 (43)

Due to the symmetry $H(q, p, \tau) = H(q, -p, \tau)$ the two global minima with nonzero p_* will stay symmetric with respect to the q-axis at later times.

It follows from (34), (40)) that the linear oscillation frequency vanishes at the bifurcation point, $\Omega_*(\tau_0) = 0$, however the energy gap $\Delta\lambda(\tau_0) \neq 0$. By solving the Schrödinger equation (5) at this point in the representation of the momentum p one can find the eigenfunctions $\tilde{\Psi}_k(p, \tau_0)$ and eigenvalues $\lambda_k(\tau_0)$ corresponding to a 1D quantum system moving in a quartic potential (cf. Eq. (41)). This analysis yields an estimate for the value of the gap, and the characteristic localization range δp for $\tilde{\Psi}_k(p, \tau_0)$

$$\Delta \lambda \sim \epsilon^{4/3}, \quad \delta p \sim \epsilon^{1/3}.$$
 (44)

The size of the energy barrier in momentum p separating the two global minima in (41) grows with time for $\tau - \tau_0$ and this leads to a rapid decrease of the energy gap. Sufficiently far from the bifurcation point, $\tau - \tau_0 \gg \epsilon^{2/3}$, each of the global minima $(q_*(\tau), p_*^{\pm}(\tau))$ gives rise to its own WKB asymptotic (35) localized at the minimum. The ground state and the first exited state correspond to their symmetric and anti-symmetric combinations, respectively

$$\Psi_k(q) = \frac{1}{\sqrt{2}} \left(\overline{\Psi}(q; q_*, p_*^+, \tau) + (-1)^k \overline{\Psi}(q; q_*, p_*^-, \tau) \right),$$

$$k = 0, 1.$$
(45)

For $\tau - \tau_0 \gg \epsilon^{2/3}$ the tunnelling splitting of energy levels for the symmetric and antisymmetric states determines the value of the gap $\Delta\lambda(\tau)$ and decreases exponentially fast with $\tau - \tau_0$. Away from the bifurcation region, $\tau - \tau_0 = \mathcal{O}(1)$, the gap scales down exponentially with n (note that $\epsilon = 2/n$).

As a result of the local bifurcation, the purely adiabatic evolution in QAA collapses. The amplitude of staying in the adiabatic ground state for $\tau < \tau_0$ is nearly equally split between the states (45) with the two lowest eigenvalues. In general, this may reduce the probability of finding a system in a ground state at $\tau = 1$ by a factor of 2. We note that the control Hamiltonian (19) is at most a cubic polynomial in n_x , n_z , and therefore the number of local bifurcation events during QAA is of the order of one. In the worst case they will cause the reduction of the success probability in QAA by a constant factor.

For a given instance of the cost function (11) defined by the coefficients β_k (or p_k) the onset of local bifurcations (41) depends on the choice of the driver Hamiltonian H_E (20).

There are a number of ways to select coefficients γ_k 's in the driver Hamiltonian (20) to avoid local bifurcations during QAA in a broad range of values of the coefficients p_k . For example, to completely suppress local bifurcations (41) one can keep in (20) only terms linear in \hat{n}_x and set

$$\gamma_2 = \gamma_3 = \gamma_6 = 0. \tag{46}$$

A. Global bifurcation

The Hamiltonian function $H = H(q, p, \tau)$ defines a 3D surface over a 2D plane (q, p) and the shape of this surface varies with time τ . We consider global bifurcations of this surface where the energies of its two minima cross each other at some instant of time $\tau = \tau_0$ while the distance between the minima on the (q, p) plane remains finite at the crossing point. For $\tau > \tau_0$ the minima exchange their roles: global minimum becomes local and vise versa. Before and after the intersection in the energy space the two minima are uniquely identified with the ground and first exited states of the system's Hamiltonian (26). The corresponding wave functions $\Psi_{0,1}(q)$ are well approximated by their asymptotic expressions(35),(36).

