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Few-body anharmonic oscillators and the matrix continued fractions

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Abstract. For both identical and distinguishable particles and for an arbitrary polynomial approximation to the realistic two-body forces, the A-body Hamiltonian may be converted into an infinite block-three-diagonal matrix in the properly arranged, translationally invariant, oscillator basis. As a consequence, the exact Green function and all the projections of eigenstates of the microscopic Schrödinger equation become expressible in terms of the matrix continued fractions. This generalises the recent reformulation of the one-dimensional $A=1$ anharmonic problem by Graffi and Grecchi. The quick convergence of this non-perturbative method of solving the many-body bound-state problem is demonstrated for the simplest three- and four-body examples. With the core-possessing type $V(r)=-r^2+r^4$ of the spin- and isospin-independent two-body interaction, only the 10^{-3} error in the three-bosonic ground-state energy arises from restricting our formulae to 5×5 dimensional matrices.

1. Introduction and summary

The microscopic description of nuclear structure is a typical situation where we must use efficient approximation techniques since the 'exact' numerical solution of the underlying microscopic Schrödinger equation

$$H\psi = E\psi \qquad H = -\sum_{i=1}^{A} \frac{\hbar^2}{2m_i}\Delta_{\vec{r}_i} + \sum_{i>j=1}^{A} V(\vec{r}_i - \vec{r}_j) \tag{1.1}$$

is extremely complicated. This is caused by the strong core of the phenomenological nucleon–nucleon forces, the long range of the Coulombic interaction, etc.

Perturbation approaches may start from the only solvable many-body model with the harmonic oscillator (HO) forces $V(\vec{r}) \sim r^2$ and often encounter formal as well as practical difficulties. The simple-minded perturbation strategy is therefore modified by alternative variational techniques adapted to the specific nature of the particular problem in question. For example, the Faddeev–Yakubovsky equations are usually considered for the few-body energies, $\exp(-S)$ formalism describes the structure of magic nuclei, etc. In the present paper we shall investigate the possibilities offered by the formalism of the matrix continued fractions (MCF, see § 2 or Znojil 1980).

Our present approach to the many-body problem is inspired by Graffi and Grecchi (1975) and their exact solution of the one-body problem with anharmonic oscillator (AHO) interactions. Our main idea lies in the replacement of any 'realistic' force by

its polynomial approximation

$$V(\vec{r}) = \sum_{m=1}^{p} g_m (\vec{r}^{\,2})^m \qquad g_p > 0, p \geq 1. \tag{1.2}$$

We shall see below that this leads to the applicability of the MCF method. Since we are interested only in the sufficiently strongly bound states, the necessary value of degree p in the AHO force (1.2) may be expected to be reasonably small. Intuitively, this may be interpreted as a consequence of the spatial confinement of the system and supports *a priori* our belief in the overall efficiency of the MCF stragegy.

In the numerical context, MCF formalism preserves some of the merits of the Lanczos algorithm. Because of the present widespread accessibility of medium-sized computers, its iterative manipulations with relatively small matrices seems to be a highly promising technique. It might also bridge the gap between the analytic and purely numerical pictures of the physical processes and resembles partially the somewhat related doorway and hallway state constructions (Feshbach *et al* 1980).

For pedagogical reasons, we first present our results for distinguishable particles (§ 3) while the realistic system of indistinguishable particles (we neglect spin variables for the sake of brevity) is studied in § 4. We show how group theory helps to elucidate the structure of the optimal basis and we emphasise the minimisation of dimensions of the continued-fraction matrices. This meets the practical requirements concerning computer capacity. One of our main conclusions is the rather unusual observation that, once the anharmonicity p in (1.2) is fixed, an increase in A, especially for the transition to the genuine many-body problem ($A=2 \to A=3 \to \ldots$), is surprisingly 'smooth' from the technical point of view, especially in the case of identical particles. Thus, although the exceptional character of the many-body HO force is even more pronounced than in the traditional one-particle problem (the AHO corrections alter the Schrödinger equation more profoundly), the formal analogy between different values of A is easily preserved. Furthermore, all the technical and numerical characteristics of the various few-body AHO calculations (increase of dimensions, rate of convergence, etc) prove to be comparable from the practical point of view. In the simplest $p=2$ examples with a 'core' we have achieved fairly good convergence of the ground-state energies for the three- and four-body bosonic AHO systems, never using matrices larger than 10×10.

Of course, for very high A, the numerical performance of the MCF formalism becomes less efficient since the dimensions in the exact Schrödinger equation grow too quickly. Nevertheless, the iterative character of our MCF representation of the Green function seems to remain at least a useful guide for making approximations, the character of which might resemble the various averagings employed in the reaction-theory context (Feshbach *et al* 1980).

Our preliminary numerical tests are very encouraging for light nuclei. We may therefore expect that some more realistic models (with $A>3$ and $p>2$ or including the spin, isospin and tensor forces) will also be exactly solvable by the present MCF technique.

2. The matrix continued-fraction method

Linear equations of the Schrödinger type may be treated by methods varying from the analytic representations of ψ and E to their purely numerical approximations.

