



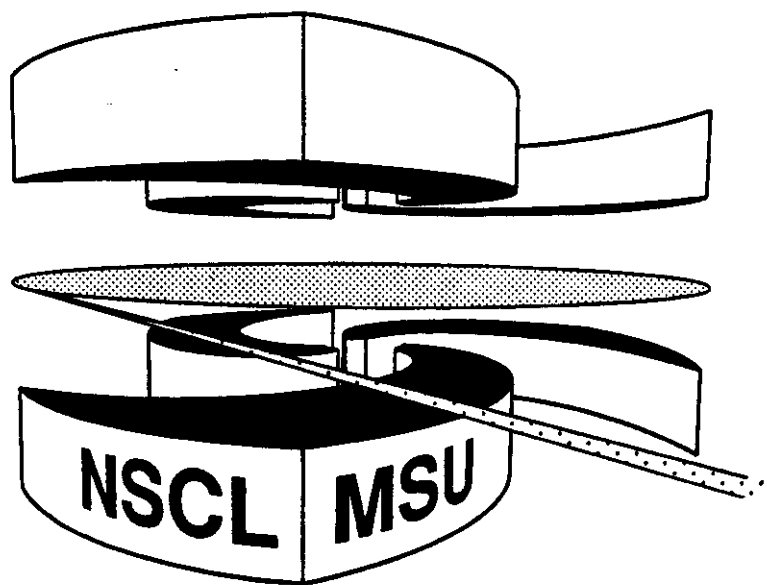
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**LEVEL CROSSINGS, EFFECTIVE GAUGE FIELDS,  
FRACTIONAL QUANTUM NUMBERS AND INSTABILITIES  
IN LARGE AMPLITUDE COLLECTIVE MOTION**

**Invited talk at "Symposium on Contemporary Physics"  
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*HAPPY BIRTHDAY ABE!*

Large Amplitude Collective Motion (LACM) theory is one subject to which Abe Klein has devoted a significant amount of his time. His recent Annals of Physics article with Niels R. Walet and Giu Do **Dang**, 208, 90 (1991) is a partial review of his and his collaborators' efforts towards solving one of the central and most difficult problems of LACM, the definition of the collective submanifold. I have been fortunate to work with him on this subject and to become one of his numerous friends. I hope that Abe will enjoy the subject I have chosen.

I shall argue here that band crossings play **a** crucial and far more subtle role in LACM than has been appreciated. The ultimate theory of LACM will have to include the dynamical effects arising from their presence. The fact that adiabaticity is violated near **a** level crossing is a textbook issue. In their classical paper [1], Hill and Wheeler **gave** a rather detailed analysis of the role of **Landau-Zener** transitions and advocated the use of **a** multisurface potential energy in the treatment **of** LACM. Similar problems arise **as** well in chemistry and condensed matter physics [2] and the presence of level crossings is linked with the onset of dissipation. In Ref. [3] I have suggested **a** similar picture, but also added a new element, dynamically generated gauge fields. Relatively recently it became evident that there is a rather unusual correction to the adiabatic theorem, the way everyone knows it from textbooks, the so-called Berry's phase. Berry and Mead [4] pointed out that gauge fields have to be added to the Born-Oppenheimer picture, whenever a level crossing is present, and that they might lead to some rather remarkable phenomena. Mead [4] coined the

term "Molecular Aharonov-Bohm effect" to designate this new class of phenomena. At the present, the prevailing attitude is that if a collective Hamiltonian can be derived it contains a kinetic energy term and a potential energy term. The Berry's phase phenomenon or the Molecular Aharonov-Bohm effect demands however, that one should introduce as well effective gauge potentials, which depending on the degree of sophistication of the theoretical approach could be either abelian or non-abelian [5]. It takes almost an insignificant change in the value of a collective variable to generate a band crossing [6].

I shall discuss now what happens at one isolated band crossing and to this end I shall introduce an idealized model, which, in spite of its simplicity, it embodies the essential physics of the phenomena taking place at or near a level crossing [7]. Let us assume that there are three slow degrees of freedom  $\mathbf{Q}$ ,  $\mathbf{P}$ , whose motion is governed by the Hamiltonian

$$H_0 = \frac{\mathbf{P}^2}{2M} + V(Q), \quad (1)$$

with a large mass and a relatively shallow potential. In particular, one can associate one variable with the quadrupole deformation and the other two with the real and imaginary parts of the pairing field. Most of the time I shall treat the slow variables as classical, however this approximation can be easily improved either at the semiclassical level or even quantum if necessary. Since I want to limit this analysis to an isolated band crossing only, e.g. the ground and an excited state bands, the fast degrees of freedom will be treated in a reduced two-dimensional Hilbert space by the Hamiltonian

$$h = \frac{1}{2} \kappa \mathbf{Q} \cdot \boldsymbol{\sigma}, \quad (2)$$

where  $\kappa$  is a coupling constant and  $\boldsymbol{\sigma}$  are the usual Pauli matrices.

