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Kinetic energy in the mass quadrupole oscillation collective model

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A simple microscopic derivation of the kinetic energy in the collective model is presented with no restriction to small vibrations. The result gives a small correction to the Bohr-Mottelson expression.

[NUCLEAR STRUCTURE Kinetic energy found in generalization of Bohr model.]

I. INTRODUCTION

Instead of depending upon the identification of the nucleus with the liquid drop, a satisfactory modern formulation of the collective model must be microscopic (see remarks of Wigner at the 1970 Solvay Conference[1]). Recently, this microscopic reformulation has been achieved by identifying the liquid drop surface coordinates $\alpha_{2\mu}$ with the spherical components of the quadrupole moment.[2,3] In this note, the kinetic energy for this reformulated collective model is determined; the result is not restricted to small vibrations.

We would like to first study the general problem of constructing the kinetic energy in a microscopically-formulated collective model and apply these considerations to the simple case of the center-of-mass coordinates. In Sec. II the collective model itself is investigated.

Let M be the configuration space for some microscopic collective coordinates. By "microscopic," we mean there is a differentiable map Φ from R^{3A}, the configuration space of a system of A particles, onto the collective space M, $\Phi : R^{3A} \to M$. For example, M may be the center-of-mass space R^3 and Φ is the map

$$\Phi : R^{3A} \to R^3 ;$$

$$(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_A) \to \vec{X} = \frac{1}{A} \sum_{n=1}^{A} \vec{x}_n . \tag{1}$$

Now a differential operator, say the Laplacian Δ, on R^{3A} transforms under Φ into a differential operator Δ^Φ on M according to

$$\Delta^\Phi(f) = \Delta(f o \Phi) o \Phi^{-1} , \tag{2}$$

for any differentiable complex-valued function f on M.

The apparent restriction here is that Φ be one-to-one so that Φ^{-1} is defined; this would then eliminate the center-of-mass case from our considerations. However, all that is necessary for Δ^Φ to be well defined is that $\Delta(f o \Phi)$ take on the same value for all elements in the inverse image $\Phi^{-1}(m)$ for all $m \epsilon M$. In other words, when the chain rule is applied to $\Delta(f o \Phi)$, the coefficients of the resulting differential operator in the collective coordinates of M depend only on these collective coordinates. For the simple center-of-mass case, these coefficients are actually constant equal to $\frac{1}{A}$:

$$\Delta^\Phi = \frac{1}{A} \sum_{i=1}^{3} \frac{\partial^2}{\partial X_i^2} . \tag{3}$$

An adequate description of a set of collective states can be reduced to the determination of collective wave functions on M provided the nuclear Hamiltonian splits

$$H = H_{\text{coll}}(\text{collective variables}) + H_{\text{int}}(\text{intrinsic variables}) + H_{\text{coup}} \tag{4}$$

for which, when acting on the collective states, H_{int} is a multiple of the identity and the coupling H_{coup} is small compared to H_{coll}. For the kinetic part of H, we see that if Δ^Φ is well defined, then, *independent of the choice of the intrinsic coordinates*, the quadratic in the collective momenta is a part of H_{coll} and definitely not a part of H_{coup}:

$$H = -\frac{1}{2m}\Delta^\Phi + V_{\text{coll}} + H_{\text{int}} + H_{\text{coup}} . \tag{5}$$

For the center-of-mass case, one can choose intrinsic coordinates for which the kinetic coupling is zero.

The importance of the splitting (5) lies in the fact that the physically appropriate choice of the intrinsic coordinates now depends entirely on whether or not the potential energy separates. The kinetic energy does not figure in the selection of the intrinsic coordinates for a microscopic collective model in which Δ^Φ is well defined.

As will be seen in Sec. II, the Bohr-Mottelson collective model may be formulated as a model in which Δ^Φ is well defined. Hence, the problem of realizing this phenomenological model as a fully microscopic theory reduces to the problem of an appropriate selection of intrinsic coordinates whereby the potential energy splits.

