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Elasticity in the Response of Nuclei

G. F. BERTSCH*

Department of Physics, Cyclotron Laboratory, Michigan State University, East Lansing, Michigan 48823

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From the RPA equations of motion, we derive macroscopic equations for the vibrations of nuclei. These equations imply the Tassie model of form factors and yield an energy for the quadrupole vibration 30% lower than the empirical. We interpret the modes as the classical vibration of an elastic solid.

1. INTRODUCTION

As part of a program to understand nuclei in macroscopic terms, we here examine the RPA equations of motion in coordinate space. The variables in the equations can then be given classical interpretations. These equations cannot be solved exactly, but the classical interpretation suggests a variational solution. This solution turns out to have similar frequencies to the corresponding variational solution of the classical problem of the vibrations of an incompressible elastic solid. The reader may wonder how it is possible for nuclei to have elastic behavior; it is well known that nuclei are liquid drops! The following points should be noted. First, even classical fluids can exhibit elastic behavior in their high frequency response. A familiar example is Silly Putty. Second, the fluid model predicts a mass dependence of vibration frequencies

$$\omega \sim R^{-(3/2)} \sim A^{-(1/2)},$$

where R is the radius of the nucleus and A is the mass number. This is at variance with empirics, which requires the milder dependence,

$$\omega \sim R^{-1} \sim A^{-(1/3)}.$$

Finally, another Fermi system, liquid He^3, is predicted to have transverse waves [1]. This can only happen if the ground state has rigidity.

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2. Quantum Mechanical Variational Principle

The derivation will proceed by Thouless's variational principle [2]. The object is to find the solution of RPA equations of motion. Working in the space of particle–hole configurations, Thouless shows that an upper bound to the frequency ω is given by

$$|\omega| \leqslant (X, Y)\begin{pmatrix}A & B\\ B & A\end{pmatrix}\begin{pmatrix}X\\ Y\end{pmatrix}\Big/(X, -Y)\begin{pmatrix}X\\ Y\end{pmatrix} \tag{1}$$

Here (X, Y) is a trial vector in the configuration space, and A and B are matrix elements of the Hamiltonian. The only requirement on the trial vector is that X and Y be separately orthogonal to any vectors with zero eigenvalue.

To sort out macroscopic variables, it is preferable to work in position space instead of particle–hole configuration space. Instead of dealing with amplitude X_{ij} for a particular particle–hole configuration $|ij^{-1}\rangle$, we consider a wavefunction perturbation on each occupied orbit j,

$$\phi^j \sim \phi_0^j(r) + e^{i\omega t}\phi_x^j(r) + \phi_y^j(r)\, e^{-i\omega t}, \tag{2}$$

where ϕ_0^j is the Hartree–Fock orbit. The relation between the X coefficients in the standard method and the perturbation ϕ_x^j is simply

$$\phi_x^j(r) = \sum_i X_{ij}\phi_i(r). \tag{3}$$

For convenience, although it is not necessary, we shall assume that the Hartree–Fock Hamiltonian $\mathscr{H}[\rho]$ is purely real. Then the wavefunction may be chosen real also, and the RPA equations in position space with the given Hamiltonian $\mathscr{H}[\rho]$ are

$$\begin{aligned}[\mathscr{H}[\rho_0] - \epsilon_j]\, \phi_x^j + \frac{\delta\mathscr{H}}{\delta\rho}\, \delta\rho\, \phi_0^j &= \omega\phi_y^j,\\ [\mathscr{H}[\rho_0] - \epsilon_j]\, \phi_y^j + \frac{\delta\mathscr{H}}{\delta\rho}\, \delta\rho\, \phi_0^j &= -\omega\phi_x^j,\end{aligned} \tag{4}$$

with

$$\delta\rho = \sum_{\substack{\text{occupied}\\ \text{orbits}}} \phi_0^j(\phi_x^j + \phi_y^j).$$

