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A RELATION BETWEEN ADIABATIC INERTIAL PARAMETERS
AND THE CUBIC INVERSE ENERGY-WEIGHTED SUM RULE*

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Abstract. In the case of a collective path generated by a constrained Hartree-Fock calculation, we derive a simple expression for the adiabatic inertial parameter. This parameter is given by the cubic inverse energy-weighted sum rule calculated in the random phase approximation around each point of the path.

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In the present letter we consider mass parameters calculated in adiabatic time-dependent Hartree-Fock theory [1]. We shall assume that the collective path is generated by a constrained Hartree-Fock calculation

$$[W_0 - \lambda \hat{Q}, \rho_0(\lambda)] = 0 \quad (1)$$

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where $\lambda\hat{Q}$ is a given external field and W_0 the Hartree-Fock field constructed from the single-particle density matrix $\rho_0(\lambda)$ (satisfying $\rho_0^2 = \rho_0$). For such a path it has been shown in reference [2] that the adiabatic inertial mass $M(\lambda)$ is given by the nuclear polarizability corresponding to the operator

$$\hat{P} = i\hbar \left[\frac{\partial \rho_0(\lambda)}{\partial \lambda}, \rho_0(\lambda) \right] . \quad (2)$$

Explicitly

$$M(\lambda) = \frac{\partial}{\partial \mu} \langle \Phi(\lambda, \mu) | \hat{P} | \Phi(\lambda, \mu) \rangle \Big|_{\mu=0} , \quad (3)$$

where $\Phi(\lambda, \mu)$ is the Hartree-Fock solution of the constrained Hamiltonian $H - \lambda\hat{Q} - \mu\hat{P}$. Since the right-hand side of eq. (3) is known to be related to the inverse energy-weighted sum rule calculated in the random-phase approximation (RPA) [3,4], we can also express $M(\lambda)$ as

$$M(\lambda) = 2 \sum_{n>0} | \langle \psi_n | \hat{P} | \psi_0 \rangle |^2 / \omega_n . \quad (4)$$

In eq. (4) ψ_n and ω_n denote RPA eigenstates and energies corresponding to the Hamiltonian $H - \lambda\hat{Q}$, ψ_0 the RPA ground state and the sum runs over positive energy states only. We will now show that the amplitudes $\langle \psi_n | \hat{P} | \psi_0 \rangle$ can be related to those of the constraining operator $\hat{Q}$.

For this purpose we define the column vectors ρ_1 , p and q whose components are

$$\rho_1(a, A) = \langle a | \frac{\partial \rho_0}{\partial \lambda} | A \rangle , \quad p(a, A) = \langle a | \hat{P} | A \rangle , \quad q(a, A) = \langle a | \hat{Q} | A \rangle , \quad (5)$$

where a is a particle state and A a hole state relative to the Hartree-Fock ground state defined by $\rho_0(\lambda)$. With this notation one has [5,6]

$$\langle \psi_n | \hat{Q} | \psi_0 \rangle = (X_n^+ \ Y_n^+) \begin{pmatrix} q \\ q^* \end{pmatrix}, \quad \langle \psi_n | \hat{P} | \psi_0 \rangle = (X_n^+ \ Y_n^+) \begin{pmatrix} p \\ p^* \end{pmatrix}, \quad (6)$$

where X_n and Y_n are the RPA amplitudes defined by [6]

$$X_n(a, A) = \langle \psi_0 | C_A^+ C_a | \psi_n \rangle, \quad Y_n(a, A) = \langle \psi_0 | C_a^+ C_A | \psi_n \rangle, \quad (7)$$

with C^+ being the particle creation operator.

As is well known, the self-consistent change $\Delta \lambda \rho_1$ in the density matrix $\rho_0(\lambda)$ induced by increasing the external field $\lambda \hat{Q}$ to $(\lambda + \Delta \lambda) \hat{Q}$ is given by [7]

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_1^* \end{pmatrix} = \begin{pmatrix} q \\ q^* \end{pmatrix}. \quad (8)$$

In eq. (8) A and B are the usual RPA matrices [5] calculated with the Hamiltonian $H - \lambda \hat{Q}$. Multiplying both sides of eq. (8) to the left by $(X_n^+ \ Y_n^+)$ we obtain

$$\omega_n (X_n^+ - Y_n^+) \begin{pmatrix} \rho_1 \\ \rho_1^* \end{pmatrix} = \langle \psi_n | \hat{Q} | \psi_0 \rangle. \quad (9)$$

Since from the definition (2) of the operator $\hat{P}$ we have

$$\langle a | \hat{P} | A \rangle = i\hbar \langle a | \rho_1 | A \rangle, \text{ i.e. } p = i\hbar \rho_1, \text{ eq. (9) reduces to}$$

$$\omega_n \langle \psi_n | \hat{P} | \psi_0 \rangle = i\hbar \langle \psi_n | \hat{Q} | \psi_0 \rangle. \quad (10)$$

Inserting this expression into eq. (4) we find that the inertial mass $M(\lambda)$ is related to the cubic inverse energy-weighted sum rule calculated in RPA:

$$M(\lambda) = 2\hbar^2 m_{-3}(\hat{Q}), \quad (11)$$

where m_k is the usual notation for the RPA moment of the distribution of multipole strength [4]

$$m_k(\hat{Q}) = \sum_{n>0} \omega_n^k |\langle \psi_n | \hat{Q} | \psi_0 \rangle|^2. \quad (12)$$

An obvious consequence of eq. (11) is that the RPA moment m_{-3} is directly obtainable by solving the constrained Hartree-Fock equations implied by expression (3). Such calculations were already performed in ref. [2] for quadrupole vibrations in Oxygen-16 and Carbon-12. More generally eq. (10) implies that $m_{-(2k+1)}$ can be obtained by performing k successive constrained Hartree-Fock calculations.

By using as a collective variable the quantity $Q = \langle \hat{Q} \rangle$ the inertial mass $M(Q)$ (satisfying $M(Q)dQ^2 = M(\lambda)d\lambda^2$) is found to be

$$M(Q) = \frac{1}{2} \hbar^2 m_{-3} / (m_{-1})^2, \quad (13)$$

since from references [3,4] we know that $dQ/d\lambda = 2m_{-1}$. This expression shows that the adiabatic inertial mass $M(Q)$ is greater than or equal to the irrotational mass defined as [8]

$$B(Q) = \frac{1}{2} \hbar^2 / m_1(\hat{Q}) \quad (14)$$

Indeed from the inequality $m_{-1}/m_{-3} \leq m_1/m_{-1}$ [4], we find that $M(Q) \geq B(Q)$, with equality occurring in the only case where the distribution of strength is concentrated into one single state. In the numerical calculations of reference [2] it was found that $M(Q)$ and $B(Q)$ are rather close for quadrupole vibrations in Oxygen-16, while significant differences occur in Carbon-12. From the above discussion we see that this result is related to the fact that the RPA quadrupole strength is more concentrated in Oxygen-16 than Carbon-12.

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