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COMMENT

Cranking, adiabatic phases and monopoles

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Abstract. Lowest-order cranking about a principal axis breaks down for a system with non-zero $\langle J_z \rangle$ along its symmetry axis. Such a system should be cranked about an axis at an angle to the symmetry axis. This can be understood in terms of the Berry phase, which acts like the field of a magnetic monopole. Possible applications are discussed.

1. Introduction

In studying molecular, nuclear or field-theoretic systems it is often convenient to start with a deformed solution to a mean-field (or Hartree-Fock) approximation. The approximate solution breaks some of the symmetries of the Hamiltonian, for example, translations or rotations. Such symmetries mean that the deformed state will be degenerate. These degeneracies will show up as 'zero modes' in the quantum fluctuations about the mean-field solution.

Eigenstates of the symmetry operators can be constructed by projection: taking an appropriate linear combination of the degenerate deformed states. Alternatively, one can introduce collective coordinates corresponding to the broken symmetries and quantise these. (For reviews of these ideas in nuclear physics and field theory, see [1-3].)

Exact projection of a deformed state can be technically very complicated, especially if large numbers of particles are involved. Hence it is often simpler to use a 'cranking' approximation to calculate the energies of the symmetry eigenstates [1, 2]. This involves minimising the energy in a frame which is rotating about a principal axis of the system. However, we have found problems with cranking when the system has a non-vanishing expectation value for one of the symmetry generators. As we show in § 2, the lowest-order cranking equations then have no finite solutions. This can be avoided if one cranks about an axis at an angle to the symmetry axis. Villars has shown this within the framework of adiabatic TDHF [4]. Here we show that the same result can be obtained directly, by regarding cranking as an approximation to variation after projection [5].

This effect can be understood in terms of an additional contribution to the phase of the rotating state, coming from the overlaps between the deformed states. This is the 'Berry phase' [6]; it acts like the field of a magnetic monopole [7], producing velocity-dependent forces on the rotating system.

In § 3 we discuss the monopole analogy in more detail. A charged particle moving in the monopole field has an additional contribution to its angular momentum proportional to its radius vector relative to the monopole. This is analogous to the non-zero $\langle J_z \rangle$ along the symmetry axis. The minimum angular momentum of the charged particle can be related to the angular frequency of small cyclotron orbits about an axis close to the symmetry axis of the particle-monopole system.

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Based on this analogy, in § 4 we discuss further the cranking of a system with non-zero $\langle J_z \rangle$. The angle between the cranking and symmetry axes is to be regarded as a variational parameter of the wavefunction. We discuss the limits of large and small $\langle J_z \rangle$ and the relation to the usual cranking.

Finally, in § 5, we mention some possible applications of these ideas, in particular to systems with symmetry groups larger than SU(2).

2. Cranking

In the self-consistent cranking approximation one looks for a time-dependent solution to the mean-field equations of motion, where the solution moves with constant velocities in the collective coordinates. The dependence of the energy on these velocities gives the inertia parameters for the collective motions. Obviously this is a semiclassical approach; it should be a good approximation to projection when the overlaps between the deformed states are sharply peaked functions of the collective coordinates [5].

The solution of the time-dependent mean-field (TDMF) equations is equivalent to minimising the expectation value of the Hamiltonian in a moving frame. To illustrate the approach we consider a deformed system which breaks rotational invariance. We assume that the system has an axis of symmetry, which we take to be the z axis. To crank the system one minimises the energy in a frame rotating with constant angular velocity ω about a principal axis:

$$\langle H' \rangle = \langle H \rangle - \omega \langle J_x \rangle. \tag{2.1}$$

The moment of inertia can then be found from

$$\langle J_x \rangle = \mathcal{I} \omega. \tag{2.2}$$

The angular velocity acts as a Lagrange multiplier which should be adjusted to give

$$\langle J_x \rangle = [J(J+1)]^{1/2}. \tag{2.3}$$

To lowest order, the rotational spectrum is then given by

$$E_{\text{rot}} = \frac{1}{2\mathcal{I}} J(J+1). \tag{2.4}$$

This should be a good approximation provided ω is small enough for this, essentially adiabatic, treatment to be valid.

We have found problems with this approach when the system has non-zero $\langle J_z \rangle$ along the symmetry axis. There are no solutions to the TDMF equations where the system rotates slowly about a principal axis. The lowest-order cranking equations have no finite solutions.