The MCF method lies somewhere between these two extremes and represents a reasonably flexible formalism comprising many specific approaches as special cases. In the present context, we may explain its structure by recalling the inspiration of our paper, namely, the solution of the one-body AHO problem in one spatial dimension as given by Graffi and Grecchi (1975). In their case, the use of the HO basis (Hermite polynomials) implies the band structure of the Hamiltonian H. In full analogy with the classical treatment of the three-diagonal (Jacobi) matrices (Wilkinson 1965) the authors arrive at the MCF representation of the Green function and identify its numerically determined poles with the AHO energy levels.

The formalism summarised here is worked out in detail by Znojil (1980). To the partitioned HO basis $|X_k^m\rangle$, $m = 1, 2, \ldots, M_k$, $k = 1, 2, \ldots$, and to the related Hamiltonian matrix in the partitioned block-three-diagonal (BTD) form

$$H = \begin{pmatrix} A_1 & B_1 & 0 & \ldots & \\ B_2^{\mathrm{T}} & A_2 & B_2 & 0 & \ldots \\ 0 & B_2^{+} & \ldots & & \\ \ldots & & & & \end{pmatrix} \qquad \begin{array}{l} A_k = A_k^{ij},\ B_k = B_k^{in}, \\ i, j = 1, 2, \ldots, M_k \\ n = 1, 2, \ldots, M_{k+1} \\ k = 1, 2, \ldots \end{array} \tag{2.1}$$

we may assign the auxiliary sequence $F_k(E)$, $k = 1, 2, \ldots$, satisfying the recurrences

$$F_k(E) = (EI - A_k - B_k F_{k+1}(E) B_k^{+})^{-1}. \tag{2.2}$$

The finite truncation of the matrix H is equivalent to the initialisation $F_{N+1}(E) = 0$ of (2.2). It is assumed that the limit $N \to \infty$ exists and defines each MCF $F_k(E)$ in the same way as the classical continued fractions are defined as limits of their finite approximants (Wall 1948). The MCF coincide with the classical continued fractions whenever $M_k = 1$, $k = 1, 2, \ldots$.

Assuming the existence of the MCF sequence $F_k(E)$ in the vicinity of the AHO energy levels $E = E_0$, we may identify $G(E) = \det F_1(E)$ with the Green function of the Schrödinger equation (1.1). Moreover, the Schrödinger equation is reduced to the finite-dimensional model-space form

$$\sum_{i=1}^{M_1} (E\delta_{ij} - \mathscr{H}_{ij}^{\mathrm{eff}}) D_1^i = 0 \qquad j = 1, 2, \ldots, M_1 \tag{2.3}$$

where the effective Hamiltonian is defined explicitly by the exact MCF expression $\mathscr{H}^{\mathrm{eff}} = A_1 + B_1 F_2(E) B_1^{+}$. Once the energies $E = E_0$ are determined numerically as the poles of $G(E)$, the projections $D_1^i = \langle X_1^i \,|\, \psi \rangle$ of the exact solution on the model-space basis may be found easily from the $M_1 \times M_1$ dimensional linear algebraic equation (2.3). As a consequence, the complete solution of (1.1) with any H of the BTD form (2.1) may be written as a compact expansion (Znojil 1980)

$$\psi = \alpha \sum_{k=1}^{\infty} \sum_{i=1}^{M_k} |X_k^i\rangle D_k^i \qquad D_{k+1} = D_k B_k F_{k+1}(E_0) \qquad k \geqslant 1. \tag{2.4}$$

The normalisation formula determining α,

$$\|\psi\| = \alpha^2 \sum_{k=1}^{\infty} \sum_{i=1}^{M_k} D_k^i D_k^i, \tag{2.5}$$

follows from the orthonormality of the HO basis.

The proofs of convergence are an important ingredient of the MCF formalism converting the formal solution into the analytical one. In the present context, they are still missing even when $A = 1$, especially for the infinite series (2.4). At the same time, their numerical $A = 1$ tests have led us to expect that the favourable numerical properties might survive the transition to the many-body AHO cases.

3. Distinguishable particles

The one- →two-body or the one- →three-dimensional extensions of (1.1) are trivial and need not be explained in detail. In a way, their further $A = 2 \to A = 3 \to \ldots$ generalisation is also a matter of mere technicality but the details are less trivial—they will be worked out in the following.

3.1. Anharmonic forces in Jacobi coordinates

The first technical question we must resolve when considering systems with $A \geqslant 2$ is the removal of the centre-of-mass (CM) degrees of freedom. This step is entirely standard—assuming for simplicity that all the particle masses are equal ($\hbar = 2m_i = 1$, $i = 1, 2, \ldots, A$), we may define the Jacobi coordinates

$$\bar{\xi}_i = (\xi_i \sin\theta_i \cos\varphi_i, \xi_i \sin\theta_i \sin\varphi_i, \xi_i \cos\varphi_i)$$
$$= [i(i+1)]^{-1/2}\left(-i\bar{r}_{i+1} + \sum_{j=1}^{i} \bar{r}_j\right) \qquad i = 1, 2, \ldots, A-1, A \tag{3.1}$$