II. KINETIC ENERGY IN THE COLLECTIVE MODEL

We wish to reformulate the Bohr-Mottelson collective model[4] as a microscopic model in the sense of Sec. I and then compute the kinetic energy Δ^Φ.

The Bohr-Mottelson (BM) model supposes that the nucleus can be characterized, for the explanation of certain collective effects, by its surface. The model nucleus, considered to have constant density throughout, is defined by the surface quadrupole deformation parameters α_μ^{BM}. With these assumptions, the BM model has taken the configuration space of the nucleus to be parametrized by the α_μ^{BM}.

However, this configuration space may equally well be coordinatized by the traceless quadrupole moment q_μ. The rather involved coordinate transformation from the α_μ^{BM} to the q_μ is explicitly given in the Appendix.

We are now in a position to naturally reformulate the BM model by taking the new configuration space to be the set of all traceless quadrupole moments for a finite system of A nucleons. The two configuration spaces are evidently identical in the continuum limit. Therefore, we may regard the reformulated model to be a generalization of the BM model applicable to a finite system.

The question that arises is whether the finite BM model is as tractable a theory as the continuum BM model. In particular, is the kinetic energy naturally given in the new model? Since the finite BM model is a microscopic collective model in the sense of Sec. I, Δ^Φ is the kinetic energy, provided it is well defined. Unfortunately, it is not well defined. However, if the trace of the quadrupole moment is included in the configuration space of the finite BM model, then Δ^Φ is well defined [Eqs. (7) and (8) and the moment of inertia Eq. (11)]. Hence, our finite BM model includes monopole vibrations.

Of course, this Δ^Φ in the simultaneous limit of small irrotational vibrations, large particle number, and decoupled monopole motion must give the usual BM result for the kinetic energy. However, Δ^Φ will also be applicable to a finite system with no restriction to small vibrations and no assumption of monopole decoupling.

Let Q be the space of positive-definite symmetric 3×3 real matrices and Φ the map

$$\begin{aligned}&\Phi : R^{3A} \to Q \,;\\ &(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_A) \to (q_{ij}) \,,\\ &q_{ij} = \sum_{n=1}^{A} x_{ni} x_{nj} \,.\end{aligned} \tag{6}$$

If the six coordinates q_{ij}, $i \geq j$, are taken as a chart for Q, then Δ^Φ is given by

$$\begin{aligned}\Delta^\Phi = \sum_{\substack{i\geq j,\\ i'\geq j'}} (\delta_{ii'} q_{jj'} + \delta_{ji'} q_{ij'} \\ + \delta_{ij'} q_{ji'} + \delta_{jj'} q_{ii'}) \frac{\partial}{\partial q_{i'j'}} \frac{\partial}{\partial q_{ij}} \\ + 2A \sum_i \frac{\partial}{\partial q_{ii}} \,.\end{aligned} \tag{7}$$

Since the coefficients of the derivatives in q_{ij} are functions on Q, the Laplacian Δ^Φ is well defined. Hence, the remarks of the Introduction apply here and the kinetic energy on many-particle space naturally defines the kinetic energy in the collective model.

Comparison with the Bohr-Mottelson kinetic energy is readily obtained by a change of coordinates on Q. Let q_μ be the spherical components of the traceless quadrupole moment (normalization given by $q_0 = 2q_{33} - q_{11} - q_{22}$) and $r = (\sum_i q_{ii})^{1/2}$ the monopole coordinate. The dimensionless collective coordinates α_μ are defined by $q_\mu = 3/\sqrt{5\pi}\, A R_0^2 \alpha_\mu^*$, where the constant R_0 is the radius of the spherical drop; we also define a dimensionless monopole parameter ρ by $r^2 = \frac{3}{5} A R_0^2 \rho$. Then, if $\pi_\mu = -i\hbar\partial/\partial\alpha_\mu$,

$$\begin{aligned}-\frac{\hbar^2}{2m}\Delta^\Phi = \frac{1}{2B}\Bigg[\rho^2[\pi\times\pi]^0 - \left(\frac{35}{8\pi}\right)^{1/2}[\pi\times\alpha^*\times\pi]^0 \\ - \frac{5}{2\pi}\frac{i\hbar}{\rho}\frac{\partial}{\partial\rho}[\alpha^*\times\pi]^0 \\ - \frac{5\hbar^2}{8\pi}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial}{\partial\rho}\right) + \frac{3A-2}{\rho}\frac{\partial}{\partial\rho}\right)\Bigg] \,,\end{aligned} \tag{8}$$

where m is the nucleon mass and $B = 3/8\pi m A R_0^2$.

