Eur. Phys. J. A **12**, 29–40 (2001)

THE EUROPEAN PHYSICAL JOURNAL A

Some considerations on the restoration of Galilei invariance in the nuclear many-body problem

Part I: Mathematical tools, spectral functions and spectroscopic factors of simple bound states

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Received: 20 February 2001 / Revised version: 22 May 2001
Communicated by D. Schwalm

Abstract. The mathematical tools to restore Galilei invariance in the nuclear many-body problem with the help of projection techniques are presented. For simple oscillator configurations recursion relations for the various elementary contractions are derived. The method is then applied to simple configurations for the ground states of ^{4}He, ^{16}O and ^{40}Ca as well as to the corresponding one-hole and one-particle states. As a first application the spectral functions and spectroscopic factors for the above-mentioned doubly even nuclei are investigated. It turns out that the conventional picture of an uncorrelated system underestimates the single-particle strengths of the hole states from the last occupied shell while that of the higher excited hole states is overestimated considerably. These results are in complete agreement with those derived by Dieperink and de Forest using different methods. Similar effects are seen for the particle states which have not been studied before. All the calculations presented here are performed analytically and thus can be checked explicitly by the interested reader.

PACS. 21.60.-n Nuclear-structure models and methods

1 Introduction

Like classical mechanics non-relativistic quantum mechanics, too, is based on three fundamental assumptions on the structure of space and time.

- Time is homogeneous. Thus the total energy of a closed system is conserved.
- Space is isotropic. Hence the total angular momentum of a closed system is conserved.
- Space is homogeneous. Consequently the total linear momentum of a closed system is a constant of motion, too.

For the conventional nuclear many-body problem which treats the nucleus as a closed system of elementary, non-relativistic nucleons interacting with each other via some suitable effective interaction these three assumptions have the consequence that the corresponding Hamiltonian, however complicated it may be,

- cannot depend explicitely on time,
- has to conserve the total angular momentum,
- can besides on spin and isospin only depend on relative coordinates and momenta but not on the center-of-mass coordinate of the nucleons and only in a trivial way on the total linear momentum.

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It will be the last of these three requirements which will be studied extensively in the present and five forthcoming papers.

Because of this requirement the Hamiltonian can be written as a sum of an internal and a center-of-momentum (COM) part

$$\hat{H} \,=\, \hat{H}_{\rm int}\left(\vec{r}_i - \vec{R}_A,\, \hat{p}_i - \frac{1}{A}\hat{P}_A,\, \sigma_i,\, \tau_i\right) + \frac{\hat{P}_A^{\,2}}{2MA}\,, \quad (1.1)$$

where we have introduced

$$\vec{R}_A \,\equiv\, \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i \qquad \text{and} \qquad \hat{P}_A \,=\, \sum_{i=1}^{A}\hat{p}_i\,, \quad (1.2)$$

for the center-of-mass coordinate and the operator of the total linear momentum of the considered A-nucleon system, respectively. As usual in the nuclear many-body problem we have assumed identical masses (M) for protons and neutrons.

Because of the separability of the Hamiltonian, its eigenstates have the form

$$|\Psi\rangle \,=\, |\Psi_{\rm int}\rangle|\vec{P}_A\rangle\,, \quad (1.3)$$

i.e., they factor into an internal state describing the relative motion of the nucleons and a trivial plane-wave state

with momentum $\vec{P}_A$ describing the motion of the nucleus as a whole. The correponding energies are

$$E = E_{\rm int} + \frac{\vec{P}_A^{\,2}}{2MA}\,. \tag{1.4}$$

Now the principle of relativity tells us that there is no absolute motion. We can always choose that inertial frame of reference in which the system is at rest. This we shall call the "center-of-momentum (COM) rest frame". Since $\vec{P}_A = 0$ in this frame, the many-body problem gets the form of an internal Schroedinger equation

$$\hat{H}_{\rm int}\,|\Psi_{\rm int}\rangle = E_{\rm int}\,|\Psi_{\rm int}\rangle \tag{1.5}$$

depending only on relative coordinates and momenta. Exactly this equation is used in few-body physics. One rewrites the Hamiltonian in relative ("Jacobi") coordinates (and the conjugate momenta) and then solves (1.5). Examples are the textbook treatment of the deuteron, the Faddeev equations for the three-, or the Faddeev-Yakubowski equations for the four-body problem.

In the nuclear many-body problem, however, this procedure can hardly be used. The reason for this is quite simple: nucleons are undistiguishable, identical fermions and thus their total wave function has to be antisymmetric with respect to arbitrary exchanges of any two of them. The relative coordinates, however, depend on all $3A$ nucleon coordinates. Thus the antisymmetrisation has to be done explicitly. This is still feasible in the three- and four-body problems, though even there it requires considerable effort. For heavier nuclei like, *e.g.*, ^{20}Ne or ^{40}Ca, however, it becomes simply impossible. Roughly speaking (*i.e.*, forgetting for the moment of all the needed angular momentum and isospin algebra) there are only $3\,! = 6$ terms for three identical fermions but $20\,! \sim 2.4 \times 10^{18}$ terms for 20 of them.

Thus, instead of solving (1.5), in many-fermion physics one usually expands the total wave function in terms of Slater determinants (or generalized Slater determinants) $|D\rangle$:

$$|\Psi\rangle = \sum_D |D\rangle\, c_D\,, \tag{1.6}$$

which respect the Pauli principle by construction. The price one has to pay is that (1.6) depends on $3A$ coordinates instead of the $3A-3$ allowed by Galilei invariance. It thus contains contaminations due to the motion of the system as a whole, so-called "spurious" admixtures. By assuming (1.6) one has sacrified Galilei invariance for the sake of the Pauli principle.

Obviously this approximation is very good, if we consider the many-electron problem in atomic physics. The mass of the nucleon is about 2000 times heavier than that of the electron and thus even in the worst case, the hydrogen atom, only a rather small error is made. In other words: in atomic physics we have a natural coordinate system with the origin, which is almost identical to the COM coordinate, fixed to the nucleus. The same is true for metallic clusters where the ion jelly is so much heavier than the electrons again, and obviously in most problems of solid-state physics, too.

In the nuclear many-body problem, however, such a "natural" center is missing (and the same holds for the non-relativistic constituent quark models). So how good is the above approximation there? In almost all textbooks on the nuclear many-body problem you will find a statement claiming that the error will be of the order of $1/A$ and thus "can savely be neglected as soon as nuclei above ^{16}O are considered" [1]. It is one of the central aims of the present series of papers to question this kind of "general belief".

The fact that there may be a problem was almost immediately recognized after the development of the nuclear shell model. There was pioneering work on oscillator configurations by Elliot and Skyrme [2] as well as by Tassie and Barker [3] and Giraud [4]. The methods devised by them how to treat the COM motion are still widely used in shell model configuration-mixing calculations (see, *e.g.*, [5]). They are, however, restricted to pure oscillator configurations and require furthermore a rather special truncation of the model space (see subsect. 2.2).

The problem of how to restore Galilei invariance for the case of arbitrary model spaces spanned by general (non-oscillator) configurations was, at least in principle, solved by some of the "giants" in the nuclear many-body problem like Peierls, Yoccoz and Thouless [6–8] and a couple of others already in the early sixties.