where $\bar{r}_{A+1} = 0$. Since the kinetic energy operator remains proportional to the sum of Laplacians in the new variables (3.1), we may put

$$H = -\Delta_{\bar{\xi}_A} + H_o \qquad \psi = \psi_0 \exp(\mathrm{i}\,\bar{k}_A \bar{\xi}_A) \qquad E = E_0 + \bar{k}_A^2 \tag{3.2}$$

and obtain the AHO Schrödinger equation (1.1) in the translationally invariant form

$$H_0\psi_0 = E_0\psi_0 \qquad H_0 = -\sum_{i=1}^{A-1} \Delta_{\bar{\xi}_i} + V_{\mathrm{AHO}}^{(A,p)}$$
$$V_{\mathrm{AHO}}^{(A,p)} = \sum_{j=1}^{A}\sum_{i=1}^{j-1}\sum_{m=1}^{p} g_m[(\bar{r}_i - \bar{r}_j)^2]^m = \sum_{m=1}^{p} g_m v_m^{(A)}(\bar{\xi}_1, \ldots, \bar{\xi}_{A-1})$$
$$v_m^{(A)} = v_m^{(A)}(\xi_1, \ldots, \xi_{A-1}, \cos\omega_{ij}) \tag{3.3}$$
$$\cos\omega_{ij} = \cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \cos(\varphi_i - \varphi_j) \qquad 1 \leqslant i < j \leqslant A-1.$$

Here, ψ_0 is independent of $\bar{\xi}_A$ and $V_{\mathrm{AHO}}^{(A,p)}$ is a genuine many-body operator.

The HO interaction ($p = 1$) is exceptional because of the removal of this many-body character of V since

$$V_{\mathrm{AHO}}^{(A,1)} = g_1 A \sum_{i-1}^{A-1} \xi_i^2.$$

Starting from the first non-degenerate (quartic, $p = 2$) case, the angular dependence

of $V_{\mathrm{AHO}}^{(A,p)}$ does not drop out and we get

$$v_2^{(3)} = \tfrac{9}{2}(\xi_1^2+\xi_2^2)^2 - 6\xi_1^2\xi_2^2 \sin^2\omega_{12}$$

$$v_2^{(4)} = 5\xi_1^4 + 5\xi_2^4 + \tfrac{16}{3}\xi_3^4 + \tfrac{10}{3}\xi_1^2\xi_2^2 + \tfrac{8}{3}\xi_1^2\xi_3^2 + \tfrac{8}{3}\xi_2^2\xi_3^2 + \tfrac{20}{3}\xi_1^2\xi_2^2\cos^2\omega_{12} + \tfrac{16}{3}\xi_1^2\xi_3^2\cos^2\omega_{13}$$
$$+ \tfrac{16}{3}\xi_2^2\xi_3^2\cos^2\omega_{23} + (16/3\sqrt{2})\xi_1^2\xi_2\xi_3\cos\omega_{12}\cos\omega_{13}$$
$$+ (8/3\sqrt{2})(\xi_1^2-\xi_2^2)\xi_2\xi_3\cos\omega_{23}$$

and so on. The derivation and structure of the general formula is rather lengthy though straightforward; we obtain

$$v_m^{(A)} = \sum_{B=2}^{A} W_m^{(B)}$$

$$W_m^{(B)} = \sum_{j=1}^{B-1}[(\bar{r}_B - \bar{r}_j)^2]^m$$
$$= \sum_{j=1}^{B-1}\left(B^2 T_{B-1} + \sum_{n=j}^{B-2} T_n + (j-1)^2 T_{j-1} + 2B\sum_{n=j}^{B-2} S_{n,B-1}\right.$$
$$\left. - 2B(j-1)S_{j-1,B-1} + 2\sum_{n=j}^{B-2}\sum_{p=j}^{n-1} S_{pn} - 2\sum_{n=j}^{B-2}(j-1)S_{j-1,n}\right)^m$$
$$T_n = \xi_n^2/[n(n+1)] \qquad n = 1,\ldots,A-1$$
$$S_{ij} = \xi_i\xi_j\cos\omega_{ij}/[ij(i+1)(j+1)]^{1/2}$$
$$1 \leqslant i < j \leqslant A-1 \qquad m = 1,2,\ldots,p.$$

We observe that the complexity of the explicit $V_{\mathrm{AHO}}^{(A,p)}$ prescription increases rather quickly with p. Nevertheless, the corresponding lengthy formulae may comfortably be generated for any fixed A and p by an appropriate symbolic-manipulation language algorithm on the computer. The general structure of $V_{\mathrm{AHO}}^{(A,p)}$ characterised by the explicit presence of the angular variables resembles strongly the case of the non-central anharmonic potential solved by the MCF technique by Znojil (1981) for $A = 1$. This is the main inspiration of the following section.

