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VIBRATING POTENTIAL MODEL FOR GIANT RESONANCES IN DEFORMED METAL CLUSTERS AND NUCLEI

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Much attention has been paid last time to giant resonances (GR) in metal clusters (MC) and their comparison with GR in nuclei (see reviews [1-5] and refs. therein). The vibrating potential model (VPM) seems to be very appropriate for investigation of GR in both these systems [6-10].This model is convenient for qualitative analysis and simultaneously provides the RPA accuracy of numerical calculations. The VPM is widely used in nuclear physics [7-10] and has recently been modified for MC [6].

Investigation of GR is rather complicated for deformed systems. In nuclear physics the (doubly) stretched coordinate method is used to simplify the task in the case of quadrupole deformation (see, for example, [10]). But this method is rather complicated for MC (due to adding the Coulomb term) [11] and is not, practically, derived for systems with other kinds of deformation. In this paper, by using the multipole expansion of the single-particle potential and electron density we obtain equations of the VPM for systems with any kind of deformation.

The VPM equations coincide with equations of the schematic RPA with separable forces. The strength constant of residual forces is determined from the self-consistency condition. For the most simple external field $f(\mathbf{r}) = r^{\lambda}Y_{\lambda\mu}$ which corresponds to a divergency free and irrotational ($rot\nabla\mathbf{f}(\mathbf{r}) = div\nabla\mathbf{f}(\mathbf{r}) = 0$) flow we have the secular (dispersion) equation [6]:

$$X_t \equiv 2\sum_{kk'} \frac{< k'|Q|k >^2 (\epsilon_k + \epsilon_{k'})}{(\epsilon_k + \epsilon_{k'})^2 - \omega_t^2} = \kappa_0^{-1} \qquad (1)$$

where

$$\kappa^{-1} = \int \nabla Q(\mathbf{r}) \cdot \nabla f(\mathbf{r}) n_0(\mathbf{r}) d\mathbf{r} = -\int Q(\mathbf{r}) \nabla f(\mathbf{r}) \cdot \nabla n_0(\mathbf{r}) d\mathbf{r} \qquad (2)$$

is the inverse strength constant and

$$Q(\mathbf{r}) = \nabla V_0(\mathbf{r}) \cdot \nabla f(\mathbf{r}) + \int \frac{\nabla n_0(\mathbf{r}') \cdot \nabla f(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}', \qquad (3)$$

is the operator of residual interaction. Here, $| k >$ and ϵ_k are the single-particle eigenstate and eigenenergy of the static hamiltonian with a single-particle potential $V_0(\mathbf{r})$, ω_t is a root of the equation (1), n_0 is a static ground state density. If the second (Coulomb) term is neglected in (3), we obtain the version of the VPM used for description of isoscalar GR in nuclei. Thus, equations (1)-(3) can be used to study GR in both MC and nuclei.

Equations (1)-(3) take place for both spherical and deformed systems. But in the deformed case they are too general to be convenient for estimations and numerical calculations. One can get more appropriate equations using the multipole expansion of single-particle potential

$$V_0(\mathbf{r}) = \sum_l \sum_{m=-l}^{l} V_{lm}(r) Y^d_{lm}(\Omega), \tag{4}$$

and ground state density

$$n_0(\mathbf{r}) = \sum_l \sum_{m=-l}^{l} n_{lm}(r) Y^d_{lm}(\Omega). \tag{5}$$

where $Y^d_{lm}(\Omega) = Y_{lm}(\Omega) + d \cdot Y^{\dagger}_{lm}(\Omega)$ and the external field is written as

$$f^d_{\lambda\mu}(\mathbf{r}) = r^{\lambda} Y^d_{\lambda\mu}(\Omega). \tag{6}$$

If $d = +1$ and -1, the functions (4)-(6) are hermitian and antihermitian, respectively. As a result, the hermiticity of the Hamiltonian is assured. It is clear that any single-particle potential and density distribution are covered by expressions (4)-(5). So, the generality of the model is not lost.