To see how this arises, consider the lowest-order cranking equations. For a many-fermion system these have the form [1, 2]

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \delta\rho \\ \delta\rho^* \end{pmatrix} = \omega \begin{pmatrix} J_x^{(\text{ph})} \\ J_x^{(ph)*} \end{pmatrix} \tag{2.5}$$

where $\delta\rho$ is the first-order change in the single-particle density matrix, and $\boldsymbol{J}^{(\text{ph})}$ denotes the particle-hole matrix elements of the angular momentum. For a soliton one has a similar set of equations [8], with changes to the mean boson fields coupled in. The (Hermitian) matrix on the LHS of (2.5) is the 'stability matrix'; it is the linearised form of the mean-field equations of motion. It also appears in the RPA equations for small-amplitude oscillations about the mean field [1, 2, 9]:

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = \varepsilon\begin{pmatrix} X \\ -Y \end{pmatrix}. \tag{2.6}$$

The RPA equations have zero-energy solutions corresponding to the symmetries broken by the mean-field solution. In particular, there is one for rotation about the y axis,

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix}\begin{pmatrix} J_y^{(\mathrm{ph})} \\ -J_y^{(\mathrm{ph})*} \end{pmatrix} = 0. \tag{2.7}$$

Hence (2.6) will have no finite solutions if the inhomogeneous term has a non-zero overlap with the zero mode. This overlap has the form

$$\begin{aligned}(J_y^{(\mathrm{ph})}, -J_y^{(\mathrm{ph})*})\begin{pmatrix} J_x^{(\mathrm{ph})} \\ J_x^{(\mathrm{ph})*} \end{pmatrix} &= \langle J_y J_x\rangle - \langle J_y J_x\rangle^* \\ &= \langle [J_y, J_x]\rangle \\ &= -\mathrm{i}\langle J_z\rangle. \end{aligned} \tag{2.8}$$

From this we see that the problem will arise whenever $\langle J_z\rangle$ is non-zero.

Note that this does not show up in the usual treatment of the intrinsic states of diatomic molecules and deformed nuclei. There, states with $J_z = \pm K$ are degenerate and one can take the intrinsic state to be an equally weighted mixture [10, 11], with $\langle J_z\rangle = 0$.

It means that when one attempts to crank about a principal axis (e.g. the x axis) the system tries to realign the cranking axis by rotating about the y axis. The origin of this behaviour can be understood by examining the angle dependence of the overlaps between rotated deformed states.

Consider, for simplicity, an intrinsic state which is an eigenstate of J_z with $J_z = K$. The rotated states are

$$|\alpha, \beta, \gamma\rangle = \exp(-\mathrm{i}\alpha J_z)\exp(-\mathrm{i}\beta J_y)\exp(-\mathrm{i}\gamma J_z)|\Phi\rangle \tag{2.9}$$

in the usual convention [12]. Projection produces a symmetry eigenstate which is a linear combination of these:

$$|JM\rangle = \left(\frac{2J+1}{8\pi^2}\right)^{1/2}\int \mathrm{d}^3\Omega\; D^J_{M,K}(\alpha, \beta, \gamma)^*|\alpha, \beta, \gamma\rangle. \tag{2.10}$$

Note that, due to the symmetry of the intrinsic state about the z axis, the integrand is independent of the Euler angle γ. Hence γ has no physical significance; different choices of γ give different phases to the wavefunctions—they correspond to different choices of gauge. A convenient choice is $\gamma = -\alpha$, giving

$$|JM\rangle = \left(\frac{2J+1}{2}\right)^{1/2}\int \sin\beta\;\mathrm{d}\alpha\;\mathrm{d}\beta\; D^J_{M,K}(\alpha, \beta - \alpha)^*|\alpha, \beta, -\alpha\rangle. \tag{2.11}$$

The energy of a projected state is

$$\begin{aligned} E_J &= \frac{\langle JM|H|JM\rangle}{\langle JM|JM\rangle} \\ &= \frac{\int \mathrm{d}^3\Omega\;\mathrm{d}^3\Omega'\; D^J_{M,K}(\Omega)\langle\Omega|H|\Omega'\rangle D^J_{M,K}(\Omega')^*}{\int \mathrm{d}^3\Omega\;\mathrm{d}^3\Omega'\; D^J_{M,K}(\Omega)\langle\Omega|\Omega'\rangle D^J_{M,K}(\Omega')^*}. \end{aligned} \tag{2.12}$$

