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2001 J. Phys. A: Math. Gen. 34 1741

(http://iopscience.iop.org/0305-4470/34/8/317)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **34** (2001) 1741–1752 www.iop.org/Journals/ja PII: S0305-4470(01)13332-9

A geometrical approach to non-adiabatic transitions in quantum theory: applications to NMR, over-barrier reflection and parametric excitation of quantum oscillator

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Received 18 April 2000, in final form 1 November 2000

Abstract

This paper deals with non-adiabatic processes (i.e. processes excluded by the adiabatic theorem) from the geometrical (group-theoretical) point of view. An approximate formula for the probabilities of the non-adiabatic transitions is derived in the adiabatic regime for the case when the parameter-dependent Hamiltonian represents a smooth curve in the Lie algebra and the quantal dynamics is determined by the corresponding Lie group evolution operator. We treat the spin precession in a time-dependent magnetic field and the over-barrier reflection problem in a uniform way using the first-order dynamical equations on $SU(2)$ and $SU(1.1)$ group manifolds, respectively. A comparison with analytic solutions for simple solvable models is provided.

PACS numbers: 0365, 0220, 0240

1. Introduction

It is well known that probabilities of transitions induced by a time dependence of the Hamiltonian are suppressed if the dependence is slow. This statement formulated and proved by Born and Fock [3] is presented in standard textbooks (e.g. by Messiah [7]) and is known as the *adiabatic theorem*. The adiabatic theorem does not prove that the transitions are forbidden, it means just that the probabilities are suppressed exponentially and vanish to any finite order of the standard perturbation theory. Transitions of this type should not be discarded, however, if they result in special phenomena, even though relatively rare ones. The over-barrier reflection and the spin-flip in a time-dependent magnetic field slowly deviating from the original direction may serve as simple examples of such phenomena. Usually, the adiabatic character of the process suggests a way to evaluate its probability, as in the quasi-classical approximation.

[1] Professor M S Marinov passed away on 17 January 2000.

Corrections to the adiabatic theorem were considered in a number of works, especially with application to physical systems with two non-degenerate energy levels. Dykhne [8] considered a Hamiltonian $\hat{H}(t)$ with two eigenstates $\Psi_1(t)$, $\Psi_2(t)$ which is analytic in time. He found the transition probability p_{12} for a system, prepared at time $-\infty$ in the eigenstate $\Psi_1(-\infty)$ to pass to the eigenstate Ψ_2 as t runs from $-\infty$ to $+\infty$. This probability is expressed by the formula

$$p_{12} \sim \exp\left(-2T\left|\operatorname{Im}\int_0^{t_c}(E_2(t) - E_1(t))\,\mathrm{d}t\right|\right). \tag{1}$$

Here t_c is a point in the complex time plane in which $E_2(t)$ and $E_1(t)$ cross, and T is a time-scale parameter (large in the adiabatic limit) over which $\hat{H}(t)$ changes essentially. A rigorous derivation of Dykhne's result was given by Davis and Pechukas [9]. Suominen and co-workers [12, 13] have applied the Dykhne, Davis and Pechukas approach to two-level solvable models. In particular, an adiabatic behaviour of the Landau and Zener [14, 15] model was considered. It appears that for this model the Dykhne, Davis and Pechukas method gives the exact answer.

From the works of Berry [2], Joye *et al* [4], Jakšić and Segert [5, 6] it becomes clear that similar to the Berry adiabatic phase [1], the transition probabilities induced by a time dependence of the Hamiltonian are connected with the geometry of the parameter space. In particular, when the evolution of a system is described by the Hamiltonian of the form

$$\hat{H}(s) = \boldsymbol{n}(s)\cdot\sigma \quad |\boldsymbol{n}(s)| = 1 \tag{2}$$

(where $\boldsymbol{n}(s)$ is a parameter-dependent unit vector and $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ are Pauli matrices) in the first-order adiabatic perturbation theory the transition (spin-flip) $W_\pm$ is determined by the Fourier transform [2, 4–6]:

$$W_\pm \sim \left|\int_{-\infty}^{+\infty}\exp(-2\mathrm{i}Ts)\chi(s)\,\mathrm{d}s\right|^2 \tag{3}$$

$$\chi(s) = \mathrm{i}/2|n'(s)|\exp(-\mathrm{i}\varsigma(s)) \tag{4}$$

where $|\boldsymbol{n}'(s)|$ is related to the Riemannian length element $\mathrm{d}l(s) = |\boldsymbol{n}'(s)|\,\mathrm{d}s$ of the unit sphere. The function $\varsigma(s)$ is given by the integral

$$\varsigma(s) = \int_0^s \kappa_g(s)\,\mathrm{d}s \tag{5}$$

and $\kappa_g(s)$ is the geodesic curvature of a path $\boldsymbol{n}(s)$:

$$\kappa_g(s) = \frac{\boldsymbol{n}''(s)\cdot(\boldsymbol{n}'(s)\times\boldsymbol{n}(s))}{|\boldsymbol{n}'(s)|^2}. \tag{6}$$

We note that the Hamiltonian (2) defines a curve in the Lie algebra $su(2)$. The corresponding evolution operator belongs to the fundamental (2×2) representation of the group $SU(2)$ and the transition probability appears to be completely determined by the geometric properties of the $SU(2)$ group homogeneous space $S^2 = SU(2)/U(1)$ (which serves as the parameter space for this particular situation).

