The Leading Order of the Theory of Strong Perturbations in Quantum Mechanics

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Abstract

We prove that, for a quantum system that undergoes a strong perturbation, the solution of the leading order equation of the strong field approximation (M. Frasca, Phys. Rev. A, 45, 43 (1992)) can be derived by the adiabatic approximation. In fact, it is shown that greatest is the perturbation and more similar the quantum system is to an adiabatic one, the solution being written as a superposition of eigenstates of the time-dependent perturbation. A direct consequence of this result is that the solution of the Schrödinger equation in the interaction picture, in the same approximation for the perturbation, coincides with the one of the leading order of the strong field approximation. The limitation due to the requirement that the perturbation has to commute at different times is so overcome. Computational difficulties could arise to go to higher orders. Beside, the method is not useful for perturbations that are constant in time. In such a case a small time series is obtained, indicating that this approximation is just an application to quantum mechanics of the Kirkwood-Wigner expansion of statistical mechanics. The theory obtained in this way is applied to a time-dependent two-level spin model, already considered for the study of the Berry’s phase, showing that a geometrical phase
could arise if a part of the hamiltonian is considered as a strong perturbation. No adiabatic approximation is taken on the parameters of the hamiltonian, while their cyclicity is retained.
1 Introduction

In a series of papers, I proposed a new perturbation approach to cope with quantum systems that experience the effect of a large time-dependent perturbation [1]. The main computational limitation that appears is originating from the leading order equation that can be written as

$$V(t)|\psi> = i\hbar \frac{d|\psi>}{dt},$$

being $V(t)$ the perturbation. A general solution for this equation does not exist unless we take $[V(t), V(t')] = 0$. This condition appears to limit the usefulness of the method to some simple systems. Actually, the situation is a little more favourable than it does not seem at a first view. We will see in a moment that the main trick to derive the perturbation series in [1], i.e. rescaling the time variable, can change the situation.

In fact, the leading order equation should be more correctly written as

$$\lambda V(t)|\psi(t)> = i\hbar \frac{d|\psi(t)>}{dt},$$

being $\lambda$ the parameter taken to run away to infinity as in [1]. In such conditions we are able to find, in any case except computational difficulties, an approximate solution to the above equation, that agrees with the strong field approximation proposed in [1], as the above equation is identical to the one of ref.[2] to prove the adiabatic theorem of quantum mechanics. To see that
this is indeed the case, with the rescaling proposed in [1] of the time variable, i.e. \( t \rightarrow \lambda t = \tau \), one gets

\[
V(\frac{\tau}{\lambda})|\psi(\frac{\tau}{\lambda})> = i\hbar \frac{d|\psi(\frac{\tau}{\lambda})>}{d\tau}
\]  \hspace{1cm} (2)

that shows as \( \lambda \), the perturbation strength, is a natural time-scale for the change of both the Hamiltonian and the wave-function. For very large \( \lambda \), the variation is very slowly and we can invoke the adiabatic approximation.

In the following we will use the no-rescaled equation as, in such a way, we are able to see directly the approximation involved. The main physical point is that the stronger the perturbation, the more indistinguishable the quantum system is from an adiabatic one. This result also gives a general approach to cope with equations in the form \( \lambda L(t)u(t) = \frac{du(t)}{dt} \), being \( \lambda \) a very large parameter and \( L(t) \) an operator depending on the parameter \( t \) and acting on the vector \( u(t) \). To our knowledge, in literature, the adiabatic theorem has never been presented from this point of view.

Some computational difficulties could arise when one tries to go to higher orders. This problem originates from the fact that the eigenstates of the perturbation are time-dependent. We hope to treat this limitation in a future paper, but we are however beyond the strong limitation discussed above.
An important case is the one of a time-independent perturbation. Here we face a difficulty of the method as we are able to get just a small time series. This difficulty is simply indicating that we are applying the high-temperature Wigner-Kirkwood method of statistical mechanics to quantum systems. However, such kind of limitations are typical of perturbation methods as one can see from the standard small-perturbation approach applied to a simple two-level model.