It is convenient to make a further definition of two new variables,

$$\eta^j = \phi_x^j + \phi_y^j$$

and

$$\zeta^j = \phi_x^j - \phi_y^j.$$

The RPA equations then become

$$[\mathscr{H}_0 - \epsilon_j]\,\eta^j + 2\,\frac{\delta\mathscr{H}}{\delta\rho}\,\delta\rho\,\phi_0{}^j = \omega\zeta^j, \tag{5a}$$

$$[\mathscr{H}_0 - \epsilon_j]\,\zeta^j = \omega\eta^j. \tag{5b}$$

We can give interpretations to the variables ζ^j and η^j which make (5b) the equation of continuity. To do this, we shall define a velocity potential

$$\Phi = \frac{\zeta^j}{\phi_0{}^j}\,\frac{1}{m}\,.$$

To see that this a a reasonable definition, we take the gradient of the potential and multiply by the density to get the momentum density

$$(\phi_0{}^j)^2\, m\vec{\nabla}\Phi = \phi_0{}^j(\vec{\nabla}\phi_x{}^j - \vec{\nabla}\phi_y{}^j) - \vec{\nabla}\phi_0{}^j(\phi_x{}^j - \phi_y{}^j).$$

This is identical to the coefficient of $e^{i\omega t}$ in the quantum mechanical expression

$$\phi^{j*}\vec{p}\phi^j.$$

if Eq. (2) is used for the wavefunctions. We now multiply Eq. (5b) by $\phi_0{}^j$ to rewrite it as

$$\phi_0{}^j\left(\frac{-\nabla^2}{2m} + V\right)\zeta_0{}^j - \zeta_0{}^j\left(\frac{-\nabla^2}{2m} + V\right)\phi_0{}^j$$
$$= \phi_0{}^j\left(\frac{-\nabla^2}{2m}\right)\zeta_0{}^j - \zeta_0{}^j\left(\frac{-\nabla^2}{2m}\right)\phi_0{}^j = \frac{-\vec{\nabla}}{m}\cdot(\phi_0{}^j)^2\,\vec{\nabla}\,\frac{\zeta^j}{\phi_0{}^j} = \omega\phi^j\eta^j = \omega\,\delta\rho.$$

With our identification of variables, the left side is the divergence of the momentum density. The right side is, of course, the time derivative of the ordinary density. This then expresses the equation of continuity

$$-\vec{\nabla}\cdot\frac{\vec{p}}{m} = \frac{d\rho}{dt}\,.$$

Equation (5a) is the dynamical equation of the system since it relates the time derivative of the velocity potential, i.e., the acceleration, to the change in density. For Bose systems, this equation can be transformed to Bernoulli's equation for fluids [3], having a fairly simple pressure term. This is not possible in Fermi systems.

Returning to the calculation of vibrations, we express the variational principle in terms of our variables as

$$|\,\omega\,| = \frac{1}{2}\,\frac{\sum_{jj'} \langle \eta^j[\delta_{jj'}(\mathscr{H}_0 - \epsilon_j) + 2(\delta V/\delta\rho)\,\phi^j\phi^{j'}]\,\eta^{j'}\rangle + \sum_j \langle \zeta^j[\mathscr{H}_0 - \epsilon_j]\,\zeta^j\rangle}{\sum_j \langle \zeta^j\eta^j\rangle}. \tag{6}$$

We now have to choose trial ζ^j and η^j. An obvious choice for a velocity potential is $r^l Y^l$, which is exact for a multipolarity l in the limit that the motion is incompressible and irrotational. Thus, we choose ζ^j as

$$\zeta^j = r^l Y^l \phi_0{}^j(r). \tag{7}$$

Such a velocity potential changes the density of the system by displacing the wavefunctions

$$\phi^j(r) \to \phi^j(\vec{r} + \alpha\vec{\nabla} r^l Y^l). \tag{8}$$

Hence we choose

$$\eta^j = \alpha(\vec{\nabla} r^l Y)\cdot\vec{\nabla}\phi^j. \tag{9}$$

The variational parameter is α, the relative amplitudes of the velocity and density fluctuations. The density fluctuation $\delta\rho = \sum_j \phi^j\eta^j$, derived from (9), is identical in shape to Tassie's form factor [4]

$$\delta\rho \sim r^{l-1}Y^l(r)\,\frac{d\rho_0}{dr} \tag{10}$$

where ρ_0 is the density of the ground state. This is not surprising, since Tassie assumes hydrodynamic equations which imply incompressible and irrotational flow. The expression to be minimized is of the form

$$\omega[\alpha] = \frac{1}{2}\,\frac{\alpha^2 A + B}{\alpha C}. \tag{11}$$

The minimum is

$$\omega\left[\left(\frac{A}{B}\right)^{1/2}\right] = \left(\frac{AB}{C^2}\right)^{1/2} \tag{12}$$

