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ENERGY-WEIGHTED MOMENTS IN THE PROBLEMS OF FRAGMENTATION

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Investigation of the interaction between simple nuclear excitations (for example, one-quasiparticle or one-phonon states) and more complex states (quasiparticle-plus-phonon or two-phonon ones) is essential for describing quantitatively the nuclear resonance width, explaining the quenching of the spin-isospin transition strength and so on. The modifications in the energetical spectrum and transition strength caused by the interaction between simple and complex states consume the main efforts in such calculations. It is convenient to express the integral characteristics of the strength distributions through their energy-weighted moments

$$S^K = \sum_{\nu} E_{\nu}^K |\langle 0|B|\psi_{\nu}\rangle|^2. \qquad (1)$$

where $\langle 0|B|\psi_{\nu}\rangle$ is the amplitude of transition from the ground $|0\rangle$ to excited state $|\psi_{\nu}\rangle$ with excitation energy E_{ν} due to the action of the transition operator B, K is nonnegative integer. The sum is taken through all the states ψ_{ν}.

The method of calculation of the energy-weighted moments for the fragmentation task to solve it in the quasiparticle-phonon nuclear model (QPNM)[1] is described. Simple states (one-quasiparticle, one-phonon, etc.) that are the eigenstates of the vibrational hamiltonian describing superconducting-type quasiparticles and separable multipole-multipole and spin-multipole-spin-multipole interactions between them are naturally selected in this model, and more complex states (quasiparticle-plus-phonon, two-phonon, etc.) are connected with them by the quasiparticle-phonon interaction, i.e.,

$$H = H_{v} + H_{vq}.$$

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$$H=H_{v}+H_{vq}.$$

H_v is the vibrational hamiltonian, H_{vq} is the hamiltonian of quasiparticle-phonon interaction. Eigenfunctions of the H

$$H\psi_\nu=E_\nu\psi_\nu \qquad (2)$$

are chosen in the form of

$$\psi_\nu=\sum_m c_m^\nu\varphi_m+\sum_n\tilde{c}_n^\nu\tilde{\varphi}_n\,, \qquad (3)$$

where φ_m are eigenstates of H_v

$$H_v\varphi_m=\omega_m\varphi_m$$

and $\tilde{\varphi}_n$ are more complex states, φ_m and $\tilde{\varphi}_n$ being mutually orthogonal.

Let us define the projection operators P and Q by

$$P\psi_\nu=\sum_m c_m^\nu\varphi_m$$

and

$$Q\psi_\nu=\sum_n\tilde{c}_n^\nu\tilde{\varphi}_n\,.$$

It is evident that

$$PQ\psi_\nu=QP\psi_\nu=0$$

and

$$(P+Q)\psi_\nu=\psi_\nu\,.$$

Using those relations (2) may be rewritten as

$$\begin{aligned}(PH_vP+PH_{vq}Q)\psi_\nu&=E_\nu P\psi_\nu\\(QH_{vq}P+QHQ)\psi_\nu&=E_\nu Q\psi_\nu\end{aligned} \qquad (2')$$

H_ϑ is the vibrational hamiltonian, $H_{\vartheta q}$ is the hamiltonian of quasiparticle-phonon interaction. Eigenfunctions of the H

$$H\psi_\nu = E_\nu \psi_\nu \qquad (2)$$

are chosen in the form of

$$\psi_\nu = \sum_m c_m^\nu \varphi_m + \sum_n \tilde{c}_n^\nu \tilde{\varphi}_n , \qquad (3)$$

where φ_m are eigenstates of H_ϑ

$$H_\vartheta \varphi_m = \omega_m \varphi_m$$

and $\tilde{\varphi}_n$ are more complex states, φ_m and $\tilde{\varphi}_n$ being mutually orthogonal.