The small vicinity of the global bifurcation point can be described within the standard 2-level avoiding-crossing picture. There $\Psi_{0,1}(q)$ are given by symmetric and antisymmetric superpositions of the WKB-asymptotic corresponding to intersecting minima. The value of the gap changes with time as $\sqrt{c^2(\tau - \tau_0)^2 + \Delta \lambda_{\min}^2}$ where c is some constant and the minimum gap is determined by the overlap of the WKB asymptotic. To logarithmic accuracy it is given by the imaginary part of the mechanical action (35) along the instanton trajectory connecting the two minima

$$-\epsilon \log \Delta \lambda_{\min} = \left| \operatorname{Im} \int_{-i\infty}^{i\infty} dt \, \dot{q}(t) p(t) \right| \tag{47}$$

$$\lim_{\tau \to \pm i\infty} q(\tau) = q_*^{1,2}, \lim_{\tau \to \pm i\infty} p(\tau) = p_*^{1,2}$$
(48)

Here q_*^k, p_*^k are coordinates of the two minima; $H(q_*^1, p_*^1, \tau_0) = H(q_*^2, p_*^2, \tau_0)$, and the instanton trajectory obeys the Eqs. (32). The analytical expression for the minimum gap was studied in [4], [9] for the case $H_E = 0$, using a simplified version of the Hamming Weight problem (10). Below we identify certain geometrical properties of the global bifurcations in the case $H_E = 0$ that will be used later in the selection of the drivers H_E for the successful QAA.

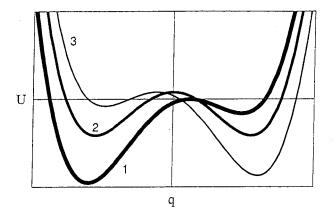


FIG. 2: The global bifurcation mechanism: the effective potential profiles $U(q, \tau)$ vs q for $\tau < \tau_0, \tau = \tau_0$ and $\tau > \tau_0$ are represented by the curves 1,2, and 3, respectively.

1. The case
$$H_E = 0$$

In the case $\gamma_j \equiv 0$ (j = 1, ...6), the Hamiltonian has a minimum at $p_*(\tau) = \pi k$ and the value of $q_*(\tau)$ corresponds to the global minimum of the effective potential $U(q, \tau)$ (39). We use Eq. (19) and also the condition $U'(q_*) = 0$ to obtain the following equation for $q_*(\tau)$

$$\frac{dq_*(\tau)}{d\tau} = -\frac{G'_P(q_*(\tau))}{(1-\tau) U''(q_*(\tau),\tau)}.$$
(49)

This equation holds until the global bifurcation point at $\tau = \tau_0$ where $q_*(\tau)$ changes discontinuously in time (see Fig. 2). At the minimum of the potential $U''(q_*) > 0$ and therefore the direction of the motion of $q_*(\tau)$ entirely depends on the direction of the "force", $-G'_P(q_*)$. At $\tau = 0$ the potential U(q, 0) has a unique minimum at the point $q = q_*(0) = 0$. It is clear that with this initial condition equation (49) can lead to a "wrong" minimum of $G_P(q)$ that lies above the global minimum, and such cases will give rise to a global bifurcation. This effect is illustrated in Fig.1 where the two different cost functions correspond to the same direction of motion for $q_*(\tau)$. The value of $q_*(\tau)$ may either smoothly approach the global minimum of the cost (curve 2), or move toward a "wrong" local minimum (curve 1), leading to the global bifurcation and exponentially small gap in QAA. Adding H_E to the control Hamiltonian can invert the direction of motion of $q_*(\tau)$ toward the global minimum of $G_P(q)$. This can be seen from the fact the Eq.(49) in presence of H_E possesses the additional term

$$-\frac{(1-\tau)}{U''(q_*,\tau)}\frac{\partial G_E(\sqrt{1-q_*^2},q_*)}{\partial q_*},$$
(50)

(here we drop for sake of brevity the argument τ in $q_*(\tau)$). Clearly, the successful G_E should not possess reflection symmetry with respect to n_z . Therefore we should only select the terms in (20) that contain odd powers of n_z . Taking into account (46) we arrive at the following form of the driver Hamiltonian

$$G_E(\hat{n}_x, \hat{n}_z) = \gamma_4 n_x n_z. \tag{51}$$

This driver can remove the potential barrier between the two competing global minima of $U(q, \tau)$ by shifting the original minimum at $\tau = 0$ towards the true global minimum of the cost function $G_P(q)$ (cf. Fig. 1). In the classical picture (26) the driver (51) corresponds to an external field parallel to z-axis which can destroy the tunnelling barrier along this direction. The mechanism of such tunnelling avoidance is similar to the one considered in [1], where the external field generated by the driver (51) compensates the effective field due to the linear term proportional to the coefficient β_1 in the problem Hamiltonian (11).