3.2. Unsymmetrised oscillator basis and MCF solvability

Preserving the full analogy with the non-central modification of the one-body AHO we may get rid of the angular variables in the next entirely standard step using the 'multipolar' partial-wave decomposition of ψ_0. Of course, when $A > 2$, the orthonormalised and complete set of spherical '$A-1$-polar' harmonics $|\{l\}\rangle$ is not unique and may be defined with different angular momentum couplings (see Varshalovitsh *et al* 1975). In the simplest arrangement

$$\bar{l}_{A-1} + \bar{l}_{A-2} = \bar{\lambda}_{A-2} \qquad \bar{\lambda}_{i+1} + \bar{l}_i = \bar{\lambda}_i$$
$$i = A-3,\ldots,2 \qquad \bar{\lambda}_2 + \bar{l}_1 = \bar{L} \tag{3.4}$$

of the vector-addition scheme corresponding to the composite index (quantum numbers)

$$\{l\} = \{l\}_{A-2} = (l_{A-1}l_{A-2}(\lambda_{A-2})l_{A-3}(\lambda_{A-3})\ldots l_1 LM)$$

we obtain the harmonics ($\Omega_i = (\cos\theta_i, \varphi_i)$)

$$\langle\Omega_1\Omega_2\ldots\Omega_{A-1}|\{l\}_{A-2}\rangle = \sum_{\substack{m_1\ldots m_{A-1}\\ \mu_2\ldots\mu_{A-2}}} C^{LM}_{l_1 m_1 \lambda_2\mu_2} C^{\lambda_2\mu_2}_{l_2 m_2 \lambda_3\mu_3}\ldots C^{\lambda_{A-2}\mu_{A-2}}_{l_{A-2}m_{A-2}l_{A-1}m_{A-1}} \times Y_{l_1m_1}(\theta_1,\varphi_1)\ldots Y_{l_{A-1}m_{A-1}}(\theta_{A-1}\varphi_{A-1}) \tag{3.5}$$

where $C^{LM}_{lm\lambda\mu}$ and $Y_{lm}(\theta,\varphi)$ denote the standard Clebsch–Gordan coefficients and the spherical harmonics, respectively. Another coupling pattern we shall need below

$$\{l\} = \{l\}_m = l_{A-1}\ldots l_{m+2}(\lambda_{m+2})l_{m+1}l_m(\lambda)(\lambda_m)l_{m-1}\ldots LM,$$

may be obtained when we replace the $(m+1)$th and mth terms in (3.4) by the vector compositions

$$\bar{l}_{m+1} + \bar{l}_m \equiv \bar{\lambda} \qquad \bar{\lambda}_{m+2} + \bar{\lambda} \equiv \bar{\lambda}_m.$$

The overlap with the original states coincides with the so-called Racah coefficients:

$$\langle\{l\}_{A-2}|\{l\}_m\rangle = (-1)^{\lambda_{m+2}+l_{m+1}+l_m+\lambda_m}(2\lambda_{m+1}+1)^{1/2}(2\lambda+1)^{1/2}\begin{Bmatrix}\lambda_{m+2} & l_{m+1} & \lambda_{m+1}\\ l_m & \lambda_m & \lambda\end{Bmatrix} \tag{3.6}$$

and is proportional to the 6-j symbol $\{\ldots\}$.

For any coupling scheme, we introduce the partial waves $\varphi_{\{l\}} = \langle\{l\}|\psi_0\rangle$ and derive the radial form of the Schrödinger equation (3.3) in the usual way. Since the action of the kinetic energy operator on the harmonics $|\{l\}\rangle$ is well known, the detailed form of the radial equation depends on the action of the angular variables S_{ij}. When we identify $\cos\omega_{ij}$ with the bipolar function—$4\pi\langle\Omega_i\Omega_j|1100\rangle/\sqrt{3}$ and employ the Clebsch–Gordan series

$$\langle\Omega_1\Omega_2|1100\rangle\langle\Omega_1\Omega_2|l_1l_2\lambda\mu\rangle = \frac{\sqrt{3}}{4\pi}\sum_{\mu,\nu=0}^{1}(-1)^{\mu+\nu}(l_1+1-\mu)^{1/2}(l_2+1-\nu)^{1/2} \times\begin{Bmatrix} l_2+1-2\nu & l_2 & 1\\ l_1 & l_1+1-2\mu & \lambda\end{Bmatrix} \times\langle\Omega_1\Omega_2|l_1+1-2\mu, l_2+1-2\nu, \lambda\mu\rangle \tag{3.7}$$

it is not difficult to specify the decomposition of S_{ij} into the finite number of $|\{l'\}\rangle$ in accord with the triangular inequalities, $l'_{i,j} = l_{i,j}$, $l_{i,j} \geqslant 1$.

Concerning the partial-wave representation of the operator H_0, we may therefore infer that the multipolar basis may be ordered in such a way that H_0 acquires the block-three-diagonal operator form resembling (2.1); an example is given in § 3.3 below.

