Adiabatic approximation, Gell-Mann and Low theorem, and degeneracies: A pedagogical example

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We study a simple system described by a 2×2 Hamiltonian and the evolution of its quantum states under the influence of a perturbation. More precisely, when the initial Hamiltonian is not degenerate, we check analytically the validity of the adiabatic approximation and verify that, even if the evolution operator has no limit for adiabatic switchings, the Gell-Mann and Low formula allows the evolution of eigenstates to be followed. In the degenerate case, for generic initial eigenstates, the adiabatic approximation (obtained by two different limiting procedures) is either useless or wrong, and the Gell-Mann and Low formula does not hold. We show how to select initial states in order to avoid such failures.

I. INTRODUCTION

Adiabatic switching is a crucial ingredient of many-body theory. It provides a way to express the eigenstates of a Hamiltonian $H = H_0 + H_1$ in terms of the eigenstates of H_0. Its basic idea is to switch the interaction H_1 very slowly, i.e., to transform H into a time-dependent Hamiltonian $H(t) = H_0 + e^{-\varepsilon|t|}H_1$ where the small parameter $\varepsilon > 0$ eventually vanishes. Under the influence of $H(t)$, an eigenstate $|Y_0\rangle$ of H_0 becomes a time-dependent wave function $|\Psi_\varepsilon(t)\rangle$, and it might be expected that an eigenstate of $H = H(0)$ is obtained by taking the limit of $|\Psi_\varepsilon(0)\rangle$ when ε tends to zero. It turns out that this naive expectation is not justified because $|\Psi_\varepsilon(0)\rangle$ has no limit when $\varepsilon \to 0$. When the initial state $|Y_0\rangle$ belongs to a nondegenerate eigenspace (isolated from the other eigensubspaces), Gell-Mann and Low [1] solved the problem by dividing out the divergence by a suitable factor. The ratio is called the Gell-Mann and Low wave function and its convergence can be proved by using the adiabatic theorem [2].

In the first part of this work, we present an exactly solvable 2×2 model that illustrates the fact that the limit $\varepsilon \to 0$ of $|\Psi_\varepsilon(0)\rangle$ does not exist. The validity of the Gell-Mann and Low wave function is shown by analytically calculating the corresponding adiabatic approximation.

It was realized 50 years ago [3] that the Gell-Mann and Low formula must sometimes be extended to the case of a degenerate initial state of H_0. This happens in many practical situations, for instance when the system contains unfilled shells. This problem has been discussed in several fields, including nuclear physics [4], solid state physics [5], quantum chemistry [6], and atomic physics [7]. In most cases, it is assumed that there is *some* eigenstate $|Y_0\rangle$ for which the Gell-Mann and Low formula holds. More precisely, if $\mathcal{V}_0$ is

the vector space generated by the eigenstates of H_0 associated with the degenerate ground state energy E_0, then the claim is that there exists some initial state $|Y\rangle$ in $\mathcal{V}_0$ whose time-evolved state $|\Psi_\varepsilon(0)\rangle$ is (up to a divergent phase) an eigenstate of H. To see that it is not possible to choose any element of $\mathcal{V}_0$ as initial state, let us forget for a moment the divergent phase and consider a perturbation H_1 that splits the degeneracy and two initial states $|Y^1\rangle$ and $|Y^2\rangle$ whose time evolutions give rise to two eigenstates of H, denoted by $|\Psi_\varepsilon^1(0)\rangle$ and $|\Psi_\varepsilon^2(0)\rangle$, with different energies E_1 and E_2. By linearity, the initial state $|Y^1\rangle + |Y^2\rangle$ evolves into $|\Psi_\varepsilon^1(0)\rangle + |\Psi_\varepsilon^2(0)\rangle$, which is not an eigenstate of H because $E_1 \neq E_2$. Therefore, $|Y^1\rangle + |Y^2\rangle$ is not a proper initial state.

When the initial state of H_0 is degenerate, we show that, even for the very simple 2×2 model considered here, the Gell-Mann and Low wave function does not have a limit for almost all initial conditions. We find, however, the specific initial states that lead to convergent wave functions. For the application of many-body methods to degenerate systems, it is crucial to find a way to select the proper initial states.