B. Bifurcation transition to the tunnelling regime

In general, one can expect that a complete suppression of the tunnelling barrier at all values of τ requires a certain magnitude (and sign) of the coefficient γ_4 depending on the choice of the coefficients β_k in the cost function $G_P(q)$.

The transition to the tunnelling regime can be described as an A_3 bifurcation point, illustrated in Fig.2. The effective potential U changes parametrically with τ , γ_4 and $\{\beta_k\}$. Near the bifurcation point $(\tau_c, \gamma_{4c}, q_c)$, the potential has the form $U = a \, \delta q^4 + b \, \delta \gamma \delta q^2 + c \, \delta q \, \delta \tau$ where $\delta \tau, \delta q, \delta \gamma$ are deviations from the bifurcation point in τ, q and γ_4 , respectively. The corresponding conditions for the A_3 bifurcation point are:

$$\frac{\partial U}{\partial q} = \frac{\partial^2 U}{\partial q^2} = \frac{\partial^3 U}{\partial q^3} = 0.$$
 (52)

Taking into account (39) and (19),(20),(51), the above equation yields

$$\tau_{c} (1 - \beta_{2}) = 1 + \frac{2}{3} \frac{\tau_{c}^{2} (1 - \tau_{c}) (\beta_{1} + \beta_{3})^{2}}{[2 - \tau_{c} (2 - \beta_{2})]^{2}},$$

$$\gamma_{4c} (1 - \tau_{c}) = \frac{(1 - \tau_{c}) (3\beta_{1} + \beta_{3}) + \tau_{c}\beta_{2}\beta_{3}}{\tau_{c}\beta_{2} - 2 (1 - \tau_{c})},$$
(53)

These equations should be solved for γ_{4c} and τ_c for the given set of the coefficients β_k . The bifurcation is avoided when

$$|\gamma_4| > |\gamma_{4c}|. \tag{54}$$

For example, in the particular case of the HWP (10) considered in [4], [1], we have

$$\beta_1 = 1/2, \quad \beta_2 = -3/2, \quad \beta_3 = -7/6,$$
(55)
 $\tau_c \approx 0.44, \quad \gamma_{4c} \approx -0.95.$

In this case the example of the driver Hamiltonian H_E that allows to avoidance of tunnelling in QAA was given in [1] where the value of $\gamma_4 = -8$ was used. According to (55) this value is way below the critical value γ_{4c} .

1. Numerical Simulations of the bifurcation boundary

We performed numerical simulations with the effective potential (39) checking for the onset of tunnelling for all $p_k \in [0,3]$, k = 1,...4. The numeric simulations confirm that the situation discussed above is typical for the general HWP, implying that (51) is the only driver term that can be fundamentally responsible for the tunnelling avoidance in a general case, if the coefficient γ_4 is defined appropriately. In particular, one of the two drivers (51) with

$$\gamma_4 \ge \gamma_c = 4.9 \quad \text{or} \quad \gamma_4 \le -\gamma_c = -4.9$$

 $p_k \in [0; 3] \quad k = 0, 1, 2, 3,$
(56)

always suppresses tunnelling in the QAA.

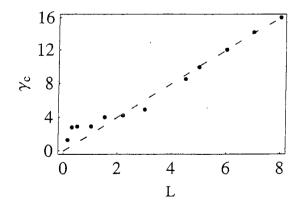


FIG. 3: The critical value γ_c vs domain size L.

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We also solve the Eqs. (53) numerically for coefficients p_k taking values on a dense grid of points in the cube $p_k \in [0; L]$ (k=0,1,2,3). For each size of the cube L we select the point with largest value of γ_{4c} denoted below as $\gamma_c \equiv \gamma_c(L)$. The results are presented in Fig.3. The critical value γ_c is monotonically increasing in L, and the dependence is close to linear for sufficiently large L, but it is non-linear in the range $0 \leq L \leq 3$. It can be inferred from Eq. (53) that a nonlinear dependence of γ_c on the scale L is due to the fact that the critical time τ_c also depends on L.

