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Abstract
In this paper we give a general method to solve a time-dependent Schrödinger
equation. The formalism developed is based on the quantum variational
principle conveniently 'averaged'. In addition, we apply our method to study
the time-dependent systems in which the Hamiltonians are linear functions of
$SU(1, 1)$ and $SU(2)$ Lie algebras.

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1. Introduction

The explicitly time-dependent quantum systems have been a long standing mathematical
problem not yet completely solved in general. Various methods have been used to obtain
approximate solutions for such time-dependent problems. The adiabatic method has been one
of the most general and frequently used approximate methods for time-dependent quantum
systems [1]. A quantum adiabatic theorem, including the recent improvements due to Berry [2]
was derived in [3]. This derivation is based on the introduction of the averaged variational
principle. The necessity of 'averaging' appears as soon as one considers a pure state $|\psi(t)\rangle$
written as a linear combination of the reference instantaneous stationary eigenstate of the
Hamiltonian $|\psi(t)\rangle = \sum_n C_n(t)|n, \vec{X}(t)\rangle$. Exploiting the decomposition of the evolution
operator method, Cheng and Fung [4] have studied the nonadiabatic generalization of Berry's
result due to Aharonov and Anandan [5].

The existence of the invariant operator, introduced by Lewis and Riesenfeld [6], for such
time-dependent quantum systems allows one to find the exact quantum states in terms of the
eigenstates of the invariant operator up to some time-dependent phase factors.

In this paper we use the variational principle approach and show that the non-adiabatic
evolution amounts to replacing this principle by a well defined averaged version of them.

In section 2, we give a derivation of the exact evolution of the quantum system by means of the 'averaged' variational principle, and our results will be compared with those of the evolution operator method of Cheng and Fung [4]. In section 3, we apply our general results to study time-dependent $SU(1, 1)$ and $SU(2)$ quantum systems [7–10] and we end with two special examples.

2. The quantum averaged variational principle

Consider a quantum system whose Hamiltonian $H(t)$ is time dependent. In order to find the evolution of the state

$$|\psi(t)\rangle = \mathcal{U}(t)|\psi(0)\rangle \tag{2.1}$$

where $\mathcal{U}(t)$ is the evolution operator, one must call for some variational principle and not for the Schrödinger equation

$$\delta\left[\int^t \langle\psi(t')|i\partial_{t'} - H(t')|\psi(t')\rangle \, dt'\right] = 0 \tag{2.2}$$

where the quantum mechanical Lagrangian $L_Q = \langle\psi(t)|i\partial_t - H(t)|\psi(t)\rangle$ is a function of the 'ket' $|\psi(t)\rangle$, its time derivative $|\dot\psi(t)\rangle$ and the 'bra' $\langle\psi(t)|$. Since $\langle\dot\psi(t)|$ does not appear in L_Q, the Euler–Lagrange equation obtained from variation with respect to $\langle\psi(t)|$ leads to the Schrödinger equation $(i\partial_t - H)|\psi(t)\rangle = 0$, if there is no restriction on $|\psi(t)\rangle$. When considering adiabatic evolution, the usual variational principle has to be replaced by an averaged version

$$\delta\left[\int^t \overline{\langle\psi(t')|i\partial_{t'} - H(t')|\psi(t')\rangle} \, dt'\right] = 0. \tag{2.3}$$

(The overbar means that one first calculates the expression in the angular brackets, then one averages over the phases of stationary states before varying the integral.) This replacement is justified in [3], where it is shown that the procedure of averaging leads to simple derivations of the standard quantum adiabatic theorem and of his extension, namely the geometrical Berry phase.

