Partial suppression of nonadiabatic transitions

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Abstract
The adiabatic following of eigenstates of time-varying Hamiltonians can serve as a useful tool in preparing or manipulating quantum states. If the time variation is not sufficiently slow, however, nonadiabatic transitions to unwanted states occur. Recently, it has been shown that the adiabatic following can be perfectly restored if the original Hamiltonian is complemented with an additional term. Although there is an explicit formula for this compensating term, typically one may not always be able to construct it in an experiment. Here we present a straightforward approach for a partial suppression of the nonadiabatic transitions applicable for any set of available Hamilton operators. We illustrate the method on several examples including interacting spin systems, interacting bosons in a double-well potential, a particle in an expanding box and a system of atoms interacting via a Rydberg-blockade. Whenever suitable compensating operators are available, the system may be evolved faster or with higher fidelity along an eigenstate of the original time-dependent Hamiltonian.

1. Introduction

In many physical situations, it is possible to prepare a target quantum state by adiabatically following an eigenstate of a slowly changing Hamiltonian. However, there may be a trade-off between speed and fidelity. If time is scarce, one needs the processes to be as fast as possible,
and if the process is slow, the system may be subject to decoherence and decay. If, on the other hand, the Hamiltonian changes fast, nonadiabatic transitions to unwanted states are induced.

Recently, much effort has been devoted to this challenge. Demirplak and Rice [1], and independently Berry [2], proposed a very elegant way to compensate the diabatic transitions by supplementing the original Hamiltonian \( H_0(t) \) with an additional term, \( H_B(t) \), such that, under the influence of \( H_0 + H_B \), the system follows the (time-varying) eigenstates of \( H_0(t) \). \( H_B(t) \) provides a ‘shortcut to adiabaticity’ studied now in numerous theoretical [3–7] and experimental [8] works (see [9] for a detailed review). Although there is a concise analytic formula for \( H_B(t) \), in many cases one does not have direct means to construct such a Hamiltonian physically.

Here we present a simple and straightforward way to construct a compensating Hamiltonian \( H_C(t) \), using any available set of physical interactions. Our presentation generalizes the approach used in our recent proposal to prepare spin squeezing and Schrödinger cat states in the atomic samples with the Rydberg blockade [10]: one combines the available operators so that their action on the chosen eigenstate of \( H_0(t) \) is as close as possible to the action of \( H_B(t) \). In [10], a combination of two available interactions was sufficient to closely emulate the Berry Hamiltonian such that the process could speed up by an order of magnitude. In this paper, we show how the method can be applied with an arbitrary number of additional operators, and we give examples for different physical systems.

2. Suppression of nonadiabatic transitions

Assume that we want an eigenstate \( |\psi_0\rangle \) of Hamiltonian \( H_0(t = 0) \) to transform adiabatically into the corresponding eigenstate of the Hamiltonian \( H_0(t) \) at later times \( t \). As shown in [2], an exact following occurs if the system is subject to a combined time-dependent Hamiltonian \( H = H_0 + H_B \), where

\[
H_B = i \hbar \sum_n (|\dot{n}\rangle \langle n| - |n\rangle \langle \dot{n}|) \tag{1}
\]

with \( |n\rangle \equiv |n(t)\rangle \) the instantaneous eigenvectors of \( H_0(t) \), \( H_0(t)|n(t)\rangle = E_n(t)|n(t)\rangle \), and the dot denoting the time derivative. Although \( H_B \) can be computed at any time, it is not always possible to construct it in an experiment. If we are able to simultaneously control the strengths of a fixed set of available Hamiltonians \( L_k \), we can combine them into a compensating Hamiltonian \( H_C \) as

\[
H_C = \sum_{k=1}^K \alpha_k L_k, \tag{2}
\]

where \( \alpha_k \) are time-dependent real numbers and \( K \) is the number of available operators. The system then evolves subject to the combined Hamiltonian \( H = H_0 + H_C \).