The linear dependence of $\gamma_c(L)$ for large L has a simple intuition. According to (11) and (12), the magnitude of $G_P(q)$ is proportional to L. According to Eq.(49), the maximal magnitude of the coefficient β_1 presents a "force" that can possibly move a system into the local minimum at small τ . From (12), we conclude that $|\beta_1|_{\max} = \max_{p_k \in [-L,L]} \beta_1 = 2L$. In the limit of large L, the role of the driver G_B in (53) becomes unimportant. Therefore, the only competing terms are the driver G_E and the problem Hamiltonian G_P . The term (50) generated by H_E compensates (50) the "force" β_1 when $|\gamma_4| \ge |\beta_1|_{\max}$, and therefore in this limit we have

$$\gamma_{c}(L) = \max_{p_{k} \in [-L,L]} \gamma_{4c} \approx |\beta_{1}|_{\max} = 2L.$$
 (57)

One should note that among the effective potentials generated by choosing different $\{p_k\}$, there are two subsets that can be mapped onto each other by means of the mirror reflection about the q-axis, $U(q, \tau) \rightarrow -U(q, t)$. We note that the same driver H_E can not simultaneously suppress tunnelling barriers in each of the two mutually symmetric potentials: if the tunnelling barriers are not suppressed with γ_c , they will be suppressed with $-\gamma_c$, and vice versa. This gives a simple intuition for the tunnelling barrier suppression boundary (54).

Finally we conclude, that it is possible to indicate the range of value of $|\gamma_4|$ such that the driver Hamiltonian $H_E = l^3 \gamma_4 \hat{n}_x \hat{n}_z$ will play the role of a **universal** driver that guarantees polynomial performance of the QAA for all instances of the generalized Hamming weight problem (10) provisory to the mirror-reflection symmetry in the possible choice of the cost functions and the common normalization factor L.

VII. PROBABILITY OF SUCCESS OF THE QAA WITH RANDOM PATHS

Using the analysis from the previous section one can estimate the probability of success for the QAA with random paths proposed in [1]. In that algorithm, the ensemble of random drivers H_E was generated using random 3×3 matrices $A_{z_i z_j z_k}$ (17). It is shown in Appendix A that for the bit-symmetric optimization problem (10) the above ensemble is identical to the ensemble of independent uniformly-distributed random coefficients γ_k (k=1 - 6) that appears in the largespin representation of the driver H_E (20). Then for any instance of optimization problem in (10) defined by the set of the coefficients $\{p_k\}$ one should compute the fraction f of the domain of the coefficients $\{\gamma_k\}$ where the following conditions are satisfied:

- (i). Condition for the nonzero effective mass (38).
- (ii). The condition (54) for the complete avoidance of the tunnelling barriers in combination with Eq.(53) for the bifurcation boundary.

Here we compute the fraction f for the particular instance of the optimization problem (10) considered in [1, 4, 9]. In this case Eq. (38) takes the form

$$\frac{\omega_x}{1-\tau} = -2 + \tau \left[\gamma_1 + 2\gamma_2 n_x + 3\gamma_3 n_x^2 + \gamma_4 q + \gamma_5 q^2 + 2\gamma_6 n_x q \right] \neq 0,$$
(58)

where $n_x = \pm \sqrt{1 - q_*^2}$ and q_* provides global minimum of $U(q, \tau)$ (39). The effective mass is non-zero if $\omega_x \neq 0$, and (58) yields an estimate on the range of $\{\gamma_k\}$ as

$$|\gamma_2| + |\gamma_6| \le 1 + 1/2 \left(|\gamma_1| + 3|\gamma_3| + |\gamma_4| + |\gamma_5| \right).$$
(59)

Following [1] we assume that the non-diagonal matrix elements $A_{z_i z_j z_k}$ are distributed in the interval [-3, 3]. Making use of (A8), we obtain

$$|\gamma_2| + |\gamma_6| \le 16, \quad |\gamma_1| + 3 |\gamma_3| + |\gamma_4| + |\gamma_5| \le 50.$$
 (60)

Therefore, the probability that inequality (59) is satisfied is estimated as $1-15^2/(50 \times 16) \approx 0.71875$. On the other hand, the values of γ_4 in (A8) belong to the range, $-12 \leq \gamma_4 \leq 12$. Using the value of $\gamma_c \approx -0.95$ given in (55) we estimate the probability of $\gamma_4 \leq -\gamma_c$ to be approximately equal to ≈ 0.46 . Making an approximation that the cases when the effective mass is non-zero are statistically independent from the cases when $\gamma_4 \leq -\gamma_c$, we obtain the total probability of success as $P_{tot} \approx 0.46 \times 0.71875 = 0.334 \approx 1/3$, which is in qualitative agreement with the numerical results of [1]. This estimate can be generalized to the case when the matrix elements $A_{z_i z_j z_k}$ are distributed in the interval [-L, L] for sufficiently large L > 3. In this case, the probability that (59) is satisfied remains the same, ≈ 0.71875 , while the probability that $\gamma_4 \leq -\gamma_c$ is estimated as

 $(4L - |\gamma_c|)/8L$. With the assumption of statistical independence, the total probability of success is $P_{tot} \approx 0.718 \times (4L - 0.95)/8L$, and in the limit of large L >> 1 we have $P_{tot} \approx 0.359$ which exceeds slightly the value for L = 3.