In the following, we extend the quantum averaged variational principle to an arbitrary evolution. A judicious parametrization of the Hilbert space consists of choosing as basis vectors the set of states $\{|n, t\rangle\}$ generated from the set $\{|n, 0\rangle\}$ by a time-dependent unitary operator $V(t)$ parametrized by certain time-dependent c-number variables, so that

$$V(t)|n, 0\rangle = |n, t\rangle \tag{2.4}$$

and writing

$$|\psi(t)\rangle = \sum_n C_n(t)|n, t\rangle. \tag{2.5}$$

Then, the trial state is parametrized by set c-number variables, the time development of which is determined through the averaged variational principle.

Before showing that the right evolution can be recovered from the variational principle conveniently averaged, it is useful to give the precise definition of the quantum averaging denoted by an overline $\overline{(\ldots)}$. To get the average $\overline{F(|\psi\rangle)}$ of any functional F of the state $|\psi\rangle$, one first replaces, in F, the state $|\psi(t)\rangle$ by its expression $|\psi(t)\rangle = \sum_n C_n(t)|n, t\rangle$. Each state $|n, t\rangle$ is then multiplied by an arbitrary phase factor $e^{i\alpha_n}$: $\sum_n C_n(t)|n, t\rangle \rightarrow \sum_n C_n(t)\,e^{i\alpha_n}|n, t\rangle$;

finally $\overline{F(|\psi\rangle)}$ is obtained by averaging over the phases $\{\alpha_n\}$ considered as independent, uniformly distributed random variables:

$$\overline{F(|\psi\rangle)} = \int_0^{2\pi} \int_0^{2\pi} \cdots \int_0^{2\pi} F\left(\sum_n C_n(t)\, \mathrm{e}^{\mathrm{i}\alpha_n} |n,t\rangle \right) \prod_n \frac{\mathrm{d}\alpha_n}{2\pi}. \qquad (2.6)$$

With the above notations and definitions at hand, we are now in position to show that the evolution of a pure quantum state can be obtained from the averaged variational principle. It is easy to verify that the averaging procedure gives

$$\delta\left[\int^t \mathrm{d}t' \sum_n \mathrm{i} C_n^* \dot{C}_n - |C_n|^2 \big(\langle n,0| V^+ H\, V - \mathrm{i} V^+ \dot{V} |n,0\rangle \big) \right] = 0. \qquad (2.7)$$

Then, the corresponding Euler–Lagrange equations with respect to the variables C_n^*, read

$$C_n(t) = C_n(0) \exp\left[-\mathrm{i} \int_0^t \mathrm{d}t' \big(\langle n,0| V^+ H\, V - \mathrm{i} V^+ \dot{V} |n,0\rangle \big) \right]. \qquad (2.8)$$

The important implication of this results is clear. The quantum averaged variational principle implies that the operator $V^+ \mathcal{U}$ is diagonal in the basis $\{|n,0\rangle\}$ with eigenvalue $\exp\left[-\mathrm{i} \int_0^t \mathrm{d}t' \big(\langle n,0| V^+ H\, V - \mathrm{i} V^+ \dot{V} |n,0\rangle \big) \right]$.

This is of similar form to equations (2.17) and (2.18) of Cheng and Fung [4]. Cheng and Fung decompose the evolution operator $\mathcal{U}$ as $V\, R$, R being chosen to be diagonal in the basis $\{|n,0\rangle\}$ so as to facilitate the calculation of $\mathcal{U}$; $|n,0\rangle$ evolves into $|n,t\rangle$ under V. In our analysis, we do not need to suppose that the operator $V^+ \mathcal{U}$ is diagonal in the basis $\{|n,0\rangle\}$, being a natural implication of the quantum averaged variational principle.

