PRACTICAL ANGULAR MOMENTUM PROJECTION METHOD IN MULTI-SHELL HARTREE-FOCK CALCULATIONS; ^{22}Na AS AN EXAMPLE

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A practical method for projecting good angular momentum from non-axial deformed HF intrinsic states involving a large number of particles and j shells, is described. The ^{22}Na example shows good results for the excitation energies, and E2 and M1 matrix elements.

The use of multi-shell deformed Hartree-Fock intrinsic states [1] has been recognised to be a powerful method for providing a microscopic description of the bulk properties of nuclei [2]. However, one should also project good angular momentum from these states in order to compute detailed properties such as energies and spins of excited states. This letter describes a fast, practical, and general projection method, applicable to large bases, and gives results for ^{22}Na as an example. A systematic investigation of all the stable nuclei with $4 \leqslant A \leqslant 40$ will be reported elsewhere.

Let $|\chi\rangle$ be a normalised intrinisic-state Slater determinant defined by N (neutron) and Z (proton) deformed HF orbitals, each having good parity. Thus $|\chi\rangle$ may violate axial, neutron-proton, and time-reversal symmetry. We do assume however that $|\chi\rangle$ has the IV group rotational symmetry so that it may be expressed in the principal axis system of the mass quadrupole tensor [3], where any two K's contained in a $|\chi\rangle$ differ by a multiple of 2. Thus we have

$$|\chi\rangle = \sum_{K=K_{\min}, K_{\min}+2\ldots}^{K_{\max}} \; \sum_{J=|K|}^{J_{\max}} |J(K)K\rangle \qquad (1)$$

where $|J(K)M\rangle$ is the unnormalised projected component of $|\chi\rangle$ with good J and $J_z = M$, and belonging to the Kth band of $|\chi\rangle$. For any two $|\chi\rangle$'s and any multipole operator of rank λ, $\hat{O}_{\lambda\mu}$, the reduced matrix elements [4] $\langle J'(K')\| O_\lambda \| J(K)\rangle$ are given by a slight generalisation of the well-known Hill-Wheeler integral of Peierls and Yoccoz [5]

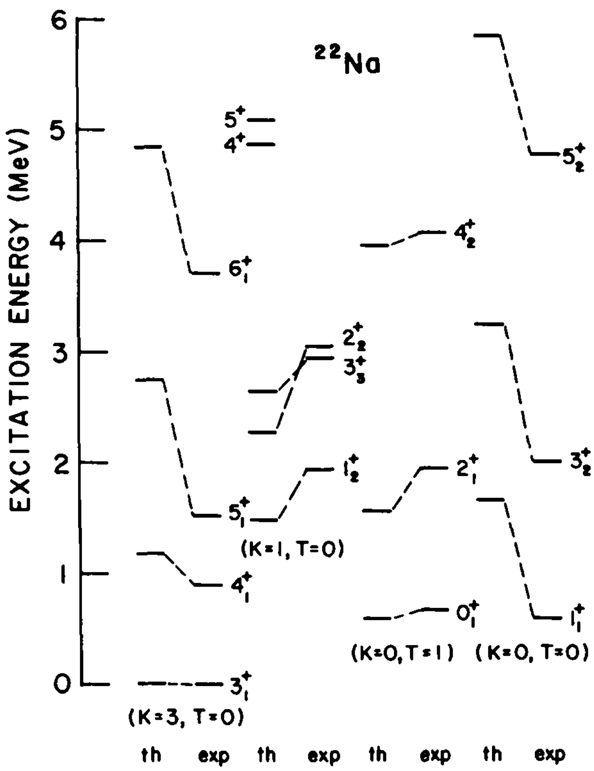

Fig. 1. Low energy spectrum of ^{22}Na.