Provided this energy depends smoothly on J, one may expand the matrix element $\langle\Omega|H|\Omega'\rangle$ in terms of derivatives with respect to the Euler angles [5]. To second order, this gives

$$\langle\Omega|H|\Omega'\rangle=(a_0+a_i\mathscr{L}_i^{\text{int}}+a_{ij}\mathscr{L}_i^{\text{int}}\mathscr{L}_j^{\text{int}}+\ldots)\langle\Omega|\Omega'\rangle \tag{2.13}$$

where $\mathscr{L}_i^{\text{int}}$ denote the intrinsic angular momentum operators acting on the Euler angles Ω. The coefficients a_0, a_i are given by

$$\begin{aligned}&a_0=\langle\Phi|H-\boldsymbol{a}\cdot\boldsymbol{J}|\Phi\rangle\\&\langle\Phi|H\boldsymbol{J}|\Phi\rangle_{\text{c}}=\langle\Phi|(\boldsymbol{a}\cdot\boldsymbol{J})\boldsymbol{J}|\Phi\rangle_{\text{c}}\end{aligned} \tag{2.14}$$

in the notation of [2].

The usual arguments [5] can be extended straightforwardly to include a non-zero expectation value for J_z, as well as J_x. Keeping terms to first order in $\mathscr{L}_i^{\text{int}}$ one obtains

$$E_J\simeq\langle\Phi|H|\Phi\rangle+\omega_x\{[J(J+1)-K^2]^{1/2}-\langle\Phi|J_x|\Phi\rangle]+\omega_z[K-\langle\Phi|J_z|\Phi\rangle\}. \tag{2.15}$$

Hence the cranked intrinsic state can be found by varying

$$\langle\Phi|H'|\Phi\rangle=\langle\Phi|H-\omega_xJ_x-\omega_zJ_z|\Phi\rangle \tag{2.16}$$

with respect to $|\Phi\rangle$. The angular velocities should be adjusted to give

$$\begin{aligned}&\langle\Phi|J_x|\Phi\rangle=[J(J+1)-K^2]^{1/2}\\&\langle\Phi|J_z|\Phi\rangle=K.\end{aligned} \tag{2.17}$$

A system with non-zero $\langle J_z\rangle$ should thus be cranked with an angular velocity which has a non-zero component along the symmetry axis. This result has also been found by Villars [4], who treated cranking as an adiabatic approximation to time-dependent Hartree-Fock.

The reason for this becomes clearer when we examine the collective motion of the system. Although we know, from symmetry considerations, that the collective wavefunctions are D functions, these could also have been obtained from the Hill-Wheeler equation corresponding to (2.12) and (2.13):

$$\int \mathrm{d}^3\Omega'(a_o+a_i\mathscr{L}_i^{\text{int}}+a_{ij}\mathscr{L}_i^{\text{int}}\mathscr{L}_j^{\text{int}}+\ldots)\langle\Omega|\Omega'\rangle f(\Omega')=0. \tag{2.18}$$

When the overlap $\langle\Omega|\Omega'\rangle$ is sharply peaked at $\Omega=\Omega'$, this reduces to a Born-Oppenheimer-type equation for the collective wavefunction $f(\Omega)$.

In the uncranked intrinsic state the expectation values of J_x and J_y vanish, and so the coefficients a_{ij} are given by [5]

$$a_{11}=a_{22}=1/2\mathscr{I}_0 \tag{2.19}$$

all others being zero. Hence the collective Hamiltonian is, to second order,

$$\mathscr{H}_{\text{coll}}=\frac{1}{2\mathscr{I}_0}[\boldsymbol{\mathscr{L}}^2-(\mathscr{L}_3^{\text{int}})^2] \tag{2.20}$$

apart from constant terms like $a_0+a_3\mathscr{L}_3^{\text{int}}$.

Since the intrinsic state is an eigenstate of J_z, the γ dependence of $\langle\Omega|$ is trivial:

$$\mathscr{L}_z^{\text{int}}\langle\Omega|=K\langle\Omega|. \tag{2.21}$$

Hence we can fix the gauge as in (2.11) by pulling out a factor of $\exp[\mathrm{i}K(\alpha+\gamma)]$ from the overlap. The gauge-fixed Hamiltonian then involves only α and β. It can be written as

$$\begin{aligned}\mathscr{H}'_{\text{coll}} &= \exp[-\mathrm{i}K(\alpha+\gamma)]\mathscr{H}_{\text{coll}}\exp[\mathrm{i}K(\alpha+\gamma)] \\ &= -\frac{\partial^2}{\partial\beta^2} - \cot\beta\frac{\partial}{\partial\beta} + \frac{1}{\sin^2\beta}\left(-\mathrm{i}\frac{\partial}{\partial\alpha} + K(1-\cos\beta)\right)^2. \end{aligned}\tag{2.22}$$