The paper is so structured. In sec.2 we present the derivation of the adiabatic theorem for strongly perturbed quantum systems and show that, in the interaction picture, the solution, for a large perturbation, can be written in the same form as for the strong field approximation. In sec.3 we consider the case of a time-independent perturbation showing that here we face a small-time development. In sec.3 we apply our result to a two-level model showing that if a part of the Hamiltonian can be considered as a large perturbation then a Berry’s phase arises as computed in [3] for the adiabatic analog of the perturbation part of the considered system.
2 A Derivation of the Adiabatic Approximation from a New Point of View

For our aims we consider the following Schrödinger equation

\[ \lambda H(t)\psi = i\frac{d\psi}{dt} \]  \hspace{1cm} (3)

having \( \lambda \to \infty \) and \( H(t) \) a time-dependent hamiltonian typical of the considered quantum system. Here and in the following we set \( \hbar = 1 \). In order to show clearly the approximations involved, we do not operate the rescaling \( t \to \lambda t \). Instead, let us make the ansatz as in the adiabatic approximation

\[ |\psi \rangle = \sum_{n} c_n(t)e^{i\gamma_n(t)}e^{-i\lambda \int_{t_0}^{t} E_n(t')dt'} |n; t\rangle \] \hspace{1cm} (4)

being

\[ H(t)|n; t\rangle = E_n(t)|n; t\rangle \] \hspace{1cm} (5)

and

\[ \dot{\gamma}_n = <n; t| i\frac{d}{dt} |n; t\rangle. \] \hspace{1cm} (6)

The probability amplitudes, \( c_n(t) \) are to be found. By a direct substitution of eq.(4) into eq.(3) one gets

\[ \dot{c}_m(t) = - \sum_{n \neq m} e^{i[\gamma_n(t) - \gamma_m(t)]}e^{-i\lambda \int_{t_0}^{t} \Omega_{nm}(t')dt'} < m; t| i\frac{d}{dt} |n; t\rangle c_n(t) \] \hspace{1cm} (7)
that is the sought equation to find the probability amplitudes. We have set

\[ \Omega_{nm}(t) = E_n(t) - E_m(t). \]

The standard approach to obtain a set of solutions to eq. (7) is to put it in integral form and iterate by taking, at the leading order, the probability amplitudes at the initial time \( t_0 \). In the limit \( \lambda \to \infty \) we have again the adiabatic approximation, that is \( c_m(t) \approx c_m(t_0) \).

In fact, at the next order, one has to evaluate the integral

\[
I_{nm}(t) = \int_{t_0}^{t} e^{i[\gamma_n(t') - \gamma_m(t')]} e^{-i\lambda \int_{t_0}^{t'} \Omega_{nm}(t'') dt''} <m; t'\mid \frac{d}{dt} \mid n; t' > dt' \quad (8)
\]

that, in the limit \( \lambda \to \infty \), has a strongly oscillating exponential. In such a case we recognize the same situation as in ref. [2] for the adiabatic theorem and we have that the integral goes to 0 at least as \( \frac{1}{\sqrt{\lambda}} \), if the energy levels cross (for a more rigorous mathematical approach to the asymptotic evaluation of integrals we refer back to refs. [4]). Then, we can conclude that the adiabatic approximation is a very good one for eq. (3).

The main problem one has to face with such a result, when applied to strongly perturbed quantum system, is the computational difficulty that arises trying to go to higher orders. This is due to the fact that, differently from the small-perturbation approach, the states are time-dependent. So, the equations derived in [1] for the strong field approximation could not be
easily solvable. Beside, our derivation does not exclude a time-independent perturbation. But, as already showed in [1], a constant perturbation gives rise to terms that depends on power of time, that is, we face a small-time development. Our aim in the next section will be just to give an indication that, at least in a simple case, the series is the quantum analog of the Kirkwood-Wigner approximation of statistical mechanics.

An interesting result we can obtain from the above discussion is that the interaction picture, for a very large perturbation, yields the same result as the leading order of the strong field approximation. So, let us consider a system with a hamiltonian $H(t) = H_0 + \lambda V(t)$ with $\lambda \to \infty$. In the interaction picture we will have

$$U^+ \lambda V(t) U \ket{\psi_I} = i \frac{d \ket{\psi_I}}{dt}$$

(9)

with

$$H_0 U = i \frac{d U}{dt}$$

(10)

and $\ket{\psi} = U \ket{\psi_I}$. By the conclusion drawn above, the solution of eq.(9) can be written down as

$$\ket{\psi_I} \approx \sum_n c_n(t_0) e^{i \gamma_n^I(t)} e^{-i \lambda \int_{t_0}^t v_n^I(t') dt'} \ket{n; t > I}$$