Now let us compare this with the Born-Oppenheimer approximation for a simple situation, when the slow degrees of freedom evolve as  $\mathbf{Q}(t) = Q_0(\sin(\omega t), 0, \cos(\omega t))$ . Formally, the quantum problem is identical to the motion of a spin 1/2 in a uniformly rotating magnetic field in the  $xz$ -plane. I shall represent the quantum state by the density matrix  $\rho$

$$\rho = \frac{1}{2} \begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix}, \quad (3)$$

where  $\mathbf{r} = (x, y, z) = Tr(\rho\sigma)$  are real, with  $r^2 = x^2 + y^2 + z^2 \leq 1$  (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  $i\dot{\rho} = [h, \rho]$  one readily obtains that

$$x(t) = \sin(\omega t) + \left\{ -\frac{\omega^2}{\Omega^2} \sin(\omega t) - \frac{\omega}{2\Omega^2} \left[ \frac{\sin(\Omega + \omega)t}{\Omega + \omega} + \frac{\sin(\Omega - \omega)t}{\Omega - \omega} \right] \right\}, \quad (4a)$$

$$y(t) = \frac{\omega}{\Omega^2} [\cos(\Omega t) - 1], \quad (4b)$$

$$z(t) = \cos(\omega t) + \left\{ -\frac{\omega^2}{\Omega^2} \cos(\omega t) - \frac{\omega}{2\Omega^2} \left[ \frac{\cos(\Omega + \omega)t}{\Omega + \omega} - \frac{\cos(\Omega - \omega)t}{\Omega - \omega} \right] \right\}, \quad (4c)$$

if  $\kappa Q_0 = 1$  (this amounts only to a redefinition of the time scale) and where  $\Omega^2 = 1 + \omega^2$ . The strictly adiabatic approximation is  $(x(t), y(t), z(t)) = (\sin \omega t, 0, \cos \omega t)$ . One can characterize the motion of  $\mathbf{r}$  as precession (with frequency  $\omega$ ) plus nutation (with frequency  $\Omega$ ). One would expect that the ATDHF theory [8] shall apply if  $\omega \ll 1$ . ATDHF theory requires terms of up to order  $\omega^2$  to be retained and it assumes that they are slowly varying functions of time. In Refs. [8] 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  $\rho_0$  (generalized coordinate) and  $\chi$  (generalized momentum) are hermitian and time-even. In the present case ( $r = 1$ ,  $r_0 = \sqrt{x^2 + z^2}$ )

$$\rho_0 = \frac{1}{2r_0} \begin{pmatrix} r_0 + z & x \\ x & r_0 - z \end{pmatrix}, \quad \chi = \frac{\arcsin(y)}{2r_0} \begin{pmatrix} -x & z \\ z & x \end{pmatrix}. \quad (5)$$

Even though the collective velocity is small when  $\omega \ll 1$ , its frequency is of order  $\Omega$  (the collective velocity is proportional to  $y(t)$ ). Similarly, the collective coordinate  $\rho_0$  has high frequency components beyond the 0-th order in  $\omega$ . Also, as one can see from Eqs. (4), a straightforward expansion in  $\omega$  is meaningless (one can not simply retain terms of up to order  $\omega^2$ , as ATDHF theory implies), 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. The above simple formulas warn us that near a band crossing the dynamics might be more complicated than a simple minded adiabatic approximation might suggest.