The remaining chore is the evaluation of A, B, and C in terms of their definitions, Eq. (6), and our trial wavefunction. We start with the overlap $C = \sum_j \langle \zeta^j\eta^j\rangle$. The functions ζ, η, represent admixtures of unoccupied orbits in the wavefunction of particles in occupied orbits, so in principle the functions should be projected onto the unoccupied orbits. However, it is easy to show that the projection is unnecessary. For suppose the orbit j' is also occupied and has nonvanishing overlap with j. Then we separate out of the sum two terms

$$\langle \zeta^j \mid j'\rangle\langle j' \mid \eta^j\rangle + \langle \zeta^{j'} \mid j\rangle\langle j \mid \eta^{j'}\rangle.$$

These terms cancel with our trial wavefunctions because

$$\langle \zeta^j \mid j' \rangle = \langle j \mid \zeta^{j'} \rangle$$

and

$$\langle \eta^j \mid j' \rangle = -\langle \eta^{j'} \mid j \rangle.$$

We can then evaluate C as

$$C = \sum_j \int d^3r\ \phi^j r^l Y^l (\vec{\nabla} r^l Y^l) \cdot \vec{\nabla} \phi^j, \tag{13a}$$

$$= \sum_j \int d^3r\ \phi^j r^l Y^l (\vec{\nabla} r^l Y^l) \cdot \left(\frac{\vec{\nabla} - \overleftarrow{\nabla}}{2} \right) \phi^j, \tag{13b}$$

$$= -\frac{1}{2} \int d^3r\ \rho_0(r) (\vec{\nabla} r^l Y^l) \cdot (\vec{\nabla} r^l Y^l), \tag{13c}$$

$$\approx -\frac{l(2l+1)}{2} \int r^2\, dr\ \rho_0(r)\, r^{2l-2}. \tag{13d}$$

In the first step we integrated by parts. The last step follows from assumption of a spherical symmetric density distribution in the ground state and some vector algebra [5].

The next term we consider is the kinetic term

$$B = \sum_j \langle \zeta^j \mid \mathscr{H}_0 - \epsilon_j \mid \zeta^j \rangle. \tag{14}$$

Again the projection on unoccupied orbits is unnecessary. The reason for the cancellation this time is that

$$\langle j' \mid \mathscr{H}_0 - \epsilon_j \mid j' \rangle = \epsilon_{j'} - \epsilon_j = -\langle j \mid \mathscr{H}_0 - \epsilon_{j'} \mid j \rangle \tag{15}$$

To evaluate this term, we write out $\mathscr{H}_0$ in terms of kinetic and potential operators

$$B = \sum_j \int d^3r\ \phi^j r^l Y^l \left[\left(-\frac{\nabla^2}{2m} + V \right) r^l Y^l \phi^j - r^l Y^l \left(-\frac{\nabla^2}{2m} + V \right) \phi^j \right] \tag{16a}$$

$$= \sum_j \int d^3r\ \phi^j r^l Y^l \left(-\frac{1}{m} \right) \vec{\nabla} r^l Y^l \cdot \vec{\nabla} \phi^j \tag{16b}$$

$$= +\frac{1}{2m} \int d^3r \sum_j (\phi^j)^2 (\vec{\nabla} r^l Y^l) \cdot (\vec{\nabla} r^l Y^l) \tag{16c}$$

$$\approx \frac{l(2l+1)}{2m} \int r^2\, dr\ \rho_0(r)\, r^{2l-2}. \tag{16d}$$

As before, the last step requires a spherical density distribution.