In fact it was shown [6] that the operator

$$\hat{C}_A(0) \equiv \int \mathrm{d}^3\vec{a}\,\hat{S}(\vec{a}\,) \equiv \int \mathrm{d}^3\vec{a}\,\exp\left[i\vec{a}\cdot\hat{P}_A\right]\,, \tag{1.7}$$

if applied to any localized state of the type (1.6), does project into the COM rest frame, *i.e.*, restores translational invariance. Note, that the restriction "localized" is here rather important. Being localized the COM has a finite momentum distribution. Consequently all the matrix elements involving the operator (1.7) will converge and the problem of projecting out something with "measure zero" is avoided. Scattering states with, *e.g.*, one nucleon in the continuum have to be treated differently. Such states will be discussed in the fourth and fifth paper of the present series.

The action of (1.7) on a localized state involves the integral over the usual "shift operator". It can be understood as a superposition of the state shifted all over normal space with equal weight. In this way zero total momentum is ensured. The procedure is quite similar to the restoration of rotational invariance. There from any deformed object in "intrinsic" space a spherical (zero angular momentum) state in the "laboratory" frame of reference can be obtained by superposing all the rotated configurations with equal weight and thus producing a result which is independent of the choice of the direction of the quantization axis.

It should be stressed, however, that in general (1.7) restores only the translational and not the full Galilei invariance. Only if either a double-projection technique [7] is applied or if the restoration is performed *before* the wave

function is determined, *e.g.*, by variation, one obtains the right mass [8,1]. Again this is rather similar to angular-momentum projection. Also here the correct moment of inertia is only obtained if the restoration of rotational invariance is performed before the variation.

Unfortunately, (1.7) is a rather complicated A-body integral operator and its application is technically rather involved. First of all, unlike rotations, which will never lead out of a chosen model space as long as in the single-particle basis for each total angular-momentum states all the magnetic substates are included, spacial shifts are not confined to any of the usual finite model spaces. They will always mix the configurations inside the chosen space with those outside. Closely connected to this complication is the second problem: as far as rotations are concerned any angular-momentum zero object remains invariant. Thus it is easy to assume some (totally occupied) "inert" core and restrict the model space to a few valence shells around the Fermi level. If one wants to restore Galilei invariance, such an assumption is not possible out of an obvious reason: whenever the total linear momentum of the "valence" nucleons is changed, this change has to be compensated by the total momentum of the "core" nucleons in order that the total linear momentum of the whole nucleus remains zero. Thus, the restoration of Galilei invariance requires necessarily that no inert core is assumed.

These complications may be the reason why, though the method was known in principle already 30 years ago, few practical calculations have been done restoring Galilei invariance in this way. Only at the beginning of the 1990's there was a first Galilei-invariant Hartree-Fock calculation by Schmid and Gruemmer [9], though only for ^{4}He, and by the same authors shortly afterwards an investigation of the effects of restoring the translational invariance on the charge densities of various nuclei [10]. Schmid and Reinhard [11] then investigated the problem of the charge densities in more detail using Hartree-Fock wave functions obtained with a particular Skyrme interaction [12]. All these papers showed first hints on the importance of treating Galilei invariance in the nuclear many-body problem correctly, were, however, restricted to rather special aspects.

The present series of papers tries to investigate the problem in a more systematic way. For this purpose we shall work in the first three articles entirely with simple oscillator configurations: the ground-state configurations of the three doubly closed shell nuclei ^{4}He, ^{16}O and ^{40}Ca as well as the one-hole states with respect to them. Configurations with one nucleon in the continuum will be treated in the articles 4 and 5. The restriction to oscillator configurations seems somewhat surprising since, as already mentioned, there are other (less general) methods to treat the COM problem in these cases, and furthermore, as we shall see in subsect. 2.2, most of these configurations factor into an internal part and a COM component with the COM in a $0s$-oscillator state and are hence "non-spurious". However, for the one-hole states with excitation energies $\geq 1\hbar\omega$ such a factorisation is not possible. Thus, we have the possibility to check the results of the projection into the COM rest frame for the non-spurious states and to investigate the effects of the restoration of Galilei invariance for those configurations containing spurious admixtures at the same time. Another advantage of using these simple configurations is that all the calculations presented here can be done analytically. Thus every reader which studies these papers carefully and has some computer algebra code installed on his home or office computer can reproduce all the results for himself. And, last but not least, using oscillator configurations in the present context is a rather "conservative" approach. The use of more realistic configurations will only increase the effects of the COM motion. Thus, the results presented here can be considered as a sort of a "lower limit" for the COM effects to be obtained in more realistic calculations.

The content of the present series of papers can be summerized as follows. In sect. 2 of this first paper we shall develop the mathematical tools needed to compute the amplitudes of general observables in between oscillator configurations with and without the projection into the COM rest frame. Much of the content of this section can be found in the literature, however, there is a lot of material which is new, *e.g.*, the recursion relations for the matrix elements of a generalized shift operator as well as for the corresponding elementary contractions. Section 3 will then be devoted to a first example: spectral functions and spectroscopic factors. These have been derived for the one-hole oscillator configurations already in 1974 by Dieperink and de Forest [13] using different methods. Besides rederiving their results we shall, however, also investigate the one-particle states. In the second paper of the present series then form factors for elastic and inelastic electron scattering and the Coulomb sum rule as well as its first and second moments will be discussed. The third paper then deals with the energies of the considered configurations computed with density-independent interactions as well as with density-dependent forces. Papers four and five will be devoted to problems with one nucleon in the continuum. In particular standard approximations for the analysis of quasi-elastic electron scattering will be investigated. Paper four will present a simple knock-out model and use Woods-Saxon partial-wave expansions for this purpose. In paper five then a more microscopic coupled-channel approach will be studied. Finally, in the sixth paper, the formalism will be extended to generalized Slater determinants of the Hartree-Fock-Bogoliubov type and combined with angular momentum, particle number and parity projections. This paper will show how, in principle, completely unrestricted Hartree-Fock-Bogoliubov calculations with symmetry projection before the variation can be done including the restoration of full Galilei invariance.

2 Mathematical tools

In this section we shall develop the mathematical tools needed to compute the expectation values and transition amplitudes of various observables with and without projection into the center-of-momentum (COM) rest frame. We shall start in subsect. 2.1 by defining the notation

we shall use for spherical three-dimensional harmonic-oscillator states. This is common textbook knowledge and hence will be sketched only briefly. In subsect. 2.2 we shall then introduce oscillator determinants as A (and $A-1$) nucleon states, discuss their COM properties and define the elementary contractions needed to calculate the unprojected matrix elements of arbitrary observables. This could obviously be done in a simpler (the normal) way, however, to compare the unprojected results directly with the COM-projected ones later on, it is preferable to represent them in a similar fashion. Subsection 2.3 then presents the elementary contractions in between shifted oscillator determinants needed to compute the COM-projected matrix elements of arbitrary observables. For this purpose a generalized shift operator modified by two recoil operators is used. This is the central part of the present section. Finally, in subsect. 2.4 we shall calculate the norm for COM-projected doubly closed major shell determinants and the COM-projected one-hole states with respect to them.