If one treats the slow variables as classical, the equations of motion for this system can be derived from the following Lagrangian [7,9]

$$\mathcal{L} = \mathbf{P} \cdot \dot{\mathbf{Q}} + \frac{z(xy - yx)}{2(x^2 + y^2)\sqrt{x^2 + y^2 + z^2}} - \left[ \frac{\mathbf{P}^2}{2M} + V(Q) + \frac{1}{2}\kappa\mathbf{Q} \cdot \mathbf{r} \right]. \quad (6)$$

The second term is the gauge field of a Dirac monopole [4], which, when integrated over a closed loop, is the exact quantum nonintegrable phase, which modifies the Bohr-Sommerfeld quantization rule. The equations of motion are

$$\dot{\mathbf{Q}} = \frac{\mathbf{P}}{M}, \quad \dot{\mathbf{P}} = -\frac{\partial V(Q)}{\partial \mathbf{Q}} - \frac{1}{2}\kappa\mathbf{r}, \quad \dot{\mathbf{r}} = \kappa\mathbf{Q} \times \mathbf{r}. \quad (7a, b, c)$$

In this form they can be thought of as fully quantum, if Eqs.(7a,b) are interpreted as Heisenberg equations of motion for the corresponding operators (Eq. (7c) 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 behaviour of an arbitrary quantum system near a level crossing. It is easy to establish the existence of the following integrals of motion

$$r = \sqrt{x^2 + y^2 + z^2}, \quad E = \frac{\mathbf{P}^2}{2M} + V(Q) + \frac{\kappa\mathbf{Q} \cdot \mathbf{r}}{2}, \quad \mathbf{J} = \mathbf{Q} \times \mathbf{P} + \frac{1}{2}\mathbf{r}. \quad (8-10)$$

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 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/real.) This fractionalization of the quantum numbers is well-known in molecular spectra [10,11].

A standard Born-Oppenheimer approach to this model corresponds to assuming  $\mathbf{Q} \cdot \mathbf{r} = \pm Q$ , ( $r = 1$ ), i.e. the "spin" is enslaved by the "magnetic field". The equations of motion for the slow variables then read

$$\dot{\mathbf{Q}} = \frac{\mathbf{P}}{M}, \quad \dot{\mathbf{P}} = -\frac{\partial V_{\pm}(Q)}{\partial \mathbf{Q}} = -\left( \frac{\partial V(Q)}{\partial \mathbf{Q}} \pm \frac{\kappa\mathbf{Q}}{2Q} \right), \quad (11a, b)$$

where  $V_{\pm}(Q) = V(Q) \pm \kappa Q/2$  represent the two adiabatic potential surfaces, the lower one being a "Mexican hat". At this level the adiabatic approximation has several deficiencies:

- Instead of  $\mathbf{J}$  only  $\mathbf{L} = \mathbf{Q} \times \mathbf{P}$  is conserved. As a result the “classical collective trajectory” is confined to a plane.
- Even though in the exact treatment the force is everywhere defined and non-singular, in the Born-Oppenheimer approximation the force is singular at the origin.
- The Bohr-Sommerfeld quantization rule ( $\hbar = 1$ )  $\oint \mathbf{P} \cdot d\mathbf{Q} = 2(n + \alpha_M)\pi$  does not include the correction coming from the Berry’s phase.  $\alpha_M$  is the correction coming from turning points or the Maslov index.

One can try to improve upon this simple Born-Oppenheimer approximation by taking into account the induced Berry’s gauge potential into the Lagrangian. This amounts to replacing the Lagrangian in Eq. (6) by

$$\mathcal{L}_{BO} = \mathbf{P} \cdot \dot{\mathbf{Q}} \pm \frac{Q_3(Q_1\dot{Q}_2 - Q_2\dot{Q}_1)}{2(Q_1^2 + Q_2^2)\sqrt{Q_1^2 + Q_2^2 + Q_3^2}} - \left[ \frac{\mathbf{P}^2}{2M} + V(Q) \pm \frac{2\kappa Q}{2} \right], \quad (12)$$

which follows from assuming  $\mathbf{Q} \cdot \mathbf{r} = \pm Q$ , ( $r = 1$ ). The ensuing equations of motion are then

$$\dot{\mathbf{Q}} = \frac{\mathbf{P}}{M}, \quad \dot{\mathbf{P}} = - \left( \frac{\partial V(Q)}{\partial \mathbf{Q}} \pm \frac{\kappa \mathbf{Q}}{2Q} \pm \frac{\mathbf{Q} \times \mathbf{P}}{2MQ^3} \right). \quad (13a, b)$$

The main difference with Eqs. (11a,b) is in the presence of the induced “magnetic force”, arising from the “Dirac monopole” at the origin. Now  $\mathbf{P}$  and  $\mathbf{Q}$  are not canonical variables anymore. One can easily check that in this improved adiabatic approximation:

- The conserved total angular momentum is

$$\mathbf{J}_{BO} = \mathbf{Q} \times \mathbf{P} \pm \frac{\mathbf{Q}}{2Q}, \quad (14)$$

which is much closer to the truth. Due to this the classical collective trajectory is not confined to a plane anymore, similarly to the exact solution.