This has precisely the form of the Hamiltonian for a charged particle moving round a magnetic monopole [13]. The components of the vector potential are

$$A_\beta = 0 \qquad A_\alpha = K(1-\cos\beta)\tag{2.23}$$

hence this is a gauge in which the Dirac string runs along the negative z axis. The potential leads to velocity-dependent forces in the effective (Born-Oppenheimer) Hamiltonian for adiabatic rotations [14]. When the system is adiabatically rotated through a closed cycle, they give a non-trivial contribution to the phase of the wavefunction—the Berry phase [6]. To complete the correspondence note that the monopole spherical harmonics [13] are identical to the D functions which are the collective wavefunctions for a rotating system with $J_z = K \neq 0$. Comparing the expressions in [13] with those in ch 2 of [12], one sees that

$$Y_{K,J,M}(\beta,\alpha) = D^J_{M,K}(\alpha,\beta,\pm\alpha)^*\tag{2.24}$$

where $\gamma = \pm\alpha$ correspond to the two choices of gauge considered in [13].

Finally, if $|K| = \frac{1}{2}$ the large mixing between $K = \pm\frac{1}{2}$ states means that this approach must be modified. As shown by Wilczek and Zee [15], such a system can be treated by including non-Abelian gauge potentials in the collective Hamiltonian.

To clarify the effects of the velocity-dependent forces on cranking, we discuss the classical charged-particle-monopole system in more detail in the next section.

3. Monopole analogy

Here we consider a charged particle moving on a sphere of radius R at whose centre there is a magnetic monopole. This illustrates the effects of the gauge potentials on cranking, which is essentially a classical approximation to the collective motion.

Classically the particle can move in circular orbits at an angle β to the axis of rotation, with angular velocity

$$\omega = \frac{qg}{mR^2\cos\beta}\tag{3.1}$$

where q, m are the charge and mass of the particle, and g is the magnetic charge of the monopole.

Note that there is a minimum angular velocity for the possible orbits,

$$\omega_c = qg/mR^2.\tag{3.2}$$

This is just the cyclotron frequency for small-radius orbits, that is, with β very small.

Another feature of the charged-particle-monopole system is that the conserved angular momentum is [16]

$$\boldsymbol{L} = m\boldsymbol{r}\times\boldsymbol{v} - qg\hat{\boldsymbol{r}}.\tag{3.3}$$

The additional contribution to the angular momentum, qg, lies along the direction from the monopole to the particle—the symmetry axis of the system. Hence it is analogous to the non-zero $\langle J_z \rangle$ of the previous section. It means that the system has a minimum angular momentum

$$K = qg \tag{3.4}$$

which is quantised to half-integer values by Dirac's condition [7].

Note that, although the minimum angular velocity and the angular momentum lie along the symmetry axis, they are still related by the moment of inertia for rotation about a perpendicular axis

$$\mathcal{I} = mR^2. \tag{3.5}$$

Although the monopole field produces velocity-dependent forces preventing the system from rotating about a principal axis, it does not affect the moment of inertia.

4. Modified cranking

We now return to the discussion of a system with non-zero $\langle J_z \rangle$, and consider cranking about an axis at an angle β to the symmetry axis. That is, we minimise

$$\langle H' \rangle = \langle H \rangle - \omega \sin \beta \langle J_x \rangle - \omega \cos \beta \langle J_z \rangle \tag{4.1}$$

where the angle β is to be regarded as an adjustable parameter,

First we consider a restricted variation keeping the mean fields fixed. In this case, the angular momentum of the cranked state is

$$\langle J_x \rangle = \mathcal{I}_0 \omega \sin \beta \tag{4.2}$$

where $\mathcal{I}_0$ is the Inglis moment of inertia [1, 2]. The expectation value of the Hamiltonian in the rotating frame has the form

$$\langle H' \rangle = \text{constant} - \tfrac{1}{2}\mathcal{I}_0 \omega^2 \sin^2 \beta - \langle J_z \rangle \omega \cos \beta. \tag{4.3}$$

We can now vary (4.3) with respect to β to determine the orientation of the system which minimises $\langle H' \rangle$:

$$\frac{\partial}{\partial \beta} \langle H' \rangle = -\mathcal{I}_0 \omega^2 \cos \beta \sin \beta + \langle J_z \rangle \omega \sin \beta = 0. \tag{4.4}$$