VIII. POLYNOMIAL QAA AND CLASSICAL DYNAMICS OF LARGE SPIN

In absence of tunnelling, the dynamics of the large spin can be characterized by classical equations of motion for the spin projections treated as c-numbers in the form [18]

$$\frac{d\vec{S}}{dt} = \left[\vec{\omega}, \vec{S}\right],\tag{61}$$

with

$$\overrightarrow{\omega} = \frac{\partial H}{\partial \overrightarrow{S}} = \left\{ \frac{\partial H}{\partial S_x}, \ \frac{\partial H}{\partial S_y}, \ \frac{\partial H}{\partial S_z} \right\}.$$
(62)

In coordinate form and in terms of the dimensionless spin projections, this yields

$$\frac{dn_x}{dt} = -\omega_z n_y,$$

$$\frac{dn_y}{dt} = \omega_z n_x - \omega_x n_z,$$

$$\frac{dn_z}{dt} = \omega_x n_y,$$
(63)

where we took into account that since H does not contain the S_y component, $\vec{\omega} = \frac{\partial H}{\partial \vec{S}} = \{\omega_x, 0, \omega_z\}$. In the case when the "effective magnetic field" $\vec{\omega}$ does not explicitly depend on time, the system (61), (62) has two independent integrals of motion

$$\vec{S}^{2} = S_{x}^{2} + S_{y}^{2} + S_{z}^{2}, \qquad (64)$$

$$J = \frac{1}{\omega} \left(\overrightarrow{\omega}, \overrightarrow{S} \right) = \frac{\omega_{x} S_{x} + \omega_{z} S_{z}}{\sqrt{\omega_{x}^{2} + \omega_{z}^{2}}}.$$

The first (64) reflects the conservation of total spin and also holds for an arbitrary time-dependent field $\vec{\omega} = \frac{\partial H}{\partial \vec{S}}$, whereas the second integral corresponds to the adiabatic invariant of the system (61), (62). Since in our case $\vec{\omega} = \frac{\partial H}{\partial \vec{S}}$ is parametrically time-dependent, the adiabatic invariant is conserved approximately for sufficiently slow parametric evolution. Note that the adiabatic solutions always play the role of "envelope solutions". This means that on average, the spin

closely follows the adiabatic solution, but there are fast oscillatory-type motions superimposed on the slow adiabatic evolution. Basically, the adiabatic approximation in the classical case is applicable when the "slow" motion is much slower than the fast oscillatory motion. This exactly corresponds to the adiabatic evolution of the spin system in the quantum case [22].

Making use of (64) and taking into account that at the instant $\tau = 0$, the total spin was parallel to the x-axis, we obtain $J/l = \frac{\omega_x n_x + \omega_z n_z}{\sqrt{\omega_x^2 + \omega_z^2}} = 1$, or

$$\overrightarrow{n} = \frac{\overrightarrow{\omega}}{\omega},\tag{65}$$

implying that the total spin is always parallel the effective magnetic field $\vec{\omega}$. Therefore, the adiabatic evolution of the large spin can be simply described as the situation when the spin follows the effective field (on average).

We note that at this level, there is a direct correspondence between the adiabatic classical solution and the quasiclassical wave functions of the large spin parallel to \vec{n} . From (65), it follows that this direction can be identified with the effective magnetic field $\vec{\omega} = \frac{\partial H}{\partial \vec{s}}$. This justifies the "variational" approach introduced in [1, 4], identifying the variational wave functions with the adiabatic ground states along the evolution paths when the total spin is parallel to $\vec{\Omega}$. Therefore, one can observe that in the absence of tunnelling, the general HWP is solved essentially by the classical paths of the QAA.