II. NONDEGENERATE INITIAL STATES

Two-dimensional matrices are the simplest nontrivial models that can be considered in quantum physics, and were indeed already used as toy models for many-body theory studies (see Ref. [8] and references therein). However, this is the first time to our knowledge that the evolution operator and its adiabatic approximation have been calculated explicitly for such a model.

We consider the two-dimensional system described by the Hamiltonian $H = H_0 + H_1$ with

$$H_0 = \begin{pmatrix} \mu - \delta & 0 \\ 0 & \mu + \delta \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & x \\ x & 0 \end{pmatrix}. \tag{1}$$

We assume that $\delta \neq 0$, so that the initial state is nondegenerate. Without restriction, it can further be assumed that $\delta > 0$. Moreover, by properly choosing the energy origin, it can also be assumed that $\mu = 0$.

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According to the usual treatment of adiabatic switching [9,10], it is convenient to transform the Schrödinger equation for the time-dependent Hamiltonian $H(t) = H_0 + e^{-\varepsilon|t|} H_1$ to the interaction picture. The dependence of the operators and wave functions on the parameter $\varepsilon > 0$ will be implicit in the following. If we denote by $\Psi_S(t)$ a solution of the Schrödinger equation

$$i \frac{\partial \Psi_S(t)}{\partial t} = H(t) \Psi_S(t),$$

the wave function in the interaction picture is defined as

$$\Psi(t) = e^{iH_0 t} \Psi_S(t).$$

It satisfies

$$i \frac{\partial \Psi(t)}{\partial t} = H_{\text{int}}(t) \Psi(t),$$

subject to the boundary condition $\Psi(-\infty) = \Upsilon$, where Υ may be an eigenstate of H_0. The Hamiltonian $H_{\text{int}}(t)$ is the Hamiltonian $H(t)$ in the interaction picture,

$$H_{\text{int}}(t) = e^{-\varepsilon|t|} e^{iH_0 t} H_1 e^{-iH_0 t}.$$

In the simple case (1) considered here, this operator reads

$$H_{\text{int}}(t) = x e^{-\varepsilon|t|} \begin{pmatrix} 0 & e^{-2i\delta t} \\ e^{2i\delta t} & 0 \end{pmatrix}. \tag{2}$$

Instead of using wave functions, it is customary to work with the evolution matrix $U(t)$ such that $\Psi(t) = U(t)\Upsilon$. We refer to [11] for sufficient conditions on the time-dependent Hamiltonian $H_{\text{int}}(t)$ in order to ensure the existence of the unitary propagator $U(t)$.

A. The evolution operator: Analytic solution and limiting behavior

We give in this section the analytic expression of the evolution matrix. This operator is the solution of the Schrödinger equation in the interaction picture,

$$i \frac{dU(t)}{dt} = H_{\text{int}}(t) U(t), \tag{3}$$

with the boundary condition $U(-\infty) = \text{Id}$. In the following, we consider $t \leq 0$, so that the switching function is $e^{\varepsilon t}$. We also assume that $x > 0$. With the matrix elements of $U(t)$ denoted by

$$U(t) = \begin{pmatrix} a(t) & b(t) \\ c(t) & d(t) \end{pmatrix},$$

Eq. (3) is equivalent to the system of equations

$$ia' = x e^{-i(2\delta + i\varepsilon)t} c,$$

$$ic' = x e^{i(2\delta - i\varepsilon)t} a,$$

$$ib' = x e^{-i(2\delta + i\varepsilon)t} d,$$

$$id' = x e^{i(2\delta - i\varepsilon)t} b, \tag{4}$$

with the boundary conditions

$$a(-\infty) = d(-\infty) = 1, \quad b(-\infty) = c(-\infty) = 0.$$

Since the functions c, d are independent of the functions a, b, and satisfy equations of the same form as for a, b, it is enough to solve the first two equations of the above system.