Completing the analogy with Znojil (1981), we introduce the A-body HO basis $|\langle n\rangle\{l\}\rangle$, $\langle n\rangle = (n_1, n_2, \ldots, n_{A-1})$ as the multipolar harmonics (3.5) multiplied by $(A-1)$tuple products of the radial $A=1$ HO states

$$\langle\xi|nl\rangle = (-1)^n\left(\frac{2\Gamma(n+1)}{\Gamma(n+l+\frac{3}{2})}\right)^{1/2}\exp(-\tfrac{1}{2}\xi^2)\xi^l L_n^{l+\frac{1}{2}}(\xi^2)$$
$$L_n^{\alpha}(x) = \frac{e^x x^{-\alpha}}{n!}\frac{d^n}{dx^n}(e^{-x}x^{\alpha+n}) \tag{3.8}$$

where $L_n^{\alpha}(x)$ are the classical Laguerre polynomials. Since they satisfy the fundamental identities (Bateman and Erdélyi 1953)

$$\begin{aligned} L_n^{\alpha-1}(x) &= L_n^{\alpha}(x) - L_{n-1}^{\alpha}(x) \\ xL_n^{\alpha+1}(x) &= (n+\alpha+1)L_n^{\alpha}(x) - (n+1)L_{n+1}^{\alpha}(x) \end{aligned} \tag{3.9}$$

the action of the radial variables T_i on any HO state (3.8) is similar to the action of the kinetic energy operator—it generates only the two other new states with $n_i' = n_i \pm 1$. At the same time, the action of the ξ linear variables S_{ij} is accompnied by the l shift—hence equations (3.9) remain applicable. This is of fundamental importance here; the action of the full operator H_0 on any state $|\langle n\rangle\{l\}\rangle$ always generates the finite number of similar states. The matrix representation of H_0 is of the form (2.1) due to the orthogonality of the HO basis. This completes the proof of our main statement, i.e., the applicability of the MCF technique of § 2 to any $A \geqslant 1$ AHO problem. In detail, we may define the Green function $G(E) = \det F_1(E)$, its poles $E = E_0$ and the HO projections $D_k(E_0)$ of ψ_0, i.e. the exact solution of the AHO many-body Schrödinger equation, provided that all the corresponding $N \to \infty$ limits exist.

We may specify the optimal ordering of the basis states. This generalised Lanczos (GL) construction leads to the minimal dimension of the blocks M_k and proceeds as follows.

(i) We choose any finite 'model-space' subset of the HO $|\langle n\rangle\{l\}\rangle$ states and denote its elements by the kets $|X_1^m\rangle$, $m = 1, 2, \ldots, M_1$.

(ii) The action of the Hamiltonian H_0 on this model space generates the finite superpositions of the new 'doorway' states $|\langle n'\rangle\{l'\}\rangle$ to be denoted as $|X_2^m\rangle$, $m = 1, 2, \ldots, M_2$.

(iii) Repeatedly, we re-numerate the full HO basis in such a way that each group $|X_{k+1}^m\rangle$, $m = 1, 2, \ldots, M_{k+1}$ of the kth 'hallway' states contains precisely the new states $|\langle n''\rangle\{l''\}\rangle$ generated from the old group $|X_k^m\rangle$, $m = 1, 2, \ldots, M_k$ by the action of H_0.

3.3. The three-body illustration

In the simplest case with $A = 3$, $p = 2$ and $L = 0$ where

$$\langle \Omega_1\Omega_2 | l_1 l_2 00\rangle = \delta_{l_1 l_2}[(-1)^l/4\pi](2l_1+1)^{1/2}P_{l_1}(\cos\omega_{12})$$

and $P_l(x)$ are the Legendre polynomials, the partial-wave expansion of ψ_0 becomes extremely simple:

$$\psi_0 = \sum_l \frac{(l+\frac{1}{2})^{1/2}}{\xi_1\xi_2}\varphi_l(\xi_1, \xi_2)P_l(\cos\omega_{12}). \tag{3.10}$$

We shall further require the $\vec{r}_1 \leftrightarrow \vec{r}_2$ symmetry of the wavefunction which is equivalent to the even parity of the summation index l in (3.10). Owing to the simplicity of this example, the radial Schrödinger equation is

$$\begin{pmatrix} H_{00}-E & \beta_0\xi_1^2\xi_2^2 & 0 & \ldots \\ \beta_0\xi_1^2\xi_2^2 & H_{02}-E & \beta_2\xi_1^2\xi_2^2 & \ldots \\ 0 & \beta_2\xi_1^2\xi_2^2 & H_{04}-E & \ldots \\ \ldots & & & \end{pmatrix} \begin{pmatrix} \varphi_0(\xi_1, \xi_2) \\ \varphi_2(\xi_1, \xi_2) \\ \varphi_4(\xi_1, \xi_2) \\ \ldots \end{pmatrix} = 0 \tag{3.11}$$

$$H_{0l} = \alpha_l \xi_1^2 \xi_2^2 + \sum_{i=1}^{2} \left(-\frac{\partial^2}{\partial \xi_i^2} + \frac{l(l+1)}{\xi_i^2} + 3g_1 \xi_i^2 + \tfrac{9}{2} g_2 \xi_i^4 \right)$$

$$\alpha_l = 6g_2 \left(1 + \frac{1}{(4l-2)(4l+6)} \right) \qquad \beta_l = 6g_2 \frac{(l+1)(l+2)}{(2l+3)(2l+1)^{1/2}(2l+5)^{1/2}}$$

and resembles strongly that of Znojil (1981). The abbreviations α_l and β_l here denote the normalised matrix elements

$$\langle l | 3g_2(1+2\sin^2 \omega_{12}) | l \rangle \text{ and } \langle l | 6g_2 \cos^2 \omega_{12} | l+2 \rangle,$$

respectively.

