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# Collective motions and single particle models†

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**Abstract.** The connection between single particle and collective motion is discussed on the basis of the generator coordinate method. Earlier and recent work on the subject is reviewed.

## 1. Introduction

There is probably no need to dwell on the question why one has to make extensive use of models when dealing with the nuclear many body problem. We simply have no chance of solving Schrödinger's equation exactly in this case.

Furthermore, models have been very successful from a phenomenological point of view. The models fall into two classes: 'collective models' and 'single particle models'. Prototypes of such models are the 'liquid drop model' and the 'shell model' respectively (Mayer and Jensen 1960). The success of two models which obviously take opposite points of view must necessarily lead to attempts to combine both models in a unified theory of nuclear structure. The first successful attempt is the so called 'unified model' of Bohr and Mottelson (1953) and Nilsson (1955). Their approach is predominantly phenomenological. The nuclear degrees of freedom are the five surface coordinates of the quadrupole deformation together with the particle coordinates in the intrinsic frame of reference. In this intrinsic coordinate system the nucleons move independently in a deformed shell model potential. Clearly five of these coordinates are redundant and if they are not eliminated subsidiary conditions result. In the 'unified model' they are neglected. At this point one may ask the question how such a successful model can be interpreted as an approximate solution of Schrödinger's equation? A first answer was given by Baranger and Kumar in a series of papers (Baranger and Kumar 1965, 1967, 1968a, 1968b, 1968c, 1968d). They start with Hartree–Fock (HF) or Hartree–Fock–Bogoljubov (HFB) theory to define a single particle basis. Collective coordinates are then introduced as expectation values of quantities like the quadrupole tensor. They are then allowed to vary slowly with time (adiabatic approximation). The time dependence is determined from time dependent HF or HFB theory. Taking the expectation value of $H$ the collective Hamiltonian is obtained as a function of collective coordinates and momenta. Finally the theory is quantized with respect to the collective coordinates. The results of this theory are in very good agreement with experiment as can be seen in figure 1. I do not think it is necessary to comment in detail on these results.

Recently Baranger and Veneroni (private communication) have generalized the theory in the sense that they have shown that time dependent HFB theory can be used as the basis of a theory of collective motion where there are no restrictions whatsoever

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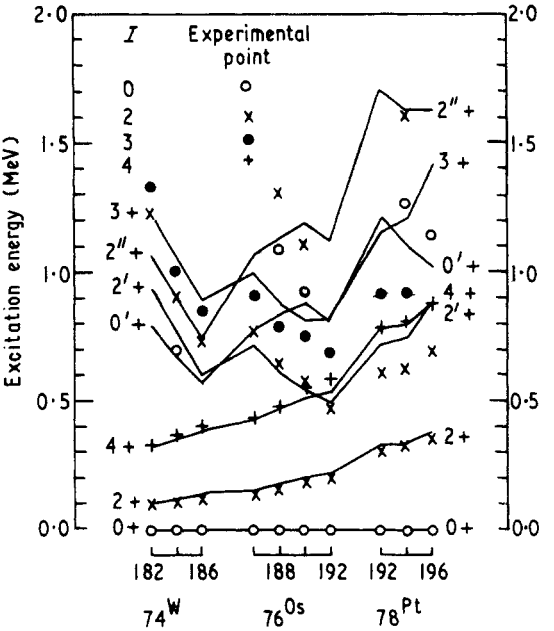


**Figure 1.** Energy levels (MeV). The calculated values are connected by straight lines. The experimental values are indicated by symbols. The figure is taken from Baranger and Kumar (1968d).

either on the nucleon–nucleon interaction or on the type of collective coordinates. Of course, the problem of quantization of the collective coordinates and hence the introduction of redundant variables remains the same as before.