1. Solution of the equation for the unknown function a

By elimination of the function c in Eq. (4), the second-order evolution equation

$$a'' + (2i\delta - \varepsilon)a' + x^2 e^{2\varepsilon t} a = 0 \tag{5}$$

is obtained. This equation can be solved by using standard techniques [[12], p. 442, Eq. (23)]. If we rewrite the unknown function a as $a(t) = e^{-i(\delta + i\varepsilon/2)t} Z_\nu(x e^{\varepsilon t}/\varepsilon)$ and introduce the variable $s = x e^{\varepsilon t}/\varepsilon$, Eq. (5) becomes the Bessel equation for $Z_\nu(s)$, with

$$\nu = 1/2 - i\delta/\varepsilon. \tag{6}$$

Since J_ν and $J_{-\nu}$ are two independent solutions of the Bessel equation when ν is not an integer [13], the function $a(t) = \bar{a}(s)$ has the general form

$$\bar{a}(s) = \left(\frac{\varepsilon s}{x}\right)^\nu [C_1 J_\nu(s) + C_2 J_{-\nu}(s)], \tag{7}$$

where the constants C_1 and C_2 are determined by the boundary conditions at $s = 0$ (i.e., in the limit $t \to -\infty$). Since $a(-\infty) = \bar{a}(0) = 1$, and by the series expansion [[13], Eq. (9.1.10)]

$$J_\nu(s) = \left(\frac{s}{2}\right)^\nu \sum_{k=0}^\infty \frac{(-s^2/4)^k}{k! \Gamma(\nu + k + 1)},$$

it follows that $C_1 = 0$ and $C_2 = 2^{-\nu} \Gamma(1 - \nu)$.

2. Solution of the equation for the other unknown functions

The function $c(t) = \bar{c}(s)$ can be obtained from the expression of $a(t) = \bar{a}(s)$, relying on the first equation in the system (4), rewritten in the s variable as $\bar{c}(s) = i(\varepsilon s/x)^{1-2\nu} \bar{a}(s)$. Since $[s^\nu J_{-\nu}(s)]' = -s^\nu J_{1-\nu}(s)$ [[13], Eq. (9.1.30)], it holds that

$$\bar{c}(s) = -iC_2 \left(\frac{\varepsilon}{x}\right)^{1-2\nu} s^{1-\nu} J_{1-\nu}(s).$$

The functions b and d satisfy the same equations as a and c, respectively, but with different boundary conditions. With the above notation, it can easily be checked that b is also a combination of Bessel functions as given by (7), but with $C_1 = -i(\varepsilon/x)^{2\nu-1} 2^{\nu-1} \Gamma(\nu)$ and $C_2 = 0$.

3. Properties of the solution

In view of the above results, the problem (4) has the analytic solution

$$a(t) = C_2 \left(\frac{x}{\varepsilon}\right)^\nu e^{\varepsilon \nu t} J_{-\nu}\left(\frac{x e^{\varepsilon t}}{\varepsilon}\right),$$

$$b(t) = C_1 \left(\frac{x}{\varepsilon}\right)^\nu e^{\varepsilon \nu t} J_\nu\left(\frac{x e^{\varepsilon t}}{\varepsilon}\right),$$
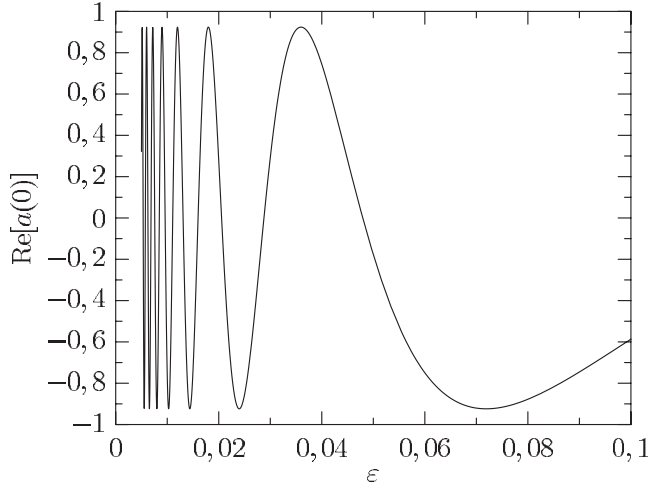
FIG. 1. Real part of $a(0)$ as a function of ε for $x=\delta=1$. For clarity, the region $x<0.005$ is not plotted.