We denote the chosen eigenstate of \( H_0(t) \) in which we want to keep the system as \( |0\rangle \equiv |0(t)\rangle \). If \( H_B \) is not available, we want \( H_0 + H_C \) to act on \( |0\rangle \) as closely as possible as \( H_0 + H_B \) would do. In particular, we require the norm of the vector \( (H_C - H_B)|0\rangle \) to be as small as possible, i.e. we want to find the set of \( \alpha_k \) that minimizes

\[
\langle 0 | \left( \sum_{k=1}^K \alpha_k L_k - H_B \right) \left( \sum_{k'=1}^K \alpha_{k'} L_{k'} - H_B \right) |0\rangle. \tag{3}
\]
This is a quadratic form that reaches minimum for $\alpha_k$s solving the set of linear algebraic equations

$$\sum_{k=1}^{K} A_{m,k} \alpha_k = C_m,$$  \hspace{1cm} (4)

where

$$A_{m,k} = \langle L_m L_k + L_k L_m \rangle,$$  \hspace{1cm} (5)

$$C_k = \langle L_k H_B + H_B L_k \rangle$$  \hspace{1cm} (6)

and the brackets denote mean values of the operators in the time-dependent state $|0\rangle$.

Equations (4)–(6) provide a simple theory to find a useful combination of the available Hamiltonian operators. Note that if all $C_k$ vanish, equation (4) suggests that no compensating Hamiltonian should be applied, and only if at least some of the $L_k$ operators do not anti-commute with $H_B$, our recipe may suppress the nonadiabatic processes.

3. Example: two spin-$\frac{1}{2}$ particles

Let us assume two spin-$\frac{1}{2}$ particles with variable interaction

$$H_0 = -B(\sigma_x^{(1)} + \sigma_x^{(2)}) + J \sigma_z^{(1)} \sigma_z^{(2)}$$  \hspace{1cm} (7)

with coefficients $B$ and $J$ being functions of time, $B = B(t)$, $J = J(t)$. This model has been used for the simulation of a quantum magnet with trapped ions [11], and is also relevant for quantum information processing in NMR (see e.g. [12] for a review). The aim is to transform the system adiabatically from the lowest-energy eigenstate of $-\sigma_x^{(1)} - \sigma_x^{(2)}$ to the lowest-energy eigenstate of $\sigma_z^{(1)} \sigma_z^{(2)}$ by switching from $J \ll B$ to $J \gg B$.

3.1. Hamiltonian diagonalization

In the basis $|\uparrow \uparrow\rangle, |\uparrow \downarrow\rangle, |\downarrow \uparrow\rangle, |\downarrow \downarrow\rangle$ the Hamiltonian has the form

$$H_0 = \begin{pmatrix}
J & -B & -B & 0 \\
-B & -J & 0 & -B \\
-B & 0 & -J & -B \\
0 & -B & -B & J
\end{pmatrix}.$$  \hspace{1cm} (8)

It is useful to express the parameters as

$$J = A \sin \varphi,$$  \hspace{1cm} (9)

$$B = \frac{A}{2} \cos \varphi$$  \hspace{1cm} (10)

with $A$ and $\varphi$ being time dependent and $\varphi \in (0, \pi/2)$. The eigenvalues are then $\pm A$ and $\pm A \sin \varphi$ with the eigenvectors

$$|\phi_1\rangle = \frac{1}{2\sqrt{1 + \sin \varphi}} \begin{pmatrix} \cos \varphi \\ 1 + \sin \varphi \\ 1 + \sin \varphi \\ \cos \varphi \end{pmatrix},$$

$$|\phi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix},$$

3
\[ |\phi_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad |\phi_4\rangle = \frac{1}{2\sqrt{1 + \sin \varphi}} \begin{pmatrix} 1 + \sin \varphi \\ -\cos \varphi \\ -\cos \varphi \\ 1 + \sin \varphi \end{pmatrix}. \tag{11} \]

### 3.2. Berry Hamiltonian

Since \(|\phi_2\rangle = |\phi_3\rangle = 0\), the Berry Hamiltonian has just two terms

\[ H_B = i\hbar |\phi_1\rangle \langle \phi_1| + i\hbar |\phi_4\rangle \langle \phi_4|, \tag{12} \]

which yields

\[ H_B = \frac{\hbar \dot{\varphi}}{4} \begin{pmatrix} 0 & -i & 0 & -i \\ i & 0 & 0 & i \\ i & 0 & 0 & i \\ 0 & -i & 0 & 0 \end{pmatrix} = \frac{\hbar \dot{\varphi}}{4} \left( \sigma_y^{(1)} \sigma_z^{(2)} + \sigma_z^{(1)} \sigma_y^{(2)} \right). \tag{13} \]