Let us define the projection operators P and Q by

$$P\psi_\nu = \sum_m c_m^\nu \varphi_m$$

and

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It is evident that

$$PQ\psi_\nu = QP\psi_\nu = 0$$

and

$$(P+Q)\psi_\nu = \psi_\nu .$$

Using those relations (2) may be rewritten as

$$\begin{aligned} (PH_\vartheta P + PH_{\vartheta q} Q)\psi_\nu &= E_\nu P\psi_\nu \\ (QH_{\vartheta q} P + QHQ)\psi_\nu &= E_\nu Q\psi_\nu \end{aligned} \qquad (2')$$

because

$$PHP\psi_\nu = PH_\vartheta P\psi_\nu$$

$$PH_\vartheta Q\psi_\nu = 0 .$$

Therefore, the problem is reduced to the eigenvalue problem for the real symmetrical matrix $\hat{H}$

$$\hat{H} \begin{Vmatrix} P\psi_\nu \\ Q\psi_\nu \end{Vmatrix} \equiv \begin{Vmatrix} PH_\vartheta P & PH_{\vartheta q}Q \\ QH_{\vartheta q}P & QHQ \end{Vmatrix} \begin{Vmatrix} P\psi_\nu \\ Q\psi_\nu \end{Vmatrix} = E_\nu \begin{Vmatrix} P\psi_\nu \\ Q\psi_\nu \end{Vmatrix}$$

or in detail

$$\omega_m c_m^\nu + \sum_{n'} \langle\varphi_m|H_{\vartheta q}|\tilde{\varphi}_{n'}\rangle \tilde{c}_{n'}^\nu = E_\nu c_m^\nu$$

$$\sum_{m'} \langle\tilde{\varphi}_n|H_{\vartheta q}|\varphi_{m'}\rangle c_{m'}^\nu + \sum_{n'} \langle\tilde{\varphi}_n|H|\varphi_{n'}\rangle \tilde{c}_{n'}^\nu = E_\nu \tilde{c}_n^\nu .$$

For each ν the unknowns c_m^ν and $\tilde{c}_n^\nu$ set the matrix $\hat{H}$ eigenvector corresponding to the eigenvalue E_ν. The norm of this vector is defined by

$$\langle\psi_\nu|\psi_\nu\rangle = \sum_m {c_m^\nu}^2 + \sum_n {\tilde{c}_n^\nu}^2 = 1 .$$

The amplitude of transition from the ground $|0\rangle$ to the excited state (3) is equal to

$$\langle 0|B|\psi_\nu\rangle = \sum_m c_m^\nu \langle 0|B|\varphi_m\rangle + \sum_n \tilde{c}_n^\nu \langle 0|B|\tilde{\varphi}_n\rangle .$$

In many tasks the direct transition to the state $\tilde{\varphi}_n$ can be neglected, i.e., it may be assumed that $\langle 0|B|\tilde{\varphi}_n\rangle = 0$. In this case

$$\langle 0|B|\psi_\nu\rangle = \sum_m c_m^\nu \langle 0|B|\varphi_m\rangle = \sum_m c_m^\nu b_m ,$$

where $b_m = \langle 0|B|\varphi_m\rangle$ and

$$S^k = \sum_\nu E_\nu^k \sum_{m,m'} c_m^\nu c_{m'}^\nu b_m b_{m'}^* =$$

$$= \sum_{m,m'} b_m b_{m'}^* \sum_\nu E_\nu^k c_m^\nu c_{m'}^\nu .$$

Based on the properties of the eigenvectors and eigenvalues of the real symmetrical matrix or more exactly on the spectral decomposition of the real symmetrical matrix ([2] and eq. (2) from the appendix), it can be shown that

$$\sum_\nu E_\nu^k c_m^\nu c_{m'}^\nu = (\hat{H}^k)_{m,m'} ,$$

where $\hat{H}^k$ is the k-th degree of the matrix $\hat{H}$. Hence,

$$S^k = \sum_{m,m'} (\hat{H}^k)_{m,m'} b_m b_{m'}^* = \langle 0|BPH^kPB^+|0\rangle . \qquad (4)$$

By using this formula and the rules of multiplication of the block matrices, it is easy to get

$$S^0 = \langle 0|BPB^+|0\rangle = \sum_m |b_m|^2$$

$$S^1 = \langle 0|BPH_\nu PB^+|0\rangle = \sum_m \omega_m |b_m|^2$$

$$S^2 = \langle 0|BP\{H_\nu^2 + H_{\nu q}QQH_{\nu q}\}PB^+|0\rangle =$$

$$= \sum_{m,m'} b_m b_{m'}^* \{\omega_m^2 \delta_{m,m'} + \sum_n \langle\varphi_m|H_{\nu q}|\tilde{\varphi}_n\rangle\langle\tilde{\varphi}_n|H_{\nu q}|\varphi_{m'}\rangle\} .$$

It is seen from those expressions that in the fragmentation tasks, if one does not take into account a possibility of a direct transition from the ground to complex states $\tilde{\varphi}_n$, the quasi-particle-phonon interaction alters neither the total transition strength nor the energy centroid (independence of S^0 and S^1 of $H_{\nu q}$) but increases the second moment, i.e., leads to the growth of the strength distribution width.

