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Evaluation of Nuclear Potential Matrix Elements in the Deformed Cartesian Basis

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A method is developed which permits a rapid computation of the nuclear potential matrix elements on the deformed Cartesian basis using the reduced matrix elements $\langle nl \mid V_{JST} \mid n'l' \rangle_\omega$ and the brackets $\langle nlm \mid n_x n_y n_z \rangle$ given by an analytic expression valid for ω_x, ω_y, ω_z, ω being nonequal.

The main features concerning the implantation of this method on a computer using the symmetry properties of the calculated terms are also given.

INTRODUCTION

It is sometimes advantageous in nuclear structure calculations to use the harmonic oscillator basis. It is then easy to build states of given (λ, μ) [1] and in the case of deformed nuclei, one can use a restricted basis with different values of ω on the three coordinate axes [2]. Nevertheless, in that case the calculation of the nuclear interaction matrix elements may necessitate the evaluation of multiple integrals with all the disadvantages involved.

We suggest an indirect method without integral calculations using the reduced matrix elements on the spherical basis. This method is specially suitable for potentials defined by matrix elements in the spherical basis, as Kuo and Brown potential, and may be used also for potentials given analytically, since the programs for the evaluation of such elements generally exist for such potentials. We use an analytic expression for the bracket $\langle n_x n_y n_z \mid nlm \rangle$ valid for a deformed Cartesian basis and symmetry properties which allow the program to be available on a small computer.

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PRINCIPAL FEATURES OF THE CALCULATION

Knowing the reduced matrix elements $\langle nl \mid V_{JST} \mid n'l' \rangle_\omega$ we compute all $\langle ij \mid V \mid \tilde{k}l \rangle$, i, j, k, l being wave functions of the Cartesian basis belonging to the $1s$, $1p$, $2s$, $1d$ shells with supplementary quantum numbers $\tau_z = \pm\frac{1}{2}$ and $\sigma_z = \pm\frac{1}{2}$. ω_x, ω_y, ω_z may have different values. Usually, the reduced matrix elements are given for

$$\begin{aligned} l, l' &= 0, 1, 2, \\ 0 &\leqslant n, n' \leqslant 7. \end{aligned} \tag{1}$$

For ω_x, ω_y, ω_z equal, $\mid n_x n_y n_z \rangle$ may be expanded on the states $\mid nlm \rangle$ of the same ω and the same major shell. Then the calculation of matrix elements $\langle ij \mid V \mid \tilde{k}l \rangle$ is done by adding the contributions of a finite number of known reduced matrix elements.

For ω_x, ω_y, ω_z nonequal, $\mid n_x n_y n_z \rangle$ has an infinite expansion on the spherical basis.

To calculate matrix elements $\langle ij \mid V \mid \tilde{k}l \rangle$ one needs to know an infinite number of reduced matrix elements. Then one has to truncate the expansion according to condition (1). The evaluation will be correct if

$$\sum_{\substack{n>7 \\ l=0,1,2 \\ -l\leqslant m\leqslant l}} |\langle nlm \mid n_x n_y n_z \rangle|^2$$

is very small. This condition may be achieved if $n_x + n_y + n_z$ is small and if ω_x, ω_y, ω_z are not too much different, so we take

$$\omega = (\omega_x \omega_y \omega_z)^{1/3}.$$

Since our program evaluates $\langle ij \mid V \mid \tilde{k}l \rangle$ in the first three major shells and takes into account the large dimension of the spherical basis used, we may hope for a good precision as regards physical deformations.

DETAILS OF THE CALCULATION

First the scalar products $\langle nlm \mid n_x n_y n_z \rangle$ are calculated. If the Cartesian basis is not deformed we obtain [3]

$$\begin{aligned} &\langle nlm \mid n_x n_y n_z \rangle \\ &\quad = (-i)^{n_y} [1 + (-)^{n_x+n_y-m}] (-)^{1/2(n-l-m+n_x-n_y)} \frac{(n_x + n_y + m/2)!}{2^{l+1}} \\ &\qquad \times \left(\frac{(2l+1)(l-m)!\, n_x!\, n_y!\, n_z!}{(n+l+1)!!\, (n-l)!!\, (l-m)!} \right)^{1/2} \delta_{n_z, n-n_x-n_y} \end{aligned}$$

$$\times \sum_{s=0}^{l} \sum_{\mu=0}^{n_x} \frac{(-)^{\mu+s}}{(n_x - \mu)!\,((n_y - n_x - m)/2 + \mu)!\,\mu!\,((n_x + n_y + m)/2 - \mu)!}$$

$$\times \frac{((n - l)/2 + s)!\,(2l - 2s)!}{((n - l + m - n_x - n_y)/2 + s)!\,s!\,(l - s)!\,(l - 2s - m)!} \tag{2}$$

For $m \geqslant 0$.