Now an important remark can be made. The operator $V(t)$ depends on time through a set of parameters $V(\vec{X}(t))$, therefore the Lagrangian function depends on two types of variables $(C_n,\ \dot{C}_n)$ and $(\vec{X},\ \dot{\vec{X}})$. The complement to equation (2.8) is obtained by making variation with respect to the parameters $\vec{X}(t)$, and the corresponding Euler–Lagrange equations give the following equations:

$$\left[\frac{\partial}{\partial X_i} \left(\langle n,0| \mathrm{i} V^+ \frac{\partial V}{\partial X_j} |n,0\rangle \right) - \frac{\partial}{\partial X_j} \left(\langle n,0| \mathrm{i} V^+ \frac{\partial V}{\partial X_i} |n,0\rangle \right) \right] \dot{X}_i$$
$$= \frac{\partial}{\partial X_j} \big(\langle n,0| V^+ H\, V |n,0\rangle \big) \qquad (2.9)$$

which determine the time evolution of external parameters characterizing the wavefunction and couple those parameters dynamically to the quantum degrees of freedom.

Before closing this section, let us consider:

(i) The basis vectors $\{|n,0\rangle\}$ are chosen to be eigenstates of the initial condition operator $I(0)$ (for example, the Hamiltonian $H(0)$) at time $t=0$ with constant eigenvalues δ_n and $V(t)|n,0\rangle = |n,t\rangle$ is an eigenstate at any time of any dynamical invariant $\mathcal{U}(t)\, I(0)\, \mathcal{U}^+(t)$ of the Hamiltonian H; the solution of the equation $\partial I / \partial t = \mathrm{i}\hbar[I, H]$. Then, according to the general theory of Lewis and Riesenfeld, the evolution operator $\mathcal{U}(t)$ will satisfy the following:

$$\mathcal{U}(t)\, |n,0\rangle = \exp\left[-\mathrm{i} \int_0^t \mathrm{d}t' \big(\langle n,0| V^+ H\, V - \mathrm{i} V^+ \dot{V} |n,0\rangle \big) \right] V(t)\, |n,0\rangle \qquad (2.10)$$

which implies that the operator $V^+ \mathcal{U}$ is diagonal in the basis $\{|n,0\rangle\}$.

(ii) If we employ the adiabatic assumption, then the state $V(t)|n,0\rangle = |n,t\rangle$ is an instantaneous eigenstate of the Hamiltonian $H(t)$ at any time with eigenvalues $E_n(t)$, then the result represented in (2.8) and (2.10) is exactly the result obtained by Berry [2].

Then as already noted [3, 4] adiabaticity implies that the operator $V^+ \mathcal{U}$ is diagonal in the basis $\{|n, 0\rangle\}$. In addition, the time-evolution of external parameters characterizing the trial wavefunction reduces to

$$\left[\frac{\partial}{\partial X_i}\left(\langle n, \vec{X}|\mathrm{i}\frac{\partial}{\partial X_j}|n, \vec{X}\rangle\right) - \frac{\partial}{\partial X_j}\left(\langle n, \vec{X}|\mathrm{i}\frac{\partial}{\partial X_i}|n, \vec{X}\rangle\right)\right]\dot{X}_i = \frac{\partial}{\partial X_j}E_n(\vec{X}). \quad (2.11)$$

Introducing a 'vector potential' in parameters space $A_j(\vec{X}) = \langle n, \vec{X}|\mathrm{i}\frac{\partial}{\partial X_j}|n, \vec{X}\rangle$, hence we can rewrite (2.11) in the form

$$F_{ij}\dot{X}_i = \frac{\partial}{\partial X_j}E_n(\vec{X}) \quad (2.12)$$

where $F_{ij} = \partial_i A_j - \partial_j A_i$ is an 'electromagnetic tensor' in parameter space.

It is quite striking to note that the averaged variational principle can be taken as a definition for adiabatic quantum motion which is an approximation to the full dynamics, when the state $|\psi(t)\rangle$ is written as a linear combination of instantaneous eigenstates of the Hamiltonian $H(t)$. However, it can also be taken as a mathematical formulation of the exact quantum evolution, when the state $|\psi(t)\rangle$ is expanded in terms of the eigenstate of the invariant operator $I(t)$.