2.1 The spherical three-dimensional harmonic oscillator

The Hamiltonian for a particle with mass M in a spherical three-dimensional harmonic-oscillator potential has the form

$$\hat{h} \,=\, \frac{\hat{\vec{p}}^{\,2}}{2M} \,+\, \frac{1}{2}M\omega^2\vec{r}^{\,2}\,, \tag{2.1}$$

where $\vec{r}$ is the space vector and $\hat{\vec{p}}$ the corresponding momentum operator. In Cartesian representation, the eigenstates of (2.1) can be written as $|\vec{n}\rangle$, where $\vec{n}$ is the vector of the numbers of oscillator quanta in the three different space directions. The corresponding eigenvalues are

$$E(\vec{n}) \equiv E_N = \left(N+\frac{3}{2}\right)\hbar\omega, \qquad \text{with } N \equiv \sum_{i=1}^{3} n_i\,. \tag{2.2}$$

The space representation of the oscillator eigenstates can be written as

$$\langle\vec{r}\,|\vec{n}\,\rangle \equiv \langle\vec{r}\,|n_1n_2n_3\rangle = \left(\frac{1}{b\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}x^2\right\}\prod_{i=1}^{3}(x_i|n_i)\,, \tag{2.3}$$

where b is the usual oscillator length ($b^2=\hbar/M\omega$) and $x \equiv |\vec{x}| \equiv |\vec{r}/b|$. For the polynomial parts of (2.3) $(x_i|n_i) \equiv R_{n_i}(x_i)$ and their derivatives we have the recursion relations

$$\begin{aligned} R_0(x_i) &= 1\,,\\ R_{n_i+1}(x_i) &= \sqrt{\frac{2}{n_i+1}}x_iR_{n_i}(x_i) - \sqrt{\frac{n_i}{n_i+1}}R_{n_i-1}(x_i)\,,\\ \frac{\mathrm{d}}{\mathrm{d}x_i}R_{n_i}(x_i) &= \sqrt{2n_i}R_{n_i-1}(x_i)\,. \end{aligned} \tag{2.4}$$

The corresponding momentum space representation is

$$\langle\vec{k}\,|\vec{n}\,\rangle \equiv \left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}\kappa^2\right\}\prod_{i=1}^{\nu}(\kappa_i|n_i)\,, \tag{2.5}$$

where $\vec{\kappa} \equiv b\vec{k}$. Here the polynomial parts are

$$(\kappa_i|n_i) \,=\, (-i)^{n_i}R_{n_i}(\kappa_i)\,. \tag{2.6}$$

For the space representation of the lowest few oscillator states one obtains

$$\begin{aligned} \langle\vec{r}\,|000\rangle &= \left(\tfrac{1}{b\sqrt{\pi}}\right)^{3/2}\exp\left\{-\tfrac{1}{2}x^2\right\}\,,\\ \langle\vec{r}\,|100\rangle &= \langle\vec{r}\,|000\rangle\sqrt{2}x_1\,,\\ \langle\vec{r}\,|010\rangle &= \langle\vec{r}\,|000\rangle\sqrt{2}x_2\,,\\ \langle\vec{r}\,|001\rangle &= \langle\vec{r}\,|000\rangle\sqrt{2}x_3\,,\\ \langle\vec{r}\,|200\rangle &= \langle\vec{r}\,|000\rangle\left\{-\tfrac{1}{\sqrt{2}}(1\,-\,2x_1^2)\right\}\,,\\ \langle\vec{r}\,|110\rangle &= \langle\vec{r}\,|000\rangle 2x_1x_2\,,\\ \langle\vec{r}\,|020\rangle &= \langle\vec{r}\,|000\rangle\left\{-\tfrac{1}{\sqrt{2}}(1\,-\,2x_2^2)\right\}\,,\\ \langle\vec{r}\,|101\rangle &= \langle\vec{r}\,|000\rangle 2x_1x_3\,,\\ \langle\vec{r}\,|002\rangle &= \langle\vec{r}\,|000\rangle\left\{-\tfrac{1}{\sqrt{2}}(1\,-\,2x_3^2)\right\}\,,\\ \langle\vec{r}\,|011\rangle &= \langle\vec{r}\,|000\rangle 2x_2x_3\,. \end{aligned} \tag{2.7}$$

Let us simplify the notation by introducing

$$\begin{aligned} |0s\rangle &\equiv |000\rangle\,,\\ |i\rangle &\equiv \{|100\rangle,\,|010\rangle,\,|001\rangle\}\,,\\ |2i\rangle &\equiv \{|200\rangle,\,|020\rangle,\,|002\rangle\}\,,\\ |i<j\rangle &\equiv \{|110\rangle,\,|101\rangle,\,|011\rangle\}\,, \end{aligned} \tag{2.8}$$

with $i,j \,=\, 1,2,3$. In this notation the momentum space representation of the states (2.7) becomes

$$\begin{aligned} \langle\vec{k}\,|0s\rangle &= \left(\tfrac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\tfrac{1}{2}\kappa^2\right\}\,,\\ \langle\vec{k}\,|i\rangle &= \langle\vec{k}\,|0s\rangle\left\{-i\sqrt{2}\kappa_i\right\}\,,\\ \langle\vec{k}\,|2i\rangle &= \langle\vec{k}\,|0s\rangle\left\{\tfrac{1}{\sqrt{2}}(1\,-\,2\kappa_i^2)\right\}\,,\\ \langle\vec{k}\,|i<j\rangle &= \langle\vec{k}\,|0s\rangle\left\{-2\kappa_i\kappa_j\right\}\,. \end{aligned} \tag{2.9}$$

In spherical coordinates one has, on the other hand,

$$\begin{aligned} \langle\vec{r}\,|nl\lambda\rangle \quad\equiv\quad & b^{-3/2}\pi^{-1/4}\exp\left\{-\frac{1}{2}x^2\right\}\\ & \times 2\sqrt{\frac{(2n+2l+1)!!}{n!2^n}}\left(\sqrt{2}x\right)^l\,Y_{l\lambda}(\hat{r})\\ \times\sum_{K=0}^{n}(-)^K & \binom{n}{K}\frac{1}{(2l+2K+1)!!}\left(\sqrt{2}x\right)^{2K}\,. \end{aligned} \tag{2.10}$$

Comparing this with the Cartesian representation, one obtains

$$\begin{aligned} |0s0\,\rangle &= |000\rangle\,,\\ \begin{pmatrix}|0p+1\rangle\\ |0p0\;\rangle\\ |0p-1\rangle\end{pmatrix} &= \begin{pmatrix}-\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0\\ 0 & 0 & 1\\ +\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0\end{pmatrix}\begin{pmatrix}|100\rangle\\ |010\rangle\\ |001\rangle\end{pmatrix}\,, \end{aligned} \tag{2.11}$$

$$\begin{pmatrix} |1s0\ \rangle \\ |0d+2\rangle \\ |0d+1\rangle \\ |0d0\ \rangle \\ |0d-1\rangle \\ |0d-2\rangle \end{pmatrix} =$$

$$\begin{pmatrix} -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ +\frac{1}{2} & -\frac{1}{2} & 0 & +\frac{i}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{6}} & +\frac{2}{\sqrt{6}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & +\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ +\frac{1}{2} & -\frac{1}{2} & 0 & -\frac{i}{\sqrt{2}} & 0 & 0 \end{pmatrix} \begin{pmatrix} |200\rangle \\ |020\rangle \\ |002\rangle \\ |110\rangle \\ |101\rangle \\ |011\rangle \end{pmatrix} .$$

It is easily checked that the transformations (2.11) are unitary.