## 2. Generator coordinates

Concerning the redundant variables there are two possible ways to attack the problem. Either the subsidiary conditions are taken into account properly or collective variables are not introduced as dynamical variables. The first possibility has been chosen by Villars and Cooper (1970). In the case of nuclear rotations they show that the result of Thouless and Valatin (1960) for the moment of inertia can be obtained after suitable approximations have been made. One of the essential assumptions is that the nucleus is well deformed and almost axially symmetric.

A good way to avoid the introduction of dynamical collective variables altogether is the use of generator coordinates which were introduced by Hill and Wheeler (1953) long ago. The method has been revived recently by Jancovici and Schiff (1964), Brink and Weiguny (1968), Onishi and Yoshida (1966) and finally Holzwarth (1970 and private communication), and Beck *et al* (1970). Also Rogerson-Schmeing and Villars (1971) have treated nuclear rotations with this method.

### *2.1. Rotations*

I shall discuss the rotational case first. A good starting point is the observation that nuclear wavefunctions which are obtained by solving a selfconsistent single particle

model are in general not eigenstates of operators like angular momentum squared $J^2$, particle number $N$ and linear momentum $\boldsymbol{P}$ even though these operators commute with the Hamiltonian. The reason is that the equations to be solved are nonlinear.

$$\begin{aligned}
&\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} A \\ B \end{pmatrix} E \\
&h = \epsilon - \lambda + \Gamma \\
&\Gamma_{lm} = \sum_{r,s,v} v_{lrms} B^*_{sv} B_{rv} \\
&\Delta_{lm} = \tfrac{1}{2} \sum_{r,s,v} v_{lmrs} B^*_{rv} A_{sv} \\
&\beta^+_v = \sum_k A_{kv} a^+_k + B_{kv} a_k \\
&|\phi\rangle = \prod_v \beta_v |0\rangle \qquad a_k|0\rangle = 0.
\end{aligned} \tag{1}$$

Such defects of the wavefunction $|\phi\rangle$ can be corrected when properly projected wavefunctions $|\psi\rangle$ are used as

$$|\psi^M_J\rangle = \hat{P}^M_J |\phi\rangle \tag{2}$$

$$\hat{P}^M_J |\phi\rangle = \left(\frac{2J+1}{8\pi}\right)^{1/2} \sum_K \int \mathring{D}^J_{MK}(\alpha\beta\gamma) \hat{R}(\alpha\beta\gamma) |\phi\rangle \, \mathrm{d}\Omega \tag{3}$$

$$\mathrm{d}\Omega = \mathrm{d}\alpha \, \mathrm{d}\gamma \, \mathrm{d}\cos\beta$$

$$\hat{R}(\alpha\beta\gamma) = \mathrm{e}^{\mathrm{i}\alpha J_3} \, \mathrm{e}^{\mathrm{i}\beta J_2} \, \mathrm{e}^{\mathrm{i}\gamma J_3}.$$

The variation principle which, when formulated with $|\phi\rangle$, leads to the HFB equations (1) must now be formulated with $|\psi^M_J\rangle$.

$$\delta \frac{\langle \psi^M_J | H | \psi^M_J \rangle}{\langle \psi^M_J | \psi^M_J \rangle} = 0. \tag{4}$$

This leads to the following equations:

$$\begin{aligned}
&E_{\text{proj}} = \frac{\sum_{KK'} \int \mathring{D}^J_{KK'} \langle \phi | H \hat{R} | \phi \rangle \, \mathrm{d}\Omega}{\sum_{KK'} \int \mathring{D}^J_{KK'} \langle \phi | \hat{R} | \phi \rangle \, \mathrm{d}\Omega} \\
&\delta E_{\text{proj}} = 0.
\end{aligned} \tag{5}$$

Obviously the three Euler angles $\alpha$, $\beta$, $\gamma$ play the role of generator coordinates. Under the assumption

$$\langle \phi | \hat{R}(\Omega) | \phi \rangle \simeq \delta(\Omega) \tag{6}$$

the original results of Bohr and Mottelson are recovered except for the fact that now all states of a rotational band turn out to be degenerate

$$\begin{aligned}
&E_J = E \\
\text{or} \qquad &\\
&\Theta \to \infty \qquad \Theta = \text{moment of inertia.}
\end{aligned} \tag{7}$$