IX. CONCLUSIONS

We apply the quantum adiabatic evolution algorithms with different paths [1] to the generalized Hamming Weight Problem that corresponds to the specific case of the random Satisfiability problem defined in (10). We show that any random evolution path produced by this algorithm for the HWP can be obtained by using 6 specific deterministic basis operators with random weights and therefore is parameterized by 6 independent random numbers. Therefore, the approach to QAA with different paths can still be reduced to the large spin dynamics for the HWP. We show that only one of these "generators" can be a "universal" driver fundamentally responsible for tunnelling suppression for arbitrary HWP and therefore the problem of constructing such a universal driver reduces to the definition of its weight γ_4 . Due to the possible reflection symmetry of the cost function, any particular case of the general HWP can be solved with one of the two values of the weight with $|\gamma_4| > \gamma_{4c}$, that is by applying one of the two universal path modifications. We analyze the nature of the wave functions along the successful paths and show that it is quasiclassical and corresponds to the dynamics of a large classical spin. Therefore, we show that the general HWP is solved by completely classical paths of the QAA and present a complete characterization of these paths.

We analyzed in details the types of bifurcations of the effective Hamiltonian function H(q, p) that lead to the collapse of the adiabatic evolution. The global bifurcations correspond to the onset of tunnelling in QAA and lead to the failure of the algorithm. In contrast, the local bifurcations while still corresponding to exponentially small minimum gap only lead to the decrease of the probability of success by a factor of 2. Since in a given problem function H(q, p) is a low degree polynomial in its arguments there are only a few local bifurcations possible. However, the phenomenon of local bifurcations may become important for more difficult random optimization problems. Assuming the number of such bifurcations M is large the probability of success is reduced by a factor of 2^{-M} . For M that scales up with n that would lead to the failure of the algorithm.

The method described in the paper, suggests an interesting extension to the case of the K-SAT HWP in the limit of large K. In the large-spin limit, the effective potential can be described as a white noise with certain intensity and the well-known methods (optimal fluctuation approach) are applicable. This leads to the complete characterization of the minimal gap statistics. In particular, there always exists a range of parameters where the gap and therefore the run-time of QAA are polynomial in n in the large-n limit.

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APPENDIX A: SPIN OPERATOR REPRESENTATION OF MATRIX A

The random real symmetric 8×8 random matrix A introduced in (17), describes the "transitions" between each of the $2^3 = 8$ states for each clause involving 3 bits [1]. This matrix has $(8 \times 8 - 8)/2 = 28$ independent matrix elements and can be presented in the form

$$A = A^{(1)} + A^{(2)} + A^{(3)}, (A1)$$

where $A^{(1)}, A^{(2)}, A^{(3)}$ correspond to the transitions involving one, two and three bits, respectively. For each realization, we have

$$A^{(1)} = a_{\alpha} \sigma_{\alpha}^{x} \frac{1}{4} \sum_{s,s'=\pm 1} b_{ss'} \left(1 + s \sigma_{\beta}^{z}\right) \left(1 + s \sigma_{\gamma}^{z}\right),$$

$$A^{(2)} = a_{\alpha\beta} \left(\sigma_{\alpha}^{+}\sigma_{\beta}^{+} + \sigma_{\alpha}^{-}\sigma_{\beta}^{-}\right) \frac{1}{2} \sum_{s=\pm 1} b_{s} \left(1 + s \sigma_{\gamma}^{z}\right) + \widetilde{a}_{\alpha\beta} \left(\sigma_{\alpha}^{+}\sigma_{\beta}^{-} + \sigma_{\alpha}^{-}\sigma_{\beta}^{+}\right) \frac{1}{2} \sum_{s=\pm 1} \widetilde{b}_{s} \left(1 + s \sigma_{\gamma}^{z}\right),$$

$$A^{(3)} = B \left(\sigma_{1}^{+}\sigma_{2}^{+}\sigma_{3}^{+} + \sigma_{1}^{-}\sigma_{2}^{-}\sigma_{3}^{-}\right) + C \left(\sigma_{1}^{+}\sigma_{2}^{+}\sigma_{3}^{-} + \sigma_{1}^{-}\sigma_{2}^{-}\sigma_{3}^{+}\right) + D \left(\sigma_{1}^{-}\sigma_{2}^{+}\sigma_{3}^{+} + \sigma_{1}^{-}\sigma_{2}^{-}\sigma_{3}^{-}\right) + E \left(\sigma_{1}^{+}\sigma_{2}^{-}\sigma_{3}^{+} + \sigma_{1}^{-}\sigma_{2}^{-}\sigma_{3}^{-}\right),$$
(A2)

