Modeling an Adiabatic Quantum Computer via an Exact Map to a Gas of Particles

A. M. Zagoskin,1,2 S. Savel’ev,1,3 and Franco Nori1,4

1Frontier Research System, The Institute of Physical and Chemical Research (RIKEN), Wako-shi, Saitama, Japan
2Department of Physics and Astronomy, The University of British Columbia, Vancouver, British Columbia, Canada
3Department of Physics, Loughborough University, Loughborough, United Kingdom
4Center for Theoretical Physics, CSCS, Department of Physics, The University of Michigan, Ann Arbor, Michigan, USA

(Received 12 December 2006; published 23 March 2007)

We map adiabatic quantum evolution on the classical Hamiltonian dynamics of a 1D gas (Pechukas gas) and simulate the latter numerically. This approach turns out to be both insightful and numerically efficient, as seen from our example of a CNOT gate simulation. For a general class of Hamiltonians we show that the escape probability from the initial state scales no faster than \(|\lambda|^\gamma\), where \(|\lambda|\) is the adiabaticity parameter. The scaling exponent for the escape probability is \(\gamma = \frac{1}{4}\) for all levels, except the edge (bottom and top) ones, where \(\gamma \approx \frac{1}{4}\). In principle, our method can solve arbitrarily large adiabatic quantum Hamiltonians.

Standard approaches to quantum computing are based on applying a sequence of unitary operations to a multi-qubit system, and the solution is encoded in an entangled superposition of its eigenstates, which is fragile with respect to decoherence. Regrettably, there is a growing realization that this approach is not feasible in the near future. An alternative promising paradigm is adiabatic quantum computing [1–3] (AQC), where the solution is encoded in the ground state of the system evolving under an adiabatically slow change of a control parameter \(\lambda\). Remaining in the ground state provides a strong, though not absolute, protection against relaxation and dephasing [4]. Limits of this protection and the ways of its improvement were investigated in Refs. [5,6].

In principle, any standard quantum circuit can be realized by an AQC [7,8]. Following the AQC approach, we reach the ground state of a complex Hamiltonian \(H_0\), which encodes the solution to a given quantum algorithm, by adding to \(H_0\) a large bias term \(ZH_b\), \(Z \gg 1\),

\[
H[\lambda(t)] = H_0 + \lambda(t)ZH_b, \quad (1)
\]
such that \(H(\lambda = 1)\) has a nondegenerate, easily achievable ground state. The intrinsic limitation imposed on AQC is the finite probability of excitation, via Landau-Zener tunneling [9,10], at any finite evolution speed (the adiabaticity parameter \(|\lambda|\)). This tunneling remains even after the effects of external and thermal noise are eliminated. Research on AQC has so far concentrated on evaluating and minimizing the probability of leaving the ground state. Both polynomial [8,11,12] and exponential [13,14] slowdown was predicted using AQC, and this important question remains open.

In this Letter we investigate what is the probability of escape from the ground state, and how far, on average, a system can deviate from the ground state during the adiabatic evolution. We do this by mapping the parametric evolution of the system (1) on the classical Hamiltonian dynamics of a 1D gas model with long-range repulsion (Pechukas gas [15,16]) and simulating the latter numerically. This approach, which had not been used so far in the field of AQC, turns out to be both physically insightful and numerically efficient way to solve (1). For a general class of Hamiltonians, the probability to stay in the same state shows a universal power-law dependence for all the energy levels except for the ground and top excited states, and this difference can be qualitatively understood within the Pechukas gas model. We also develop a kinetic theory that could, in principle, solve arbitrarily large adiabatic Hamiltonians.