Of special interest is the case when among $\tilde{\varphi}_n$ there are states that are not directly coupled with simple ones, i.e. described $\langle\varphi_m|H_{\nu q}|\tilde{\varphi}_n\rangle = 0$ or

$$Q\psi_\nu = (Q_1 + Q_2)\psi_\nu$$

and

$$Q_2 H_{\nu q} P\psi_\nu = PH_{\nu q} Q_2 \psi_\nu .$$

In this case matrix $\hat{H}$ appears as

$$\hat{H} = \left\| \begin{matrix} PH_\nu P & PH_{\nu q}Q_1 & 0 \\ Q_1H_{\nu q}P & Q_1HQ_1 & Q_1HQ_2 \\ 0 & Q_2HQ_1 & Q_2HQ_2 \end{matrix} \right\| .$$

Evidently,

$$S^2 = \langle 0|BP\{H_\nu^2 + H_{\nu q}Q_1Q_1H_{\nu q}\}PB^+|0\rangle ,$$

$$S^3 = \langle 0|BP\{H_\nu^3 + H_{\nu q}Q_1Q_1H_{\nu q}PPH_\nu +$$

$$+ H_{\nu q}Q_1Q_1HQ_1Q_1H_{\nu q} + H_\nu PPH_{\nu q}Q_1Q_1H_{\nu q}\}PB^+|0\rangle ,$$

i.e., S^2 and S^3 do not depend on the interaction between sub-spaces $Q_1\psi$ and $Q_2\psi$. It follows that the total width of strength distribution is defined by those complex states that are directly coupled with simple ones.

Limiting ourselves to one simple state φ_0 and assuming $b_m = \delta_{m,0}$, we can receive the result of paper [3] which has been obtained in the second perturbation order.

While calculating fragmentation one has strongly to limit due to technical reasons a number of complex states $\tilde{\varphi}_n$ taken into account. The influence of neglected configurations may be estimated by using the energy-weighted moments; their definition by formula (4) does not need diagonalizing of the large-order matrix. The table shows the energy-weighted moments S^2 and S^3 of the Gamov - Teller states strength distribution on ^{90}Zr [4] defined for different number of two-phonon states. In all, more than 11000 two-phonon states were used. The states were chosen from them for which the matrix element of the interaction hamiltonian with one-phonon states exceed a certain threshold given in the first column of the table. The table shows that the main contribution to S^2 and S^3 comes from less than 30% of two-phonon states, i.e., two-phonon basis may strongly be truncated without great loss.

Table. Dependence of S^2 and S^3 for the Gamov-Teller states on ^{90}Zr on the number of two-phonon states taken into account

Threshold value of matrix element in % of the maximal one	Number of two-phonon state in % of the maximal one	S^2 [a] in % of the maximal value	S^3 [b] in % of the maximal value
0	100	100	100
0.001	94	100	100
0.01	70	99.9	99.8
0.1	29	98.5	96.3
1.0	4	93.6	84.7
10	0.27	86.6	69.0
50	0.036	83.3	61.3

a) Contribution of $\sum_m \omega_m^2 b_m b_m^*$ to S^2 amounts to 82%.

b) Contribution of $\sum_m \omega_m^3 b_m b_m^*$ to S^3 amounts to 52%.

If the amplitudes $\langle 0/B/\tilde{\varphi}_n\rangle$ cannot be neglected in the calculation of $\langle 0/B/\Psi_\nu\rangle$ amplitude, the expression

$$S^K = \langle 0/B\tilde{P}H^K\tilde{P}B^+/0\rangle$$

should be used instead of (4). Here $\tilde{P}$ is the projection operator onto those states φ_m and $\tilde{\varphi}_n$, the amplitude of transition to which from the ground state is not equal to zero.

