Level Crossings, Adiabatic Approximation, and Beyond

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We present an analysis of the phenomena occurring whenever a level crossing is encountered. Besides Landau-Zener transitions and the quantum nonintegrable phase, fractionalization of quantum numbers and chaotic behavior emerge as intrinsically intertwined phenomena.

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In the analysis of essentially any complex system one identifies one way or another the slow and fast degrees of freedom and the subsequent discourse continues using these concepts. However, problems arising from the occurrence of so-called level crossings are not yet understood and solved in a satisfactory manner. Hill and Wheeler [1] gave a rather detailed discussion of the effects which might occur if a level crossing is encountered during the time evolution of the slow (collective) variables. Near such a configuration one often describes the behavior in terms of the well-known Landau-Zener transition. However, not so long ago another phenomenon, the so-called molecular Aharonov-Bohm effect [2] or Berry's nonintegrable quantum phase [3], was put in evidence. It is peculiar that two such remarkable phenomena occur under similar circumstances. More attention should be paid to level crossings than usually is done; at least one reason is that they are encountered very often [1,4–6]. Dissipation and the ever elusive quantum chaos are likely to be manifested due to the existence of real or avoided level crossings. On the other hand, the standard theory of (large amplitude) collective motion [7] never explicitly treats these phenomena, even though microscopically computed quantities (inertial parameters, potential energy) are rapidly varying or singular in the vicinity of avoided or real level crossings. We analyze in this paper a very simple model, which, in spite of its simplicity, embodies the essential physics of the phenomena taking place at or near a level crossing.

Let us assume that there are three slow degrees of freedom $\mathbf{Q},\mathbf{P}$, whose motion is governed by the Hamiltonian

$$H=\frac{\mathbf{P}^2}{2M}+\frac{M\omega^2\mathbf{Q}^2}{2}, \tag{1}$$

with a large mass and small angular frequency. Most of the time we will treat the slow variables as classical; however, this approximation can be easily improved to either the semiclassical level or even the quantum level if necessary. On the other side, the fast degrees of freedom will be treated in a reduced two-dimensional Hilbert space by the Hamiltonian

$$h=\tfrac{1}{2}\kappa\mathbf{Q}\cdot\boldsymbol{\sigma}, \tag{2}$$

where κ is a coupling constant and $\boldsymbol{\sigma}$ are the usual Pauli matrices. This particular form of the Hamiltonian(s) will not restrict the generality of our conclusions. The standard approach is the Born-Oppenheimer approximation. Let us assume that the slow degrees of freedom evolve as

$$\mathbf{Q}(t)=Q_0(\sin(\omega t),0,\cos(\omega t)). \tag{3}$$

We have chosen this particular form for two reasons: (i) one can solve exactly the time-dependent Schrödinger equation [8,9] and (ii) in this case Berry's gauge potential is identically zero, even though the quantum nonintegrable phase is nonvanishing. Formally, the quantum problem is identical to the motion of a spin $\frac{1}{2}$ in a uniformly rotating magnetic field in the x-z plane. We shall represent the quantum state by the density matrix ρ,

$$\rho=\frac{1}{2}\begin{pmatrix}1+z & x-iy\\ x+iy & 1-z\end{pmatrix}, \tag{4}$$

where $\mathbf{r}=(x,y,z)=\mathrm{Tr}(\rho\boldsymbol{\sigma})$ is real, with $r^2=x^2+y^2+z^2\le 1$ (equality for the case of a pure state only, $\rho^2=\rho$). Assuming that initially $z=1$ and constructing the solution of the time-dependent equation $i\dot\rho=[h,\rho]$ as a power series in t, one readily obtains that

$$x(t)\simeq\tfrac{1}{6}\omega t^3,\quad y(t)\simeq-\tfrac{1}{2}\omega t^2,\quad z(t)\simeq1-\tfrac{1}{8}\omega^2t^4, \tag{5}$$

if $\kappa Q_0=1$ (this amounts only to a redefinition of the time scale), which should be compared with the standard Born-Oppenheimer approximation,

$$[h,\rho]=0\rightarrow\mathbf{r}(t)=(\sin(\omega t),0,\cos(\omega t)),$$

$$x(t)\simeq\omega t,\quad y(t)\equiv0,\quad z(t)\simeq1-\tfrac{1}{2}\omega^2t^2. \tag{6}$$

