Supporting materials

A. Proof of Theorem II.1.

Recurrence (8) readily implies

$$|\psi_n\rangle = \frac{1}{n!} P_n \, |\psi_0\rangle, \tag{1}$$

where $P_n = P_n(A, B)$ are operators defined via recurrence

$$\begin{array}{rcl} P_0 & = & I \\ P_1 & = & A \\ \vdots & & \\ P_{n+1} & = & AP_n + nBP_{n-1} \quad \text{for } n \geq 1. \end{array} \tag{2}$$

Note that we have $\|P_0\| = 1$, $\|P_1\| = a$, and $\|P_{n+1}\| = \|AP_n + nBP_{n-1}\| \leq a\|P_n\| + nb\|P_{n-1}\|$. We wish to estimate the rate of growth of $\|P_n\|$. To this end let us consider an auxiliary scalar sequence (p_n) defined via recurrence

$$\begin{array}{rcl} p_0 & = & 1 \\ p_1 & = & a \\ \vdots & & \\ p_{n+1} & = & ap_n + nbp_{n-1} \quad \text{for } n \geq 1. \end{array} \tag{3}$$

Since $p_0 = \|P_0\|, p_1 = \|P_1\|$ and p_n grows at least as fast as $\|P_n\|$, we clearly have

$$\|P_n\| \leq p_n. \tag{4}$$

Next, we undertake to estimate the growth rate of (p_n). First, observe that $p_n = p_n(a, b)$ may be viewed as a polynomial in two variables, e.g. $p_2 = a^2 + b$, $p_3 = a^3 + 3ab$, etc. It is easily seen that the general form of the polynomials is

$$p_n = c_0[n]a^n + c_1[n]a^{n-2}b + c_2[n]a^{n-4}b^2 + c_3[n]a^{n-6}b^3 + \ldots = \sum_{k=0}^{[\frac{n}{2}]} c_k[n] \, a^{n-2k}b^k, \tag{5}$$

where the coefficients $c_k[n]$ remain to be found. Note that the last term of the polynomial is either $c_{n/2}[n] \, b^{n/2}$ (when n is even) or $c_{[n/2]}[n] \, ab^{[n/2]}$ (when n is odd), with $[x]$ denoting the integer part of x. Moreover, it is easily seen that (3) implies

$$\begin{array}{rcl} c_0[n] & = & 1 \\ c_1[n] & = & \binom{n}{2} \\ \vdots & & \\ c_k[n] & = & c_k[n-1] + (n-1)c_{k-1}[n-2] \end{array} \tag{6}$$

Using this, and applying induction one readily obtains an explicit formula

$$c_k[n] = (2k-1)!! \binom{n}{2k}, \tag{7}$$

where $(2k-1)!! = 1 \cdot 3 \cdot 5 \cdot \ldots (2k-1)$. In light of this (5) yields

$$\frac{1}{n!} \, p_n = \sum_{k=0}^{[\frac{n}{2}]} \frac{1}{k!(n-2k)!} a^{n-2k} \frac{b^k}{2^k}. \tag{8}$$

Next, we make the following observation

$$k!(n-2k)! \geq \left[\frac{n}{3}\right]! \quad \text{for } k = 0, 1, 2, \ldots, [n/2]. \tag{9}$$

Indeed, we either have $k \geq \left[\frac{n}{3}\right]$ or else $n - 2k > n - 2\left[\frac{n}{3}\right] \geq \left[\frac{n}{3}\right]$. In either case (9) follows trivially.

Next, we obtain from (8) and (9):

$$\begin{aligned} \tfrac{1}{n!}\, p_n &= \sum_{k=0}^{[\frac{n}{2}]} \tfrac{1}{k!(n-2k)!} a^{n-2k} \tfrac{b^k}{2^k} \\ &\leq \tfrac{1}{[\frac{n}{3}]!} a^n \{1 + \tfrac{b}{2a^2} + \left(\tfrac{b}{2a^2}\right)^2 + \left(\tfrac{b}{2a^2}\right)^3 + \ldots + \left(\tfrac{b}{2a^2}\right)^{[n/2]}\} \\ &\leq \tfrac{1}{[\frac{n}{3}]!} a^n (1 + \tfrac{b}{2a^2})^{n/2}. \end{aligned} \tag{10}$$

As is well known, $\left(\left[\frac{n}{3}\right]!\right)^{1/n} \to \infty$ as $n \to \infty$. Thus, recalling definition (1), we obtain

$$\|\psi_n\|^{1/n} \leq \|\frac{1}{n!} P_n\|^{1/n} \|\psi_0\|^{1/n} \leq \left(\frac{1}{n!}\, p_n\right)^{1/n} \|\psi_0\|^{1/n} = \frac{1}{\left(\left[\frac{n}{3}\right]!\right)^{1/n}} a \left(1 + \frac{b}{2a^2}\right)^{1/2} \|\psi_0\|^{1/n} \to 0, \tag{11}$$

which by (9) implies $R_c = \infty$. □

Remark 1. Consider the unitary map $U(s)$ defined by the adiabatic Schrödinger equation:

$$\frac{d}{ds} U(s) = -i(T/\hbar)\, H(s)\, U(s), \qquad \text{so that } U(s)|\psi(0)\rangle = |\psi(s)\rangle.$$