It is the main purpose of this work to establish a relation between the probabilities of the non-adiabatic transitions and the geometry of the parameter space in a way which is more general than the above-mentioned case. Namely, we consider a situation when the commutator algebra of the Hamiltonian operators $\hat{H}(s)$ at different values of the parameter s is closed for all s, constituting an arbitrary Lie algebra $\mathcal{G}$. This condition makes it possible to reformulate the original problem about the evolution of a quantum state in terms of a first-order dynamic equation on the group manifold (section 2). The adiabatic solution of this equation is constructed in section 3, and the integral expression for the Lie algebra element, determining transition probabilities, is derived. In section 4 our approach is applied to the spin precession in a variable external field. The adiabatic approximation for the spin precession [2, 4–6] is reconstructed. Applied to the ordinary one-dimensional Schrödinger equation, our method gives the well known WKBJ solution as the first adiabatic approximation. In the leading (second-)order approximation our approach leads to Bremmer's formula [18] for the over-barrier reflection (section 5). In section 6 an expression for the transition probability due to a parametric excitation of a quantum oscillator is obtained from our results. Section 7 is devoted to a comparison of our calculations with exact solutions for a number of analytically solvable models.

2. Dynamic equation on group manifolds

We consider the linear operator (matrix) equation of the form

$$\partial\hat{G}/\partial t = \hat{B}(t)\hat{G} \qquad \hat{G}(t_0) = \hat{I} \tag{7}$$

where $\hat{I}$ is the unit operator and $\hat{B}(t)$ has a given time dependence. This is a pattern for a number of physical problems, including the one-dimensional Schrödinger equation and the spin precession in a time-dependent magnetic field. If the commutator algebra of operators $\hat{B}(t)$ is closed for all t, constituting a Lie algebra $\mathcal{G}$, one actually deals with the first-order dynamical equations on the Lie group G, generated by $\mathcal{G}$. Now the problem can be written in terms of the Cartan–Maurer 1-form,

$$\mathrm{d}g\, g^{-1} = b(t)\,\mathrm{d}t \qquad g(t) \in \mathsf{G} \quad b \in \mathcal{G} \tag{8}$$

with the initial condition $g(0) = e$, i.e. the unit element of G. Special problems are those where $b(t)$ belongs to a Cartan subalgebra of $\mathcal{G}$, i.e. $b(t) \in \mathcal{H} \subset G, \forall t$. In a case like that, equation (8) is integrated immediately,

$$g(t) = \exp\left[\int_{t_0}^{t} b(\tau)\,\mathrm{d}\tau\right] \in \mathsf{H} \tag{9}$$

where H is the corresponding Abelian subgroup of G. In general, equation (8) is a set of (nonlinear) differential equations which cannot be reduced to quadratures. It is notable that the desired group element may be shifted by a properly chosen amount $g_0(t)$, so the equation is rewritten in an equivalent form, $g = g_0(t)g_1$,

$$\mathrm{d}g_1\, g_1^{-1} = b_1(t)\,\mathrm{d}t \qquad b_1(t)\,\mathrm{d}t = g_0^{-1}\left(b\,\mathrm{d}t - \mathrm{d}g_0\, g_0^{-1}\right) g_0 \in \mathcal{G}. \tag{10}$$

Thus the problem may be reduced to a more tractable one.

Let us restrict ourselves to problems where $b(t)$ approaches a Cartan subalgebra $\mathcal{H}$ asymptotically, as $t \to \pm\infty$, and evaluate the transition probability between eigenstates of operators representing $\mathcal{H}$. The S-operator given by the following limit may be used (provided this limit exists):

$$\hat{S} = \lim_{t,t_0\to\pm\infty} \exp\left[-\int_0^t \hat{B}_+(\tau)\,\mathrm{d}\tau\right] \hat{G}_{t_0}(t) \exp\left[-\int_{t_0}^{0} \hat{B}_-(\tau)\,\mathrm{d}\tau\right] \tag{11}$$

where $\hat{B}_\pm(t) \in \mathcal{H}$, and $\lim_{t,t_0\to\pm\infty} \|\hat{B}(t) - \hat{B}_\pm(t)\| = 0$. The probability of a transition between the states given by the density operators $\hat{P}_\pm$ at $t \to \pm\infty$ is

$$W_\pm \equiv \lim_{t,t_0\to\pm\infty} \mathrm{Tr}\left[\hat{P}_+\hat{G}(t)\hat{P}_-\hat{G}^\dagger(t)\right] = \mathrm{Tr}\left(\hat{P}_+\hat{S}\hat{P}_-\hat{S}^\dagger\right) \tag{12}$$

since we assume that $\hat{P}_\pm$ commute with $\hat{B}_\pm$.