Now nucleons are spin-(1/2) fermions and come in two species, protons and neutrons. Thus in addition to $|\vec{n}\rangle$ one has to specify spin and isospin quantum numbers. The corresponding creation operators, creating from the particle vacuum $|0\rangle$ a fermion with spin and isospin quantum numbers $1 \equiv \sigma_1, \tau_1$ in an oscillator eigenstate $|\vec{n}\rangle$ are denoted by

$$b^\dagger_{\vec{n}\,1}|0\rangle \equiv |\vec{n}\rangle|1\rangle\,. \tag{2.12}$$

2.2 Harmonic-oscillator determinants and elementary contractions

From (2.1) one can construct a many-body Hamiltonian for A-independent particles moving in three-dimensional harmonic-oscillator states:

$$\hat{H}_0 \equiv \sum_{i=1}^{A} \hat{h}(i) = \frac{1}{2M}\sum_{i=1}^{A} \hat{\vec{p}}^{\,2}(i) + \frac{1}{2}M\omega^2 \sum_{i=1}^{A} \vec{r}^{\,2}(i) =$$
$$\frac{1}{2M}\sum_{i=1}^{A}\left(\hat{\vec{p}}(i) - \frac{1}{A}\hat{\vec{P}}_A\right)^2 + \frac{1}{2}M\omega^2\sum_{i=1}^{A}\left(\vec{r}(i) - \vec{R}_A\right)^2$$
$$+\frac{\hat{\vec{P}}_A^{\,2}}{2MA} + \frac{1}{2}MA\omega^2\vec{R}_A^{\,2} \equiv \hat{H}_0^{\rm inv}(A) + \hat{H}_0^{\rm com}(A)\,, \tag{2.13}$$

where we have introduced the center of mass and the total momentum of the system according to eq. (1.2).

The eigenstates of this Hamiltonian are oscillator Slater determinants

$$|D\rangle = \prod_{\vec{n}\,1\,\in D}^{A} b^\dagger_{\vec{n}\,1}|0\rangle \tag{2.14}$$

and can be classified by the number of occupied quanta

$$N_{\rm tot}(D) = \sum_{\vec{n}1\in D}^{A} N(\vec{n}) = \sum_{\vec{n}\in D}\sum_{1}^{(\vec{n})}\left(\sum_{i=1}^{3} n_i\right) \tag{2.15}$$

(2.13) does not mix configurations with different $N_{\rm tot}$. Because of the separation of the Hamiltonian into a Galilei invariant internal and a COM part, each of the Slater determinants (2.14) can furthermore be written as a linear combination

$$|D\rangle = \sum_{N_{\rm com}=0}^{N_{\rm tot}} |(N_{\rm tot} - N_{\rm com})_{\rm inv}\rangle|(N_{\rm com})_{\rm com}\rangle f_{N_{\rm com}}\,. \tag{2.16}$$

From this the so-called "non-spurious" part (*i.e.*, the component with the COM in its $|(0s)_{\rm com}\rangle$ ground state) may be obtained as already proposed by Giraud [4] via diagonalizing $\hat{H}_0^{\rm com}$ in the space of all $|D\rangle$ belonging to the same $N_{\rm tot}$ and keeping only those eigenstates with $N_{\rm com} = 0$. This procedure is applied, *e.g.*, in some shell model approaches [5].

If all shells up to a maximum $N_{\rm max}(\vec{n}) = N-1$ are filled and the remaining ("valence") particles are confined to the shell with N quanta, then the COM is fixed in its ground-state configuration. This holds, *e.g.*, for the oscillator ground-state configurations $|\,\rangle$ of doubly closed major shell nuclei as well as for the one-hole states with respect to them, provided the hole is made in the last shell. In these cases

$$\left\langle\left|\frac{\hat{\vec{P}}_A^{\,2}}{2MA}\right|\right\rangle = \frac{1}{2}\langle|\hat{H}_0^{\rm com}(A)|\rangle = \frac{3}{4}\hbar\omega \tag{2.17}$$

and, for $\vec{n}$ and $\vec{n}\,'$ out of the last major shell

$$\left\langle\left| b^\dagger_{\vec{n}\,1}\frac{\hat{\vec{P}}^{\,2}_{A-1}}{2M(A-1)} b_{\vec{n}\,'\,2}\right|\right\rangle =$$
$$\frac{1}{2}\langle\,|b^\dagger_{\vec{n}\,1}\hat{H}_0^{\rm com}(A-1)b_{\vec{n}\,'\,2}|\,\rangle = \delta_{\vec{n}\vec{n}\,'}\Delta_{12}\frac{3}{4}\hbar\omega\,, \tag{2.18}$$

where $\Delta_{12} \equiv \delta(\sigma_1,\sigma_2)\delta(\tau_1,\tau_2)$ and the oscillator state $\vec{n}$ with the spin-isospin quantum numbers σ_1, τ_1 has to be occupied in the determinant $|\,\rangle$. In both equations (2.17) and (2.18) $\hbar\omega$ is the oscillator energy out of eq. (2.2). As we shall see, for holes in deeper shells (*i.e.*, those with excitation energies $\geq 1\hbar\omega$), the relation (2.18) does not hold. Here (as will be demonstrated in part 3 of the present series of papers) one has to project into the center-of-momentum rest frame.

We shall furthermore define three-dimensional plane-wave states with spin and isospin quantum numbers $1 = \sigma_1, \tau_1$ by

$$c^\dagger_{\vec{k}_1\,1}|0\rangle \equiv |\vec{k}_1\rangle|1\rangle\,, \tag{2.19}$$

with

$$\langle\vec{r}\,|\vec{k}_1\rangle = (2\pi)^{-3/2}\exp\{i\vec{k}_1\cdot\vec{r}\,\} \tag{2.20}$$

and introduce the notation Hh with capital H denoting the oscillator state ($|\vec{n}\rangle$ or $|nl\lambda\rangle$) and small h the corresponding spin and isospin quantum numbers for all the occupied states in the spin- and isospin-saturated

determinants

$$|\,\rangle = \prod_{Hh=1}^{A} b^\dagger_{Hh}|0\rangle = \left\{ \begin{array}{cc} |(0s)^4\rangle & \text{for } ^4\text{He} \\ |(0s)^4(0p)^{12}\rangle & \text{for } ^{16}\text{O} \\ |(0s)^4(0p)^{12}(1s0d)^{24}\rangle & \text{for } ^{40}\text{Ca} \end{array} \right\} . \quad (2.21)$$

Particle states with respect to (2.21) will be denoted by Pp, respectively.