$$c(t) = -iC_2\left(\frac{x}{\varepsilon}\right)^{\nu} e^{\varepsilon(1-\nu)t} J_{1-\nu}\left(\frac{xe^{\varepsilon t}}{\varepsilon}\right),$$

$$d(t) = iC_1\left(\frac{x}{\varepsilon}\right)^{\nu} e^{\varepsilon(1-\nu)t} J_{\nu-1}\left(\frac{xe^{\varepsilon t}}{\varepsilon}\right),$$

with

$$C_1 = -i(\varepsilon/x)^{2\nu-1} 2^{\nu-1}\Gamma(\nu), \quad C_2 = 2^{-\nu}\Gamma(1-\nu),$$

and where ν is defined in (6). As a consistency check, it is possible to verify that the matrix U is unitary. This follows from $|C_1|^2=|C_2|^2=\Gamma(\nu)\Gamma(1-\nu)/2=\pi/(2\sin\nu\pi)$ and $J_\nu(s)J_{1-\nu}(s)+J_{-\nu}(s)J_{\nu-1}(s)=2\sin(\nu\pi)/(\pi s)$ [see [13], Eq. (9.1.15)].

The series expansion of the Bessel functions gives

$$\bar{a}(s) = 1 + \sum_{k=1}^{\infty} \frac{(-s^2/4)^k}{k!\Pi_{j=1}^{k}(j-\nu)},$$

$$\bar{b}(s) = ie^{-2i\delta t}\frac{s}{2}\sum_{k=0}^{\infty} \frac{(-s^2/4)^k}{k!\Pi_{j=1}^{k+1}(j+\nu-1)},$$

$$\bar{c}(s) = -ie^{2i\delta t}\frac{s}{2}\sum_{k=0}^{\infty} \frac{(-s^2/4)^k}{k!\Pi_{j=1}^{k+1}(j-\nu)},$$

$$\bar{d}(s) = 1 + \sum_{k=1}^{\infty} \frac{(-s^2/4)^k}{k!\Pi_{j=1}^{k}(j+\nu-1)}.$$

Note that these solutions are valid for all values of x, $\delta\neq 0$, and $\varepsilon>0$. We have the symmetries $a(t,-\delta)=d(t,\delta)$ and $c(t,-\delta)=-b(t,\delta)$, $a(t)^*=d(t)$ and $b(t)^*=c(t)$. Moreover, $a(t)$ and $d(t)$ are even in x, while $b(t)$ and $c(t)$ are odd in x.

4. Limiting behavior of the evolution operator

Figure 1 illustrates the divergence of $a(0)$ as a function of ε. The above analytic expressions therefore show that the

evolution operator does not have a limit when $\varepsilon\rightarrow 0$. Rather, as illustrated by Fig. 1, a strongly oscillatory behavior is observed. This is the reason that the phase factor has to be canceled out by considering a renormalized wave function in the Gell-Mann and Low fashion, as explained in the next section.

B. The Gell-Mann and Low wave function

Rigorous proofs of the Gell-Mann and Low formula rely on the adiabatic approximation. Therefore, we first compute the adiatic approximation for the problem (1), and then the Gell-Mann and Low wave functions.

1. The adiabatic approximation

The adiabatic approximation consists in approximating the evolution operator in the interaction picture $U(t)$ by the adiabatic operator in the interaction picture:

$$U_a(t) = e^{itH_0}A(\tau)\bar{\Phi}_\varepsilon(\tau), \tag{8}$$

with

$$\bar{\Phi}_\varepsilon(\tau) = \lim_{\tau_0\rightarrow-\infty} \Phi_\varepsilon(\tau,\tau_0)e^{-it_0 H_0},$$

where $\tau=\varepsilon t<0$ and $\tau_0=\varepsilon t_0$ [14,15]. The unitary matrices A and Φ_ε are calculated from the eigenprojectors of $H(\tau)=H_0+e^\tau H_1$, as explained below [see formulas (10) and (11)].