The driving force in the vibration is provided by the first term

$$A = \sum_{j,j'} \left\langle \eta^j \left[\delta_{jj'}(\mathscr{H}_0 - \epsilon_j) + \frac{\delta V}{2\delta\rho} \phi^j \phi^{j'} \right] \eta^{j'} \right\rangle. \tag{17}$$

We shall neglect the residual interaction $\delta V/\delta\rho$ as well as the derivatives of the central potential V_0 in $\mathscr{H}_0$. For incompressible flows, these terms are only significant on the nuclear surface, where they give rise to a capillary restoring force. The theory of capillarity in RPA is given in [3]. For giant resonances in nuclei, capillarity is of slight importance above $A > 100$. With this approximation we have

$$\begin{aligned} A &\sim \sum_j \langle \eta^j [\mathscr{H}_0 - V_0 - \epsilon_j + \langle j \mid V_0 \mid j \rangle] \eta^j \rangle \\ &\sim \sum_j \int d^3r\, \vec{\nabla}\phi^j \cdot \vec{\nabla} r^l Y^l \left[-\frac{\nabla^2}{2m}, \vec{\nabla} r^l Y^l \cdot \vec{\nabla} \right] \phi^j. \end{aligned} \tag{18}$$

Following algebraic manipulations identical to those performed previously, we arrive at the expression

$$\begin{aligned} A = {} & \frac{1}{2m} \int d^3r \sum_j \nabla_\mu \phi^j (\nabla_\mu r^l Y^l\, \nabla_{\mu'} \nabla_\lambda r^l Y^l - \nabla_{\mu'} r^l Y^l\, \nabla_\mu \nabla_\lambda r^l Y^l)\, \nabla_{\mu'} \nabla_\lambda \phi^j \\ & + \frac{1}{2m} \int d^3r \sum_j \nabla_\mu \phi^j (\nabla_\lambda \nabla_\mu r^l Y^l) \cdot (\nabla_\lambda \nabla_{\mu'} r^l Y^l)\, \nabla_{\mu'} \phi^j, \end{aligned} \tag{19}$$

where the derivatives are summed over the Cartesian indices μ, μ', and λ. For spherically symmetric ground states the first term vanishes. Evaluation of the second term requires specific knowledge of the wavefunctions. Note that in a Bose system the integral would be nearly zero because the wavefunction is constant in the interior. For nuclei, we shall describe the wavefunctions in the interior by the Fermi gas model

$$\sum_j (\nabla_\mu \phi^j)(\nabla_\lambda \phi^j) = \rho_0 \int_0^{k_F} \frac{k^2\, dk}{k_{F/3}^3} \int \frac{d\cos\theta}{2} k_\mu(\theta)\, k_\lambda(\theta) = \rho_0 \frac{k_F{}^2}{5} \delta_{\mu\lambda}, \tag{20}$$

where k_F is the Fermi momentum. Equation (19) then becomes

$$A = \frac{1}{2m} \frac{k_F{}^2}{5} l(2l+1)(l-1)(2l-1) \int r^2\, dr\, \rho(r)\, r^{2l-4}. \tag{21}$$

We can now combine Eqs. (12), (13d), (16d), and (21) to get

$$\omega = \frac{\hbar}{m} \left(\frac{k_F{}^2 (l-1)(2l-1) \langle r^{2l-4} \rangle}{5 \langle r^{2l-2} \rangle} \right)^{1/2}. \tag{22}$$

Inserting numerical values, $k_F \simeq 1.34$, and $\langle r^2 \rangle \sim \frac{3}{5}\,((1.2)\,A^{1/3})^2$ we find for the quadrupole resonance

$$\omega_{l=2} \sim \frac{46}{A^{1/3}}, \tag{23}$$

which is 30 % lower than the experimentally observed frequency [6, 7].

3. Further Remarks

The classical formula corresponding to Eq. (22) may be derived from Rayleigh's [9] classical variational principle. The variational principle may be stated as follows. Consider an arbitrary field of displacements $\vec{u}(r)$ associated with some vibrational motion. A bound on the vibrational frequency ω is given by

$$\omega^2 \leqslant \frac{W[u]}{\frac{1}{2}\int \rho u \cdot u \, d^3r}, \tag{24}$$

where $W[u]$ is the strain energy associated with the displacement field $\vec{u}$ and $\rho(r)$ is the mass density of the vibrating system. The strain energy is given in terms of Lamé's coefficients of elasticity λ, μ by [10]

$$W = \int \left[\frac{1}{2}\lambda(\nabla \cdot u)^2 + \mu \sum_{ij} (\nabla_i u_j)(\nabla_\mu u_\lambda)\right] d^3r. \tag{25}$$

Assuming a displacement field of the form $\vec{u} = \vec{\nabla} r^l Y^l$, we obtain the following bound on the vibrational frequency.

$$\omega \leqslant \left(\frac{2\mu(l-1)(2l-1)\langle r^{2l-4}\rangle}{m\rho\langle r^{2l-2}\rangle}\right)^{1/2} \tag{26}$$

Comparing Eq. (26) with (22), we see that the functional forms are the same, the only difference being that the quantum equation has the value of the shear modulus specified.