Let us note that the strength of the Berry Hamiltonian (13) depends only on the rate of change \(\dot{\varphi}\) and not on the strength \(A\) of the original Hamiltonian. For \(\varphi = \omega t\) with a constant \(\omega\), the Berry Hamiltonian is time independent. Setting \(A = 0\), the Hamiltonian (13) indeed makes the transition between the initial and final states, regardless of what happens with the ‘adiabatic’ variables. This can be checked by calculating \(\exp(-i H_B t / \hbar)\) at the relevant time \(t = \pi / (2\omega)\),

\[ \exp \left( -\frac{i \pi H_B}{2\hbar \omega} \right) = \exp \left[ -i \frac{\pi}{8} \left( \sigma_y^{(1)} \sigma_z^{(2)} + \sigma_z^{(1)} \sigma_y^{(2)} \right) \right] \]

\[ = \frac{2 + \sqrt{2}}{4} - \frac{2 - \sqrt{2}}{4} \sigma_y^{(1)} \sigma_z^{(2)} - i \frac{\sqrt{2}}{4} \left( \sigma_y^{(1)} \sigma_z^{(2)} + \sigma_z^{(1)} \sigma_y^{(2)} \right), \tag{14} \]

which makes the transition from \(|\rightarrow \rangle\) (both spins pointing in the same \(x\) direction) to \(|\uparrow \downarrow\rangle + |\downarrow \uparrow\rangle\) (superposition of the two possible states with the spins pointing in the opposite \(z\) direction).

### 3.3. Partial compensation

If the operator \(\sigma_y^{(1)} \sigma_z^{(2)} + \sigma_z^{(1)} \sigma_y^{(2)}\) is not available, one can try to compensate with other operators. Nonzero values in equation (6) result from any combination with the arbitrary real parameters \(p\) and \(q\) of \(\sigma_y^{(1)} \sigma_z^{(2)}\) and \(\sigma_z^{(1)} \sigma_y^{(2)}\),

\[ L = p \sigma_y^{(1)} \sigma_z^{(2)} + q \sigma_z^{(1)} \sigma_y^{(2)}. \tag{15} \]

The choice, \(p = q\), yields the full operator \(H_B\) while for \(p = 0\) only \(\sigma_z^{(1)} \sigma_y^{(2)}\) is present, and similarly for \(q\) and \(\sigma_y^{(1)} \sigma_z^{(2)}\). It is interesting to study the achievements of the operator (15) for which we have

\[ \langle \phi_1| L^2 |\phi_1\rangle = (q + p)^2, \tag{16} \]

\[ \langle \phi_1| L H_B + H_B L |\phi_1\rangle = (q + p)\hbar \dot{\varphi}, \tag{17} \]

so that

\[ \alpha = \frac{\langle \phi_1| L H_B + H_B L |\phi_1\rangle}{2 \langle \phi_1| L^2 |\phi_1\rangle} = \frac{\hbar \dot{\varphi}}{2 (q + p)}. \tag{18} \]
The compensating Hamiltonian is then
\[ H_C = \alpha L = \hbar \dot{\psi} \frac{p\sigma_y^{(1)}\sigma_y^{(2)} + q\sigma_z^{(1)}\sigma_z^{(2)}}{2(q + p)}. \]  
(19)

For \( q = p \), \( H_C = H_B \), while it can be checked that for any choice of values for \( q \) and \( p \),
\[ H_C|\phi_1\rangle = H_B|\phi_1\rangle, \]
(20)
\[ H_C|\phi_4\rangle = H_B|\phi_4\rangle, \]
(21)
which means that the compensation is perfect, and if the system starts in any of the two states \( |\phi_{1,4}\rangle \) it exactly follows these eigenstates of the time dependent Hamiltonian \( H_0 \) of equation (8) as if it were complemented with the Berry Hamiltonian \( H_B \). However, under the influence of \( H_0 + H_C \) (with \( p \neq q \)), oscillations between states \( |\phi_2\rangle \) and \( |\phi_3\rangle \) are induced.