where

$$a_{\alpha}, b_{ss'}, a_{\alpha\beta}, b_s, \widetilde{a}_{\alpha\beta}, b_s, B_{\alpha\beta\gamma}, C_{\alpha\beta\gamma}, D_{\alpha\beta\gamma}, E_{\alpha\beta\gamma}$$
(A3)

are the real coefficients. The indices $(\alpha, \beta, \gamma) \in \{1, 2, 3\}$ label the bits, σ_{α}^{\pm} , σ_{α}^{x} and σ_{α}^{z} are the Pauli sigma-matrices of raising/lowering, x-projection and z-projection, respectively and $s = \pm 1$ is a spin projection variable. Note that the operator $\frac{1}{2}(1 + s \sigma_{k}^{z})$ is a projector onto the spin state s for the bit k. Clearly, the number of independent parameters in (A2) is $3 \times 4 + 6 \times 2 + 4 = 28$, where the three terms of the sum correspond to $A^{(1)}, A^{(2)}$ and $A^{(3)}$, respectively. Note that this number of parameters equals the number of independent matrix elements of A estimated above.

In the matrix form, the representation (A2) yields

$$A_{C} = \begin{bmatrix} 0 & a_{3}b_{++} & a_{2}b_{++} & \tilde{a}_{23}\tilde{b}_{+} & a_{1}b_{++} & \tilde{a}_{13}\tilde{b}_{+} & \tilde{a}_{12}\tilde{b}_{+} & B \\ 0 & \tilde{a}_{23}\tilde{b}_{+} & a_{2}b_{+-} & \tilde{a}_{13}\tilde{b}_{+} & a_{1}b_{+-} & C & a_{12}b_{-} \\ 0 & a_{3}b_{+-} & \tilde{a}_{12}\tilde{b}_{+} & D & a_{1}b_{-+} & a_{13}b_{-} \\ 0 & E & \tilde{a}_{12}\tilde{b}_{-} & \tilde{a}_{13}\tilde{b}_{-} & a_{1}b_{--} \\ 0 & a_{3}b_{-+} & a_{2}b_{-+} & a_{23}b_{-} \\ 0 & \tilde{a}_{23}\tilde{b}_{-} & a_{2}b_{--} \\ 0 & a_{3}b_{--} & 0 \end{bmatrix},$$
(A4)

where the vector $\boldsymbol{\xi}$ of 8 basis states is

$$\boldsymbol{\xi} = [+++; ++-; +-+; ++-; -++; -+-; --+; ---]^{T}, \quad (A5)$$

and the lower left portion of the symmetric matrix A_C is obtained by reflection with respect to the diagonal.

The driver H_E is obtained by summation over all clauses. In doing this summation, we take into account that now the bit indices $\{i, j, k\} \in \{1, 2, ...n\}$ run through all n bits, whereas the indices $(\alpha, \beta, \gamma) \in \{1, 2, 3\}$ characterizing the realization of A_C still run through the 3 bits (since the same realization of A_C is applied to all triples of bits). The driver H_E is given by

$$H_E = H_E^{(1)} + H_E^{(2)} + H_E^{(3)},$$
(A6)

where $H_E^{(1)}$, $H_E^{(2)}$, $H_E^{(3)}$ correspond to the transitions involving one, two and three bits, analogous to (A1).

$$H_E^{(1)} = \sum_{\alpha, i, j, k} a_\alpha \, \sigma_i^x \, \frac{1}{4} \sum_{s, s' = \pm 1} b_{ss'} \left(1 + s \, \sigma_j^z \right) \left(1 + s \, \sigma_k^z \right), \tag{A7}$$

$$\begin{split} H_{E}^{(2)} &= \sum_{\alpha,\beta,i,j,k} a_{\alpha\beta} \left(\sigma_{i}^{+}\sigma_{j}^{+} + \sigma_{i}^{-}\sigma_{j}^{-} \right) \; \frac{1}{2} \sum_{s=\pm 1} b_{s} \left(1 + s \; \sigma_{k}^{z} \right) \\ &\quad + \widetilde{a}_{\alpha\beta} \left(\sigma_{i}^{+}\sigma_{j}^{-} + \sigma_{i}^{-}\sigma_{j}^{+} \right) \; \frac{1}{2} \sum_{s=\pm 1} \widetilde{b}_{s} \left(1 + s \; \sigma_{k}^{z} \right) , \\ H_{E}^{(3)} &= \sum_{i,j,k} B \left(\sigma_{i}^{+}\sigma_{j}^{+}\sigma_{k}^{+} + \sigma_{i}^{-}\sigma_{j}^{-}\sigma_{k}^{-} \right) + C \left(\sigma_{i}^{+}\sigma_{j}^{+}\sigma_{k}^{-} + \sigma_{i}^{-}\sigma_{j}^{-}\sigma_{k}^{+} \right) \\ &\quad + D \left(\sigma_{i}^{-}\sigma_{j}^{+}\sigma_{k}^{+} + \sigma_{i}^{+}\sigma_{j}^{-}\sigma_{k}^{-} \right) + E \left(\sigma_{i}^{+}\sigma_{j}^{-}\sigma_{k}^{+} + \sigma_{i}^{-}\sigma_{j}^{+}\sigma_{k}^{-} \right) . \end{split}$$