This becomes an exact result for the number of particles tending towards infinity. Under the less restrictive assumptions

$$\begin{aligned}
&\langle\phi|J^2|\phi\rangle \gg 1\\
&|\phi\rangle = C\exp(\tfrac{1}{2}\sum_{i,k} C_{ik}\beta_i^+\beta_k^+)|\phi_0\rangle\\
&J_3|\phi_0\rangle = 0 \qquad J_3\beta_i^+|\phi_0\rangle = K_i\beta_i^+|\phi_0\rangle\\
&K_i + K_k = \pm 1\\
&\exp(i\pi J_1)|\phi\rangle = |\phi\rangle
\end{aligned} \tag{8}$$

one obtains the equations of the selfconsistent cranking model.

$$\begin{aligned}
E^J_{\text{proj}} &= \langle\phi|H|\phi\rangle - \frac{\langle\phi|J_2^2|\phi\rangle}{\Theta_Y} + \omega[\{J(J+1)\}^{1/2} - \langle\phi|J_1|\phi\rangle]\\
&\quad + \frac{1}{2\Theta_Y}(\{J(J+1)\}^{1/2} - \langle\phi|J_1|\phi\rangle]^2\\
\omega &= \frac{\langle\phi|(H-\langle H\rangle)J_1|\phi\rangle}{\langle\phi|J_2^2|\phi\rangle}\\
\frac{1}{\Theta_Y} &= \frac{\langle\phi|(H-\langle H\rangle)J_2^2|\phi\rangle}{\langle\phi|J_2^2|\phi\rangle^2}\\
\delta E^J_{\text{proj}} &= 0
\end{aligned} \tag{9}$$

is achieved by

$$\begin{aligned}
&\delta\left(\langle\phi|H|\phi\rangle - \frac{\langle\phi|J_2^2|\phi\rangle}{\Theta_Y}\right) = 0\\
&\langle\phi|J_1|\phi\rangle = \{J(J+1)\}^{1/2}.
\end{aligned} \tag{10}$$

The additional term which appears gives the lowering of the energy due to angular momentum projection.

Projection of the number of particles can be treated analogously but also in a completely rigorous way which allows a check on the approximations made. Such additional terms in the energy are not very important for well deformed nuclei and those which have large energy gaps. On the other hand for so called transition nuclei and nuclei in the vicinity of closed shells where deformations and pair correlations are not yet well developed, projection of angular momentum and particle number may change results drastically.

Summarizing one may say that for well deformed nuclei the cranking model provides a rather good completely microscopic description of ground state rotational bands up to rather high values of the angular momentum. Furthermore there is hope that the restrictive condition $\langle J^2\rangle \gg 1$ can be lifted without complicating formulae very much. This would allow an extension of the cranking model to nuclei which are not well deformed.

### *2.2. Vibrations*

I will now discuss the question of nuclear vibrations. A standard method for treating nuclear vibrations is the random phase approximation (RPA). Starting from a

selfconsistent single particle model one may derive the RPA equations by using generator coordinates (Jancovici and Schiff 1964).

The wavefunction is expressed as

$$|\psi\rangle = \int f(z_{ik}) \exp(\tfrac{1}{2} \sum_{i,k} z^*_{ik} \beta_i^+ \beta_k^+) |\phi\rangle \prod_{r,s} \mathrm{d}z_{rs}. \tag{11}$$