4. Example: four spin-\( \frac{1}{2} \) particles

The adiabatic following of eigenstates has been applied to demonstrate the emergence and frustration of magnetism with variable-range interactions in a quantum simulator based on laser controlled trapped ions [13]. Although for larger numbers of spins and general position dependence of the spin–spin interaction, one cannot get simple analytical results, with reasonably small spin numbers one can find a compensation procedure numerically. For an illustration, we assume a linear chain of four spin \( \frac{1}{2} \) particles under the influence of the Hamiltonian
\[ H_0 = -B(t) \sum_{j=1}^{4} \sigma^{(j)}_x + J_0 \sum_{j=1}^{3} \sigma^{(j)}_z \sigma^{(j+1)}_z. \]  
(22)

\( B(t) \) corresponds to an external magnetic field in the \( x \) direction and to keep a close connection to the procedure of Islam et al [13], we assume \( B(t) \) to be ramping down toward zero from some initial value \( B_0 \gg J_0 \). Initially, the first term on the right-hand side is dominant and the lowest-energy eigenstate is \( \rightarrow \rightarrow \rightarrow \rightarrow \) with all four spins pointing in the \( x \) direction. When \( B \) goes to zero, the interaction of the neighboring spins in the first term is dominant and the lowest-energy eigenstate is \( \uparrow \downarrow \downarrow \downarrow + \downarrow \uparrow \uparrow \uparrow \), i.e. an entangled antiferromagnetic state with neighboring spins pointing in the opposite \( z \) direction. Since for small \( B \) the energy levels of \( H_0 \) become close to degeneration, the adiabatic procedure has to be slow. To speed the process up, one finds \( H_B \) numerically as a \( 16 \times 16 \) matrix by a straightforward evaluation of equation (1). However, the structure of \( H_B \) is rather complicated, involving multi-particle interactions. Instead, we try here to construct a suitable \( H_C \) by using only two-particle interactions.

Different two-particle interaction operators combining the \( y \) and \( z \) spin components can be synthesized by the laser driving of the ions, and we shall consider the achievements of the following operators:
\[ L_1 = \sigma_y^{(1)} \sigma_z^{(2)} + \sigma_z^{(3)} \sigma_y^{(4)}, \]
(23)
\[ L_2 = \sigma_z^{(1)} \sigma_y^{(2)} + \sigma_y^{(3)} \sigma_z^{(4)}, \]
(24)
\[ L_3 = \sigma_y^{(2)} \sigma_z^{(3)} + \sigma_z^{(2)} \sigma_y^{(3)}, \]
(25)
\[ L_4 = \sigma_z^{(1)} \sigma_y^{(4)} + \sigma_y^{(1)} \sigma_z^{(4)}. \]
(26)

5
In figure 1(a), we show the eigenvalues of Hamiltonian (22) with the magnetic field ramping down as $B(t) = B_0 \exp(-2.4t/t_0)$ with $B_0 = 5J_0$ and $t_0 = \hbar/J_0$ (note that comparing the values with those in [13], where $J_0/\hbar \approx 1$ kHz, we have $t_0 \approx 160 \mu$s, which is shorter than the time $\approx 400 \mu$s used in [13]). The ramp down is too fast, and the final state fidelity $F(t) = \langle \langle 0(t) | \psi(t) \rangle \rangle^2$ for a state $|\psi(t)\rangle$ evolving solely under the influence of $H_0$ drops to 63% as shown by the lower curve in figure 1(b). Taking advantage of the full set of operators $L_1 \cdots L_4$ in equations (23)–(26) and the time-dependent values of $\alpha_k$ shown in figure 2(a) to construct $H_C$, the state fidelity may be kept at 100% throughout the process governed by $H_0 + H_C$. If a smaller set of compensating operators $L_k$ is applied the fidelity is less than unity but better than in the case of no compensation, as shown by the intermediate curves in figure 1(b).

We observe for example that reasonable compensation and a fidelity around 90% can be achieved when the two operators, $L_1$ and $L_3$ are used with the time dependent strengths $\alpha_k$ shown in figure 2(b).
5. Example: two interacting bosons in two wells

A prominent application of adiabatic processes is the transition between the superfluid state and the Mott insulator ground state of a bosonic system [14]. The process can be studied with a simple model that consists of two indistinguishable particles occupying two sites. The dynamics depends on two parameters—interaction energy $U$ and hopping energy $J$. The Hamiltonian is

$$H_0 = \frac{U}{2} \sum_{j=1}^{2} n_j(n_j - 1) - J \left(a_1^\dagger a_2^\dagger + a_1^\dagger a_2\right),$$