3. The adiabatic approximation

At any given time t, the driving force $b(t) \in \mathcal{G}$ may be reduced to a Cartan subalgebra $\mathcal{H}$, and the group element is decomposed as

$$b(t) = v(t)\beta(t)v(t)^{-1} \qquad \beta(t) \in \mathcal{H} \tag{13}$$

$$g(t) = w(t)h(t)w(t)^{-1} \qquad h(t) \in \mathsf{H}. \tag{14}$$

Remarkably, if v has no t dependence, that would fix the subalgebra $\mathcal{H}$ for all t, and g would be obtained immediately, like in equation (9). We consider the problems where $b(t)$ belongs to the Cartan subalgebra asymptotically, at $t \to \pm\infty$, so $\lim v(t) = e$. The equation resulting from (8) would be

$$w\left(\mathrm{d}h\, h^{-1} + w^{-1}\,\mathrm{d}w - hw^{-1}\,\mathrm{d}w\, h^{-1}\right)w^{-1} = v\beta v^{-1}\,\mathrm{d}t. \tag{15}$$

Splitting this equation into the subalgebras $\mathcal{H}$ and $\mathcal{G}\setminus H$, we obtain a set of differential equations for h and w. We find an approximate solution of equation (15) for *adiabatic* processes, where the t dependence of v is slow, the derivative $\mathrm{d}v/\mathrm{d}t$ is small, and the condition

$$\|v^{-1}\,\mathrm{d}v/\mathrm{d}t\| \ll \|\beta\| \tag{16}$$

is satisfied. Here the norm $\|y\|$ for an arbitrary element y of the Lie algebra $\mathcal{G}$ is introduced,

$$\|y\| = \sqrt{\mathrm{Tr}(YY^\dagger)} \qquad y \in \mathcal{G} \tag{17}$$

and Y is the matrix belonging to the adjoint representation of the Lie algebra $\mathcal{G}$ and corresponding to the Lie algebra element y. When the condition (16) holds, w is always close to v, and the deviation of $g(\infty)$ from the subgroup $\mathcal{H}$ is negligible. This is the meaning of the adiabatic theorem: the eigenstates of operators belonging to the subalgebra $\mathcal{H}$ are not subject to transitions.

The unknown group element may be replaced by $w = v\exp(-\omega)$, and it is assumed that $\omega \in \mathcal{G}\setminus H$. Small deviations from the adiabatic limit, producing non-adiabatic transitions, are obtained if we consider the first approximation in ω, which is expected to be of the order of $v^{-1}\,\mathrm{d}v$, discarding all higher-order terms. The result is

$$\mathrm{d}h\,h^{-1} - R(h)(v^{-1}\,\mathrm{d}v - \mathrm{d}\omega) = [\beta + (\omega\beta - \beta\omega)]\,\mathrm{d}t \tag{18}$$

where $R(h)\eta \equiv h\eta h^{-1} - \eta, \forall\eta \in \mathcal{G}$ (note that $R(h)\eta = 0$, if $\eta \in \mathcal{H}$). Separating the zero- and the first-order terms, we obtain two equations

$$\mathrm{d}h_0\,h_0^{-1} = \beta(t)\,\mathrm{d}t \qquad \text{so} \quad h_0 = \exp\left[\int_{t_0}^t \beta(\tau)\,\mathrm{d}\tau\right] \in \mathsf{H} \tag{19}$$

$$R(h_0)\partial\omega/\partial t + [h_0^{-1}\partial h_0/\partial t, \omega] = R(h_0)(v^{-1}\partial v/\partial t). \tag{20}$$

The latter equation is also integrated immediately,

$$R(h_0^{-1})\omega = \int_{t_0}^t R(h_0^{-1})(v^{-1}\dot{v})\,\mathrm{d}\tau \qquad \dot{v} \equiv \partial v/\partial t|_{t=\tau}. \tag{21}$$

In the asymptotics, as soon as $t, t_0 \to \pm\infty$, we obtain

$$\gamma \equiv \lim_{t,t_0\to\pm\infty} R(h_0^{-1})\omega = \int_{-\infty}^{\infty} R(h_0^{-1})(v^{-1}\dot{v})\,\mathrm{d}\tau \tag{22}$$

and this element of $\mathcal{G}$ determines the transition probability amplitude. In order to see that, let us insert the asymptotic value of the operator representing the group element

$$g = v\exp(-\omega)h\exp(\omega)v^{-1} \approx (e-\omega)h_0(e+\omega) \approx h_0(e - R(h_0^{-1})\omega) \tag{23}$$

in equation (12) for the transition probability. Assuming that $\hat{P}_+$ and $\hat{P}_-$ represent different (orthogonal) eigenstates of operators corresponding to $\mathcal{H}$, so that $\hat{P}_+\hat{P}_- = 0 = \hat{P}_-\hat{P}_+$, one obtains the following expression for the transition probability in the leading (second) order:

$$W_\pm = \mathrm{Tr}(\hat{P}_+\hat{\Gamma}\hat{P}_-\hat{\Gamma}) \tag{24}$$

where $\hat{\Gamma}$ is the operator representing $\gamma \in \mathcal{G}$ in equation (22). Note that any value may be taken for t_0 in equation (28); changing it, say, to t_0', would result in a constant gauge substitution of γ for γ',

$$\gamma' = (h_0')^{-1}\gamma h_0' \qquad h_0' = \exp\left[\int_{t_0'}^{t_0}\beta(\tau)\,\mathrm{d}\tau\right]. \tag{25}$$

That would not change the probability in (24). The convergence of the integral in (22) depends on how fast the driving force $b(t)$ is approaching its asymptotics in $\mathcal{H}$. It is noteworthy that the present result extends the standard perturbation theory. If $b(t) = \beta_0 + \lambda b_1(t)$, where $b_1(t) \to 0$ at $\pm\infty$, then to the first order in λ one has to set $h_0(\tau) = \exp(\beta_0\tau)$ in (22), and the result is an extension of the Born approximation. In general, γ indicates the deviation from the adiabatic limit. Even if the perturbation is not small absolutely, γ may be small because of two different reasons:

(a) the change of v is slow, though it may be not close to unity, which is the case for small perturbations;
(b) the deviation of $b(t)$ from $\mathcal{H}$ takes place during a small time interval, and the integral is small as a result of that.