Obviously $\beta = 0$ is always a solution to (4.4). Provided

$$\omega > \langle J_z \rangle / \mathcal{I}_0 \equiv \omega_c \tag{4.5}$$

there is another solution given by

$$\cos \beta = \omega_c / \omega. \tag{4.6}$$

If we examine the stability of the $\beta = 0$ solution, we find

$$\left. \frac{\partial^2}{\partial \beta^2} \langle H' \rangle \right|_0 = \mathcal{I}_0 \omega (\omega_c - \omega) \tag{4.7}$$

and so for $\omega < \omega_c$ the solution is stable. The system sits with its symmetry axis along the cranking axis, a situation which does not correspond to a physical rotation. But for $\omega > \omega_c$ this solution becomes unstable. The minimum of $\langle H' \rangle$ is the solution given by (4.6), which is a physical rotation about the cranking axis. Hence ω_c plays the same role here as the cyclotron frequency (3.2) does for the monopole system.

For cases where ω is very close to ω_c (i.e. β is small), self-consistent variation of the mean fields will not change this. To see this, note that if $\omega \sin \beta$ is small enough we can use first-order cranking. However, $\beta = 0$ is an extremum of $\langle H' \rangle$ and so is a solution to the linearised equations of motion. The lowest-order cranking solution will thus try to realign the symmetry and cranking axes. It will have the form of the zero mode for rotation about the y axis and can be dropped since we have already treated the zero mode by the β variation.

Higher-order cranking effects will of course be present. These can change the coefficient of β^4 in $\langle H' \rangle$ and so can affect the value of β at which the minimum occurs for a given ω. However, they will not change the moment of inertia (the coefficient of $\omega^2\beta^2$).

The softness of the zero mode means that it is not amenable to low-order cranking. If one restricts the changes in the fields to be orthogonal to the zero mode, these may be treated perturbatively provided ω is small compared to the intrinsic excitation energies of the system. In general, one must combine this with a variation with respect to β.

There is another limit in which things simplify: when $\langle J_z \rangle$ is small compared with the total angular momentum. Then we have $\beta \simeq \frac{1}{2}\pi$ and, to lowest order, the $\cos \beta$ term can be neglected. If ω is small enough, we can still use standard lowest-order cranking, provided we are careful to remove the singular zero-mode piece from the cranking equations (2.5). The zero mode could then be handled by varying β. This would require the inclusion of terms which are higher order in ω, but would not affect the moment of inertia.

5. Discussion

We have found that the lowest-order cranking equations have no finite solution for systems with $\langle J_z \rangle \neq 0$. This can be understood in terms of the adiabatic phases which appear in such a system. These produce velocity-dependent forces which prevent the system from rotating freely about a principal axis. The behaviour is analogous to that of a charged particle moving around a magnetic monopole. If it occurs one should use a cranking axis at an angle to the symmetry axis. The angle should be varied to minimise the energy of the rotating system.

The effects do not appear in the standard cranking approach as applied to intrinsic states of deformed nuclei or diatomic molecules. This is due to the degeneracy of states with $J_z = \pm K$ which allows one to form intrinsic states with $\langle J_z \rangle = 0$. It could show up if there were a large *CP* violation breaking this degeneracy. However, this does not correspond to a realistic situation.

More important applications are likely to be in systems with larger symmetry groups than SU(2). For example, we have found this behaviour in cranking a chiral soliton with three flavours of quark [17]. The model has an SU(3) flavour symmetry, but this is broken by the choice of intrinsic state. This state is taken to have a hedgehog structure [18], constructed from non-strange quarks and mesons. It is symmetric under hypercharge rotations, but not under the operation of the other generators of SU(3). The hypercharge of the non-strange quarks in the hedgehog acts like a non-zero angular momentum along the symmetry axis and has similar effects. In this case one cannot form states with zero net hypercharge since a soliton with the opposite intrinsic hypercharge would correspond to an antibaryon.

Similar effects should occur in SU(3) versions of the Skyrme model [19]. There the Wess–Zumino term [20], which acts as a surrogate for the quarks, is linear in time derivatives of the fields and leads to velocity-dependent forces of the type discussed here. Since the Wess–Zumino term can be obtained from an adiabatic approximation to the fermion action, it has a structure which explicitly reflects the monopole-like form of the adiabatic phases [20].

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