(27)

where $n_j$ is the occupation number and $a_j$ is the annihilation operator for particles at the $j$th site. Assuming a Hilbert subspace with exactly two particles, in the occupation number basis $|2, 0\rangle$, $|1, 1\rangle$ and $|0, 2\rangle$ the Hamiltonian has the form

$$H_0 = \begin{pmatrix} U & -\sqrt{2}J & 0 \\ -\sqrt{2}J & 0 & -\sqrt{2}J \\ 0 & -\sqrt{2}J & U \end{pmatrix} = U A - \sqrt{2} J B,$$

(28)

where we define

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

(29)

When the hopping is dominant ($U \ll J$), the ground state is $\frac{1}{\sqrt{2}} |2, 0\rangle + \frac{1}{\sqrt{2}} |1, 1\rangle + \frac{1}{\sqrt{2}} |0, 2\rangle$, which corresponds to the ‘superfluid’ state with the particle number fluctuation at each site $\Delta n_1 = \Delta n_2 = 1/\sqrt{2}$. When the repulsive interaction is dominant ($U \gg J$), the ground state is $|1, 1\rangle$ corresponding to the ‘Mott insulator’ state with $\Delta n_1 = \Delta n_2 = 0$. Varying $U$ and $J$ slowly in time, the system can undergo an adiabatic transition between these two extreme cases. Similarly as in the preceding sections, we want to speed up this transition.

To diagonalize the Hamiltonian (28) and to find corresponding $H_B$, it is useful to use the parameterization

$$U = E_0 \cos \varphi,$$

(30)

$$J = \frac{E_0}{4} \sin \varphi,$$

(31)

where both $E_0$ and $\varphi$ are functions of time. The Hamiltonian can then be written as

$$H_0 = E_0 \begin{pmatrix} \cos \varphi & -\frac{1}{2\sqrt{2}} \sin \varphi & 0 \\ -\frac{1}{2\sqrt{2}} \sin \varphi & 0 & -\frac{1}{2\sqrt{2}} \sin \varphi \\ 0 & -\frac{1}{2\sqrt{2}} \sin \varphi & \cos \varphi \end{pmatrix},$$

(32)

with the eigenenergies

$$E_1 = \frac{E_0}{2} (\cos \varphi - 1),$$

(33)

$$E_2 = E_0 \cos \varphi,$$

(34)

$$E_3 = \frac{E_0}{2} (\cos \varphi + 1).$$

(35)
and the eigenvectors

\[ |\phi_1\rangle = \left( \frac{1}{2} \sqrt{1 - \cos \varphi} \right) \]

\[ |\phi_2\rangle = -\frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 0 \\ -1 \end{array} \right) \]

\[ |\phi_3\rangle = \left( \frac{1}{2} \sqrt{1 + \cos \varphi} \right) \]

Calculating the time derivatives of \(|\phi_1\rangle\) and \(|\phi_3\rangle\), one finds the Berry Hamiltonian

\[ H_B = \frac{\hbar \dot{\varphi}}{2\sqrt{2}} \left( \begin{array}{ccc} 0 & i & 0 \\ -i & 0 & -i \\ 0 & i & 0 \end{array} \right) \]

Although the Berry Hamiltonian takes a very simple form, it may be challenging to find a physical interaction that would produce it. One could attempt to take advantage of the fact that this operator is proportional to the commutator of \(A\) and \(B\),

\[ H_B = \frac{\hbar \dot{\varphi}}{2\sqrt{2}} [A, B]. \]

This suggests that a rapid modulation of the atom interaction and the hopping potential can produce an effective Hamiltonian of the form (40). If we switch on Hamiltonians \(\Delta U_A, \sqrt{2} \Delta J_B, -\Delta U A\) and \(-\sqrt{2} \Delta J B\), each for a short time interval \(\Delta t\), to second order in \(\Delta t\), the system evolves under the effective Hamiltonian \(i\sqrt{2} \Delta t/(4\hbar) \Delta U \Delta J [A, B]\) for the total time period \(4\Delta t\). The modulated operators thus implement the Berry Hamiltonian if

\[ \Delta U \Delta J = \frac{\hbar^2 \dot{\varphi}}{\Delta t}. \]