The difference between Eqs. (5) and (6) is at least unexpected. Instead of following the driving field, the quantum state lags behind, and moreover it moves in the Hilbert space at first into an unexpected direction (y). The exact solution is in this case

$$x(t)=\sin(\omega t)+\left\{-\frac{\omega^2}{\Omega^2}\sin(\omega t)-\frac{\omega}{2\Omega^2}\left[\frac{\sin(\Omega+\omega)t}{\Omega+\omega}+\frac{\sin(\Omega-\omega)t}{\Omega-\omega}\right]\right\}, \tag{7a}$$

$$y(t)=\frac{\omega}{\Omega^2}[\cos(\Omega t)-1], \tag{7b}$$

$$z(t)=\cos(\omega t)+\left\{-\frac{\omega^2}{\Omega^2}\cos(\omega t)-\frac{\omega}{2\Omega^2}\left[\frac{\cos(\Omega+\omega)t}{\Omega+\omega}-\frac{\cos(\Omega-\omega)t}{\Omega-\omega}\right]\right\}, \tag{7c}$$

where $\Omega^2=1+\omega^2$. One can characterize the motion of $\mathbf{r}$ as precession (with frequency ω) plus nutation (with frequency Ω). One would expect that the adiabatic time-dependent Hartree-Fock (ATDHF) theory [7] shall apply if $\omega \ll 1$ (the splitting between the two levels in these units is exactly 1 for $\omega \to 0$). In Ref. [7] it was shown that one can define collective coordinates and momenta by introducing the following representation of the density matrix: $\rho=\exp(i\chi)\rho_0\exp(-i\chi)$, where both ρ_0 (generalized coordinate) and χ (generalized momentum) are Hermitian and time even. In the present case $[r=1,\ r_0=(x^2+z^2)^{1/2}]$,

$$\rho_0=\frac{1}{2r_0}\begin{pmatrix} r_0+z & x \\ x & r_0-z \end{pmatrix},\quad \chi=\frac{\arcsin(y)}{2r_0}\begin{pmatrix} -x & z \\ z & -x \end{pmatrix}. \tag{8}$$

Even though the collective velocity is small when $\omega \ll 1$, its frequency is of order Ω [the collective velocity is proportional to $y(t)$]. Similarly, the collective coordinate ρ_0 has high-frequency components beyond the zeroth order in ω. Also, as one can see from Eqs. (7) and (8), a straightforward expansion in ω is meaningless (one cannot simply retain terms of up to order ω^2), since the slow and fast modes are intertwined in a nontrivial way. In studying the collective motion, one is interested in situations where $\omega t \sim 1$, which enters in a rather complicated way into the arguments of the trigonometric functions. In the ATDHF theory there is, however, a rather subtle prescription on how to pick the "collective path" [7]. Instead of the equation $[h,\rho_0]=0$, one should solve a slightly modified one (cranked Hartree-Fock). [We tacitly assume that such a procedure was already used to "derive" the collective Hamiltonian in Eq. (1). Consequently, our disucssion applies, in particular, to the interaction between the ground state and one excited band or two excited bands near a funnel [1] or a diabolical point [3].] In the present case this amounts to going to the rotating frame, i.e., $[h-\omega/2\sigma_y,\rho_0]=0$. For such a choice of the collective path the amplitude of "nutation" is vanishing and the "spin" is enslaved by the "magnetic field," but is slightly out of the x-z plane (see the similar case treated in Ref. [9]).

The above solution deserves a lengthier analysis. We shall only mention that the Landau-Zener effect comes from the solution of a similar problem with the only difference being that one considers one slow coordinate and one pass near the level crossing, which will correspond to such situations as fission and dissociation. Our analysis is characteristic of bound collective motion instead. We shall now proceed to the analysis of the full system, i.e., coupled slow and fast degrees of freedom. For the sake of simplicity of the analysis, we shall assume that the motion of our system is governed by the Hamiltonian

$$H=\tfrac{1}{2}(\mathbf{P}^2+\mathbf{Q}^2)+\tfrac{1}{2}\mathbf{Q}\cdot\boldsymbol{\sigma}. \tag{9}$$

Constants like the inertial parameters of the slow variables, ω,κ, can be absorbed easily into $\mathbf{Q}$, $\mathbf{P}$, and t through an appropriate redefinition of the units and canonical transformations. The fact that the coupling $\mathbf{Q}\cdot\boldsymbol{\sigma}$ vanishes at the same point where the potential $\mathbf{Q}^2/2$ is centered can be easily modified, as well as the form of the coupling and/or of the potential, without essentially modifying our subsequent discussion. If one treats the slow variables as classical, the equations of motion for this system can be derived from the following Lagrangian [10]:

$$\mathcal{L}=\mathbf{P}\cdot\dot{\mathbf{Q}}+\frac{z(x\dot{y}-y\dot{x})}{2(x^2+y^2)(x^2+y^2+z^2)^{1/2}} -[\tfrac{1}{2}(\mathbf{P}^2+\mathbf{Q}^2)+\tfrac{1}{2}\mathbf{Q}\cdot\mathbf{r}]. \tag{10}$$