We can now calculate the elementary contractions within these configurations. Obviously,

$$\langle\, |b^\dagger_{Hh} b_{H'h'}|\,\rangle \;=\; \delta_{H'H}\Delta_{h'h} \quad (2.22)$$

for all the states $|Hh\rangle$ which are occupied in $|\,\rangle$. Furthermore,

$$\langle\, |c^\dagger_{\vec{k}_1\,1} b_{H'h'}|\,\rangle = \sum_{H_1h_1} \langle H_1h_1|\vec{k}_1\,1\rangle \langle\, |b^\dagger_{H_1h_1} b_{H'h'}|\,\rangle = \langle H'h'|\vec{k}_1\,1\rangle = \sqrt{\frac{b^3}{\pi\sqrt{\pi}}} \exp\left\{-\frac{1}{2}\kappa_1^2\right\} \Delta_{h'\,1}\,(H'|\vec{\kappa}_1)\,, \quad (2.23)$$

while

$$\langle\, |b^\dagger_{Hh} c_{\vec{k}_2\,2}|\,\rangle = \sum_{H_2h_2} \langle \vec{k}_2\,2|H_2h_2\rangle \langle\, |b^\dagger_{Hh} b_{H_2h_2}|\,\rangle = \langle \vec{k}_2\,2|Hh\rangle = \sqrt{\frac{b^3}{\pi\sqrt{\pi}}} \exp\left\{-\frac{1}{2}\kappa_2^2\right\} \Delta_{2\,h}\,(\vec{\kappa}_2|H) \quad (2.24)$$

and, finally,

$$\langle\, |c^\dagger_{\vec{k}_1\,1} c_{\vec{k}_2\,2}|\,\rangle = \sum_{H_1h_1H_2h_2} \langle \vec{k}_2\,2|H_2h_2\rangle \langle H_1h_1|\vec{k}_1\,1\rangle \langle\, |b^\dagger_{H_1h_1} b_{H_2h_2}|\,\rangle = \frac{b^3}{\pi\sqrt{\pi}} \exp\left\{-\frac{1}{2}(\kappa_1^2+\kappa_2^2)\right\} \Delta_{2\,1} \sum_H (\vec{\kappa}_2|H)(H|\vec{\kappa}_1) \equiv \frac{b^3}{\pi\sqrt{\pi}} \exp\left\{-\frac{1}{2}(\kappa_1^2+\kappa_2^2)\right\} \Delta_{2\,1}\, y(\vec{\kappa}_2,\,\vec{\kappa}_1)\,. \quad (2.25)$$

The polynomial parts $(\kappa_2|H)$ are given in (2.9). For the function y we obtain immediately

$$y(\vec{\kappa}_2,\,\vec{\kappa}_1) \;= \left\{ \begin{array}{cc} 1 & \text{for } ^4\text{He} \\ 1+2\vec{\kappa}_1\cdot\vec{\kappa}_2 & \text{for } ^{16}\text{O} \\ \frac{5}{2}-(\vec{\kappa}_1-\vec{\kappa}_2)^2+2(\vec{\kappa}_1\cdot\vec{\kappa}_2)^2 & \text{for } ^{40}\text{Ca} \end{array} \right\} . \quad (2.26)$$

The elementary matrix elements (2.22) to (2.25) are sufficient to compute the unprojected matrix elements of arbitrary observables in between the determinants (2.21) and the one-hole excitations with respect to them.

2.3 Shifted-oscillator determinants and elementary contractions

For the calculation of the corresponding COM-projected matrix elements we consider a generalized version of the A-body shift operator in (1.7) modified by two recoil operators

$$\hat{Z}_A \equiv \exp\{iA\vec{q}_1\cdot\vec{R}_A/b\}\exp\{i\vec{\alpha}\cdot b\hat{\vec{P}}_A\} \times \exp\{-iA\vec{q}_2\cdot\vec{R}_A/b\} = \prod_{i=1}^{A} \exp\{i\vec{q}_1\cdot\vec{x}\,(i)\}\exp\{i\vec{\alpha}\cdot b\hat{\vec{p}}\,(i)\} \times \exp\{-i\vec{q}_2\cdot\vec{x}\,(i)\} = \prod_{i=1}^{A} \hat{\mathbf{z}}(i)\,, \quad (2.27)$$

where $\vec{q}_1$ and $\vec{q}_2$ are two dimensionless momenta and $\vec{\alpha} \equiv \vec{a}/b$ is the dimensionless shift vector. The matrix element of (2.27) in between two arbitrary Slater determinants is then given by the determinant of the single-particle matrix elements of $\hat{\mathbf{z}}$ in between the occupied states of these determinants. Note, that this operator does not mix states with different spin and isospin quantum numbers. Thus, we can write

$$\langle \vec{n}\,1|\hat{\mathbf{z}}|\vec{n}\,'\,2\rangle \;=\; \Delta_{12}\langle\vec{n}|\hat{\mathbf{z}}|\vec{n}\,'\rangle \;\equiv\; Z_{\vec{n}\vec{n}\,'}\,. \quad (2.28)$$

The matrix elements $Z_{\vec{n}\vec{n}\,'}$ can be calculated easily. One obtains

$$Z_{\vec{n}\vec{n}\,'} \equiv \langle\vec{n}|\exp\{i\vec{q}_1\cdot\vec{x}\}\exp\{i\vec{\alpha}\cdot b\hat{\vec{p}}\}\exp\{-i\vec{q}_2\cdot\vec{x}\}|\vec{n}\,'\rangle = \exp\Big\{-\frac{1}{4}\alpha^2-\frac{i}{2}(\vec{q}_1+\vec{q}_2)\cdot\vec{\alpha}-\frac{1}{4}(\vec{q}_1-\vec{q}_2)^2\Big\}\, z_{\vec{n}\vec{n}\,'} \equiv Z_{00}\, z_{\vec{n}\vec{n}\,'}\,. \quad (2.29)$$

Again the polynomial parts can be written as

$$z_{\vec{n}\vec{n}\,'} \;\equiv\; \prod_{i=1}^{3} \zeta_{n_i n_i'}\,. \quad (2.30)$$

Defining

$$\vec{\beta} \equiv \frac{1}{\sqrt{2}}\Big(\vec{\alpha} - i[\vec{q}_1 - \vec{q}_2]\Big)$$

$$\text{and} \qquad \vec{\beta}\,' \equiv \frac{1}{\sqrt{2}}\Big(\vec{\alpha} + i[\vec{q}_1 - \vec{q}_2]\Big)\,, \quad (2.31)$$

one obtains the recursion relations

$$\zeta_{00} = 1\,,$$

$$\zeta_{n_i+1 n_i'} = \frac{-\beta_i}{\sqrt{n_i+1}}\,\zeta_{n_i n_i'} + \sqrt{\frac{n_i'}{n_i+1}}\,\zeta_{n_i n_i'-1}\,,$$

$$\zeta_{n_i n_i'+1} = \frac{+\beta_i'}{\sqrt{n_i'+1}}\,\zeta_{n_i n_i'} + \sqrt{\frac{n_i}{n_i'+1}}\,\zeta_{n_i-1 n_i'}\,. \quad (2.32)$$

For (doubly) closed oscillator major shells (all shells up to N_F fully occupied) we obtain then

$$\langle\, |\hat{Z}_A|\,\rangle \;=\; \det Z_A \;=\; (Z_{00})^A\,, \quad (2.33)$$

with the determinant of the "reduced overlap matrices" $\mathbf{z}$ out of eq. (2.30) being identical to one. The corresponding minors are

$$\langle\,|b^\dagger_{Hh}\hat{Z}_{A-1}b_{H'h'}|\,\rangle\;=\;(Z_{00})^{A-1}\;\Delta_{h'h}\,z^{-1}_{H'H}\,. \qquad (2.34)$$