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$$\langle J'(K')\|O_\lambda\|J(K)\rangle = \frac{2J+1}{8\pi^2}\sum_{\mu} C^{J\lambda J'}_{K'-\mu,\,\mu K'}$$

$$\times \int d^3\Omega\, D^{J\,*}_{K'-\mu,K}(\Omega)\,\langle\chi'|\hat{O}_{\lambda\mu}\hat{R}(\Omega)|\chi\rangle\ , \qquad (2)$$

where $\Omega = (\alpha, \beta, \gamma)$ denotes the three Euler angles, $\hat{R}(\Omega)$ is the rotation operator, $D^{J}_{MN}(\Omega)$ is a rotation matrix,

$$\int d^3\Omega = \int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_{-1}^{+1} dx, \quad x = \cos\beta\ ,$$

and C denotes a Clebsch-Gordan coefficient. In particular, the overlap and normalisation coefficients of the projected states are obtained from eq. (2) by using the unit operator $\hat{O}_{oo} = 1$. Now the α and γ integrations can not be performed analytically because of the non-axiality of $|\chi\rangle$; in fact, one needs an optimal method to compute the $\int d^3\Omega$ integrals since the integrands are time consuming to evaluate, especially when $\hat{O}_{\lambda\mu}$ is a two-body operator such as the Hamiltonian and a large basis is used. One can show that this may be done through the use of Gaussian quadrature formulae. Thus the β integration is replaced by the familiar formula

$$\int_{-1}^{+1} f(x)\,dx = \sum_{i=1}^{N_\beta} f(x_i)w_i\ , \qquad (3)$$

where N_β is the number of different J states contained in $|\chi\rangle$ and $|\chi'\rangle$, $f(x)$ is the integrand in eq. (2), and x_i and w_i are the nodes and weights of the N-point Gaussian quadratures. The γ integration is replaced by a not so well-known identity

$$\frac{1}{2\pi}\int_0^{2\pi} f(\gamma)d\gamma = \frac{1}{m}\sum_{r=0}^{m-1} f\left(\frac{\pi r}{m}\right)\ , \qquad (4)$$

$$2m = K_{\max} - K_{\min} + 2\ ,$$

which can be shown to hold exactly for all the integrands in eq. (2). A similar equation holds for the α integral. The above results only make useof the $\Delta K = 2$ rule and are thus valid for both even and odd nuclei. The required number of independent values of the integrand can be reduced by the judicious use of symmetries. For example, if $|\chi'\rangle = |\chi\rangle$, then from $(\hat{O}_{\lambda\mu})^+ = (-1)^{\lambda-\mu+c}\,\hat{O}_{\lambda-\mu}$ instead of m^2N_β only $\frac{1}{2}m(m+1)N_\beta$ evaluations of the integrand need be made. For even-even nuclei with IV group invariant ground state configurations, one reduces this last number by nearly an additional factor of four.

Although there are several ways [1,6] of calculating the matrix elements $\langle\chi'|\hat{O}_{\lambda\mu}\hat{R}(\Omega)|\chi\rangle$ occurring in eq. (2), we have found the cross-density matrix method of Löwdin [7] to be the most suitable one for our purpose. Since the details of the method can be found in ref. [7], we only remark here that an algorithm can be found such that the method may still be used even when $|\chi\rangle$ and $|\chi'\rangle$ are orthogonal by one or two particle-hole pairs [8], as is the case in β-decay transitions.

We now turn to our ^{22}Na example. We use a five major shell basis [2] with $\hbar\omega = 13.5$ MeV, the Saunier-Pearson No.2 N-N interaction [9], the two-body Coulomb interaction, and the kinetic energy with respect to the center-of-mass. All twenty-two single-nucleon orbits are different from each other. The HF intrinsic state is obtained iteratively and the projected energy is computed. The method of variation after projection is also used to perturb this intrinsic state until the lowest projected energy is obtained; further details of this procedure will be given elsewhere. As a result, it emerges that the low-lying positive parity states can be represented adequately by one non-axial state containing components with* $K = 5, 3, 1, -1$ and one axial $K = 0$ ($|\chi_0\rangle$) state. The non-axial state is mostly $K = 3$ and will be called $|\chi_3\rangle$. This state yields the lowest 3^+ state at $E_b = 159.93$ MeV, which is identified with the experimental 3^+ ground state at $E_{b,\exp} = 174.15$ MeV. Fig. 1 shows a comparison between the calculated and experimental positive parity excitation spectra [10,11]. The theoretical excitation energies are all taken relative to E_b and the spectrum is separated into four bands for convenience only, since the K and T values shown are only approximate due to the nonaxiality [12] and the Coulomb force [2]. The $K = 3$, and $K = 1$ bands are projected from $|\chi_3\rangle$ while the other two come from $|\chi_0\rangle$. Whereas the $K = 3$ band spectrum shows a marked dilation, the spacings of the other bands are good, with the possible exception of the missing Coriolis inversion of the $2^+_2, 3^+_3$ levels in the $K = 1$, $T = 0$ band. Although Coriolis decoupling is automatically included in the projection method its strength is being underestimated here. The higher excitation energy of the $K = 0$, $T = 0$ band head compared to the $K = 0$, $T = 1$ one is interesting and may indicate a possible defect in the relative strengths of the $T = 0$ to $T = 1$ components

* The number of K's in a given χ can be determined by studying the reduced matrix elements of the zero-body identity operator.