Pechukas gas dynamics.—In this approach we consider the instantaneous eigenstates, \(|n(\lambda)\rangle\), and eigenvalues, \(E_n(\lambda)\), of the Hamiltonian (1): \(H(\lambda)|n\rangle = E_n(\lambda)|n\rangle\). The Hamiltonian \(H_0\) is at all times fully determined by the set of its instantaneous matrix elements, \(\langle m|H_0|n\rangle = E_n(\lambda)\delta_{mn} - \lambda\langle m|ZH_b|n\rangle\). The latter can be determined from the closed set of differential equations (see Refs. [15,16]):

\[
\frac{d}{d\lambda} x_m = v_m; \quad \frac{d}{d\lambda} v_m = 2\sum_{m+n=0} |l_{mn}|^2 \left(\frac{1}{(x_m - x_n)^2} - \frac{1}{(y_m - y_n)^2}\right), \quad (2)
\]

where \(x_n(\lambda) = E_n(\lambda)\), \(v_n(\lambda) = \langle n|ZH_b|n\rangle\), and \(l_{mn}(\lambda) = [E_m(\lambda) - E_n(\lambda)]\langle m|ZH_b|n\rangle\). Equations (2) describe the classical Hamiltonian dynamics of a 1D gas with repulsion, where \(\lambda\) plays the role of time, and the nth “particle” has a position \(x_n(\lambda)\) and velocity \(v_n(\lambda)\). The particle-particle repulsion is determined by the “relative angular momenta” \(l_{mn}(\lambda)\).

The mapping of AQC to the classical dynamics of Eq. (2) is exact and applies to any Hamiltonian. All the information about the Hamiltonian \(H_0\) is contained in the initial values, \(x_m(\lambda = 1)\), \(v_m(\lambda = 1)\), and \(l_{mn}(\lambda = 1)\). Those are given by the appropriate matrix elements of
the Hamiltonian (1) at \( \lambda = 1 \), \( H(1) = H_0 + ZH_b = Z(H_b + Z^{-1}H_0) \). By choice, \( H(1) \) has nondegenerate, well separated levels, with an easily reachable ground state. The initial conditions for Eq. (2) can be obtained perturbatively in \( Z^{-1} \) to any accuracy.

CNOT gate.—Consider a specific example of an AQC. An arbitrary \( N \)-step, \( M \)-qubit quantum algorithm can be encoded in \( H_0 \) using the “ground state quantum computing” approach [17], whereby every qubit is represented by an array of \( 2 \times (N + 1) \) quantum dots sharing a single electron. The state of the \( m \)th qubit on the \( (n + 1) \)st step of the algorithm is given by the probability amplitude to find the electron on either the quantum dot \((m, n, 0)\) or \((m, n, 1)\).

The solution is determined by the ground state probability amplitudes on the quantum dots \((m, N, 0)\) and \((m, N, 1)\).

For a simple universal quantum gate, the CNOT (where \( N = 1, M = 2 \)), \( H_0 \) can be written as [8,17]

\[
H_{\text{CNOT}} = (c_{010}^\dagger c_{11}^\dagger c_{00}^\dagger c_{10}^\dagger) (C_{11} c_{010} - C_{10} c_{000})
+ (c_{011}^\dagger c_{11}^\dagger c_{01}^\dagger c_{10}^\dagger) (C_{11} c_{011} - C_{10} c_{001})
+ C_{00} c_{001}^\dagger c_{11}^\dagger + C_{01} c_{011}^\dagger c_{10}^\dagger,
\]

where \( c_{mn}^\dagger \) creates an electron on the corresponding dot, \( c_{mn}^\dagger = (c_{m0}^\dagger c_{m1}^\dagger) \), and \( \sigma^z \) is a Pauli matrix. The ground state energy of (3) is zero. To specify the initial state of the qubits before the operation, a small correction must be added.

The results shown in Fig. 1(a) correspond to CNOT \([00] \rightarrow [00]\). To achieve this, the term \( \delta H = \varepsilon (c_{000}^\dagger c_{000} + c_{100}^\dagger c_{100}) \), with \( \varepsilon = -0.1 \), was added to \( H_0 \). Remarkably, even though the initial conditions for the Pechukas equations (2) were only calculated to first order in \( Z^{-1} = 0.1 \), the results agree with the exact diagonalization to four significant figures, indicating a high efficiency of the approach. The same accuracy holds for the CNOT acting on all the other basis states. All the degeneracies of the Hamiltonian (3) are precisely reproduced in our approach. Since any 1D gas with repulsive interactions naturally expands, the decrease of the bias potential \( \lambda ZH_b \) corresponds to a contraction from \( H \) to \( H_0 \) and can be considered a Loschmidt time reversal [18] of the natural evolution. Note that while the levels generally repel, certain groups of levels can cross, due to the symmetries of the Hamiltonian (3).