In order to compare Δ^Φ with the BM kinetic energy we must (1) decouple the monopole coordinate, (2) take the continuum limit, (3) make a change of coordinates from α_μ to the surface parameters α_μ^{BM}, and (4) take the small vibration limit. If the monopole coordinate ρ is decoupled, then the kinetic energy simplifies to

$$T_{\mathrm{coll}} = \frac{\rho^2}{2B}[\pi\times\pi]^0 - \frac{1}{2B}\left(\frac{35}{8\pi}\right)^{1/2}[\pi\times\alpha^*\times\pi]^0 \,, \tag{9}$$

where ρ is now a constant. This expression is independent of the particle number so that it is directly applicable to the continuum model. If the change of coordinates is made to the surface parameters and the small vibration limit is taken

$\alpha_\mu \to \alpha_\mu^{\mathrm{BM}} \to 0$, then

$$T_{\mathrm{coll}} \to \frac{\rho^2}{2B}[\pi^{\mathrm{BM}} \times \pi^{\mathrm{BM}}]. \tag{10}$$

Since the BM model has $\rho \to 1$ for small vibrations (see Appendix), the kinetic energy T_{coll} yields the BM kinetic energy $T_{\mathrm{coll}}^{\mathrm{BM}} = 1/2B[\pi^{\mathrm{BM}} \times \pi^{\mathrm{BM}}]^0$ in the small vibration limit. In particular, observe that B is the mass parameter for irrotational motion in the BM model.

We would like to make several observations concerning the collective kinetic energy T_{coll}. Firstly, in order to have exact correspondence with the BM model, the monopole coordinate must be completely decoupled, i.e., ρ is constant in Eq. (9). However, if so desired, the coupling can be partially taken into account by letting ρ be a function of α_μ^{BM} (see Appendix). This has been done below for the moment of inertia [Eq. (11)].

Secondly, it should be emphasized that T_{coll} is independent of the particle number. Hence, the expression for T_{coll} applies to both the finite and continuum BM models.

Thirdly, this expression for T_{coll} is limited neither to small vibrations nor to irrotational motion.

Finally, if the kinetic energy is needed by the reader in the surface coordinates, then a further change of variables must be made from α_μ to α_μ^{BM}. As the formulas of the Appendix make clear, the kinetic energy T_{coll} expressed in the surface coordinates is a complicated second order differential operator, which we have not determined. Hence, if possible, it would be advantageous to work with the quadrupole coordinates. This does seem possible and desirable for various reasons: (i) In addition to the simpler expression that the kinetic energy takes, all other physical quantities of the collective model find a natural expression in terms of the quadrupole moment, e.g., the shape of the nucleus and the K quantum number.[6] Moreover, the collective physical quantities are now given in microscopic coordinates, an obvious theoretical improvement. (ii) The calculations performed in the collective model have customarily been made with the small deformation restriction. Therefore, such computational results apply directly to the collective model on Q space with the same restriction to small vibrations. (iii) The model on Q space gives a natural bridge[7] between the collective model and the algebraic models of collective motion.[8]

If we make yet a further coordinate change to the Euler angles and β, γ deformation parameters, then the moment of inertia may be calculated to be

$$I_K = \frac{4B\beta^2 \sin^2[\gamma - k(2\pi/3)]}{\rho^2 + (5/4\pi)^{1/2}\beta\cos[\gamma - k(2\pi/3)]} \tag{11}$$