Because of the non-spuriousity of holes within the last shell, the inverse of the reduced overlap matrices can be computed by simple (matrix) recursion relations. Denoting by "1" all the oscillator states $\{\vec{n}\,;\,N(\vec{n})\leq N_F\}$ up to the shell N_F and by "2" all states $\{\vec{n}\,;\,N(\vec{n})=N_F+1\}$ out of the shell N_F+1 and the corresponding reduced matrices out of eq. (2.34) within these states by boldface characters one obtains

$$\begin{aligned}
&z^{(N_F=0)^{-1}}_{00}=1\,,\\
&\mathbf{z}^{(N_F+1)^{-1}}_{22}=\mathbf{1}_{22}\,,\\
&\mathbf{z}^{(N_F+1)^{-1}}_{12}=-\mathbf{z}^{(N_F)^{-1}}_{11}\,\mathbf{z}_{12}\,,\\
&\mathbf{z}^{(N_F+1)^{-1}}_{21}=-\mathbf{z}_{21}\,\mathbf{z}^{(N_F)^{-1}}_{11}\,,\\
&\mathbf{z}^{(N_F+1)^{-1}}_{11}=\mathbf{z}^{(N_F)^{-1}}_{11}\;+\;\mathbf{z}^{(N_F+1)^{-1}}_{12}\mathbf{z}^{(N_F+1)^{-1}}_{21}\,. \qquad (2.35)
\end{aligned}$$

For the additional elementary contractions we obtain

$$\begin{aligned}
&\langle\,|c^\dagger_{\vec{k}_1\,1}\hat{Z}_{A-1}b_{H'h'}|\,\rangle\;=\\
&\quad\Delta_{h'1}\,(Z_{00})^{A-1}\left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}\kappa_1^2\right\}\\
&\quad\times\sum_{H\leq F}z^{-1}_{H'H}(H|\vec{\kappa}_1)\equiv\\
&\quad\Delta_{h'1}\,(Z_{00})^{A-1}\left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}\kappa_1^2\right\}\tilde{r}_{H'}\,(\vec{\kappa}_1), \qquad (2.36)
\end{aligned}$$

where the sum ($H\leq F$) runs over all states $\vec{n}$ which are occupied in $|\,\rangle$. Furthermore

$$\begin{aligned}
&\langle\,|b^\dagger_{Hh}\hat{Z}_{A-1}c_{\vec{k}_2\,2}|\,\rangle\;=\\
&\quad\Delta_{2h}\,(Z_{00})^{A-1}\left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}\kappa_2^2\right\}\\
&\quad\times\sum_{H'\leq F}(\vec{\kappa}_2|H')z^{-1}_{H'H}\equiv\\
&\quad\Delta_{2h}\,(Z_{00})^{A-1}\left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}\kappa_2^2\right\}r_H\,(\vec{\kappa}_2) \qquad (2.37)
\end{aligned}$$

and, finally,

$$\begin{aligned}
&\langle\,|c^\dagger_{\vec{k}_1\,1}\hat{Z}_{A-1}c_{\vec{k}_2\,2}|\,\rangle\;=\\
&\quad\Delta_{21}\,(Z_{00})^{A-1}\left(\frac{b}{\sqrt{\pi}}\right)^{3}\exp\left\{-\frac{1}{2}(\kappa_2^2+\kappa_1^2)\right\}\\
&\quad\times\sum_{H',\,H\leq F}(\vec{\kappa}_2|H')z^{-1}_{H'H}(H|\vec{\kappa}_1)=\\
&\quad\Delta_{21}\,(Z_{00})^{A-1}\left(\frac{b}{\sqrt{\pi}}\right)^{3}\exp\left\{-\frac{1}{2}(\kappa_2^2+\kappa_1^2)\right\}x\,(\vec{\kappa}_2,\,\vec{\kappa}_1)\,.
\end{aligned} \qquad (2.38)$$

Again there exist recursion relations for the vectors $\tilde{\mathbf{r}}$ and $\mathbf{r}$ and for the scalar x. Using the the matrices out of eq. (2.35), we obtain

$$\begin{aligned}
&\tilde{r}^{(0)}_0(\kappa_1)=1,\\
&\tilde{\mathbf{r}}^{(N_F+1)}_2(\kappa_1)=(\mathbf{2}|\vec{\kappa}_1)-\mathbf{z}^{(N_F+1)}_{21}\tilde{\mathbf{r}}^{(N_F)}_1(\vec{\kappa}_1),\\
&\tilde{\mathbf{r}}^{(N_F+1)}_1(\kappa_1)=\tilde{\mathbf{r}}^{(N_F)}_1(\kappa_1)+\mathbf{z}^{(N_F+1)^{-1}}_{12}\tilde{\mathbf{r}}^{(N_F+1)}_2(\kappa_1), \qquad (2.39)
\end{aligned}$$

while

$$\begin{aligned}
&r^{(0)}_0(\kappa_2)=1,\\
&\mathbf{r}^{(N_F+1)}_2(\kappa_2)=(\vec{\kappa}_2|\mathbf{2})-\mathbf{r}^{(N_F)}_1(\vec{\kappa}_2)\mathbf{z}^{(N_F+1)}_{12},\\
&\mathbf{r}^{(N_F+1)}_1(\kappa_2)=\mathbf{r}^{(N_F)}_1(\kappa_2)+\mathbf{r}^{(N_F+1)}_2(\kappa_2)\mathbf{z}^{(N_F+1)^{-1}}_{21}, \qquad (2.40)
\end{aligned}$$

and

$$\begin{aligned}
&x^{(0)}\,(\vec{\kappa}_2,\,\vec{\kappa}_1)=1\,,\\
&x^{(N_F+1)}\,(\vec{\kappa}_2,\,\vec{\kappa}_1)=x^{(N_F)}\,(\vec{\kappa}_2,\,\vec{\kappa}_1)\\
&\qquad\qquad+\mathbf{r}^{\,(N_F+1)}_{\,2}\,(\kappa_2)\;\cdot\;\tilde{\mathbf{r}}^{\,(N_F+1)}_{\,2}(\kappa_1)\,, \qquad (2.41)
\end{aligned}$$

where in the last line the scalar product of the vectors $\mathbf{r}$ and $\tilde{\mathbf{r}}$, restricted to the components out of the shell N_F+1, is meant.