Let us admit that the third particle is distinguishable from the remaining two bosons so that the Pauli principle is satisfied in a trivial way. Then, we may formulate the following.

Proposition. Assuming that the auxiliary MCF quantities are convergent, equations (2.3) and (2.4) with $M_k = k(2k-1)$ represent the exact solution of our three-body quartic AHO example.

Proof. Denoting the basis states by $|n_1, n_2, l\rangle$, the matrix H_0 is three-diagonal in l and its infinite submatrices $H_{lln_2n_2+2}$, $H_{lln_2n_2+1}$, $H_{ll+2n_2n_2}$ and $H_{lln_2n_2}$ contain one, three, three lower and five non-zero diagonals, respectively. Hence, each HO state is coupled to at most $5+(2\times3)+(2\times1)+(2\times3\times3)=31$ other HO states. We may choose the one-dimensional model space with $|X_1^1\rangle = |000\rangle$ and generate the GL ordering with $M_1 = 1$, $M_2 = 6$, $M_3 = 15, \ldots$ in accord with § 3.2.

4. Identical particles

4.1. Action of the Pauli principle

The complete set of the commuting operators H_0 (Hamiltonian), L^2 (square of the full angular momentum) and L_z (its projection), characterises an intrinsic state ψ_0 of the A-body system provided that the particles are distinguishable. The more interesting cases (identical bosons or fermions, without spin for simplicity) necessitate an addition of the projectors $\sigma_{(A)}^{(\pm)}$ (symmetriser or antisymmetriser, respectively). It is a matter of simple algebra to verify that the symmetrisation/antisymmetrisation operator $\sigma_{(A)}^{(\pm)}$ may be defined by the recurrent formula

$$\sigma_{(A)}^{(\pm)} = W_{(A)}^{(\pm)} W_{(A-1)}^{(\pm)} \ldots W_{(2)}^{(\pm)} / A!$$

$$W_{(A)}^{(\pm)} = 1 \pm W_{(A-1)}^{(\pm)} P_{(A)} \qquad W_1^{(\pm)} = 1 \pm P_{(2)} \tag{4.1}$$

in the bosonic/fermionic case. Here the operator $P_{(i)}$ corresponds to the interchange of the neighbouring particles $\vec{r}_{i-1}$ and $\vec{r}_i$.

The most important property of factorisation (4.1) is the simplicity of its Jacobi coordinate representation. First, the trivial algebra implies that $P_{(m+2)}$ will be represented by the (pseudo)orthogonal and real symmetric transformation

$$\begin{pmatrix} \vec{\xi}_m' \\ \vec{\xi}_{m+1}' \end{pmatrix} = \begin{pmatrix} \cos\varphi_m & \sin\varphi_m \\ \sin\varphi_m & -\cos\varphi_m \end{pmatrix} \begin{pmatrix} \vec{\xi}_m \\ \vec{\xi}_{m+1} \end{pmatrix} \qquad \cos\varphi_m = \frac{1}{(m+1)} \tag{4.2}$$

involving just the two coordinates ($\bar{\xi}_m = \bar{\xi}'_m = 0$ for $m = 0$). The quantities φ_m in (4.2) are the 'Euler' angles in the general rotation

$$\mathcal{R}(\bar{r}_i \leftrightarrow \bar{r}_{i+j}) = P_{(i+1)}P_{(i+2)} \ldots P_{(i+j)}P_{(i+j-1)} \ldots P_{(i+1)}.$$

Next, the elementary rotation (4.2) may be re-interpreted as the 'unequal-mass' transition from the 'CM' coordinates $\bar{\xi}_m = \bar{R}$, $\bar{\xi}_{m+1} = \bar{r}$ to the 'one-particle' variables $\bar{r}_1 = \bar{\xi}'_m$ and $\bar{r}_2 = \bar{\xi}'_{m+1}$. If we also change the coupling of the angular momenta in accord with (3.6), then (4.2) degenerates to a transformation of a certain two-particle subset of the full HO basis. Of course, the $P_{(m+2)}$ matrix may be represented by the Moshinski brackets $\langle \ldots | \ldots \rangle_D$ with the mass ratio $D = \tan^2 \varphi_m$:

$$\begin{aligned}\langle \xi'_m | n'_m l'_m \rangle \langle \xi'_{m+1} | n'_{m+1} l'_{m+1} \rangle \langle \ldots \Omega'_m \Omega'_{m+1} \ldots | \{l\}_m \rangle \\ = \sum_{n_m l_m n_{m+1} l_{m+1}} \langle n_{m+1} l_{m+1} n_m l_m ; \lambda | n'_m l'_m n'_{m+1} l'_{m+1} ; \lambda \rangle_{1/m(m+2)} \\ \times \langle \xi_m | n_m l_m \rangle \langle \xi_{m+1} | n_{m+1} l_{m+1} \rangle \langle \ldots \Omega_m \Omega_{m+1} \ldots | \{l\}_m \rangle \end{aligned} \tag{4.3}$$