When expressed in the surface deformation parameters β^{BM}, γ^{BM}, this moment reduces to the Bohr-Mottelson inertia tensor in the limit of small vibrations, $I_K \to I_K^{\mathrm{BM}} = 4B(\beta^{\mathrm{BM}})^2 \sin^2[\gamma^{\mathrm{BM}} - k(2\pi/3)]$. However, the change in the moment from the Bohr-Mottelson irrotational estimate is relatively small—about a 30% increase for prolate ($\gamma^{\mathrm{BM}} = 0$) states:

$$I/I^{\mathrm{BM}} = 1 + 1.036\beta^{\mathrm{BM}} - 0.339(\beta^{\mathrm{BM}})^2 + 0(|\beta^{\mathrm{BM}}|^3). \tag{12}$$

III. CONCLUSION

We have succeeded in deriving the kinetic energy in the collective model without any restrictive assumption to small vibrations. The result, [Eq. (9)] predicts a moment of inertia [Eq. (11)] which differs only slightly from the liquid drop model. Nevertheless, if the details of the collective model spectrum are required, then the correction given here to the Bohr-Mottelson kinetic energy must be included.

Such a small modification to the kinetic energy would seem to support the claim that the potential is largely responsible for the large increase in the moment from the irrotational estimate. However, it has been shown by Gulshani and Rowe[5] that a reasonable choice of intrinsic coordinates [a smooth transversal of $GL(3)$] naturally introduces terms from the intrinsic and coupled kinetic energy which very well might be responsible for the increased inertia tensor.

A collective model for the order λ multipole moment can be obtained by taking the collective space M to be the polynomials of degree λ in x_{ni}. However, since the coefficients of Δ^Φ are polynomials of degree $2\lambda - 2$, Δ^Φ is not well defined unless $\lambda = 1, 2$.

APPENDIX

In this Appendix, explicit formulas are given for the change of coordinates from the nuclear surface coordinates to the quadrupole coordinates.

The nuclear surface $R(\theta, \phi)$ as a function of the directional angles (θ, ϕ) is given in terms of the constant equilibrium radius R_0 and the surface deformation coordinates α_μ^{BM}:

$$R(\theta, \phi) = R_0[1 + \sum_\mu \alpha_\mu^{\mathrm{BM}} Y_{2\mu}(\theta, \phi)]. \tag{A1}$$

Assuming constant density and noting that conservation of particle number defines the density in terms of the surface parameters, we may compute the traceless quadrupole moment $q_\mu = 3/\sqrt{5\pi}\, A R_0{}^2 \alpha_\mu^*$:

$$\alpha_\mu = \left(\frac{4\pi}{5}\right)^{1/2} \frac{\int dg\, \mathfrak{D}^{(2)}_{\mu 0}(g)^* [1 + (5/4\pi)^{1/2} \sum_\nu \alpha_\nu^{\mathrm{BM}} \mathfrak{D}^{(2)}_{\nu 0}(g)]^5}{\int dg [1 + (5/4\pi)^{1/2} \sum_\nu \alpha_\nu^{\mathrm{BM}} \mathfrak{D}^{(2)}_{\nu 0}(g)]^3} . \tag{A2}$$

Hence, α_μ is a rational function of the α_μ^{BM}. If the change of coordinates from α_μ to α_μ^{BM} is made in the expression for Δ^Φ [Eq. (8)] then the resulting kinetic energy in the surface coordinates is a second order differential operator with rational coefficients in α_μ^{BM}.

We also wish to give the transformation from the surface rotational-vibrational coordinates (Ω^{BM}, β^{BM}, γ^{BM}), Ω = Euler angles, to the quadrupole rotational-vibrational coordinates (Ω, β, γ):

$$\begin{aligned} &\alpha_\mu^{\mathrm{BM}} \equiv \sum_\nu \mathfrak{D}^{(2)}_{\mu\nu}(\Omega^{\mathrm{BM}})^* a_\nu^{\mathrm{BM}}, \quad a_0 = \beta^{\mathrm{BM}} \cos\gamma^{\mathrm{BM}}, \\ &a_{\pm 1} = 0, \\ &a_{\pm 2} = \frac{1}{\sqrt{2}} \beta^{\mathrm{BM}} \sin\gamma^{\mathrm{BM}}, \end{aligned} \tag{A3}$$

and similarly for α_μ. From the invariance of the integral in (A2), one obtains

(a) $\Omega = \Omega^{\mathrm{BM}}$, i.e., the Euler angles are identical;