The eigenvalues of $H(\tau)$ are

$$e_\pm(\tau) = \pm\lambda, \quad \lambda = \sqrt{\delta^2 + x^2 e^{2\tau}}.$$

With the notation $y=xe^\tau/\delta$ the corresponding eigenprojectors read

$$P_\pm(\tau) = \frac{1}{2\sqrt{1+y^2}}\begin{pmatrix} \sqrt{1+y^2}\mp 1 & \pm y \\ \pm y & \sqrt{1+y^2}\pm 1 \end{pmatrix}.$$

Defining the Hermitian matrix [15]

$$K(\tau) = i\sum_{\sigma=\pm} \frac{dP_\sigma(\tau)}{d\tau}P_\sigma(\tau) = \frac{iy}{2(1+y^2)}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},$$

the matrix A appearing in (8) satisfies the equation

$$A'(\tau) = -iK(\tau)A(\tau), \tag{9}$$

with the boundary condition $A(-\infty)=\text{Id}$. The unique solution is

$$A(\tau) = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{1+\alpha} & \sqrt{1-\alpha} \\ -\sqrt{1-\alpha} & \sqrt{1+\alpha} \end{pmatrix} \tag{10}$$

with $\alpha=(1+y^2)^{-1/2}\in[0,1]$.

The phase matrix $\Phi_\varepsilon(\tau,\tau_0)$ is obtained from the integral of the eigenvalues

$$\Phi_\varepsilon(\tau,\tau_0) = \sum_{\sigma=\pm} \exp\left(-\frac{i}{\varepsilon}\int_{\tau_0}^{\tau} e_\sigma(\tau')d\tau'\right)P_\sigma(\tau_0).$$

For large negative τ_0, up to $O(e^{\tau_0})$ terms coming from the approximation $P_\sigma(\tau_0)\simeq P_\sigma(-\infty)$,

$$\Phi_\varepsilon(\tau, \tau_0) = \begin{pmatrix} e^{i\phi(\tau,\tau_0)/\varepsilon} & 0 \\ 0 & e^{-i\phi(\tau,\tau_0)/\varepsilon} \end{pmatrix}, \quad (11)$$

where

$$\phi(\tau, \tau_0) = \int_{\tau_0}^{\tau} \sqrt{\delta^2 + x^2 e^{2\sigma}} d\sigma = F(\tau) - F(\tau_0),$$

with

$$F(\tau) = \sqrt{\delta^2 + x^2 e^{2\tau}} - \frac{\delta}{2} \ln\left(\frac{\sqrt{\delta^2 + x^2 e^{2\tau}} + \delta}{\sqrt{\delta^2 + x^2 e^{2\tau}} - \delta} \right).$$

Note that $F(\tau_0)$ has no finite limit for $\tau_0 \to -\infty$. However, because the computations are done in the interaction picture, the phase matrix $\Phi_\varepsilon(\tau, \tau_0)$ is multiplied by the unitary operator $e^{-it_0 H_0}$, and the operator so obtained has a limit when $\tau_0 \to -\infty$. Indeed,

$$\begin{aligned} \bar{\Phi}_\varepsilon(\tau) &= \lim_{t_0 \to -\infty} \Phi_\varepsilon(\tau, \tau_0) e^{-iH_0 t_0} \\ &= \begin{pmatrix} \exp[i\phi(\tau)/\varepsilon] & 0 \\ 0 & \exp[-i\phi(\tau)/\varepsilon] \end{pmatrix}, \end{aligned}$$

where

$$\phi(\tau) = \lim_{t_0 \to -\infty} \phi(\tau, \tau_0) + \delta\tau_0 = F(\tau) - \delta\left(1 - \ln\frac{2\delta}{x}\right).$$

At $t=0$, we obtain the adiabatic approximation

$$U_a(0) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi(0)/\varepsilon}\sqrt{1+\alpha} & e^{-i\phi(0)/\varepsilon}\sqrt{1-\alpha} \\ -e^{i\phi(0)/\varepsilon}\sqrt{1-\alpha} & e^{-i\phi(0)/\varepsilon}\sqrt{1+\alpha} \end{pmatrix},$$

where α is now $(1 + x^2/\delta^2)^{-1/2}$.