so that the complete symmetrisation/antisymmetrisation matrix $\sigma^{(\pm)}_{(A)}$ must remain diagonal with respect to the energy quantum number $\mathcal{N} = \sum_{i=1}^{A-1} (2n_i + l_i)$ and the parity of $\sum_{i=1}^{A-1} l_i$. As a consequence, the BTD structure of H_0 survives its symmetrisation/antisymmetrisation: $\sigma^{(\pm)}_{(A)} H_0 \sigma^{(\pm)}_{(A)} = H_{0s/a}$.

4.2. Symmetrised oscillator basis

Let us start this section with a short summary. We may assign the MCF solution as described in § 2 to the many-body Schrödinger equation with the AHO two-particle interactions. This is a consequence of the BTD structure of the Hamiltonian H_0 or $H_{0s/a}$ in the unsymmetrised GL-ordered HO basis.

Unfortunately, the product construction (3.5)×(3.8) of this basis cannot reflect the singular character of the projectors $\sigma_{(A)}$. In other words, the action of $H_{0s/a}$ on $|\langle n \rangle \{l\}\rangle$ generates only a few independent new states. They must be represented as superpositions of a large number of the unsymmetrised products $|\langle n \rangle \{l\}\rangle$. In this way, $H_{0s/a}$ in the form of the original BTD matrix H_0 multiplied by the BTD matrix $\sigma_{(A)}$ will be characterised by an inadequate increase of the block dimensions M_k for higher k.

The key to the problem lies in the symmetrisation of the basis itself, $|X^i_k\rangle \sim |\langle n \rangle \{l\}\rangle \rightarrow |X^i_k\rangle \sim \sigma_{(A)} |\langle n \rangle \{l\}\rangle$. In the more general setting, we may construct the basis states as such superpostiions of $|\langle n \rangle \{l\}\rangle$ which also possess, besides the fixed total energy $\mathcal{N}$ and angular momentum L, the fixed quantum number $[f]$ (Young tableau) characterising the irreducible representations of the permutation group. We emphasise that the fixed symmetry pattern $[f]$ is the most important ingredient in the present modification of the basis. It has two aspects:

(a) we may simplify the evaluation of the matrix elements of H_0 in the standard way and consider each particular component $V(r_i - r_j)$ of the potential $V^{(A,p)}_{\mathrm{AHO}}$ separately. Formally, the commutation of H_0 and $\sigma_{(A)}$ is taken fully into account;

(b) we may simply extend our discussion to particles with spin.

Of course, H_0 is diagonal with respect to $\mathcal{N}$, L and $[f]$ so that the new symmetrised basis will be more appropriate for our purposes. Some new technical problems arise with the complete classification and algebraic construction of this basis. This was

discussed by Kramer and Moshinski (1966) introducing further quantum numbers $(\lambda\mu)$ and Λ numbering the representations of the groups SU(3) and O_{A-1} respectively. Concerning the general case, see Majling *et al* (1974, 1979) for details.

4.3. The three- and four-body examples

For $p=2$ and the three identical spinless bosons in the s state, each old group $|X_k^m\rangle$, $m=1,2,\ldots,M_k$ as specified in § 3.3 contains k different fixed-energy subgroups with $\mathcal{N}=2k-2,\ 2k,\ldots,4k-4$. The partition dimensions of the symmetrised operator $\sigma_{(3)}^{(+)}H_0\sigma_{(3)}^{(+)}$, $M_k=\frac{1}{12}2^k(2^{k+1}-1)(7\times 2^{k-1}-5)$, grow extremely quickly even for the low cut-offs ($M_1=1$, $M_2=21$, $M_3=230,\ldots$), due to the non-diagonality of $\sigma_{(3)}^{(+)}$. Even the fixed-energy re-partitioning with $M_k=\frac{1}{3}k(2k-1)(4k-1)$ or, alternatively, $M_k=\frac{1}{3}k(2k+1)(4k+1)$ is rather inefficient ($M_3=140$ or 91, respectively). At the same time the $A=3$ classification of Kramer and Moshinski (1966)

$$|\mathcal{N}(\lambda\mu)LM\Lambda[f]\rangle=\sum_{n_1l_1n_2l_2}|n_1n_2l_1l_2LM\rangle\left(\begin{matrix}(n_10)(n_20)\\ l_1\quad l_2\end{matrix}\middle|\begin{matrix}(\lambda\mu)\\ L\end{matrix}\right)d^{\lambda/2}_{(n_1-n_2)/2,\Lambda/2}(\pi/2) \qquad (4.4)$$

with the Wigner function d and the SU(3) Clebsh–Gordan coefficients $(\cdots|\cdots)$ appears to be complete and sufficiently simple for practical purposes (Makharadze and Mikhelashvili 1971). Its introduction reduces the block dimensions M_k significantly below the values of § 3 (cf table 1).