- The scalar potential force is identical to the one in standard Born-Oppenheimer approximation, but the “induced magnetic force” is even more singular at the

origin. However, since in the adiabatic approximation  $\kappa \rightarrow \infty$  and  $\dot{Q} \rightarrow 0$ , the role of the “magnetic force” is rather small, except in the immediate vicinity of the origin. The strength of this induced “magnetic force” is independent of  $\kappa$  and its role is merely to ensure the conservation of the “correct total angular momentum”. The fact that the strength of this induced “magnetic force” is independent of the coupling strength between the slow and fast degrees of freedom is obviously not a very pleasant feature. Its strength should somehow vanish when  $\kappa \rightarrow 0$  and increase in the opposite limit. This fact alone should shed strong doubts on the limits of validity of this improved adiabatic approximation, which has been widely discussed in the literature lately, in connection with the Berry’s phase phenomenon or the Molecular Aharonov-Bohm effect. This form of the effective magnetic field follows simply from the kinematical constraint imposed on the “spin” variables.

- The Bohr–Oppenheimer quantization rule now reads

$$\oint \left[ \mathbf{P} \cdot d\mathbf{Q} \pm \frac{Q_3(Q_1 dQ_2 - Q_2 dQ_1)}{2(Q_1^2 + Q_2^2)\sqrt{Q_1^2 + Q_2^2 + Q_3^2}} \right] = 2(n + \alpha_M)\pi, \quad (15)$$

and it includes the contribution from the Berry’s phase as it should. However, the range of validity of this formula is very likely limited (see above the comment).

One should expect this improved Born–Oppenheimer approximation to be valid only for extremely low potential energies, where the “spin” is almost perfectly antialigned with the “magnetic field” and the total energy is almost identical to  $V_-(Q)$ . This is a rather strong limitation for the purposes of LACM. Even though the potential  $V(Q)$  might be rather shallow, the amplitude of the motion is large and the potential energy  $V(Q)$  can undergo rather large variations. There is no reason to expect that along the collective trajectory the kinetic energy is always small. This amounts to the fact that the “spin” cannot remain antialigned with the “magnetic field” and strong deviations from the (improved) adiabatic approximation will occur.

The nonlinear coupling between the fast and slow degrees of freedom leads to chaotic trajectories [11,12]. I lack the space here to go into more details, but I want

to draw attention to a rather simple consequence of the chaotic behaviour. Since the slow and fast degrees of freedom seem to influence each other in a nontrivial way, one cannot expect that the Landau-Zener formula for the transition probability from one level to another to be applicable. The Landau-Zener probability is a monotonic function of the slow velocity and diabatic behaviour sets in rather quickly. In the presence of a strong chaotic source, the behaviour of the transition probability, or the population of the two levels ( $\rho_{11}$  and  $\rho_{22}$ ), will be extremely irregular functions of the asymptotic values of the energy (far from the band crossing). This should lead to a rather unusual character of the dissipation in LACM.

In Fig. 1 one has an example of a multisurface potential energy of a "realistic" nucleus (many-fermionic system), which undergoes large amplitude collective motion, not merely small amplitude vibrations around a local minimum. In particular, the potential energy of a fissioning nucleus will have a similar appearance. In a simplified picture, one can imagine that at each band crossing there is a "Dirac magnetic monopole". The "effective magnetic field" generated by each "monopole" is felt in the immediate neighborhood of each funnel or diabolic point mainly.

Let us assume that the motion starts with almost vanishing collective velocity near the top of the barrier towards the ground state configuration. Once it reaches the first band crossing, depending on the particular values of the collective coordinates and momenta and the population of the two adjacent bands, after passing past the funnel [1] or diabolical point [4], the system can end up in any state. In the absence of a "magnetic force" the system will most likely follow the valley of the lower potential energy surface. The "magnetic force" will however curve the trajectory (or even capture the system for a while) and at the same time the "spin" (which is related with the relative population of the two adjacent bands) can turn around. Near the funnel or diabolical point, the collective and intrinsic degrees of freedom are strongly coupled and the motion is essentially chaotic. One cannot expect either the adiabatic or the diabatic picture to be a truthful representation of the reality. An essential element is of course the fact that the collective motion is really multi-dimensional, one cannot limit the analysis to only one degree of freedom, since the "magnetic field" will propel the system into additional directions. The final picture