2. Quality of the adiabatic approximation

The rigorous adiabatic theorem (see Ref. [16] for a recent account) states that the adiabatic evolution operator U_a defined by Eq. (8) is such that

$$\sup_{t \leq 0} \|U(t) - U_a(t)\| \leq C\varepsilon,$$

for some constant C. In particular, for $t=0$, $\|U(0) - U_a(0)\| \leq C\varepsilon$. Figure 2 shows that this result is indeed verified in the case considered here, and allows a numerical estimate to be given for the constant C.

3. The Gell-Mann and Low limit

The Gell-Mann and Low formula describes how an eigenvector of the reference (unperturbed) Hamiltonian H_0 evolves under an added perturbation H_1. Starting from one of the initial eigenstates of H_0, namely,

$$|\Upsilon^1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\Upsilon^2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad (12)$$

the associated Gell-Mann and Low wave functions

$$|\Psi^i(0)\rangle = \lim_{\varepsilon \to 0} \frac{U(0)|\Upsilon^i\rangle}{\langle \Upsilon^i | U(0) | \Upsilon^i \rangle} = \lim_{\varepsilon \to 0} \frac{U_a(0)|\Upsilon^i\rangle}{\langle \Upsilon^i | U_a(0) | \Upsilon^i \rangle}$$

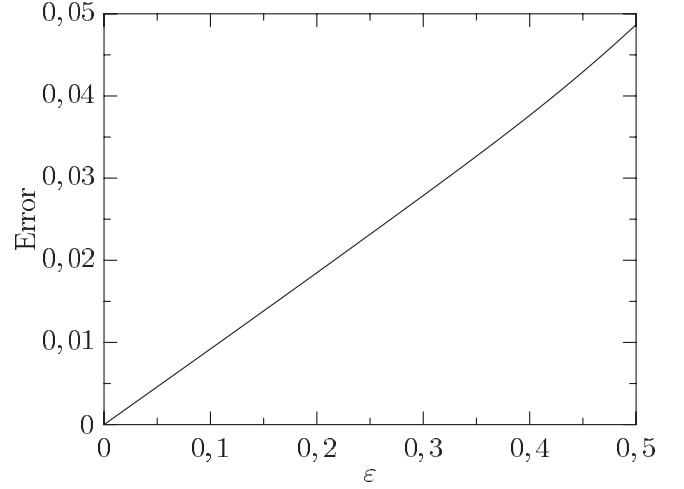can be computed using (8). They read, respectively,

FIG. 2. Modulus of the difference between $a(0)$ and its adiabatic approximation as a function of ε for $x = \delta = 1$.

$$\begin{pmatrix} 1 \\ a_{21}(0) \\ a_{11}(0) \end{pmatrix} = \begin{pmatrix} 1 \\ -\frac{x}{\sqrt{x^2 + \delta^2} + \delta} \end{pmatrix}$$

and

$$\begin{pmatrix} a_{12}(0) \\ a_{22}(0) \\ 1 \end{pmatrix} = \begin{pmatrix} \frac{\sqrt{x^2 + \delta^2} + \delta}{x} \\ 1 \end{pmatrix},$$

where $a_{ij}(\tau)$ are the matrix elements of $A(\tau)$ given by (10). It is easy to check that these vectors are indeed eigenstates of H for the eigenvalues $-\sqrt{x^2 + \delta^2}$ and $\sqrt{x^2 + \delta^2}$, respectively. These eigenvalues can be obtained by the energy-shift formula ([10], p. 200). The difference ΔE between the energy of an eigenstate of $H_0 + H_1$ and that of the corresponding eigenstate $|\Upsilon_0\rangle$ of H_0 is

$$\Delta E = \lim_{\varepsilon \to 0} i\varepsilon x \frac{d}{dx} \ln\langle \Upsilon_0 | U(0) | \Upsilon_0 \rangle$$

$$= \lim_{\varepsilon \to 0} i\varepsilon x \frac{d}{dx} \ln\langle \Upsilon_0 | U_a(0) | \Upsilon_0 \rangle.$$

We find indeed that $\Delta E = \delta - \sqrt{x^2 + \delta^2}$ for $|\Upsilon^1\rangle$ and $\Delta E = -\delta + \sqrt{x^2 + \delta^2}$ for $|\Upsilon^2\rangle$.