4. Spin-flip in a variable magnetic field

The spin precession in a time-dependent magnetic field, the fundamental problem for NMR [10], is determined by the Bloch equation for the spinor wavefunction,

$$\mathrm{i}\,\mathrm{d}\psi/\mathrm{d}t = (\mathcal{B}\cdot\sigma)\psi \tag{26}$$

where $\mathcal{B} \equiv \mu\boldsymbol{B}(t)$, $\boldsymbol{B}(t)$ is a variable magnetic field vector, μ is the particle magnetic moment, and σ are the Pauli matrices. The fundamental solution of equation (26) is given by a unitary 2×2 matrix, so the group is $SU(2)$. The matrix $\hat{G}$ is given by equation (7) with $\hat{B} = -\mathrm{i}(\mathcal{B}\cdot\sigma)$.

Let us consider, for instance, the case where a pulse is applied in the x-direction, while the z-component is constant, $\boldsymbol{B} = \{B_1(t), 0, B_0\}$, and $B_1(t) \to 0$ as $\to \pm\infty$. The adiabatic approximation holds if $B_1(t)$ is a slow function of t. The elements which appear in (13) are

$$\beta(t) = 2\mu[B_0^2 + B_1^2(t)]^{1/2}J_3 \qquad v(t) = \exp(\theta J_2) \tag{27}$$

where $\tan\theta = -B_1(t)/B_0$, and J_a is the basis in $\mathcal{G}$, represented by $\frac{1}{2}\mathrm{i}\sigma_a$. For this particular representation, we find from equation (17), that

$$\|v^{-1}\,\mathrm{d}v/\mathrm{d}t\| = |\mathrm{d}\theta/\mathrm{d}t| \qquad \|\beta\| = \mu[B_0^2 + B_1^2(t)]^{1/2} \tag{28}$$

and the general condition of applicability (16) leads to

$$|\mathrm{d}\theta/\mathrm{d}t| \ll \mu[B_0^2 + B_1^2(t)]^{1/2}. \tag{29}$$

The spin-flip, as given by equation (22), is determined by $\gamma = A_{+-}J_2$, and

$$A_{+-} = \int_{-\infty}^{\infty} \mathrm{e}^{2\mathrm{i}\alpha(\tau)}\dot{\theta}\,\mathrm{d}\tau \qquad \alpha(\tau) = \mu\int_{\tau_1}^{\tau}[B_0^2 + B_1^2(t)]^{1/2}\,\mathrm{d}t. \tag{30}$$

The spin probability is $W_{+-} = |A_{+-}|^2$. The accuracy of the approximation has been checked for a field where the exact analytical solution is available (see section 7).

In the formula (30) $\mathrm{d}l(\tau) = \dot{\theta}\,\mathrm{d}\tau$ is the Riemannian length element on the path $\boldsymbol{n}(\tau) = (\sin\theta, 0, \cos\theta)$. The geodesic curvature determined by equation (6), is equal to zero. In a more general case of the magnetic field configuration $\boldsymbol{B} = |B|(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ the group element g_0 leading to equation (10) will be chosen as $g_0 = \exp(-2\phi J_3)$. This transformation alters the phase $\alpha(\tau)$ in equation (30) to $\mu\int_{\tau_1}^{\tau}[\sin^2\theta + (\cos\theta - \dot{\phi}/|B|)^2]^{1/2}|B|\,\mathrm{d}t$. An expansion of $\alpha(\tau)$ to the lowest-order non-vanishing in $\dot{\phi}/|B|$ leads to Berry [2], Joye *et al* [4], Jakšić and Segert [5, 6] result for the spin-flip probability.

5. Over-barrier reflection

The Schrödinger equation, $\Psi'' - U(x)\Psi = -k^2\Psi$ is equivalent to the following first-order problem for the two-component function $\psi(x)$, satisfying the equation

$$\frac{\mathrm{d}\psi}{\mathrm{d}x} = \hat{B}(x)\psi$$

where

$$\psi = \begin{pmatrix} \Psi' - \mathrm{i}k\Psi \\ \Psi' + \mathrm{i}k\Psi \end{pmatrix} \qquad \hat{B}(x) \equiv -\mathrm{i}\begin{pmatrix} k - U/2k & U/2k \\ -U/2k & -k + U/2k \end{pmatrix}. \tag{31}$$