The boson approximation (ie $\beta_l^+ \beta_m^+$, $\beta_m \beta_l$ are considered as boson operators) leads to the following set of equations:

$$\begin{aligned}
&\int (H(zz') - EN(zz')) f(z') \, \mathrm{d}z' = 0 \\
&z \equiv \{z_{ik}\} \qquad z' \equiv \{z'_{ik}\} \\
&H(zz') = \langle z|H|z'\rangle \qquad N(zz') = \langle z|z'\rangle \\
&|z\rangle = \exp(\tfrac{1}{2} \sum_{i,k} z^*_{ik} \beta_i^+ \beta_k^+) |\phi\rangle \\
&N(zz') = \exp(\tfrac{1}{2} \sum_{lm} z'^*_{lm} z_{lm}) \qquad \text{(boson approximation)}
\end{aligned} \tag{12}$$

$$\begin{aligned}
&G(z) = \int N(zz') f(z') \, \mathrm{d}z' \\
&\left\{ \sum_{\nu,\rho} P_{\nu\rho} z_\nu \frac{\partial}{\partial z_\rho} + \frac{1}{2} R_{\nu\rho} \left( \frac{\partial^2}{\partial z_\nu \, \partial z_\rho} + z_\nu z_\rho \right) - (E - E_0) \right\} G(z) = 0 \\
&\nu \equiv k, l \qquad \rho \equiv m, n \qquad k < l \qquad m < n \\
&P_{klmn} = \langle \phi | [H, \beta_k \beta_l] \beta_m^+ \beta_n^+ | \phi \rangle \\
&R_{klmn} = \langle \phi | [H, \beta_k^+ \beta_l^+] \beta_m^+ \beta_n^+ | \phi \rangle
\end{aligned} \tag{13}$$

$$\begin{aligned}
&B^+ = uz + v \frac{\partial}{\partial z} \\
&B = u \frac{\partial}{\partial z} + vz
\end{aligned} \qquad \left( \begin{array}{c} \text{transformation to decoupled} \\ \text{bosons in matrix notation} \end{array} \right) \tag{14}$$

$$\begin{aligned}
&uP - vR = \hbar\omega u \\
&uR - vP = \hbar\omega v
\end{aligned} \qquad \text{(thus decoupling is achieved)} \tag{15}$$

$$\begin{aligned}
&\left( \sum_\sigma \hbar\omega_\sigma (B_\sigma^+ B_\sigma + \tfrac{1}{2}) - \tfrac{1}{2} \operatorname{tr} P - (E - E_0) \right) G = 0 \\
&B_\sigma G_0 = 0 \qquad \text{(boson vacuum)} \qquad E^0 = E_0 - \tfrac{1}{2} (\operatorname{tr} P - \sum_\sigma \hbar\omega_\sigma).
\end{aligned} \tag{16}$$

For details see Jancovici and Schiff (1964). Of course, a nuclear wavefunction which is obtained in this way suffers from the same defects as the HFB solution with which one started. Therefore one combines the use of generator coordinates with angular momentum projection. This means three of the generator coordinates are the Euler angles (Holzwarth 1970 and private communication). The dependence of the weightfunction $f(z)$ on these three angles is known, *a priori*. Concerning the remaining coordinates one

best uses ones intuition to select a suitable finite set. Naturally one begins quite modestly with 'quadrupole bosons' (Holzwarth 1970 and private communication)

$$B^+_{2,K} = \sum_{j_1,j_2,m} b^K_{j_1 j_2} G(j_1 j_2 2; mK-m)\beta^+_{j_1 m}\beta^+_{j_2 K-m}. \tag{17}$$

If only $K = 0$ is taken into account one has the equations

$$\begin{aligned} |\psi^M_J\rangle = {} & \left(\frac{2J+1}{8\pi^2}\right)^{1/2} \int \hat{D}^J_{M0}(\Omega)\hat{R}(\Omega) \int \Gamma(z) \exp z^* B^+_{2,0}|\phi\rangle \, \mathrm{d}z \, \mathrm{d}\Omega \\ & \times \int P_J(\cos\beta) \int \Gamma(z')(\langle z| \, \mathrm{e}^{\mathrm{i}\beta J_2} H|z'\rangle - E^J\langle z| \, \mathrm{e}^{\mathrm{i}\beta J_2}|z'\rangle) \\ & \times \mathrm{d}z' \, \mathrm{d}\cos\beta \\ |z\rangle = {} & \exp z^* B^+_{2,0}|\phi\rangle. \end{aligned} \tag{18}$$