III. DEGENERATE CASE

Initial degenerate states for the model (1) are obtained when $\delta = 0$. In this case, the evolution operator can still be computed analytically, and actually has a simpler expression than the one obtained in Sec. II A in the nondegenerate case:

$$U(t) = \begin{pmatrix} \cos(xe^{\varepsilon t}/\varepsilon) & -i\sin(xe^{\varepsilon t}/\varepsilon) \\ -i\sin(xe^{\varepsilon t}/\varepsilon) & \cos(xe^{\varepsilon t}/\varepsilon) \end{pmatrix}. \quad (13)$$

In particular,

$$U(0) = \begin{pmatrix} \cos(x/\varepsilon) & -i\sin(x/\varepsilon) \\ -i\sin(x/\varepsilon) & \cos(x/\varepsilon) \end{pmatrix}.$$

A. Failure of the adiabatic approximation and the Gell-Mann and Low formula

1. Adiabatic approximation

There are two ways to calculate the adiabatic approximation, depending on the order of the limits $\delta \to 0$ and $\tau_0 \to -\infty$. If we first carry out the limit $\delta \to 0$, the computation of Sec. II B 1 can be repeated by starting from the Hamiltonian H_0 with $\delta = 0$. The eigenvalues corresponding to $H(\tau)$ are $\pm x e^\tau$, and the eigenprojectors are constant:

$$P_\pm(\tau) = \frac{1}{2}\begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix}.$$

Thus, $K(\tau) = 0$, so that $A(\tau)$ is constant and equal to its boundary value $A(\tau) = \mathrm{Id}$. The computation of $\bar{\Phi}_\varepsilon(\tau)$ is therefore straighforward and leads to the adiabatic approximation

$$U_a(t) = U(t),$$

where $U(t)$ is given by Eq. (13). The adiabatic approximation is therefore exact but, as we shall see, the Gell-Mann and Low wave function has no limit for the initial states Υ^1 and Υ^2 when $\varepsilon \to 0$.

Taking first the limit $\tau_0 \to -\infty$ amounts to taking the limit $\delta \to 0$ in the adiabatic evolution operator (8). For the operator A, the limit is

$$A(\tau) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \tag{14}$$

for any $\tau \leq 0$. Notice that the boundary condition at $\tau = -\infty$ for Eq. (9) on A is therefore not satisfied. For the matrix $\Phi_\varepsilon(\tau)$, the limit is

$$\Phi_\varepsilon(\tau) = \begin{pmatrix} \exp(ixe^\tau/\varepsilon) & 0 \\ 0 & \exp(-ixe^\tau/\varepsilon) \end{pmatrix}.$$

The limit of the adiabatic evolution operator reads now

$$U_a(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} \exp(ixe^{\varepsilon t}/\varepsilon) & \exp(-ixe^{\varepsilon t}/\varepsilon) \\ -\exp(ixe^{\varepsilon t}/\varepsilon) & \exp(-ixe^{\varepsilon t}/\varepsilon) \end{pmatrix}. \tag{15}$$

It is, however, not an approximation of $U(t)$.

The discrepancy between the two approaches clearly shows that the two limits $\delta \to 0$ and $\tau_0 \to -\infty$ do not commute for degenerate systems.