In order to eliminate the complex coefficient $(-i)^{n_y}$ we use the Cartesian basis kets with a coefficient $(-i)^{n_y}$ as geometrical basis states. If the Cartesian basis is deformed we write

$$\langle nlm \mid n_x n_y n_z \rangle = \sum_{n_x' n_y' n_z'} \langle nlm \mid n_x' n_y' n_z' \rangle \langle n_x' n_y' n_z' \mid n_x n_y n_z \rangle.$$

Here the $\mid n_x' n_y' n_z' \rangle$ are the kets of the Cartesian basis with the same ω as $\mid nlm \rangle$ and belong to the same major shell. $\langle nlm \mid n_x' n_y' n_z' \rangle$ is then evaluated with the previous formula,

$$\langle n_x n_y n_z \mid n_x' n_y' n_z' \rangle = \langle n_x \mid n_x' \rangle \langle n_y \mid n_y' \rangle \langle n_z \mid n_z' \rangle.$$

Writing

$$\alpha = (\omega_x/(\omega_x + \omega))^{1/2} \qquad \beta = (\omega/(\omega_x + \omega))^{1/2},$$

we have

$$\langle n_x \mid n_x' \rangle = ((\omega_x + \omega)\,\pi n_x!\,n_x'!\,2^{n_x + n_x'})^{-1/2} \int_{-\infty}^{+\infty} \exp(-x^2/2)\,H_{n_x}(\alpha x)\,H_{n_x'}(\beta x)\,dx.$$

In order to calculate the last integral we integrate the product of $\exp(-x^2/2)$ and the generating functions of $H_{n_x}(\alpha x)$ and $H_{n_x'}(\beta x)$

$$I_1 = \int_{-\infty}^{+\infty} \exp(-x^2/2)\exp(-s^2 + 2s\alpha x - t^2 + 2t\beta x)\,dx$$

$$= (2\pi)^{1/2} \exp(s^2(2\alpha^2 - 1) + t^2(2\beta^2 - 1) + 4\alpha\beta st).$$

This integral may be expanded in the following way:

$$I_1 = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{s^m t^n}{m!\,n!} \int_{-\infty}^{+\infty} \exp(-x^2/2)\,H_m(\alpha x)\,H_n(\beta x)\,dx.$$

By identifying with the expansion of I_1 after integration we obtain for $m + n$ even

$$\int_{-\infty}^{+\infty} \exp(-x^2/2)\,H_{n_x}(\alpha x)\,H_{n_x'}(\beta x)\,dx$$

$$= (2\pi)^{1/2}\,n_x!\,n_x'! \sum_{q=0}^{\min(n_x, n_x')} \frac{2^{2q}}{(n_x + n_x'/2)!}\,(2\alpha^2 - 1)^{(n_x - q)/2}$$

$$(2\beta^2 - 1)^{(n_x' - q)/2}\,(\alpha\beta)^q\,C^q_{n_x + n_x'} C^{(n_x' - q)/2}_{(n_x + n_x')/2 - q}$$

The summation over q is done for q values being such that $q + n_x$ is even. Knowing the brackets $\langle nlm \mid n_x n_y n_z \rangle$ we calculate the matrix elements

$$\langle n_x n_y n_z S S_z \mid V_{TS} \mid n_x' n_y' n_z' S S_z' \rangle$$
$$= \sum_{lml'm'JJ_z} \langle n_x n_y n_z \mid nlm \rangle \langle lSmS_z \mid JJ_z \rangle \langle nlJ \mid V_{TS} \mid n'l'J \rangle$$
$$\langle JJ_z \mid l'Sm'S_z' \rangle \langle n'l'm' \mid n_x' n_y' n_z' \rangle .$$

Finally we calculate $\langle ij \mid V \mid \tilde{k}\tilde{l} \rangle$.

The spatial wave functions $\phi_i \phi_j \phi_k \phi_l$ associated to i, j, k, l are expanded in the C.M. and relative coordinate systems.