One should note that the second term on the r.h.s. for $H_E^{(2)}$ gives a contribution, which is diagonal in S_z representation and therefore leads to the effective "re-definition" of the cost function.

Following the logic of [1], we disregard such terms. Also, the commutation relations between the total spin components give contributions $\sim 1/l$ to the effective potential and can be neglected in the large-spin limit. Taking this into account, we obtain from (A7) in the large-spin limit

$$H_E = \left(\frac{n}{2}\right)^3 \left(\gamma_1 n_x + \gamma_2 n_x^2 + \gamma_3 n_x^3 + \gamma_4 n_x n_z + \gamma_5 n_x n_z^2 + \gamma_6 n_x^2 n_z\right),$$

where $n_a = S_a/l$ is a dimensionless spin projection on *a*-axis and the coefficients $\{\gamma_k\}$ are given by

$$\begin{split} \gamma_{1} &= \frac{1}{6} \left(\sum_{\alpha} a_{\alpha} \right) \left(\sum_{s,s'} b_{ss'} \right) + \frac{1}{3} \left(C + D + E - 3B \right), \\ \gamma_{2} &= \frac{2}{3} \left(\sum_{\alpha,\beta} a_{\alpha\beta} \right) \left(b_{+} + b_{-} \right), \\ \gamma_{3} &= \frac{1}{3}B, \\ \gamma_{4} &= \frac{2}{3} \left(\sum_{\alpha} a_{\alpha} \right) \left(b_{++} - b_{--} \right), \\ \gamma_{5} &= \frac{1}{3} \left(\sum_{\alpha} a_{\alpha} \right) \left(b_{++} + b_{--} - b_{-+} - b_{+-} \right) - \frac{1}{3} \left(C + D + E - 3B \right), \\ \gamma_{6} &= \frac{2}{3} \left(\sum_{\alpha,\beta} a_{\alpha\beta} \right) \left(b_{+} - b_{-} \right). \end{split}$$
(A8)

In particular, the deterministic driver considered in [1] corresponds to $b_{-+} = b_{+-} = \{b_s\} = \{a_{\alpha\beta}\} = B = C = D = E = 0$, $a_{\alpha} = 1$ and $b_{++} = -b_{--} = -2$. It follows from (A8) that in this case, the only non-zero coefficient in (A8) is $\gamma_4 = -8$. This corresponds to $H_E = -4nS_xS_z$, which is equivalent to $H_E = -2n(S_xS_z + S_zS_x)$ in the large-spin limit according to the above discussion.

APPENDIX B: BIFURCATION POINT ANALYSIS

Taking into account only the γ_4 term in H_E and expanding up to the 4th order, we obtain the conditions U' = U'' = U''' = 0 for the A_3 bifurcation point { τ_c, γ_c, x } in the form [24] (cf. (52))

$$\tau_{c} \left(\beta_{1} + 2\beta_{2}x + 3\beta_{3}x^{2}\right) = -(1 - \tau_{c}) \left[2x - x^{3} + \gamma_{c}\tau_{c}\left(1 - \frac{3}{2}x^{2}\right)\right],$$

$$\tau_{c} \left(2\beta_{2} + 6\beta_{3}x\right) = -(1 - \tau_{c}) \left[2 - 3x^{2} + \gamma_{c}\tau_{c}\left(-3x\right)\right],$$
(B1)

$$6\tau_{c}\beta_{3} = (1 - \tau_{c}) \left(6x + 3\gamma_{c}\tau_{c}\right),$$

which have to be solved for γ_c , τ_c and x for the given $\{\beta_k\}$. Solving for x, we obtain condition (53) in the text.

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