2. Nonvalidity of the general Gell-Mann and Low formula

When $\delta = 0$, the unperturbed Hamiltonian is $H_0 = 0$ and any initial state $|\Upsilon_0\rangle$ is an eigenstate of H_0 (with eigenvalue 0). Thus, there seems to be some arbitrariness in the choice of the initial state. However, we shall see that most initial states lead to divergent Gell-Mann and Low wave functions. If for instance $|\Upsilon_0\rangle = |\Upsilon^1\rangle = \binom{1}{0}$ as in Sec. II B 3, the Gell-Mann and Low wave function

$$\frac{U(0)|\Upsilon_0\rangle}{\langle \Upsilon_0|U(0)|\Upsilon_0\rangle} = \begin{pmatrix} 1 \\ -i\tan(x/\varepsilon) \end{pmatrix}$$

has no limit when $\varepsilon \to 0$. This shows that the Gell-Mann and Low formula fails for the initial state $|\Upsilon^1\rangle$. It fails also for $|\Upsilon^2\rangle$.

Similarly, the energy shift would be given by the limit for $\varepsilon \to 0$ of

$$\Delta E = i\varepsilon x \frac{d}{dx}\ln\langle \Upsilon^1|U(0)|\Upsilon^1\rangle = -ix\tan(x/\varepsilon).$$

But this has no limit when $x \neq 0$. The question is then whether there are some initial states for which the Gell-Mann and Low wave function has a limit, and how those states can be characterized.

B. Selection of the proper initial states

In this section, we try to find initial states that are eigenstates of H_0 and that lead to convergent Gell-Mann and Low wave functions. Any initial state $|\Upsilon_0\rangle$ for the model (1) in the degenerate case is of the general form (up to a trivial scaling changing this state into $-|\Upsilon_0\rangle$)

$$|\Upsilon_0\rangle = \cos\theta|\Upsilon^1\rangle + \sin\theta|\Upsilon^2\rangle,$$

where $0 \leq \theta < \pi$ and $|\Upsilon^1\rangle$ and $|\Upsilon^2\rangle$ are defined in (12). Straightforward computations show that

$$\frac{U(0)|\Upsilon_0\rangle}{\langle \Upsilon_0|U(0)|\Upsilon_0\rangle}$$

has a limit if and only if $\theta = \pi/4$ or $3\pi/4$. This defines two proper initial states

$$|\Upsilon_\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix},$$

with associated Gell-Mann and Low wave functions

$$\frac{U(0)|\Upsilon_\pm\rangle}{\langle \Upsilon_\pm|U(0)|\Upsilon_\pm\rangle} = \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix},$$

which obviously have limits in the regime $\varepsilon = 0$. Since $H_0 = 0$ in this very simple setting, the proper initial states form a basis diagonalizing H_1, as expected.

Moreover, in the basis $(|\Upsilon_-\rangle, |\Upsilon_+\rangle)$, the evolution operator becomes

$$U(t) = \frac{1}{\sqrt{2}}\begin{pmatrix} \exp(ixe^{\varepsilon t}/\varepsilon) & \exp(-ixe^{\varepsilon t}/\varepsilon) \\ -\exp(ixe^{\varepsilon t}/\varepsilon) & \exp(-ixe^{\varepsilon t}/\varepsilon) \end{pmatrix}. \tag{16}$$

Similarly, the energy-shift formula gives now the correct result $\Delta E_\pm = \pm x$.

Interestingly, the adiabatic operator given in Eq. (15) is equal to the evolution operator in the basis $(|\Upsilon_-\rangle, |\Upsilon_+\rangle)$.

IV. CONCLUSION

The adiabatic theorem was investigated here by using an exactly solvable model. Within this model, the adiabatic theorem is valid when the initial state of the system is nondegenerate. When it is degenerate, our simple model exhibits several problems that are generally present for an arbitrary initial state: the Gell-Mann and Low wave function does not converge, the energy-shift formula is not valid, and the adiabatic approximation becomes ambiguous. Moreover, our toy model shows that these problems cannot be solved by arbi-

trarily lifting the degeneracy (resorting to $\delta \neq 0$) and then taking $\delta \rightarrow 0$, because in that case the adiabatic approximation is generally not valid.

However, we show that the degeneracy problems are solved by properly choosing the initial state. At least since the work of Tolmachev [17], it has been conjectured that the Gell-Mann and Low formula is valid for properly chosen initial states when the system is degenerate. Until now, this conjecture has not been rigorously proved and no practical method has been given to select the proper initial states. We intend to come back to this question in a forthcoming presentation.

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