Although this result suggests that the Berry operator is realizable for this scheme, the rapid variation of the very same interaction terms that constitute our ‘slowly’ varying Hamiltonian is against the underlying idea to ensure adiabatic evolution and it rather reflects the nonholonomic controllability of the quantum system under two adjustable Hamiltonians [15]. Also, the procedure would not be practical: if the available time is short, one would need a rather strong modulation of \(\Delta U\) and \(\Delta J\). But if one can apply strong \(U\) and \(J\), then the adiabatic theorem works sufficiently well and one does not need to compensate for the diabatic transitions. One can quantify it as follows. Let us assume that \(E_0\) is constant. The adiabatic transition occurs for times \(T_{\text{tot}}\) satisfying \(E_0 T_{\text{tot}} > 2\hbar\). Let us assume that we are just near to this value, \(E_0 = 2\hbar/T_{\text{tot}}\), and the argument \(\varphi\) in (30) and (31) changes with constant rate between 0 and \(\pi/2\) such that \(\dot{\varphi} = \pi/(2T_{\text{tot}})\). Let us also assume that the ratio of the modulation amplitude to the maximum value of the corresponding operator is the same for both \(U\) and \(J\), and let us assume that the period of the cycle switching between operators \(\Delta U A, \sqrt{2} \Delta J B, -\Delta U A\) and \(-\sqrt{2} \Delta J B\) is
$T_{\text{period}} ( \equiv 4 \Delta t)$ such that the total number of cycles is $N = T_{\text{tot}} / T_{\text{period}}$. Then it follows from (41) that

$$\Delta U = \sqrt{2\pi N} E_0, \quad \Delta J = \sqrt{2\pi N} \frac{E_0}{4},$$

i.e. the modulated fields must be $\sqrt{2\pi N}$ times stronger than the fields just suitable for the adiabatic transition. Thus, even though $H_B$ can be constructed as a virtual operator resulting from the fast switching between other operators, to find a suitable realization of $H_B$ remains a challenge for this scheme.

### 6. Example: particle in an expanding box

An instructive example of the Berry Hamiltonian has been discussed by Jarzynski [7] who considered a particle in an infinitely deep potential well with one of the walls moving as described by the Hamiltonian

$$H_0 = \frac{p^2}{2m} + U(x)$$

with

$$U(x) = \begin{cases} \infty & \text{for } x < 0, \\ 0 & \text{for } 0 < x < D(t), \\ \infty & \text{for } D(t) < x. \end{cases}$$

As discussed in [7], the Berry Hamiltonian in this case takes the form

$$H_B = \frac{\dot{D}}{2D} (xp + px).$$

If such a Hamiltonian were available, one could expand or compress the box arbitrarily fast, and simply scale the quantum state wave function or density matrix by the same factor in position space and by the reciprocal factor in momentum space. Since it may be highly nontrivial to construct $H_B$, we ask whether there are operators readily available to provide a satisfactory partial compensation of the diabatic transitions.

One such operator is the momentum, $L = p$, which has a nonzero anti-commutator with $H_B$ is $p$, and for which equation (4) yields $\alpha = \dot{D}/2$, so that we have

$$H_C = \frac{\dot{D}}{2} p.$$ 

Physically, this Hamiltonian pertains if the system is transformed to a coordinate system in which the center of the potential moves with velocity $-\dot{D}/2$, i.e. where the well expands symmetrically with both the walls moving in opposite directions with the same speed $\dot{D}/2$.

The adiabatic eigenstates of the potential (45) are standing waves $\phi_n(x) = \sqrt{2/D} \sin(n\pi x / D)$. The matrix elements of the Hamiltonian $H_C$ coincide with those of $H_B$ for parity changing transitions, and they are zero otherwise:

$$\langle \phi_k | H_B | \phi_n \rangle = (-1)^{k+n} \frac{2i \hbar n \dot{D}}{k^2 - n^2 D}, \quad k \neq n,$$

$$\langle \phi_n | H_B | \phi_n \rangle = 0.$$
Figure 3. Probability of finding the system in the ground state of the instantaneous Hamiltonian of an expanding box as a function of time. During the time interval the box doubles its size from $D_0$ to $2D_0$, with $T_0 \equiv 4mD_0^2/(3\pi\hbar)$ being the round-trip time for a superposition of the two lowest eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$ of a box of length $D_0$.

$$\langle \phi_k | H_C | \phi_n \rangle = -\frac{2i \hbar k n}{k^2 - n^2} \frac{D}{D}, \quad k+n \text{ odd},$$

$$\langle \phi_k | H_C | \phi_n \rangle = 0, \quad k+n \text{ even}. \quad (49)$$

Changing to the frame where the box is centered at the origin and expands symmetrically, these eigenfunctions are $\propto \cos(n\pi x/D)$ for $n$ odd and $\propto \sin(n\pi x/D)$ for $n$ even, and one can get an intuitive picture of how the compensation works by noting that in the single-piston case the highest rate of diabatic transitions occurs between neighboring eigenstates ($k = n \pm 1$), while under the symmetric expansion, parity is conserved, and these transitions are thus completely suppressed by $H_C$.