Using the notation out of (2.8) and the recursion relations (2.32), we obtain for the reduced shifted overlap matrix elements (2.32) up to the $1s0d$-shell

$$\begin{aligned}
&z_{00}=1\,, && z_{0k}\;=\;+\beta'_k\,,\\
&z_{02k}=+{\beta'_k}^2/\sqrt{2}\,, && z_{0k<l}\;=\;\beta'_k\beta'_l\,,\\
&z_{i0}=-\beta_i\,, && z_{ik}\;=\;\delta_{ik}-\beta_i\beta'_k\,,\\
&z_{i2k}=\beta'_k(2\delta_{ik}-\beta_i\beta'_k)/\sqrt{2}\,,\\
&z_{ik<l}=\beta'_k\delta_{il}+\beta'_l\delta_{ik}-\beta_i\beta'_k\beta'_l\,,\\
&z_{2i0}=+{\beta_i}^2/\sqrt{2}\,, && z_{2ik}=-\beta_i(2\delta_{ik}-\beta_i\beta'_k)/\sqrt{2}\,,\\
&z_{2i2k}=\delta_{ik}[1-2\beta_i\beta'_k]+\beta_i^2{\beta'_k}^2/2\,,\\
&z_{2ik<l}=-\sqrt{2}(\beta_i\beta'_l\delta_{ik}+\beta_i\beta'_k\delta_{il}-\beta_i^2\beta'_k\beta'_l/2)\,,\\
&z_{i<j0}=\beta_i\beta_j\,, && z_{i<jk}=-\beta_i\delta_{jk}-\beta_j\delta_{ik}+\beta_i\beta_j\beta'_k\,,\\
&z_{i<j2k}=-\sqrt{2}(\beta_j\beta'_k\delta_{ik}+\beta_i\beta'_k\delta_{jk}-{\beta'}^2_k\beta_i\beta_j/2)\,,\\
&z_{i<jk<l}=\delta_{ik}\delta_{jl}-\beta_i\beta'_k\delta_{jl}-\beta_i\beta'_l\delta_{jk}\\
&\qquad-\beta_j\beta'_k\delta_{il}-\beta_j\beta'_l\delta_{ik}+\beta_i\beta_j\beta'_k\beta'_l\,. \qquad (2.42)
\end{aligned}$$

Using (2.35), we obtain assuming the usual oscillator occupations (2.21) of ^{4}He, ^{16}O and ^{40}Ca for the matrix elements $z^{-1}_{H'H}$ out of eq. (2.34) subsequently

$$z^{-1}_{00}\;=\;1 \qquad (2.43)$$

for ^{4}He, while, for ^{16}O,

$$\begin{aligned}
&z^{-1}_{00}=1-\vec{\beta}\cdot\vec{\beta}\,'\,, && z^{-1}_{k0}\;=\;+\beta_k\,,\\
&z^{-1}_{0i}=-\beta'_i\,, && z^{-1}_{ki}\;=\;\delta_{ki}\,, \qquad (2.44)
\end{aligned}$$

and, finally, for ^{40}Ca

$$
\begin{aligned}
z_{00}^{-1} &= 1-\vec{\beta}\cdot\vec{\beta}\,'+(\vec{\beta}\cdot\vec{\beta}\,')^2/2\,,\\
z_{k0}^{-1} &= \beta_k(1-\vec{\beta}\cdot\vec{\beta}\,')\,,\\
z_{2k0}^{-1} &= +\beta_k^2/\sqrt{2}\,, \qquad z_{k<l0}^{-1} = \beta_k\beta_l\,,\\
z_{0i}^{-1} &= -\beta_i'(1-\vec{\beta}\cdot\vec{\beta}\,')\,,\\
z_{ki}^{-1} &= \delta_{ki}(1-\vec{\beta}\cdot\vec{\beta}\,')-\beta_k\beta_i'\,,\\
z_{2ki}^{-1} &= +\sqrt{2}\beta_k\delta_{ki}\,, \qquad z_{k<li}^{-1} = \delta_{ki}\beta_l+\delta_{li}\beta_k\,,\\
z_{02i}^{-1} &= +\beta\,'^2_i/\sqrt{2}\,, \qquad z_{k2i}^{-1} = -\sqrt{2}\beta_i'\delta_{ki}\,,\\
z_{2k2i}^{-1} &= \delta_{ki}\,, \qquad z_{k<l2i}^{-1} = 0\,,\\
z_{0i<j}^{-1} &= \beta\,'_i\beta\,'_j\,, \qquad z_{ki<j}^{-1} = -\delta_{ki}\beta_j'-\delta_{kj}\beta_i'\,,\\
z_{2ki<j}^{-1} &= 0\,, \qquad z_{k<li<j}^{-1} = \delta_{ki}\delta_{lj}\,.
\end{aligned}
\tag{2.45}
$$

Note, that $z_{H'H}^{-1} = z_{H'H}^{-1}(\vec{\beta},\,\vec{\beta}\,')$ with $\vec{\beta}$ and $\vec{\beta}\,'$ given by eq. (2.31). Defining

$$
\vec{\beta}_{\,1} \equiv \vec{\beta} + i\sqrt{2}\,\vec{\kappa}_1 \quad \text{and} \quad \vec{\beta}\,'_2 \equiv \vec{\beta}\,' + i\sqrt{2}\,\vec{\kappa}_2 \tag{2.46}
$$

and using the recursion relations (2.39), (2.40) and (2.41), we obtain for ^{4}He (since $H = H' = 0$)

$$
\tilde{r}_0\,(\vec{\beta}_1,\,\vec{\beta}\,') = r_0\,(\vec{\beta}\,'_2,\,\vec{\beta}\,) = x(\vec{\beta}\,'_2,\,\vec{\beta}_1\,) = 1\,, \tag{2.47}
$$

while, for ^{16}O

$$
\tilde{r}_{H'}\,(\vec{\beta}_1,\,\vec{\beta}\,') = \left\{ \begin{array}{ll} 1-\vec{\beta}\,'\cdot\vec{\beta}_1 & \text{for } H'=0 \\ \beta_{1k} & \text{for } H'=k \end{array} \right\}\,, \tag{2.48}
$$

$$
r_H\,(\vec{\beta}\,'_2,\,\vec{\beta}\,) = \left\{ \begin{array}{ll} 1-\vec{\beta}\,'_2\cdot\vec{\beta} & \text{for } H=0 \\ -\beta\,'_{2i} & \text{for } H=i \end{array} \right\}\,, \tag{2.49}
$$

$$
x(\vec{\beta}\,'_2,\,\vec{\beta}_1\,) = 1-\vec{\beta}_1\cdot\vec{\beta}\,'_2\,, \tag{2.50}
$$

and, for ^{40}Ca

$$
\tilde{r}_{H'}\,(\vec{\beta}_1,\,\vec{\beta}\,') = \left\{ \begin{array}{ll} 1-\vec{\beta}\,'\cdot\vec{\beta}_1+(\vec{\beta}\,'\cdot\vec{\beta}_1)^2/2+\beta\,'^2/2 & \text{for } H'=0 \\ \beta_{1k}(1-\vec{\beta}\,'\cdot\vec{\beta}_1)-\beta\,'_k & \text{for } H'=k \\ +(1+{\beta_{1k}}^2)/\sqrt{2} & \text{for } H'=2k \\ \beta_{1k}\beta_{1l} & \text{for } H'=k<l \end{array} \right\} \tag{2.51}
$$

$$
r_H\,(\vec{\beta}\,'_2,\,\vec{\beta}\,) = \left\{ \begin{array}{ll} 1-\vec{\beta}\cdot\vec{\beta}\,'_2+(\vec{\beta}\cdot\vec{\beta}\,'_2)^2/2+\beta^2/2 & \text{for } H=0 \\ -\beta\,'_{2i}(1-\vec{\beta}\cdot\vec{\beta}\,'_2)+\beta_i & \text{for } H=i \\ +(1+{\beta\,'_{2i}}^2)/\sqrt{2} & \text{for } H=2i \\ \beta\,'_{2i}\beta\,'_{2j} & \text{for } H=i<j \end{array} \right\} \tag{2.52}
$$

$$
x(\vec{\beta}\,'_2,\vec{\beta}_1) = 5/2+(\vec{\beta}_1-\vec{\beta}\,'_2)^2/2+(\vec{\beta}_1\cdot\vec{\beta}\,'_2)^2/2\,. \tag{2.53}
$$