Table 1. Increase of the matrix dimensions needed in the MCF method ($L=0$).

	Two-body		Three-body					Four-body	
Symmetry $[f]$	[2]		[3]					[4]	
Anharmonicity p	2	3	2	3	2	2	2	2	3
Λ	—	—	—	—	0	6	12	—	—
Cut-off N $[\hbar\omega]$									
0	1	1	1	1	1	0	0	1	1
2	2	2	2	2	2	0	0	2	2
4	2	3	3	4	3	0	0	4	5
6	2	3	5	6	4	1	0	9	10
8	2	3	7	9	5	2	0	17	20
10	2	3	9	12	6	3	0	29	35
12	2	3	12	16	7	4	1	60	71

The non-trivial optimisation of the new basis is still possible since, rather suprisingly, H_0 becomes diagonal with respect to the rotational quantum number Λ which was originally introduced purely for classification purposes. In this way, we obtain the final form of the symmetrised HO basis:

$$|X_k^i\rangle=|\mathcal{N}(\lambda\mu)LM\Lambda[f]\rangle$$

with fixed $L=0$, $[f]=[3]$, $\Lambda=0$ and k is the integer part of $\frac{1}{4}(\mathcal{N}+6)$. In this basis, our numerical tests of the MCF convergence of the MCF representation of the Green function $\det F_1(E)$ were performed.

For the monotonic potentials ($g_1 > 0$ and $g_2 > 0$), the convergence proved to be extremely rapid. However, from the physical point of view, similar potentials are less interesting than the more realistic models of the nucleonic forces with the repulsive core. *A priori* our choice of the core-simulating values of $g_1 = -g_2 = -10$ will worsen the convergence—it is therefore well suited for illustration purposes. A sample of the corresponding results is presented here in table 2 and figure 1. It shows that the small-matrix algorithms are sufficient to achieve convergent results and that the energy calculations are still easily manageable even on small computers. Figure 1 illustrates in more detail the typical core-induced oscillatory dependence of energies on the variation of scale ('spring constant') of the HO basis and its smoothing for higher cut-offs. Notice the similarity of this feature in all the two-, three- and four-body systems.

Table 2. Sample of convergence: ground-state energies (MeV) of the quartic three-bosonic oscillators with $V(r) = -10\,r^2 + 10\,r^4$.

dim $\hbar\omega$	1.4	3.0	3.5	6.5	7.0	7.5	9.0
1	27.355	2.000	1.577	5.489	6.376	7.250	9.889
2	8.345	1.456	1.575	1.617	2.015	2.484	4.100
3	3.286	1.258	1.048	0.945	0.993	1.104	1.797
4	1.712	0.962	0.905	0.896	0.895	0.899	1.045
5	1.287	0.897	0.900	0.883	0.883	0.884	0.897
6	1.217	0.884	0.883	0.882	0.882	0.882	0.883
7	1.189	0.882	0.882	0.882	0.882	0.882	0.882

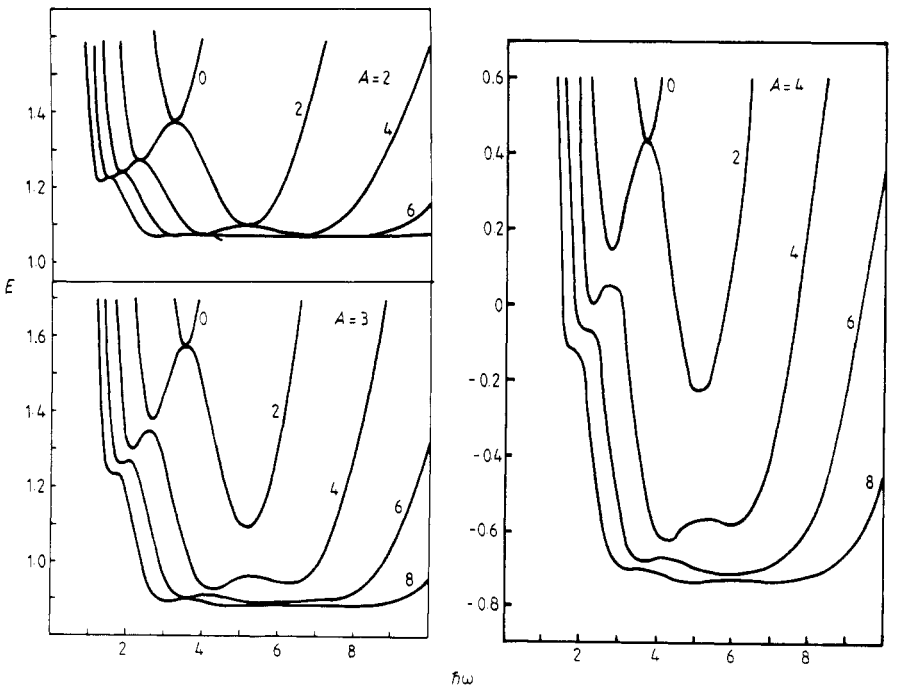

Figure 1. Pattern of the basis dependence for the calculated ground-state energies of the few-body quartic oscillators.

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