The classical shear modulus of a Fermi gas will now be derived. We consider a box of sides x, y, z, filled with the gas. The pressure on the xy face, P_{xy}, is the derivative of the kinetic energy with respect to z, divided by the area of the xy face. Since $k_z \sim 1/z$, we find

$$P_{xy} = \frac{\hbar^2}{2m}\frac{1}{xy}\frac{\partial \overline{k_z^2}}{\partial z} = \frac{\hbar^2}{m}\frac{\overline{k_z^2}}{xyz} \tag{27}$$

The moduli of elasticity are given by [10]

$$2\mu + \lambda = \frac{z\,\partial P_{xy}}{\partial z} \qquad \text{and} \qquad \lambda = \frac{x\,\partial P_{xy}}{\partial x}. \tag{28}$$

From Eqs. (27) and (28) and the $1/z$ dependence of $\overline{k_z^2}$, it is simple to show that

$$\lambda = \mu = \frac{\hbar^2}{m} \overline{k_z^2} \rho = \frac{\hbar^2}{5m} k_F^2 \rho. \tag{29}$$

This modulus is twice the value implied by Eqs. (22) and (26). However, the derivation of Eq. (22) is suspect: An integration by parts was carried out over wavefunctions of infinite extent.

An exact numerical solution for the quadrupole vibrations of a sphere is given by Lamb [8], quoted in Love's treatise (12). With elasticity parameters from Eq. (29), Lamb's solution is

$$\omega = \frac{2.64}{R} \left(\frac{\mu}{\rho}\right)^{1/2} \sim \frac{55}{A^{1/3}}.$$

This is in better agreement with experiment.

In the nuclear physics literature one can find calculations of the bulk coefficient of compressibility K

$$K = \frac{\partial P}{\partial V} = \lambda + \frac{2}{3} \mu = \frac{1}{3} \frac{\hbar^2}{m} k_F^2 \rho. \tag{30}$$

This is occasionally related to a vibrational mode using the equation for sound velocity v in a gas,

$$v^2 = K/\rho. \tag{31}$$

However, when $\mu \neq 0$ we should consider both shear and compressional waves

$$\begin{aligned} v^2 &= \frac{\lambda + 2\mu}{\rho} \qquad \text{(compressional)}, \\ v^2 &= \frac{\mu}{\rho} \qquad \text{(shear)}. \end{aligned} \tag{32}$$

Lamb also calculated the $l = 0$ compressional mode for an elastic sphere. The numerical result in this case is

$$\omega = \frac{2.56}{R} \left(\frac{\lambda + 2\mu}{\rho}\right)^{1/2} \sim \frac{92}{A^{1/3}}.$$

This is much higher than the quadrupole frequency. Experimentally, there is some ambiguity whether the observed state is quadrupole or monopole; the present theory strongly favors the quadrupole interpretation.

Unfortunately, the sense in which any of the equations (31) and (32) can describe motions of the system is limited. For an accurate description of the dynamics we would use a theory such as the Landau theory which includes interactions as well as damping of the excitations. The above macroscopic equations are then correct only in the following peculiar sense. The energy-weighted sum rule and the reciprocal energy-weighted sum rule for appropriate operators corresponding to longitudinal and transverse excitations may be calculated in the Landau theory. Their ratio is

$$\frac{\langle \omega \rangle}{\langle 1/\omega \rangle} \sim Aq^2,$$

with A given by (32), if there are no interactions between the particles. Of course, there are no sharp states in this limit. On the other hand, Eq. (31) is correct with a sharp state for sufficiently low frequencies, when the ground state is superfluid [11]. In this light, it is remarkable that reasonably sharp quadrupole states are possible in nuclei.

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