Note that recurrence (2) applied in the special case — i.e. $A = -i(T/\hbar)\, H_i$, $B = -i(T/\hbar)\,(H_f - H_i)$ — provides a constructive description or simulation of $U(s)$ via the formula

$$U(s) = \sum_{n=0}^{\infty} \frac{1}{n!}\, P_n.$$

In particular this description of the semigroup $s \mapsto U(s)$ may be used to simulate the evolution of mixed states (13). Indeed,

$$\frac{d}{ds} \rho(s) = -i(T/\hbar)\, [H(s), \rho(s)] \quad \Longrightarrow \quad \rho(s) = U(s) \rho(0) U(s)^*.$$

Remark 2. Note that when $b < 2a^2$ (valid in the adiabatic regime) estimate (10) may be replaced by a more efficient one. Indeed in such a case

$$1 + \frac{b}{2a^2} + \left(\frac{b}{2a^2}\right)^2 + \left(\frac{b}{2a^2}\right)^3 + \ldots \leq \frac{1}{1 - \frac{b}{2a^2}}$$

If in addition $a < 1$, then terms $p_n/n!$ diminish very fast which ensures fast convergence of series (5) when $s = 1$, also in the numerical sense. However, this is not of interest in the current problem as it represents the anti-adiabatic limit, as the number of spin flips during the evolution is of order a. In the special case of interest $a = (T/\hbar)\|H_i\|, b = (T/\hbar)\|H_i - H_f\|$ and the condition $a < 1 \,\&\, b < 2a^2$ is equivalent to

$$\hbar\, \frac{\|H_i - H_f\|}{2\, \|H_i\|^2} < T < \hbar\, \frac{1}{\|H_i\|}, \text{ which implies } \|H_i - H_f\| < 2\, \|H_i\|.$$

This assumption on T ensures the most efficient computation of series (5). However, we do not claim that this restriction delineates the only regimes in which computation is effective.

B. Algorithm efficiency

We will utilize elements of the proof given in part A to analyze the numerical efficiency of the recurrence algorithm (8) with the specific problem constituents (18–19).

First, in order to estimate the efficiency of a recurrence one needs to establish a stopping condition. It is desirable to stop recurrence when the approximation error is sufficiently small. However, little is known a priori about the solution that is sought in (8) and so the calculus methods do not seem to provide an easy estimate for the dependence of error on the degree of approximation n. As a substitute we propose the following stopping condition:

$$\text{Compute } \Psi_k \text{ for } k = 1, 2, \dots n, \text{ where } n \text{ is the smallest index such that } \|\Psi_n\|^{1/n} \leq \varepsilon. \tag{12}$$

Here, ε is regarded as a preset measure of accuracy. In light of the proof of Theorem II.1 we know that n defined by (12) is bound to be finite. Moreover, since the solution $\Psi(s)$ is an analytic function in the complex plane this is expected to provide a good estimate of the remainder error when s is bounded, e.g. $s \sim 1$.

Next, consider the particular case $T = 1$ (recall also $\hbar = 1$). Let us assume that the Taylor series is centered at s_0 (see remarks in the opening of Section IV). In such a case $a = \|H_i + s_0(H_i - H_f)\| = O(\|H_f\|) = O(N^2)$, $b = \|H_i - H_f\| = O(\|H_f\|) = O(N^2)$ which readily implies

$$a\left(1 + \frac{b}{2a^2}\right)^{1/2} = \left(a^2 + \frac{1}{2}b\right)^{1/2} = O(N^2). \tag{13}$$

It now follows from(11), (12) and the Sterling formula that

$$a\left(1 + \frac{b}{2a^2}\right)^{1/2} \sim \varepsilon \left(\left[\frac{n}{3}\right]!\right)^{1/n} \sim \varepsilon\, n^{1/3}, \quad \text{i.e. } n \sim \frac{1}{\varepsilon^3} O(N^6)$$

Now, let us consider $T >> 1$. As explained at the end of section IV, the best course of action is to carry out the computation in $\sim T$ steps. Note that the estimate (13) holds at every step, which ensures that every step requires $O(N^6)$ operations.

Finally, it is easily seen that the number of arithmetical operations necessary to find n Taylor coefficients is of rank $O(n2^N)$. Thus, the overall number of arithmetical operations required to carry out the computation is of rank $O(T \cdot n \cdot 2^N) = O(T \cdot N^6 \cdot 2^N) = O(2^N)$. This is a polynomial time algorithm when measured against the classical problem size 2^N. Naturally, and not very surprisingly, it is exponential in the number of qubits. The important feature of this algorithm is that it scales linearly with time T.

Remark 3. While the formal analysis above suggests that the constant of proportionality between the number of Taylor coefficients n and N^6 may be very large ($\sim \varepsilon^{-3}$), numerical evidence suggests that a rigid *a priori* number, say $n = 50...90$ is typically sufficient to ensure numerical convergence. However, for a small fraction of a percentage of Ising Hamiltonians there is no convergence under these conditions. Nevertheless, in the type of experiment considered in this article those cases are statistically insignificant and may be discarded.

Remark 4. We note that the recurrence algorithm does not require that all the Taylor series coefficient terms be kept in the memory. Indeed, in the case of unitary evolution with the dynamic variable being a vector Ψ of length 2^N, the memory requirement is of rank $3 \cdot 2^N$, regardless of the number of coefficients n that are kept in the approximation. Indeed, we only need to keep in the memory the variable Ψ, which is continually updated, and the two last Taylor coefficients, Ψ_k and Ψ_{k-1} as k runs from 2 to n. For a similar reason the memory requirement in the non-unitary case, when the dynamic variable is ρ of size 2^{2N}, is of rank $3 \cdot 2^{2N}$. In light of this the limitations on problem size that can be handled with the proposed method stem from the machine memory resource rather than the computational algorithm itself.