Omitting tedious mathematical transformations we present the final expressions for the operator (3) and strength constant (2) (for ion distribution the jellium approximation is used):

$$Q^{(d)}_{\lambda\mu}(\mathbf{r}) = \sum_{LM} Y_{LM}(\Omega) \cdot \sum_{lm} (C^{LM}_{lm\lambda\mu} + d(-1)^{\mu} C^{LM}_{lm\lambda-\mu})(Q^{(v)}_{\lambda Llm}(r) + Q^{(c)}_{\lambda Llm}(r)) \tag{7}$$

where

$$Q^{(v)}_{\lambda Llm}(r) = (2\lambda+1)\sqrt{\frac{\lambda(2\lambda-1)}{4\pi(2L+1)}} \cdot [M^{(1)}_{\lambda Ll}\frac{dV_{lm}}{dr} r^{\lambda-1} - M^{(2)}_{\lambda Ll} V_{lm} r^{\lambda-2}], \tag{8}$$

$$Q^{(c)}_{\lambda Llm}(r) = (2\lambda+1)\sqrt{\frac{\lambda(2\lambda-1)}{4\pi(2L+1)}} \cdot (-\frac{4\pi}{2L+1})$$

$$\cdot [M^{(3)}_{\lambda Ll} r^{-(L+1)} \int_0^r n_{lm}(r_1) r_1^{\lambda+L} dr_1 + M^{(4)}_{\lambda Ll} r^L \int_r^{\infty} n_{lm}(r_1) r_1^{\lambda-L-1} dr_1]. \tag{9}$$

Here $C^{LM}_{lm\lambda\mu}$ is the Clebsch-Gordan coefficient, expressions for $M^{(i)}_{\lambda Ll}$ are given in the Appendix. In the atomic nuclei case only term (8) should be considered.

In principle, the strength constant $\kappa^{-1}_{\lambda\mu d}$ can be calculated within methods of numerical integrating by using expressions (2), (4)-(9). But for qualitative estimations the analytical expression for $\kappa^{-1}_{\lambda\mu d}$ can be useful. This expression has the form

$$\kappa^{-1}_{\lambda\mu d} = -\sum_{lm}\sum_{l'm'}\sum_{LM} (-1)^M C^{LM}_{lm\lambda\mu} \cdot (C^{L-M}_{lm\lambda\mu} + d(-1)^{\mu} C^{L-M}_{lm\lambda-\mu})$$

$$\cdot (L^{lml'm'(v)}_{\lambda L} + L^{lml'm'(c)}_{\lambda L}) \tag{10}$$

where

$$L^{lml'm'(v)}_{\lambda L} = \frac{\lambda(2\lambda-1)(2\lambda+1)^2}{2\pi(2L+1)} \int_0^{\infty} dr r^{2\lambda-2}$$

$$\cdot [L^{(1)}_{\lambda Ll'} \frac{dn_{l'm'}}{dr}\frac{dV_{lm}}{dr} r^2 + L^{(2)}_{\lambda Ll'} n_{l'm'} \frac{dV_{lm}}{dr} r + L^{(3)}_{\lambda Ll'} n_{l'm'} V_{lm}], \tag{11}$$

$$L^{lml'm'(c)}_{\lambda L} = \frac{2\lambda(2\lambda-1)(2\lambda+1)^2}{(2L+1)^2} \cdot \int_0^{\infty} dr r^{\lambda}$$

$$\cdot [L^{(4)}_{\lambda Ll'} n_{l'm'}(r) n_{lm}(r) r^{\lambda} + L^{(5)}_{\lambda Ll'} n_{l'm'}(r) \cdot r^{-(L+1)} \int_0^r n_{lm}(r_1) \cdot r_1^{\lambda+L} dr_1$$

$$+L^{(6)}_{\lambda Ll l'} n_{l'm'}(r)\cdot r^L \int_r^\infty n_{lm}(r_1)\cdot r_1^{\lambda-L-1} dr_1]. \qquad (12)$$

The coefficients $L^{(i)}_{\lambda Ll l'}$ are given in the Appendix.