(11)
being

\[ U^+ V(t) U |n; t > = v_n^I(t) |n; t > \] (12)

and

\[ \dot{\alpha}_n(t) = <n; t| U_H^t |n; t >. \] (13)

It is not difficult to see that eq.(12) can be rewritten as

\[ V(t)(U|n; t >) = v_n^I(t)(U|n; t >) \] (14)

that shows that \( U|n; t > \) is an eigenstate of \( V(t) \). So, using the equation \( V(t)|n; t > = v_n(t)|n; t > \), we can make the identifications \( v_n^I(t) = v_n(t) \) and

\[ U|n; t > = e^{i\alpha_n(t)}|n; t > \] (15)

being the phase \( \alpha_n(t) \) to be determined. This can be accomplished by computing explicitly eq.(13) using eq.(13) yielding

\[ \dot{\alpha}_n(t) = <n; t| U_H^t |n; t > = - <n; t|H_0|n; t > \] (16)

and \( \dot{\gamma}_n(t) = <n; t| U^{t'}_H |n; t > = \dot{\gamma}_n(t) \). The final result is then

\[ |\psi > \approx \sum_n c_n(t_0)e^{i\gamma_n(t)}e^{-i \int_{t_0}^t dt' [\langle <n; t'|H_0|n; t' > + \lambda v_n(t')]}|n; t >. \] (17)

This will be a solution of eq.(1) if the term \( <n; t|H_0|n; t > \) can be neglected respect to \( v_n(t) \). This can happen by a very large perturbation. For an application of this result we refer back to ref.[5].
3 The Time-Independent Perturbation and the Kirkwood-Wigner Expansion

In order to see the relation between the theory of strong perturbations and the Kirkwood-Wigner series of statistical mechanics, we consider a one-dimensional particle of mass $m$ moving on a segment of length $L$. This particle undergoes the effect of a potential $V(x)$, so that we consider the Schrödinger equation

$$i\frac{\partial \psi(x,t)}{\partial t} = -\frac{1}{2m} \frac{\partial^2 \psi(x,t)}{\partial t^2} + V(x)\psi(x,t)$$

(18)

with the initial condition $\psi(x,0) = \frac{1}{\sqrt{L}}$. It is quite easy, using the result of re.[1], to get till first order

$$\psi(x,t) = \frac{1}{\sqrt{L}} \left\{ 1 - i \frac{t^3}{6m} [V'(x)]^2 + \frac{t^2}{4m} V''(x) \right\} e^{-itV(x)}$$

(19)

where we see the polynomial dependence on $t$ that makes meaningless the series for very long time. But, if we make the substitution $it = \beta = \frac{1}{k_BT}$, with $k_B$ the Boltzmann constant, we recover the series in ref.[6], that is, the Kirkwood-Wigner expansion. This is an indication that we are applying the same approximation in quantum mechanics, giving some insight into the
strongly perturbed quantum systems. It should also be clear that a direct
application of our above results to this case can cause some difficulties.

4 An Application: Berry’s Two-level Model

As an example, we consider the one used by Berry in [3]

\[ H(t) = \frac{1}{2}(X(t)\sigma_X + Y(t)\sigma_Y + Z(t)\sigma_Z) \]  

being \( \sigma_X, \sigma_Y, \sigma_Z \) the Pauli matrices and now we just retain the cyclicity of
the parameters \( X, Y \) and \( Z \) while no adiabatic hypothesis is made. If we
have as a strong perturbation the following part of the hamiltonian

\[ V(t) = \frac{1}{2}(X(t)\sigma_X + Z(t)\sigma_Z), \]

we will fall in the same case as considered in [3], that is, due to the above
results, the quantum system acquires a Berry’s phase on a cycle given by \( \pi \)
and the wave function changes sign on a full cycle of the parameter space.
This effect could easily be put to a test.
5 Conclusions

We have seen that the class of strongly perturbed system can be enlarged because, as the perturbation becomes stronger, the quantum system approaches even more an adiabatic one. So, the adiabatic approximation can be applied. We have also pointed out that our approximation can be an application to quantum mechanics of the Kirkwood-Wigner expansion of statistical mechanics. Beside, a fairly interesting example concerns the Berry’s phase. A geometrical phase could appear for a strongly perturbed quantum system as in the example given in the above section. To conclude we stress that this enlargement of applicability of the adiabatic theory could solve some interesting problems of field theory and quantum chaos, giving some new and unexpected results.
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