3. $SU(1, 1)$ and $SU(2)$ time-dependent quantum systems

We now want to apply the results of the previous section to the extensively studied [7–10] time-dependent $SU(1, 1)$ and $SU(2)$ quantum systems, described by the Hamiltonian

$$H(t) = \omega(t)K_0 + G(t)\left(K_+\mathrm{e}^{\mathrm{i}\varphi(t)} + K_-\mathrm{e}^{-\mathrm{i}\varphi(t)}\right) \quad (3.1)$$

where $\omega(t)$, $G(t)$, and $\varphi(t)$ are functions of time. K_0 is a Hermitian operator, while $K_+ = (K_-)^+$. The commutation relations of the operators are

$$\left[K_0, K_\pm\right] = \pm K_\pm \qquad \left[K_+, K_-\right] = DK_0. \quad (3.2)$$

The Lie algebra of $SU(1, 1)$ and $SU(2)$ consists of the generators K_0 and $K_\pm$ corresponding to $D = -2$ and 2 in the commutation relations (3.2), respectively.

Since the time evolution operator $\mathcal{U}$ can be expressed as an exponential of linear combination of Lie algebra of $SU(1, 1)$ and $SU(2)$ generators and can also be factorized in a variety of ways [8, 11], it is natural to consider our $V(t)$ in the form

$$V(t) = \exp\left\{\frac{\lambda(t)}{2}\left(K_+\mathrm{e}^{-\mathrm{i}\beta(t)} - K_-\mathrm{e}^{\mathrm{i}\beta(t)}\right)\right\} \quad (3.3)$$

that corresponds to the coherent states generator of the $SU(1, 1)$ and $SU(2)$ Lie algebras [12]. The functions $\lambda(t)$ and $\beta(t)$ are arbitrary real time-dependent parameters. If we now choose as basis vectors the eigenstate $|n\rangle$ of K_0, i.e. $(K_0|n\rangle = k_n|n\rangle)$ and writing the test vector as $|\psi(t)\rangle = \sum_n C_n(t) V(t) |n\rangle$, then, with the results (2.8) and (2.9) in mind, one gets

$$C_n(t) = C_n(0)\exp\left[-\mathrm{i}\int_0^t \mathrm{d}t\, D\left(\frac{\omega}{D} + (\dot{\beta} - \omega)\frac{4}{g^2}\sin^2\frac{g}{4}\lambda - \frac{2}{g}G\sin\frac{g}{2}\lambda\cos(\varphi + \beta)\right)\right] \quad (3.4)$$

and the complement (equation (2.9)) to this equation gives the auxiliary equations by which λ and β are determined for given values of G, φ and ω,

$$\begin{aligned}\dot{\lambda} &= 2G\sin(\varphi + \beta)\\ \frac{-\omega - \dot{\beta}}{g}\sin\frac{g}{2}\lambda &= G\cos\frac{g}{2}\lambda\cos(\varphi + \beta)\end{aligned} \quad (3.5)$$

where $g = \sqrt{2D}$. In the derivation of equations (3.4) and (3.5) use is made of commutation relations (3.2) and of the following identities:

$$V^+ K_+ V = K_+ \cos^2 \frac{g}{4}\lambda - K_- e^{2i\beta} \sin^2 \frac{g}{4}\lambda - \frac{D}{g} K_0 e^{i\beta} \sin \frac{g}{2}\lambda$$

$$V^+ K_- V = K_- \cos^2 \frac{g}{4}\lambda - K_+ e^{-2i\beta} \sin^2 \frac{g}{4}\lambda - \frac{D}{g} K_0 e^{-i\beta} \sin \frac{g}{2}\lambda$$

$$V^+ K_0 V = K_0 \cos \frac{g}{2}\lambda + \frac{1}{g}\left(K_+ e^{-i\beta} + K_- e^{i\beta}\right) \sin \frac{g}{2}\lambda$$

$$iV^+ \frac{\partial V}{\partial t} = -2K_0 \dot\beta \sin^2 \frac{g}{4}\lambda + K_+ e^{-i\beta}\left(i\frac{\dot\lambda}{2} + \frac{\dot\beta}{g}\sin\frac{g}{2}\lambda\right) + K_- e^{i\beta}\left(-i\frac{\dot\lambda}{2} + \frac{\dot\beta}{g}\sin\frac{g}{2}\lambda\right).$$