This can be seen in figures 3 and 4. They illustrate situations when the box expanded from the initial size $D_0$ to $2D_0$ by moving the wall(s) with constant speed. The motion is rather fast, as the whole process is completed within $0.3 T_0$ where $T_0 \equiv 4mD_0^2/(3\pi\hbar)$ is the oscillation period for a superposition of the two lowest eigenstates $|\phi_1\rangle$ and $|\phi_2\rangle$ in a box of the original length $D_0$. Figure 4(a) corresponds to the case when just one of the walls is moving, whereas figure 4(b) corresponds to the symmetric motion of both walls, in both cases the system starts in the ground state. The fast motion of the walls induces diabatic transitions to excited states, however, in the symmetric case these transitions are much weaker.

7. Example: Multiparticle entanglement by Rydberg blockade

7.1. Original Hamiltonian

Preparation of a multiparticle spin entangled state by means of the Rydberg blockade was discussed in [16]: let us consider $N$ atoms whose dynamics involve two lower states $|1\rangle$ and $|2\rangle$ and a Rydberg state $|r\rangle$ (see figure 5(a)). States $|1\rangle$ and $|2\rangle$ are coupled by a laser field with the Rabi frequency $\Omega_1$, and the states $|2\rangle$ and $|r\rangle$ are coupled by a laser field with Rabi
frequency $\Omega_r$. The laser is assumed to interact with all the atoms in the same way such that the collective atomic state is symmetric with respect to all permutations. Moreover, due to a strong interaction between the Rydberg excited atoms, states with more than one Rydberg excitations would become off-resonant from the laser field. As a result, the dynamics occur in the Hilbert subspace spanned by symmetric states with 0 or 1 Rydberg excitation. The total Hamiltonian is

$$ H_0(t) = H_{Jx}(t) + H_{JC}(t), $$

where

$$ H_{Jx} = -\frac{\hbar}{2} \left( a_{1}^\dagger a_{2} + a_{2}^\dagger a_{1} \right) $$

and

$$ H_{JC} = -\frac{\hbar}{2} \left( a_{2}^\dagger \sigma^+ + a_{2} \sigma^- \right). $$

Here the operators $a_j$ remove one atom in state $j$, $a_j |n_j\rangle = \sqrt{n_j} |n_j-1\rangle$, $j = 1, 2$, and $|n_j\rangle$ represents a symmetric state with $n_j$ atoms in state $|j\rangle$. The subscript in $H_{Jx}$ refers to the operator $J_x = \frac{1}{2} (a_{1}^\dagger a_{2} + a_{2}^\dagger a_{1})$ analogous to the $x$-component of the angular momentum operator. The operator $\sigma^+$ creates a symmetric superposition with one atom in the Rydberg state. The subscript in $H_{JC}$ refers to the Jaynes–Cummings (JC) model [17], however, the role of the single two-level atom in the original JC model is now played by the (collectively shared) Rydberg excitation, and the electromagnetic-field mode of the original JC is replaced by the atoms occupying state $|2\rangle$. As shown in [16], if one starts with all atoms in state $|1\rangle$ and adiabatically switches the Hamiltonian from $H_{JC}$ to $H_{Jx}$ (following, e.g. the Rabi frequencies as in figure 5(b)), the system ends up in an eigenstate of $J_x$ with $J_x = 0$. Note that in contrast to the examples discussed in the preceding sections, here the target eigenstate of the Hamiltonian is not the ground state but the central eigenstate with eigenenergy in the middle of the energy ladder.