The boson expansion of the Hamiltonian is achieved by

$$\begin{aligned} \frac{\langle z|H|z'\rangle}{\langle z|z'\rangle} &= \sum_{\rho,\sigma} A_{\rho,\sigma} z^\rho z'^{*\sigma} \\ H &= \sum_{\rho,\sigma} A_{\rho,\sigma} (B^+_{2,0})^\rho (B_{2,0})^\sigma. \end{aligned} \tag{19}$$

Now all relevant quantities can be calculated explicitly. For instance

$$\begin{aligned} \langle z| \, \mathrm{e}^{\mathrm{i}\beta J_2}|z'\rangle &= \exp z z'^* P_2(\cos\beta) \\ \langle z|(B^+_{2,0})^\rho (B_{2,0})^\sigma \, \mathrm{e}^{\mathrm{i}\beta J_2}|z'\rangle &= z^\rho (z'^* P_2)^\sigma \langle z| \, \mathrm{e}^{\mathrm{i}\beta J_2}|z'\rangle. \end{aligned} \tag{20}$$

The solution of the integral equation (18) can now be reduced to the diagonalization of a hermitian matrix. Details are given in Holzwarth (1970 and private communication).

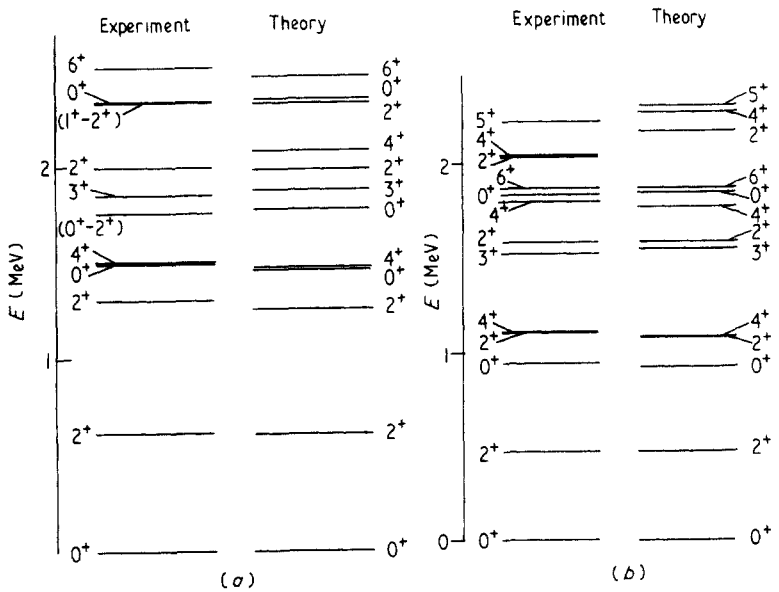


**Figure 2.** Schematic diagram of energy levels of (*a*) $^{78}$Se and (*b*) $^{102}$Ru.

In this most simple case only $K = 0$ is taken into account and the coefficients $b^K_{j_1 j_2}$ are considered as known. Thus there is just one generator coordinate ($z$) left besides the angles $\alpha, \beta, \gamma$. Moreover in applications the boson expansion of the Hamiltonian was not really carried out. Instead the coefficients $A_{\rho\sigma}$ of this expansion were varied in order to see how solutions of the variational equation depend on the magnitude of just these coefficients.

In the same way the more general case with all $K$ taken into account was treated. Results of a fit of the boson expansion to experimental data are given in figure 2 (Holzwarth 1970 and private communication).

## 3. Concluding remarks

There remain some open problems: (i) starting from a nuclear Hamiltonian the boson expansion must be carried out. (ii) The formalism should be generalized to allow the treatment of deformed nuclei and hence give a theory of rotation–vibration coupling.

One may nevertheless conclude somewhat optimistically that a completely microscopic theory of collective motion is in sight.

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