For the spherical case ($l = m = 0$, $L = \lambda$), expressions (7) and (10) are very simplified:

$$Q^{(d)}_{\lambda\mu}(\mathbf{r}) = \lambda/\sqrt{4\pi}[Y_{lm}(\Omega) + d\cdot Y^{\dagger}_{lm}(\Omega)]z[\frac{dV_0}{dr} r^{\lambda-1} - 4\pi r^{-(\lambda+1)} \int_0^r n_0(r_1) r_1^{2\lambda} dr_1] \qquad (13)$$

and

$$\kappa^{-1}_{\lambda\mu d} = -\frac{\lambda^2 d}{2\pi}(1+\delta_{\mu,0}) \int_0^\infty [\frac{dn_0}{dr}\frac{dV_0}{dr} + 4\pi n_0^2(r)] r^{2\lambda} dr. \qquad (14)$$

For systems with a large number of particles the direct solving of the RPA equations takes a considerable computer time. This is especially true for deformed systems. For investigation of GR in such systems the strength function method is very useful. Within this method we can avoid finding roots of the secular equation (1) and get information about GR through the strength function [12]

$$b(E\lambda\mu,\omega) = \sum_t B(E\lambda\mu, gr \to \omega_t)\rho(\omega-\omega_t) \qquad (15)$$

with the weight function

$$\rho(\omega-\omega_t) = \frac{1}{2\pi}\cdot\frac{\Delta}{(\omega-\omega_t)^2 + (\Delta/2)^2}. \qquad (16)$$

Here, $B(E\lambda\mu, gr \to \omega_t)$ is the reduced probability of $E\lambda\mu$ transition from the ground state to the one-phonon state with excitation energy ω_t, determined from the secular equation (1). The quantity Δ is an averaging parameter. Following the prescription [12], where the strength function for atomic nuclei is considered in detail, for MC we obtain

$$b(E\lambda\mu,\omega) = \frac{1}{\pi}\left(Im\left(\frac{\tilde{X}_t^2(z)}{X_t(z) - \kappa^{-1}_{\lambda\mu d}}\right)_{z=\omega+i\Delta/2}\right.$$

$$\left. +\Delta\sum_{k<k'} p^{\lambda\mu}_{kk'}\left(\frac{1}{(\omega-(\epsilon_k+\epsilon_{k'}))^2+(\Delta/2)^2} - \frac{1}{(\omega+(\epsilon_k+\epsilon_{k'}))^2+(\Delta/2)^2}\right)\right) \qquad (17)$$

where

$$\tilde{X}_t = 2\sum_{kk'} \frac{<k'|Q|k> p^{\lambda\mu}_{kk'}(\epsilon_k+\epsilon_{k'})}{(\epsilon_k+\epsilon_{k'})^2 - \omega_t^2} \qquad (18)$$

and $p^{\lambda\mu}_{kk'}$ is the single-particle element for the operator of $E\lambda$ transition.

If all collective strength is assumed to be concentrated in one peak (one-pole approximation), we can get the estimation

$$\omega^2_{\lambda\mu} = (\omega^{(0)}_{\lambda\mu})^2 + \frac{\int(\nabla Q_{\lambda\mu}(\mathbf{r}))^2\cdot n_0(\mathbf{r})d\mathbf{r}}{(\int Q(\mathbf{r})_{\lambda\mu}\nabla f(\mathbf{r})\cdot\nabla n_0(\mathbf{r})d\mathbf{r})} \qquad (19)$$

where $\omega_{\lambda\mu}$ and $\omega^{(0)}_{\lambda\mu}$ are the energy of the collective peak and its unperturbed value, respectively. Using a spherical jellium approximation for electron density, the oscillator form for single-particle potential

$$V_0(r) = 1/2\cdot\omega_0^2 r^2 \qquad (20)$$

and the estimation $\omega^{(0)}_\lambda = \lambda\omega_0$ for unperturbed energy, we obtain the simple expression for excitation energy of $E\lambda$ GR in spherical MC:

$$\omega_\lambda = \sqrt{\frac{\lambda}{2\lambda+1}\omega_p^2 + \omega_0^2\lambda(\lambda-1)}. \qquad (21)$$

where ω_p is the plasma frequency. This expression exactly reproduces the estimations for frequencies of E1 and E2 GR, obtained within the sum rule approach [6,13], but the λ dependence in the second term of (21) is in contradiction with the $\sim(2\lambda+1)(\lambda-1)$ dependence in [13,14] (in [13] also the spherical jellium approximation for electron density was used). This discrepancy could be caused by the use for the static potential in (21) of the oscillator form which is not consistent with the ground state electron density distribution. This could mean that the oscillator potential can not be appropriate for description of GR with large multipolarity.