(b) $$a_\mu = \left(\frac{4\pi}{5}\right)^{1/2} \frac{\int dg\, \mathfrak{D}^{(2)}_{\mu 0}(g)^* [1 + (5/4\pi)^{1/2} \sum_\nu a_\nu^{\mathrm{BM}} \mathfrak{D}^{(2)}_{\nu 0}(g)]^5}{\int dg [1 + (5/4\pi)^{1/2} \sum_\nu a_\nu^{\mathrm{BM}} \mathfrak{D}^{(2)}_{\nu 0}(g)]^3} . \tag{A4}$$

The vibrational coordinates (β, γ) are defined in terms of the surface vibrational parameters (β^{BM}, γ^{BM}) by $\beta = (a_0{}^2 + 2a_2{}^2)^{1/2}$ and $\tan\gamma = \sqrt{2}\, a_2/a_0$.

Hence, the kinetic energy in the surface rotational-vibrational coordinates is a second order differential operator whose coefficients are "solvable by radicals," i.e., rational functions with square roots.

The exact formulas for (β, γ) in terms of (β^{BM}, γ^{BM}) are clearly very complicated. However, Taylor series formulas can be given:

$$\begin{aligned} \frac{\beta}{\beta^{\mathrm{BM}}} &= 1 + \frac{2}{7}\left(\frac{5}{\pi}\right)^{1/2} \beta^{\mathrm{BM}} \cos 3\gamma^{\mathrm{BM}} \\ &\quad + \frac{1}{14\pi}\left(\frac{103}{14} - \frac{20}{7} \cos^2 3\gamma^{\mathrm{BM}}\right) (\beta^{\mathrm{BM}})^2 + O(|\beta^{\mathrm{BM}}|^3), \\ \cos(\gamma - \gamma^{\mathrm{BM}}) &= 1 - \frac{10}{49\pi} (\beta^{\mathrm{BM}})^2 \sin^2\gamma^{\mathrm{BM}} \\ &\quad \times (1 + 2\cos 2\gamma^{\mathrm{BM}})^2 + O(|\beta^{\mathrm{BM}}|^3), \\ \sin(\gamma - \gamma^{\mathrm{BM}}) &= -\frac{2}{7}\left(\frac{5}{\pi}\right)^{1/2} \beta^{\mathrm{BM}} \sin\gamma^{\mathrm{BM}} (1 + 2\cos 2\gamma^{\mathrm{BM}}) \\ &\quad + \frac{20}{49\pi} (\beta^{\mathrm{BM}})^2 \tan\gamma^{\mathrm{BM}} (1 + 2\cos 2\gamma^{\mathrm{BM}}) \\ &\quad \times (\cos^2 2\gamma^{\mathrm{BM}} - \sin^2\gamma^{\mathrm{BM}}) + O(|\beta^{\mathrm{BM}}|^3). \end{aligned} \tag{A5}$$

The nuclear surface defines all shape observables in terms of the deformation parameters. In particular, the trace of the quadrupole moment is given by

$$\begin{aligned} \rho &= \frac{\int dg [1 + (5/4\pi)^{1/2} \sum_\nu a_\nu^{\mathrm{BM}} \mathfrak{D}^{(2)}_{\nu 0}(g)]^5}{\int dg [1 + (5/4\pi)^{1/2} \sum_\nu a_\nu^{\mathrm{BM}} \mathfrak{D}^{(2)}_{\nu 0}(g)]^3} \\ &= 1 + \frac{7}{4\pi} (\beta^{\mathrm{BM}})^2 + \frac{9}{14\pi} (5/4\pi)^{1/2} (\beta^{\mathrm{BM}})^3 \cos 3\gamma^{\mathrm{BM}} \\ &\quad + O(|\beta^{\mathrm{BM}}|^4). \end{aligned} \tag{A6}$$

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