Statistics of level occupation.—Unlike the simple example of a CNOT gate presented above, when considering a general AQC case, we would benefit from the knowledge of the statistical behavior, for a given class of AQC problems (i.e., Hamiltonians \( H_b \)). An ensemble of Hamiltonians \( H_b \) corresponds to a distribution of initial conditions in the Pechukas dynamics in Eq. (2), over which an appropriate averaging must be taken. We choose a set described by one of the random matrix theory (RMT) Gaussian ensembles [19]. This, in particular, means that the distribution of \( x_\mu(\lambda = 1) \), \( v_\mu(\lambda = 1) \) and \( \langle m | ZH_b | n \rangle(\lambda = 1) \) is Gaussian. Such an assumption about the behavior of a large collection of qubits with varied couplings is reasonable and was used recently in [12,13], but must still be taken cum grano salis. For example, the numerical calculations in Ref. [14] show that for the 3-SAT problem, RMT describes well only the bulk of the spectrum. In the case of, e.g., flux qubits threaded by a magnetic field, the natural choice is the Gaussian unitary ensemble (GUE) of general Hermitian matrices. (If the system has time-reversal sym-
FIG. 2 (color online). (a) Probability \( P(n|n) \) for the system to remain in the initial state \( |n⟩ \), as a function of \( 1/T \), during the adiabatic evolution (i.e., decreasing the external field with constant speed \( |\lambda| = 1/T \)). The data are averaged over 400 GUE realizations with \( N = 50 \). The power-law dependence \( P \propto T^γ \) is clearly seen, with two distinct exponents: (i) \( γ = \frac{1}{3} \) for all the bulk states and (ii) \( γ \approx \frac{1}{2} \) for the edge states. For example, for \( N = 50 \): \( γ = \frac{1}{3} \) for \( n = 2(49) \), solid (empty) purple circles; \( n = 5(45) \), solid (empty) green triangles; \( n = 10(40) \), solid (empty) upturned magenta triangles; \( n = 25 \), black diamonds; but \( γ = \frac{1}{2} \) for the ground state (\( n = 1 \), red squares) and the highest excited state (\( n = 50 \), empty blue squares). For \( N = 150 \) (left inset): \( γ = \frac{1}{3} \) for \( n = 2 \) (purple stars), \( n = 75 \) (black pluses); but \( γ = \frac{1}{2} \) for the ground state (\( n = 1 \), red crosses). However, the average number of avoided level crossings (right inset) is a smooth function of the level number for both \( N = 50 \) (red) and \( N = 150 \) (black). As expected in the absence of external noise, the probability \( P(n|n) \) saturates at 1 as \( 1/T → 0 \) (when \( 1/T < 0.01 \)).

(b) The standard deviation \( \langle (n-n_0)^2 \rangle^{1/2} \) of the system from the initial state \( n = n_0 \) during the adiabatic evolution, as a function of \( 1/T \) (\( N = 50 \)). The scaling is approximately power law, but with the exponent smoothly dependent on the initial state. (Inset) Probability \( P(n|n_0) \) to occupy level \( |n⟩ \) at the end of the evolution, starting from level \( n_0 = 1, 25, 50 \) (\( N = 50 \)). Different curves correspond (top to bottom peaks) to \( 10^3 \times |\lambda| = 1, 2.5, 5, 10, 25, 50, 75 \).
complex system (e.g., a spin glass) with classical annealing algorithms generally depends on $1/\varepsilon$ exponentially (see Ref. [20], and references therein). It is therefore tempting to conclude that the adiabatic evolution of a quantum computer could provide an exponential speedup, on average, for this type of problem. To confirm this conjecture and establish the limits of its validity, we need to consider larger systems. Then the brute force approach to solving the set (2) becomes inefficient. We can instead identically rewrite it as a chain of computer could provide an exponential speedup, on average, to conclude that the adiabatic evolution of a quantum change of two anticrossing levels due to Landau-Zener standard; the collision integral describes the population ex-

\[ f_{ij} = \int \frac{d\alpha}{\alpha} + v \frac{d}{dx} \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]

\[ f_{ij} = \langle f_1 \rangle_v, \]