**Figure 4.** Probability density $\rho(x)$ (green line) of finding a particle in a box whose size expanded from $D_0$ to $2D_0$ by moving a single piston (a) and expanding the box symmetrically (b), compared with the probability density $\rho_1(x)$ (blue) of the lowest eigenstate of the final box. The speed of expansion corresponds to that in figure 3. Inset: probability $P_n$ of finding the particle in the $n$th eigenstate of the Hamiltonian.
7.2. Compensating operators

It turns out that the Berry Hamiltonian contains couplings between states differing by even numbers of atoms in states $|1\rangle$ and $|2\rangle$ with the same number of Rydberg excitations, and also couplings between states with different Rydberg excitations that are not coupled by $H_{JC}$. This leads us to the choice of operators suitable for a possible compensation of diabatic transitions. To produce terms coupling states with different numbers of Rydberg excitations, one could use an additional laser field tuned to resonance with the $|1\rangle \leftrightarrow |\bar{r}\rangle$ transition. It turns out that the proper phases are given by the operator

$$L_1 = \frac{i}{2} \left( a_1 \sigma^+ - a_1^\dagger \sigma^- \right) .$$

Generating an interaction that changes the atomic numbers in individual states by more than one is more challenging. One possibility is the ‘two-axis countertwisting’ proposed in [18] for the generation of spin squeezing, which may be accomplished by off-resonant multiphoton processes via the Rydberg state [19] that yields

$$L_2 = \frac{i}{2} \left( a_1^{12} a_2^2 - a_1^{a2} a_1^{1+} \right) .$$

The results of the compensation procedure can be seen in figures 5 and 6. For illustration, we have used the same situation as in [16]: $N = 6$ atoms are treated with $\sin^2$ pulses of the duration 3 $\mu$s each. The strength of the pulses does not allow a full adiabatic following of the states, and if no compensation of the diabatic transitions is applied, the final probability of staying in the zero eigenstate is close to 50% (blue line in figure 6(a)). The fidelity is improved to $\sim 80\%$ if compensation by $L_1$ (red line) or $L_2$ (magenta) or both (green line) is applied. As can be seen, either $L_1$ or $L_2$ help to a comparable amount, and their combination improves the final result only very slightly in comparison to the case when only one is used. Figure 6(b) shows the values of the coefficients $\alpha_{1,2}$ multiplying the operators $L_{1,2}$, both in the case when a single operator is used and in the case of their combined action.

The main reason why $L_{1,2}$ do not provide full compensation is that they do not couple all pairs of states that are coupled by $H_B$. In particular, $L_1$ couple states that differ by 1 in $n_1$ and
Figure 6. (a) Time evolution of the probability of staying in the zero eigenstate of the instantaneous Hamiltonian for multiparticle entanglement by Rydberg blockade with \( N = 6 \) atoms (same as in [16]). The different curves correspond to no compensation of the diabatic transitions, and to compensation by means of operators \( L_1, L_2 \) and their combination. (b) Corresponding time evolution of the parameters \( \alpha_{1,2} \).

in the Rydberg population, and \( L_2 \) couple states that differ by 2 in \( n_1 \) and \( n_2 \) while keeping the Rydberg population unchanged. On the other hand, \( H_B \) can change \( n_1 \) and \( n_2 \) by any even number while keeping the Rydberg population, or change \( n_1 \) by any odd number while changing the Rydberg population (and changing \( n_2 \) correspondingly). These more general coupling terms could be very hard to realize experimentally, nevertheless even the partial compensation can improve the results of the process significantly.

8. Discussion and conclusion

The proposed method of counterbalancing nonadiabatic transition is very simple and straightforward. In some cases it allows for the analytic expression of the compensating functions (e.g. STIRAP, two spin \( \frac{1}{2} \) systems, particle in an expanding box), while for more complicated systems a numerical evaluation of operator mean values and solution of a matrix inversion problem may be necessary. The method allows for further generalizations, and we are currently investigating the prospects for putting additional constraints on the amplitudes of the compensating operators or to adjust their values to push the states toward \( |0\rangle \) rather than merely trying to keep the overlap unchanged, when it has already been reduced. As a result, the method combines the advantages of the adiabatic procedures (especially robustness) with the requirements of speed. It is also not confined to a few relatively simple systems, but allows for a straightforward generalization to more complicated ones. The only essential requirement is a physical realization of operators having a reasonable overlap with the Berry Hamiltonian, i.e. having nonzero \( \langle H_B L + L H_B \rangle \) in the target eigenstate of \( H_0 \). The challenge is to find the suitable operators in more complicated systems, e.g. to generalize the few-particle examples to multiparticle systems and to identify the physical procedures enabling us the shortcuts to adiabaticity.
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