Thus the coordinate x plays the role of the time parameter t. For the plane wave moving in the positive direction, $\Psi = C\exp(\mathrm{i}kx)$, so the upper component of ψ vanishes, and reflection is like the spin-flip. The problem of barrier penetration is represented by equation (7), where $\hat{B}^\dagger = -\sigma\hat{B}\sigma$ ($\sigma \equiv \sigma_3$ is the diagonal Pauli matrix). Thus $\hat{G}^\dagger = \sigma\hat{G}^{-1}\sigma$, the probability current $j \equiv -\frac{1}{2k}\bar{\psi}\sigma\psi = -\frac{1}{2}\mathrm{i}(\Psi'\bar{\Psi} - \Psi\bar{\Psi}')$ is conserved, so we are dealing with the two-dimensional representation of the group $\mathsf{G} = SU(1,1)$. For $U(x)$ decreasing rapidly as $x \to \pm\infty$, one has the transfer matrix

$$\hat{T} \equiv \lim_{x,x_0\to\pm\infty}\hat{G}(x) = \begin{pmatrix} a & \bar{b} \\ b & \bar{a} \end{pmatrix} \qquad |a|^2 - |b|^2 = 1. \tag{32}$$

The penetration probability amplitude is $1/|a|^2$ and the reflection probability is $|b/a|^2$.

As soon as $\det\hat{B} = k^2 - U(x) \equiv p^2(x)$, the Abelian subgroup is $\mathsf{H} = U(1)$ in the region where $p^2 > 0$, and $\mathsf{H} = \mathsf{R}$ under the barrier, where $p^2 < 0$. The 2×2 matrix diagonalizing $\hat{B}$ is

$$\hat{V} = \begin{pmatrix} \cosh\eta & \sinh\eta \\ \sinh\eta & \cosh\eta \end{pmatrix} \qquad \exp(2\eta) \equiv \frac{p}{k}. \tag{33}$$

Applied to the plane wave, moving in the positive direction, the group element in the first-order adiabatic approximation $g \approx v h_0 v^{-1}$ leads to the following expression for the wavefunction:

$$\Psi(x) = C\left[\cosh\eta(x)\exp\left\{-\eta(x) + \mathrm{i}\int_{x_0}^{x} p(\xi)\,\mathrm{d}\xi\right\}\right.$$
$$\left.+\sinh\eta(x)\exp\left\{-\eta(x) - \mathrm{i}\int_{x_0}^{x} p(\xi)\,\mathrm{d}\xi\right\}\right]. \tag{34}$$

In the limit $x \to +\infty$ the parameter $\eta(x)$ goes to zero,

$$\lim_{x\to+\infty}\Psi(x) = C\exp\left(\mathrm{i}\int_{x_0}^{x} p(\xi)\,\mathrm{d}\xi\right) \tag{35}$$

and the over-barrier reflection is absent in the first-order adiabatic approximation. Note that within the framework of this approximation the elements of the matrix $\hat{V}$ are considered to be slowly dependent on x, and $\exp(-\eta(x)) = \sqrt{k/p(x)}$. Thus a familiar WKBJ expression for the wavefunction

$$\Psi(x) = C_1\sqrt{\frac{k}{p}}\exp\left(\mathrm{i}\int_{x_0}^{x} p(\xi)\,\mathrm{d}\xi\right) + C_2\sqrt{\frac{k}{p}}\exp\left(-\mathrm{i}\int_{x_0}^{x} p(\xi)\,\mathrm{d}\xi\right) \tag{36}$$

is reconstructed. Remarkably, v belongs to a one-parameter subgroup of $SU(1,1)$, which makes the calculations simpler than in the general problem of spin precession (cf section 4). The over-barrier reflection is determined by (22), where the element v is represented by the 2×2 matrix $\hat{V}$, and h_0 by the matrix

$$\hat{H}_0 = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\int_{x_0}^{x} p\,\mathrm{d}x} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\int_{x_0}^{x} p\,\mathrm{d}x} \end{pmatrix}. \tag{37}$$

The probability of the over-barrier reflection is $R = |A|^2$, where

$$A = \frac{1}{4}\int_{-\infty}^{+\infty} \mathrm{e}^{2\mathrm{i}\int_{x_0}^{x} p\,\mathrm{d}x}\,\frac{U'(x)}{k^2 - U(x)}\,\mathrm{d}x. \tag{38}$$

The proposed method is valid when the inequality (16) is satisfied. This leads to the same condition of applicability as in the WKBJ approximation,

$$|\mathrm{d}p(x)/\mathrm{d}x| \ll p^2(x). \tag{39}$$

Equation (38) coincides with the over-barrier reflection amplitude obtained by Bremmer [18]. Bremmer's approximation was to divide a smooth potential into a large number of small layers. The momentum $p(x)$, being different in different layers, was assumed to be constant throughout a range of a particular layer. The ordinary WKBJ solution equation (36) was then obtained by discarding all reflections of the incident wave at any layer's boundary. Assuming that only single reflections at all boundaries of the layers take place, Bremmer found the over-barrier reflection amplitude.

An advantage of our procedure is that leading to the same result (equation (38)) as Bremmer's approach, our derivation does not demand any assumptions about the qualitative character of the wave reflection. Thus our method shows that the usual condition for the validity of the WKBJ approximation (equation (36)) is only needed in order to obtain Bremmer's formula.