Therefore, based on the spectral decomposition of symmetrical real matrix, one can construct an economical (from the computing point of view) method to determine the energy-weighted moments which can be used to study the integral characteristics of strength distributions to control the errors caused by truncation of the complex states basis.

In conclusion I should like to express my deep gratitude to Prof. V.G.Soloviev and Drs. N.Yu.Shirikova, A.I.Vdovin, V.V.Voronov and L.A.Malov for reading this paper and making critical remarks.

Appendix

It is known[2] that the real symmetrical matrix $\hat{A}$ with dimension $N\times N$ has N linearly-independent eigenvectors which can be orthonormalized, i.e.,

$$\hat{A}\vec{x}^i = \lambda_i \vec{x}^i \qquad i = 1,\dots,N$$

and

$$(\vec{x}^i, \vec{x}^j) = \delta^{ij},$$

where $(\vec{a},\vec{b}) = \sum_{l=1}^{N} a_l b_l$ is the scalar product of the vectors $\vec{a}$ and $\vec{b}$. Since an arbitrary N-dimensioned vector can be decomposed in N linearly independent vectors $\vec{x}^i$

$$\hat{A}\vec{y} = \hat{A}\sum_{i=1}^{N}(\vec{x}^i,\vec{y})\vec{x}^i = \sum_{i=1}^{N}\lambda_i \vec{x}^i(\vec{x}^i,\vec{y})$$

and the matrix $\hat{A}$ can be expressed as

$$\hat{A} = \sum_{i=1}^{N}\lambda_i \cdot \hat{E}^i, \qquad (1)$$

should be used instead of (4). Here $\widetilde{P}$ is the projection operator onto those states φ_m and $\widetilde{\varphi}_n$, the amplitude of transition to which from the ground state is not equal to zero.

Therefore, based on the spectral decomposition of symmetrical real matrix, one can construct an economical (from the computing point of view) method to determine the energy-weighted moments which can be used to study the integral characteristics of strength distributions to control the errors caused by truncation of the complex states basis.

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and the matrix $\hat{A}$ can be expressed as

$$\hat{A} = \sum_{i=1}^{N}\lambda_i \hat{E}^i, \qquad (1)$$

where $(\hat{E}^i)_{\ell\ell'} = x^i_\ell x^i_{\ell'}$. Defined in such a manner matrices $\hat{E}^i$ satisfy

$$\hat{E}^i \hat{E}^j = \delta^{ij}\hat{E}^i$$

and

$$\sum_{i=1}^{N}\hat{E}^i = \hat{I},$$

where $\hat{I}$ is the unit matrix. Matrix $\hat{E}^i$ is called the projection matrix [2] and (1) is called the spectral decomposition of the real symmetrical matrix[2]. Based on the properties of $\hat{E}^i$ matrices, it is easy to show that

$$\hat{A}^K = \sum_{i=1}^{N}\lambda_i^K \hat{E}^i$$

here K is a non-negative integer.

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Кузьмин В.А. E4-86-179

Энергетически-взвешенные моменты в задачах фрагментации

Задача фрагментации простых ядерных состояний по более сложным сводится к нахождению собственных векторов и собственных значений вещественной симметричной матрицы. На основе спектрального разложения этой матрицы получен простой и экономичный с вычислительной точки зрения алгоритм определения энергетически-взвешенных моментов силовой функции. Это позволило исследовать чувствительность решения задачи фрагментации к ограничению базиса сложных состояний. Показано, что полная ширина силовой функции определяется только теми сложными состояниями, которые непосредственно связаны с простыми.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Kuzmin V.A. E4-86-179

Energy-Weighted Moments in the Problems of Fragmentation

The problem of fragmentation of simple nuclear states on the complex ones is reduced to real symmetrical matrix eigenvalue problem. Based on spectral decomposition of this matrix the simple and economical from computing point of view algorithm to calculate energetically-weighted strength function moments is obtained. This permitted one to investigate the sensitivity of solving the fragmentation problem to reducing the basis of complex states. It is shown that the full width of strength function is determined only by the complex states connected directly with the simple ones.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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