Table 1
Electromagnetic decay properties of low lying states in ^{22}Na

	Branching ratio (%)		B(E2)(e^2 fm^4)		B(M1)(μ_0^2)		mixing ratio		lifetime	
$J_i \rightarrow J_f$	exp[a]	th[b]	exp	th	exp	th	exp	th[b]	exp	th[b]
$4_1^+ \rightarrow 3_1^+$	100	100	98 ± 8	111	$5.4 \pm 1.2 \times 10^{-4}$	4.07×10^{-3}	-3.19 ± 0.26	-1.23	13.6 ±1.0ps	7.87ps
$5_1^+ \rightarrow 4_1^+$	5	13	78 ± 42	103	$5.5 \pm 3.0 \times 10^{-4}$	5.99×10^{-3}	$\pm 2.00 \pm 0.15$	-0.70	80 ± 27ps	32.2 ps
$\rightarrow 3_1^+$	95	87	25 ± 9	27.1					4.3 ± 1.4ps	3.62ps
$6_1^+ \rightarrow 5_1^+$	35 ± 10	37	135 ± 61	82.4		6.62×10^{-3}		-2.03	52 ×17fs	60.2 fs
$\rightarrow 4_1^+$	65 ± 10	63	57 ± 21	48.1						
$0_1^+ \rightarrow 1_1^+$	100	100				7.91				17.7 ps
$2_1^+ \rightarrow 1_1^+$	100	100		0.0017		3.12		-2.7×10^{-4}		7.1 fs
$\rightarrow 0_1^+$	0	0		64.7						
$3_2^+ \rightarrow 2_1^+$	0	0.4		0.0035		3.33		-1.5×10^{-4}	1.74 ± 0.34ps	1.82ps
$\rightarrow 1_1^+$	100	99.6	90 ± 18	82.9						
$4_2^+ \rightarrow 3_2^+$	100	100		0.010		3.36		-9.5×10^{-4}		1.9 fs
$\rightarrow 2_1^+$	0	0		92.0						
$5_2^+ \rightarrow 4_2^+$	40	46		0.010		3.37		-8.9×10^{-4}		30.0 fs
$\rightarrow 3_2^+$	60	54		97.1						

a) Experimental data are from ref. [10], and references quoted therein. Weighted means are taken if several pieces of recent data are available for one transition.
b) Empirical energies [10,11] are used to compute branching ratios, mixing ratios and lifetimes.

of the N-N interaction used here [9]. Since this effect is a small fraction of the total binding energy it may be that a minor change in the force parameters could produce the required shift without appreciably changing the wave-functions.

Finally we show, in table 1, some E2 and M1 decay parameters. The E0 (isometric shifts) M3 and E4 matrix elements have also been computed but will be discussed elsewhere. The agreement with experiment is generally good except for a factor of 10 error in the $\Delta T = 0$, M1 transitions in the $K = 3$ band. These are computed to be hindered by three orders of magnitude instead of the measured four orders of magnitude. This is responsible for the calculated rates of the transitions $4_1^+ \rightarrow 3_1^+$ and $5_1^+ \rightarrow 4_1^+$ being two or three times faster than the observed rates. The magnetic moments of the 3_1^+ and 1_1^+ (0.583 MeV) states were computed to be 1.805 and 0.526 nm, whereas experiment [10] yields 1.746 ± 0.01 and 0.54 ± 0.01 respectively. For comparison, the values 1.578 and 0.721 nm were calculated for the magnetic moments of the 3_2^+ and 1_2^+, respectively. The calculated electric quadrupole moment of the 3_1^+ state was $+22.81$ e fm^2 and that of the 1_1^+ was -11.08 e fm^2. To summarise we see that the present method appears to account for both bulk [2] and detailed nuclear properties without using any adjustable parameters other than those used in the basic nucleon-nucleon two-body effective interaction [9].

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