The reflection amplitude (38) may be compared with that given by Maitra and Heller [19]. These authors use a perturbative approach with the WKBJ states as the unperturbed basis. According to Maitra and Heller the approximated reflection amplitude A_{MH} is given by the matrix element of an effective potential between the usual WKBJ wavefunctions, i.e.

$$A_{MH} = \int_{-\infty}^{+\infty} U_{eff}(x,k) \frac{\mathrm{e}^{2\mathrm{i}\int^x p(y)\,\mathrm{d}y}}{p(x)}\,\mathrm{d}x. \tag{40}$$

The effective potential of Maitra and Heller is given by the formula

$$U_{eff}(x,k) = \frac{-3(p'(x))^2}{4p^2(x)} + \frac{p''(x)}{2p(x)}. \tag{41}$$

Once Maitra and Heller use the perturbative arguments their expression for the reflection amplitude should be valid when the effective potential is small, i.e.

$$|U_{eff}(x,k)| \ll k^2. \tag{42}$$

Comparing the above conditions with that of the applicability of our approximation we can see that our approach has a wider range of validity since inequality (42) follows from equation (36).

In the limit of $k^2 \gg U(x)$ the momentum $p(x)$ becomes approximately equal to k. Neglecting $U(x)$ in comparison with k^2 in the integral (38), and integrating by parts, we obtain the result which corresponds to perturbation theory:

$$A_{pert} = \frac{1}{2\mathrm{i}k} \int_{-\infty}^{+\infty} \mathrm{e}^{2\mathrm{i}kx} U(x)\,\mathrm{d}x \tag{43}$$

6. Parametric excitation of a quantum oscillator

The parametric excitation of a quantum oscillator is the excitation of the oscillator under change of its parameters $m = m(t)$ and $\Omega = \Omega(t)$. The general case with a time-dependent $m(t)$ and $\Omega(t)$ may be easily reduced to $m =$ constant by changing variables $t' = \int \frac{\mathrm{d}t}{m(t)}$, $\Omega' = m\Omega$. The Schrödinger equation for the wavefunction of the quantum oscillator has the following form:

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}\Omega^2(t)x^2\psi. \tag{44}$$

For $\Omega(t)$ the asymptotic conditions

$$\Omega(t) \longrightarrow \Omega_\pm \qquad t \longrightarrow \pm\infty \tag{45}$$

are assumed. The asymptotic stationary states are

$$\phi_n^\pm(x,t) = \phi_n(x,\Omega_\pm)\,\mathrm{e}^{-\mathrm{i}(n+\frac{1}{2})\Omega_\pm t} \tag{46}$$

$$\phi_n(x,\Omega_\pm) = \left(\frac{1}{2^n n!}\sqrt{\frac{\Omega_\pm}{\pi}}\right)^{1/2} \exp\left(-\frac{\Omega_\pm x^2}{2}\right) H_n(\sqrt{\Omega_\pm}x). \tag{47}$$

The time dependence of the quantum oscillator parameters $m(t)$ and $\Omega(t)$ allows for the transitions between different stationary states.

A typical problem is to calculate the probability of transitions W_{mn} from the state ψ_n with the asymptotic $\phi_n^{(-)}(x,t)$ at $t \to -\infty$ to the asymptotic state $\phi_m^{(+)}(x,t)$ at $t \to +\infty$. As is well known (e.g. Baz' *et al* [17]), in order to determine this probability of transitions W_{mn} it is sufficient to calculate the quantum mechanical coefficient θ of the over-barrier reflection from the one-dimensional potential of a particle with momentum $p(x) = \sqrt{k^2 - U(x)} = \Omega(x)$, where $\Omega(x)$ is the frequency function of the quantum oscillator. However, the analytic solution of the over-barrier reflection problem is known only for a number of special cases. When it is impossible to find an analytic solution for the problem of the over-barrier reflection, our approximated approach developed in section 5 may be applied. The approximated expression for the quantum mechanical coefficient θ is given by the formula (38), i.e.

$$\vartheta = \frac{1}{4}\left|\int_{-\infty}^{+\infty} \mathrm{e}^{2\mathrm{i}\int_{t_0}^{t}\Omega(t)\,\mathrm{d}t} \frac{\Omega'(t)\,\mathrm{d}t}{\Omega(t)}\right|^2. \tag{48}$$

When the parameter θ is determined, the probability of transitions W_{mn} may be calculated using the Perelomov and Popov [16] formula:

$$W_{mn} = \frac{n_<!}{n_>!}\left|\sqrt{1-\vartheta}\,P_{|m+n|/2}^{|m-n|/2}(\sqrt{1-\vartheta})\right|^2 \tag{49}$$

where $n_< = \min(m, n)$, $n_> = \max(m, n)$ and $P_n^m(x)$ are the associated Legendre functions.

7. Comparison with exact solutions

7.1. Spin precession in a magnetic field

The exact solution of the spin precession problem of section 4 is known [11] for the magnetic field

$$\boldsymbol{B}(t) = \frac{1}{T}\left(\frac{\beta_1}{\cosh(t/T)}, 0, \beta_0\right). \tag{50}$$