Within the same approximations the estimation [6] for the splitting of E1 GR in spheroidal MC with a quadrupole deformation δ is reproduced:

$$\omega^{z}_{\lambda=1} = \omega_p/\sqrt{3}\cdot(1-\frac{2}{5}\delta), \tag{22}$$

$$\omega^{z}_{\lambda=1} = \omega_p/\sqrt{3}\cdot(1+\frac{1}{5}\delta). \tag{23}$$

Finally, the equations of the VPM [6] are derived to make them suitable for description of GR in systems (MC and atomic nuclei) with any deformation. Any single-particle potentials and electron (nucleon) densities for which the coefficients of the multipole expansion are known can be used within this model. The RPA calculations within this version of the VPM are now in progress.

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Appendix

The coefficients used above have the following form:

$$M^{(1)}_{\lambda Ll} = A_{\lambda Ll} - B_{\lambda Ll},$$

$$M^{(2)}_{\lambda Ll} = l\cdot A_{\lambda Ll} - (l+1)\cdot B_{\lambda Ll},$$

$$M^{(3)}_{\lambda Ll} = (l+\lambda+L+1)\cdot A_{\lambda Ll} + (l-\lambda-L)\cdot B_{\lambda Ll},$$

$$M^{(4)}_{\lambda Ll} = (l+\lambda-L)\cdot A_{\lambda Ll} + (l-\lambda+L+1)\cdot B_{\lambda Ll}$$

where

$$A_{\lambda Ll} = \sqrt{(l+1)(2l+3)}\begin{pmatrix} l+1 & \lambda-1 & L \\ \lambda & l & 1 \end{pmatrix}\cdot C^{L0}_{l+10\lambda-10},$$

$$B_{\lambda Ll} = \sqrt{l(2l-1)}\begin{pmatrix} l-1 & \lambda-1 & L \\ \lambda & l & 1 \end{pmatrix}\cdot C^{L0}_{l-10\lambda-10}.$$

Further,

$$L^{(1)}_{\lambda Lll'} = M^{(1)}_{\lambda Ll'}\cdot M^{(1)}_{\lambda Ll},$$

$$L^{(2)}_{\lambda Lll'} = M^{(1)}_{\lambda Ll'}\cdot M^{(2)}_{\lambda Ll} - M^{(2)}_{\lambda Ll'}\cdot M^{(1)}_{\lambda Ll},$$

$$L^{(3)}_{\lambda Lll'} = ((2\lambda-1)M^{(1)}_{\lambda Ll'} + M^{(2)}_{\lambda Ll'})\cdot M^{(2)}_{\lambda Ll},$$

$$L^{(4)}_{\lambda Lll'} = ((L-\lambda)M^{(1)}_{\lambda Ll'} - M^{(2)}_{\lambda Ll'})\cdot M^{(3)}_{\lambda Ll},$$

$$L^{(5)}_{\lambda Lll'} = ((\lambda+L+1)M^{(1)}_{\lambda Ll'} + M^{(2)}_{\lambda Ll'})\cdot M^{(4)}_{\lambda Ll},$$

$$L^{(6)}_{\lambda Lll'} = M^{(1)}_{\lambda Ll'}\cdot(M^{(3)}_{\lambda Ll} - M^{(4)}_{\lambda Ll}).$$

For spherical systems we have $l = m = 0, L = \lambda$ and

$$B_{\lambda\lambda 0} = M^{(2)}_{\lambda\lambda 0} = M^{(4)}_{\lambda\lambda 0}$$

$$= L^{(2)}_{\lambda\lambda 00} = L^{(3)}_{\lambda\lambda 00} = L^{(4)}_{\lambda\lambda 00} = L^{(5)}_{\lambda\lambda 00} = 0,$$

$$M^{(1)}_{\lambda\lambda 0} = A_{\lambda\lambda 0} = \sqrt{\frac{\lambda}{(2\lambda-1)(2\lambda+1)}},$$

$$M^{(3)}_{\lambda\lambda 0} = A_{\lambda\lambda 0}(2\lambda+1) = \sqrt{\frac{\lambda(2\lambda+1)}{(2\lambda-1)}},$$

$$L^{(1)}_{\lambda\lambda 00} = A^2_{\lambda\lambda 0} = \frac{\lambda}{(2\lambda-1)(2\lambda+1)},$$

$$L^{(6)}_{\lambda\lambda 00} = A^2_{\lambda\lambda 0}(2\lambda+1) = \frac{\lambda}{(2\lambda-1)}.$$

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