These expansions are factorizables on the three axes, the expansion coefficients being given by the relation [4]

$$\langle n_x , \bar{n}_x \mid n, N \rangle = \left(\frac{n_x ! \, \bar{n}_x ! \, n! \, N!}{2^{n+N}} \right)^{1/2} \delta(n_x + \bar{n}_x - n - N)$$
$$\sum_{\alpha} \frac{(-)^{\alpha}}{(n_x - n + \alpha)! \, (\bar{n}_x - \alpha)! \, (n - \alpha)! \, \alpha!} .$$

For each term of the expansion all S, S_z , T, T_z are coupled to the i, j, k, l spins and isospins with the addition of the different contributions. We also add to the nuclear interaction the C.M. kinetic energy two body contribution

$$- \frac{1}{mA} \sum_{i<j} \mathbf{p}_i \mathbf{p}_j .$$

A is the mass number of the nucleus

$$\mathbf{p}_1 \mathbf{p}_2 = p_{1x} p_{2x} + p_{1y} p_{2y} + p_{1z} p_{2z} .$$

On $0x$, for instance, we have [5]

$$\langle n_\alpha n_\beta \mid p_{1x} p_{2x} \mid n_\gamma n_\delta \rangle = - \tfrac{1}{4} m \hbar \omega_x [\delta_{n_\gamma - 1, n_\alpha (2n_\gamma)^{1/2}} - \delta_{n_\gamma + 1, n_\alpha \{2(n_\gamma + 1)\}^{1/2}}]$$
$$\times \, [\delta_{n_\delta - 1, n_\beta (2n_\delta)^{1/2}} - \delta_{n_\delta + 1, n_\beta \{2(n_\delta + 1)\}^{1/2}}].$$

Symmetry Properties Used in the Calculation

The use of several symmetrie properties is necessary for making the program available on an IBM 360-40.

$-\langle nlm \mid n_x n_y n_z \rangle$ is different from 0 only if $n_x + n_y + n_z + l$ and $n_x + n_y + m$ are even. Then $\langle n_x n_y n_z \mid nlm \rangle$ may belong to the four series:

Series	1	2	3	4
$(-)^{n_x+n_y}$	+	−	−	+
$(-)^{n_z}$	+	−	+	−
l	0 2 −2	−1	−1	1
m	0 0 2	1	1	0

$$-\langle n_x n_y n_z S_z \mid V_{ST} \mid n_x' n_y' n_z' S_z' \rangle$$

It may be shown by a rotation of π around 0_x in the triplet case that

$$\langle n_x n_y n_z S_z \mid V_{ST} \mid n_x' n_y' n_z' S_z' \rangle = (-)^{n_x+n_x'} \langle n_x n_y n_z - S_z \mid V_{ST} \mid n_x' n_y' n_z' - S_z' \rangle.$$

Moreover a matrix element may differ from 0 only if $n_z + n_z' + S_z + S_z'$ is even. Then only the following elements are computed:

$n_z + n_z'$ even	$n_z + n_z'$ odd
$S_z = 1\ S_z' = 1$	$S_z = 1\ S_z' = 0$
$S_z = 1\ S_z' = -1$	$S_z = 0\ S_z' = 1$
$S_z = 0\ S_z' = 0$	

Singlet

$$-\langle ij \mid V \mid \tilde{k}l \rangle$$

The Cartesian basis is numbered so that odd states have numbers greater than even states. An element $\langle ij \mid V \mid \tilde{k}l \rangle$ may generate seven other elements by permutations of i and j, k and l, ij and kl. Then we compute only elements $\langle ij \mid V \mid \tilde{k}l \rangle$ such that

$$n^0\phi_i \geqslant n^0\phi_j\ n^0\phi_k \geqslant n^0\phi_l\ n^0\phi_i \geqslant n^0\phi_k\,. \tag{3}$$

There are only four possible series of elements to be calculated:

ϕ_i	ϕ_j	ϕ_k	ϕ_l
even	even	even	even
odd	even	odd	even
odd	odd	odd	odd
odd	odd	even	even

The fourth series is useless for Hartree Fock calculations with parity eigenstates orbitals.

Sets of $\phi_i\phi_j\phi_k\phi_l$ satisfying (3) are called successively. The calculation of all the $\langle ij \mid V \mid kl \rangle$ built by making spins and isospins of i, j, k, l equal to $\pm\frac{1}{2}$ is then performed and the values are written on a magnetic tape. The whole calculation requires only 15 minutes on an IBM 360-40.

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