Here β_0/T is the asymptotic precession frequency, T is the pulse duration. The applicability condition equation (29) allows for the application of our approach, when the inequality

$$\beta_1/\beta_0 \ll \sqrt{\beta_1^2 + \beta_0^2} \tag{51}$$

is satisfied. When $\beta_0 > 1$, the inequality (51) holds for all β_1 and the process would be adiabatic. Respectively, the perturbation theory can be applied for $\beta_1 \ll \beta_0$. As known from the analytical solution of equation (7) given in terms of the hypergeometric function,

$$W_{+-} = [\sin(\pi\beta_1)/\cosh(\pi\beta_0)]^2. \tag{52}$$

Calculating the integrals in (30), it is useful to change the variables as follows:

$$\beta_1/\beta_0 = \tan k \qquad \cos k \sinh(t/T) = \sinh\xi. \tag{53}$$

Taking the integral for α with $\tau_1 = 0$, we have

$$\alpha(\xi) = \beta_0\xi + \beta_1 \arctan(\tan k \tanh\xi) \tag{54}$$

$$A_{+-} = \sin k \int_0^{\infty} \sin[2\alpha(\xi)] \frac{\tanh\xi\,\mathrm{d}\xi}{(\cosh^2\xi - \sin^2 k)^{1/2}}. \tag{55}$$

The latter integral is reduced to a real form, as the pulse is symmetrical under the time inversion, so $\dot{\theta}$ is odd. The numerical calculation shows a wonderful accuracy of the approximation, namely,

$$A_{+-} \approx \frac{\sin(\pi\beta_1)}{\cosh(\pi\beta_0)} \tag{56}$$

even for moderate values of β_0, over a wide range of β_1 (see figure 1).

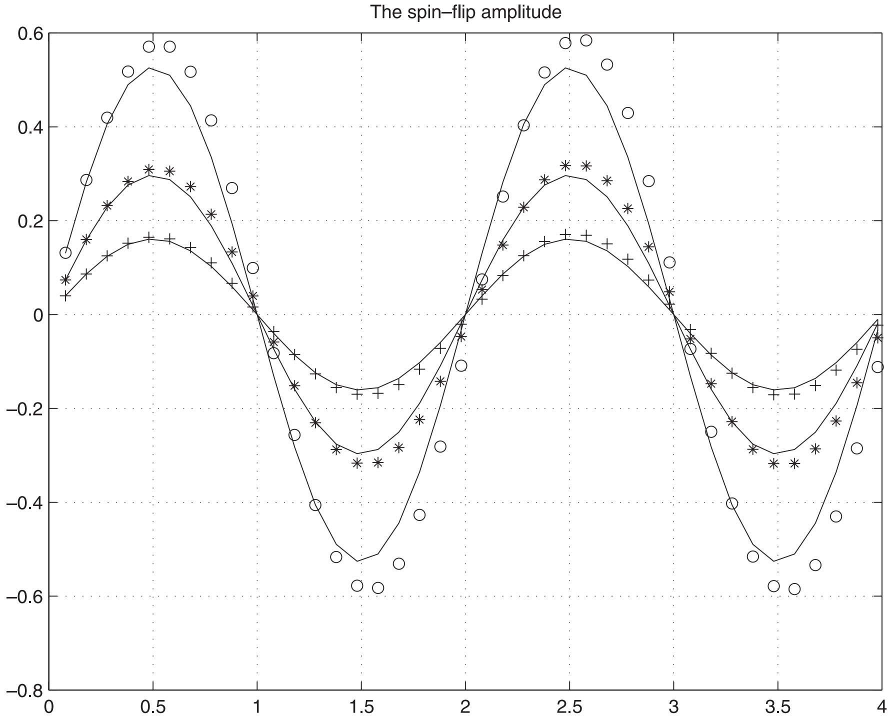

Figure 1. The spin-flip probability amplitude, for the magnetic field $\boldsymbol{B}(t) = \frac{1}{T}\left(0, \frac{\beta_1}{\cosh(t/T)}, \beta_0\right)$. The exact (equation (52)) and approximated (equation (55)) amplitudes of the spin-flip as functions of β_1 under different parameters β_0 are represented. $\beta_0 = 0.8, 0.6, 0.4$ correspond to +, $*$, $\circ$, and the exact amplitudes are given by the full curve.

7.2. Over-barrier reflection for the potential $U = U_0/(1 + \mathrm{e}^{-\gamma x})$.

The analytic expression for the reflection amplitude is

$$A = \frac{\sinh(\pi\alpha(1 - \sqrt{1-\beta}))}{\sinh(\pi\alpha(1 + \sqrt{1-\beta}))}. \tag{57}$$

In the above formula the parameters $\alpha = k/\gamma$ and $\beta = U_0/k^2$ were introduced. Perturbation theory may be applied when $k \gg U_0$, i.e. $0 < \beta \ll 1$. In that case the reflection probability is equal to

$$\rho \simeq \frac{\pi\alpha^2\beta^2}{4\sinh^2(2\pi\alpha)}. \tag{58}$$

Next, we consider the situation when $k^2 \geqslant U(x)$. As follows from the inequality (39), in the cases when

$$\beta/\alpha \ll 1 - \beta \tag{59}$$

the over-barrier probability amplitude may be calculated by our method. It is suitable to change the variables $z = \mathrm{e}^{\gamma x}$ and calculate the integral in the exponent of formula (38). We obtain the following integral expression for the over-barrier reflection probability amplitude:

$$A = \frac{\beta}{4}\int_0^{+\infty} \frac{z^{2\mathrm{i}\alpha-1}\left(2\sqrt{1-\beta}\sqrt{(z+1)((1-\beta)z+1)} + 2(1-\beta)z + 2 - \beta\right)^{2\mathrm{i}\alpha\sqrt{1-\beta}}\,\mathrm{d}z}{\left(2\sqrt{(z+1)((1-\beta)z+1)} + (2-\beta)z + 2\right)^{2\mathrm{i}\alpha}(1+z)((1-\beta)z+1)}. \tag{60}$$