(3.6)

The auxiliary equations (3.5) can be easily linearized by the following changes of variables $(2/g)tg(\lambda g/4)e^{-i\beta} = \{ig^2\dot q e^{i\varphi}\}/\{G\,q\}$ which reduces the problem to finding a complex function $q(t)$ solution of the following second-order linear differential equation:

$$\ddot q - \left\{\frac{\dot G}{G} - i(\dot\varphi + \omega)\right\}\dot q + \frac{4}{g^2}G^2 q = 0 \qquad (3.7)$$

which is in fact crucial for solving the exact quantum evolution. This is the equation of motion for a time-dependent generalized damped oscillator [13] when $g = \pm 2$ ($SU(2)$ systems). But when $g = \pm 2i$ ($SU(1, 1)$ systems) this equation corresponds to the time-dependent generalized inverted damped oscillator [14]. Here the friction is imaginary, $1/G$ and G^2 correspond to the mass and the frequency, respectively. We can see that the solution of the quantum problem may be solved either in terms of the classical solution of the equation of motion associated with the generalized Caldirola–Kanai Hamiltonian, or associated to the inverted one. After solving this equation, its solution $q(t)$ gives $\lambda(t)$ and $\beta(t)$. As a matter of practical interest we assume that $\varphi(t)$ has the form

$$\varphi(t) = -\int_0^t dt'\,\omega(t') \qquad (3.8)$$

with this choice of φ equation (3.7) has the special solution

$$q(t) = q(0)\cos\left(\int_0^t \frac{2G}{g}\,dt + \theta_0\right) \qquad (3.9)$$

and consequently

$$\lambda(t) = \pm 2\int_0^t G(t')\,dt' \qquad \beta(t) = \mp\frac{\pi}{2} + \int_0^t dt'\,\omega(t'). \qquad (3.10)$$

Substitution of (3.10) into (3.4) yields

$$C_n(t) = C_n(0)\exp\left[-ik_n\int_0^t dt'\,\omega(t')\right]. \qquad (3.11)$$

We shall now consider two special examples, the bosonic realization of the $SU(1, 1)$ Lie algebra in terms of creation and annihilation operators a^+ and a:

$$K_+ = \tfrac{1}{2}(a^+)^2 \qquad K_- = \tfrac{1}{2}(a)^2 \qquad K_0 = \tfrac{1}{2}(a^+a + \tfrac{1}{2}) \qquad (3.12)$$

and the realization of the $SU(2)$ Lie algebra in terms of spin operators J

$$K_\pm = J_\pm \qquad K_0 = J_3. \qquad (3.13)$$

In fact, $\langle n|K_0|n\rangle$ should be substituted by $n + 1/2$ or $n + 3/4$ in the boson realization of $SU(1, 1)$ Lie algebra (3.12) and by n in the realization of $SU(2)$ Lie algebra (3.13). If the characteristic parameters G, ω are constant and $\varphi = -\omega t$, the first example reduces to a well

known model in nonlinear quantum optics, namely the degenerate parametric oscillator with classical pumps, and the second to a familiar model in magnetic resonance, a particle with spin J in a magnetic field which consists of a static field along the z-axis plus a time-dependent rotating one perpendicular to it with frequency ω. Therefore, the exact quantum solution can be obtained from the classical solutions (3.8) and (3.9) as

$$q(t) = q(0) \cos((2G/g)t + \theta_0) \qquad \lambda(t) = \pm 2\, Gt \qquad \beta(t) = \mp \frac{\pi}{2} + \omega t \qquad (3.14)$$

for both $SU(1, 1)$ and $SU(2)$ systems depending on $D = \pm 2$.

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