Here one can see the appearance of the "effective gauge field of a Dirac monopole" [10,11], which, when integrated over a closed loop, is the exact quantum nonintegrable phase [2,3], which modifies the Bohr-Sommerfeld quantization rules [9–12]. The equations of motion are

$$\dot{\mathbf{Q}}=\mathbf{P}, \tag{11a}$$

$$\dot{\mathbf{P}}=-\mathbf{Q}-\tfrac{1}{2}\mathbf{r}, \tag{11b}$$

$$\dot{\mathbf{r}}=\mathbf{Q}\times\mathbf{r}. \tag{11c}$$

In this form they can be thought of as fully quantum, if Eqs. (11a) and (11b) are interpreted as Heisenberg equations of motion for the corresponding operators (Eq. (11c) is already the Schrödinger equation $i\dot{\rho}=[h,\rho]$ in a disguised form). One can safely say that the above equations describe the "correct" time behavior of an arbitrary quantum system near a level crossing. It is easy to establish the existence of the following integrals of motion:

$$r=(x^2+y^2+z^2)^{1/2}, \tag{12}$$

$$E=\tfrac{1}{2}(\mathbf{Q}^2+\mathbf{P}^2)+\tfrac{1}{2}\mathbf{Q}\cdot\mathbf{r}, \tag{13}$$

$$\mathbf{J}=\mathbf{Q}\times\mathbf{P}+\tfrac{1}{2}\mathbf{r}. \tag{14}$$

In the case of a pure state for the fast variables, $r=1$ and the first integral of motion simply expresses the conservation of the norm of the wave function. The second integral of motion is nothing else but the total energy of the system. The last integral of motion has a most unusual structure. It looks like the angular momentum for the slow degrees of freedom, except for the last term. If the slow motion is quantized J is half integer. (If the fast modes are in a mixed state, then $r<1$ and consequently J becomes fractional and real.) J also has the right commutation relations expected from a total angular momentum operator. In the space (x,y,z) (or ρ_{kl} in other words) there is a well defined symplectic structure [10], the Poisson brackets are defined [10–13], and $\mathbf{r}/2$ behaves like an angular momentum quantity. Upon quantizing the slow variables one obviously obtains the right commutation relations for the "orbital" part of J, while for $\mathbf{r}/2$

one has to retain the "classical" commutation relations. However, one can (re)introduce the usual Pauli matrices instead of $\mathbf{r}$ as well.

These equations of motion display some unusual discrete symmetries. Time-reversal invariance can be defined in several ways:

$$(\mathbf{Q},\mathbf{P},\mathbf{r}) \rightarrow (-\mathbf{Q},\mathbf{P},-\mathbf{r}), \quad (15)$$

$$(Q_1,Q_{2,3},P_1,P_{2,3},x,y,z) \rightarrow (-Q_1,Q_{2,3},P_1,-P_{2,3},-x,y,z), \quad (16)$$

up to obvious permutations in Eq. (16). Parity invariance also can be defined in several ways:

$$(\mathbf{Q},\mathbf{P},\mathbf{r}) \rightarrow (\mathbf{Q},\mathbf{P},\mathbf{r}), \quad (17)$$

$$(Q_1,Q_{2,3},P_1,P_{2,3},x,y,z) \rightarrow (Q_1,-Q_{2,3},P_1,-P_{2,3},x,-y,-z), \quad (18)$$

with again obvious permutations in Eq. (18). It seems that the enumerated cases exhaust all possible situations.

A standard adiabatic solution of Eqs. (11) has as a conserved quantity only the orbital part of the angular momentum. This leads to the fact that the collective trajectory is planar. In the exact solution, the trajectory is no longer confined to a plane and can become chaotic. Chaoticity was observed in triatomic molecules, which are described by similar equations of motion, with the only distinction that there are only two slow degrees of freedom [14]. If one describes a situation where the collective trajectory never comes close to the level crossing, then $\mathbf{Q}$ dominates over $\mathbf{r}/2$ in Eq. (11b) and the orbital angular momentum is approximately equal to the total angular momentum. However, whenever a trajectory has a low impact parameter with respect to the level crossing, the orbital angular momentum can be comparable in magnitude with $\mathbf{r}/2$ and the trajectory becomes essentially chaotic. The normal to the instantaneous trajectory plane can be anywhere in a solid angle $\pi[2J-(4J^2-1)^{1/2}]/J$, if $J \geq \frac{1}{2}$, $r=1$, centered around $\mathbf{J}$.

Negele [15], in his imaginary-time-dependent Hartree-Fock analysis of the fission of ^{32}S into two ^{16}O nuclei, displays a collective path in the quadrupole-octupole space, which has exactly the type of characteristics one should expect, in the light of the present discussion, from the presence of a level crossing. To understand Negele's result one probably needs two collective degrees of freedom only. This will amount to replacing the vector $\mathbf{J}$ with its "third" component, if the Hamiltonian for the slow variables conserves the orbital angular momentum. In the absence of such a symmetry one still has to consider an equation of the type (11b) for the slow momenta, where the presence of "fast coordinates" will modify in an essential way the dynamics. As far as we are aware, this calculation is the only one available in the nuclear literature where the fast degrees of freedom were treated without any constraints and as a result the presence of the level crossing manifested itself in such a striking way.

We find it remarkable that so many features, namely, the Landau-Zener transitions, fractionalization of quantum numbers, occurrence of dynamically generated gauge fields (effective Dirac monopoles), and chaotic behavior, emerge in the framework of this approach. Even though most of the time we refer directly to nuclear dynamics, it should be obvious that our discussion covers a larger range of physical situations.

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