The Effective Potential Energy Surface for the CVM

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A method is proposed for calculating the effective potential-energy surface (PES) which corresponds to each wave function calculated in the cluster-vibration model (CVM)[1]. This method would enable us to see to what extent clusters act as "rocks in the sea which smooth out the neighbouring waves"[2], generating in this way effective anharmonicities. Our method is based on the decomposition of the total quadrupole operator $\bar{B}$

$$\bar{B} = \bar{\alpha} + \bar{q}$$

where $\bar{\alpha}$ presents the collective and $\bar{q}$ the cluster quadrupole operator. Then the expectation values of the following operators are needed[3]: B^2, B^4, B^6, $B^3 \cos 3G$, $B^6 \cos^2 3G$, with respect to the CVM wave functions. Then, for example, $\langle CVM||B^2||CVM\rangle = \langle||(\bar{\alpha}\times\bar{\alpha})^0 + (\bar{q}\times\bar{q})^0 + 2(\bar{\alpha}\times\bar{q})^0||\rangle$. Each matrix element is factorized into the collective and cluster-factor. In order to carry out this factorization, the mixed operators are rewritten in the form

$$(\bar{\alpha}\times\bar{q})^0(\bar{\alpha}\times\bar{q})^0 = \sum_{\ell} c_1 |(\bar{\alpha}\times\bar{\alpha})^{\ell}(\bar{q}\times\bar{q})^{\ell}|^0 .$$

In this way, all matrix elements can be decomposed by a completeness relation.

1) G. Alaga, Rendiconti Scuola Internazionale, 40 Corso, Varenna 1967, p. 28.
2) S.G. Nilsson, private communication.
3) B.R. Mottelson, private communication.