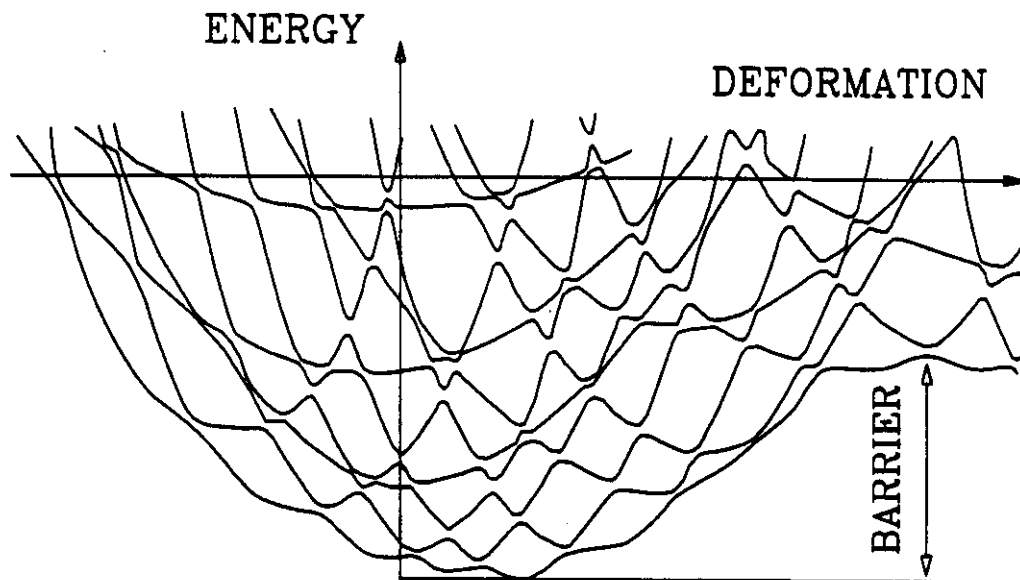


Figure 1: This figure has been adapted from W.Swiatecki, Nucl. Phys. A 488, 375 (1988). It represents the potential energy of a many-fermion system ("nucleus") as a function of one collective variable (e.g.  $\beta$ ). One can distinguish several intersecting parabolas, corresponding to different occupation numbers. Due to residual interactions (pairing, axial or octupole deformation, etc) instead of real crossings there are avoided band crossings. However, these avoided band crossings will become real band crossings when one will move into the direction of another collective variables at some point. One has to view this figure as a section of a multisurface potential energy for fixed collective variables, except one.

will be even more complicated by the fact that one has to consider actually the propagation of a packet of initial conditions, if the motion is really chaotic. In such a case quantum interference effects in the slow variables will also become important. The system can start near one band crossing and reach another one, after passing near several intermediate ones through a variety of paths. Then the interference among different trajectories should be included and (due to the essentially random distribution of funnels or diabolical points) very likely is destructive in character [2c]. The trajectory will also have a quite complicated pattern, since near every funnel or diabolical point, it will be bend or even forced to make a few turns. As a result the actual length of the trajectory can become very large and the time required to get away from the initial coordinates rather long. On a coarse scale it can appear as a random walk, in spite of the fact that very little dissipation is actually present. This is due to the fact that a system is very "unwilling" to get very far from an initial configuration, and not because it gets excited and there is a strong dissipation of the collective energy, but rather due to "Anderson localization", a characteristic behaviour of quantum particles in a random potential. The motion seems to be slower than one would expect, even though the nucleus might not get very excited by the time it reaches the potential minimum.

The number of essential elements entering this emerging picture and of related phenomena is truly astounding: i) one has to introduce several collective degrees of freedom; ii) one has to include a multisurface potential energy; iii) using a loose language, one has to introduce "effective magnetic fields"; iv) the motion becomes chaotic; v) interference phenomena should be properly taken into account for long trajectories; vi) the quantum numbers become fractional; vii) very likely, in a correct description one has to resort to a non-abelian gauge description; viii) dissipation or friction are likely much more intricate phenomena than we have suspected until now; ix) quasilocalization in collective coordinates; and the list seems simply to keep growing. The nice thing about all this range of phenomena is the obvious importance of the subject not only to nuclear physics but to chemistry, condensed matter physics, atomic clusters and likely field theoretical models as well.

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