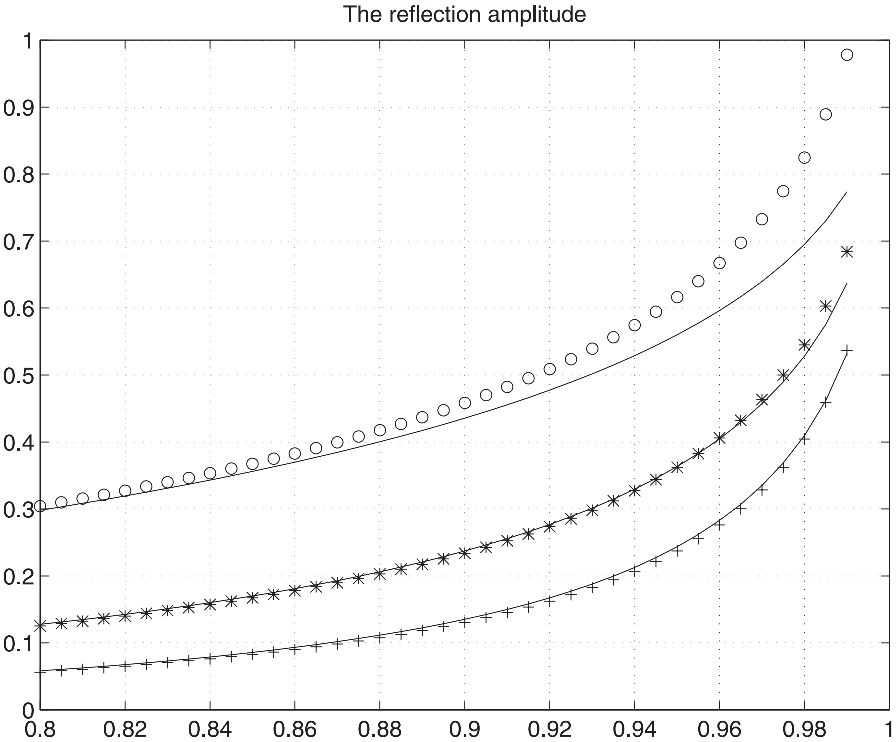

Figure 2. The reflection over the potential barrier $U = U_0/(1 + \exp(-\gamma x))$. The exact (equation (57)) and approximated (equation (60)) amplitudes of the reflection as functions of $\beta = U_0/k^2$ under different parameters $\alpha = k/\gamma$ are represented. $\alpha = 1.0, 0.7, 0.3$ correspond to $+$, $*$, $\circ$, and the exact amplitudes are given by the full curve.

A comparison of the exact and approximate (see figure 2) probability amplitudes demonstrates the very good accuracy of the approximation (38), namely

$$|A| \simeq \frac{\sinh \pi\alpha(1 - \sqrt{1-\beta})}{\sinh \pi\alpha(1 - \sqrt{1+\beta})}. \tag{61}$$

8. Conclusions

In this paper we have proposed an adiabatic approach to the calculation of probabilities for quantum transitions. In the case when the one-parameter-dependent Hamiltonian represents a smooth curve in a Lie algebra, the original Schrödinger equation was interpreted as the dynamical equation on the corresponding group manifold. The main result of this work is expressed by equation (22) that determines the Lie algebra element responsible for the non-adiabatic transitions.

The problem of over-barrier reflection in one-dimensional quantum mechanics is very similar in our approach to the problem of a spin-flip in a variable magnetic field (the difference lies in the fact that for the over-barrier reflection problem the introduced evolution operator is an element of the group $SU(1.1)$, and not of $SU(2)$, as for the spin evolution operator).

We have tested our approach on simple problems for which approximate solutions are known. In the case of a spin in a time-dependent magnetic field our procedure leads to a spin-flip amplitude equation (30). In the adiabatic limit equation (30) would coincide with the Berry [2], Joye *et al* [4], Jakšić and Segert [5, 6] result for the spin-flip probability amplitude. The application of our procedure to the over-barrier reflection gives Bremmer's formula [18] in the leading (second-)order approximation. It is remarkable that in order to obtain Bremmer's result, only the usual condition of the validity of the WKBJ approximation (equation (36)) is needed.

Having checked for two solvable models (the spin-flip in the Rosen–Zener magnetic field and the over-barrier reflection for the potential $U = U_0/(1 + \mathrm{e}^{-\gamma x})$), our adiabatic approximation not only gives the exponentially small character of the probabilities of the non-adiabatic processes, but completely describes the qualitative behaviour of these probabilities as functions of the external parameters. The integrals (30) and (38) show the same behaviour under variation of the magnetic field amplitude (the amplitude of the potential) as the exact solutions. It is interesting to note that in spite of the same condition of applicability as the WKBJ approximation, our approach is very successful in the calculation of the over-barrier reflection, while the usual WKBJ approximation gives a zero answer to all orders. The reason is that the WKBJ approximation is an asymptotic series that is unable to take the exponentially small variables into account.

Acknowledgments

We are grateful to J Avron, B Block, N Krauss, D Owen and B Segev for valuable comments and discussions that have contributed to this work.

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