2.4 Normalisation

From the above formulas the norms of the considered COM-projected determinants can be calculated easily. For $\vec{q} = \vec{q}\,' = 0$ the operator (2.27) reduces to the usual shift operator $\hat{S}_A(\vec{a})$, which appears in the projector to the COM rest frame $\hat{C}_A(0)$, defined by eq. (1.7). For the normalisation of the A-nucleon states $|\,\rangle$ we obtain therefore

$$
\begin{aligned}
N_A \equiv \langle\,|\hat{C}_A(0)|\,\rangle &= \int \mathrm{d}^3\vec{a}\langle\,|\hat{S}_A(\vec{a})|\,\rangle = \\
& b^3\pi\sqrt{\pi}\frac{1}{\pi\sqrt{\pi}}\int \mathrm{d}^3\vec{\alpha}\;(S_{00})^A = \\
& b^3\pi\sqrt{\pi}\frac{1}{\pi\sqrt{\pi}}\int \mathrm{d}^3\vec{\alpha}\;\exp\left\{-\frac{A}{4}\alpha^2\right\} = \left(\frac{4\pi b^2}{A}\right)^{3/2},
\end{aligned}
\tag{2.54}
$$

where we have used (2.33) and (2.29).

In the same way the integrated overlap matrices within one-hole states can be calculated. Here one obtains

$$
\begin{aligned}
&(N_{A-1})_{H'h'Hh} \equiv \langle\,|b^\dagger_{Hh}\hat{C}_{A-1}(0)b_{H'h'}|\,\rangle = \\
&\int \mathrm{d}^3\vec{a}\langle\,|b^\dagger_{Hh}\hat{S}_{A-1}(\vec{a})b_{H'h'}|\,\rangle = \\
&b^3\pi\sqrt{\pi}\frac{1}{\pi\sqrt{\pi}}\int \mathrm{d}^3\vec{\alpha}\;\exp\left\{-\frac{A-1}{4}\alpha^2\right\} \\
&\quad\times\,\Delta_{h'h}\,s^{-1}_{H'H}(\vec{\beta}=\vec{\beta}\,'=\vec{\alpha}/\sqrt{2}) = \\
&\left(\frac{4\pi b^2}{A-1}\right)^{3/2}\frac{1}{\pi\sqrt{\pi}}\int \mathrm{d}^3\vec{z}\exp\{-z^2\} \\
&\quad\times\,\Delta_{h'h}\,s^{-1}_{H'H}\left(\vec{\beta}=\vec{\beta}\,'=\sqrt{\frac{2}{A-1}}\,\vec{z}\right).
\end{aligned}
\tag{2.55}
$$

Using (2.43) to (2.45) as well as the unitary transformations (2.11) one obtains for $A = 4$

$$
(N_{A-1})_{H'h'Hh} = \left(\frac{4\pi b^2}{A-1}\right)^{3/2}\Delta_{h'h}\,, \tag{2.56}
$$

while for $A = 16$ the only non-vanishing matrix elements are

$$
(N_{A-1})_{H'h'Hh} = \left(\frac{4\pi b^2}{A-1}\right)^{3/2} \times\Delta_{h'h}\left\{ \begin{array}{ll} \frac{4}{5} & \text{for } H=H'=0s \\ 1 & \text{for } H=H'=0p\lambda \end{array} \right\} \tag{2.57}
$$

and for $A = 40$ we get as non-trivial results

$$
(N_{A-1})_{H'h'Hh} = \left(\frac{4\pi b^2}{A-1}\right)^{3/2} \times\Delta_{h'h}\left\{ \begin{array}{ll} \frac{941}{1014} & \text{for } H=H'=0s \\ -\frac{1}{39}\sqrt{\frac{3}{2}} & \text{for } H=0s,\ H'=1s \\ -\frac{1}{39}\sqrt{\frac{3}{2}} & \text{for } H=1s,\ H'=0s \\ 1 & \text{for } H=H'=1s \\ \frac{35}{39} & \text{for } H=H'=0p\lambda \\ 1 & \text{for } H=H'=0d\lambda \end{array} \right\}. \tag{2.58}
$$

Non-diagonal matrix elements appear only for the s-holes in ^{40}Ca. For these we do a Cholesky decomposition. Denoting the $1s$-state with "1", the $0s$-state with "2", we can write

$$\begin{pmatrix} 1 & -\frac{1}{39}\sqrt{\frac{3}{2}} \\ -\frac{1}{39}\sqrt{\frac{3}{2}} & \frac{941}{1014} \end{pmatrix} = \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} L_{11} & L_{21} \\ 0 & L_{22} \end{pmatrix}. \quad (2.59)$$

From these equations we obtain easily

$$L \equiv \begin{pmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -\frac{1}{39}\sqrt{\frac{3}{2}} & \sqrt{\frac{940}{1014}} \end{pmatrix}. \quad (2.60)$$

The inverse matrix can be calculated easily, too. Here one obtains

$$L^{-1} = \begin{pmatrix} 1 & 0 \\ \frac{1}{\sqrt{940}} & \sqrt{\frac{1014}{940}} \end{pmatrix}. \quad (2.61)$$

Using these results, we obtain for the normalized internal A-nucleon states in the center-of-mass rest frame

$$|\,,(0)\rangle \equiv \hat{C}_A(0)|\,\rangle \left(\frac{A}{4\pi b^2}\right)^{3/4}, \quad (2.62)$$

while for the corresponding internal one-hole states

$$|(Hh)^{-1},(0)\rangle \equiv \hat{C}_{A-1}(0) b_{Hh}|\,\rangle \left(\frac{A-1}{4\pi b^2}\right)^{3/4} \times \begin{Bmatrix} 1 & \text{for } H=0s \text{ in } ^4\text{He} \\ 1 & \text{for } H=0p\lambda \text{ in } ^{16}\text{O} \\ \sqrt{\frac{5}{4}} & \text{for } H=0s \text{ in } ^{16}\text{O} \\ 1 & \text{for } H=1s \text{ in } ^{40}\text{Ca} \\ 1 & \text{for } H=0d\lambda \text{ in } ^{40}\text{Ca} \\ \sqrt{\frac{39}{35}} & \text{for } H=0p\lambda \text{ in } ^{40}\text{Ca} \end{Bmatrix} \quad (2.63)$$

and for the (with respect to the $1s$-hole) Gram-Schmidt–orthogonalized $0\tilde{s}$-hole in ^{40}Ca we have

$$|(0\tilde{s},h)^{-1},(0)\rangle \equiv \hat{C}_{A-1}(0) \times \left(b_{0s0h}|\,\rangle\sqrt{\frac{1014}{940}} + b_{1s0h}|\,\rangle\frac{1}{\sqrt{940}}\right)\left(\frac{A-1}{4\pi b^2}\right)^{3/4}. \quad (2.64)$$

Now we have all the mathematical ingrediences needed for the following and can start our task to investigate the effects of the restoration of Galilean invariance on various observables.

3 Spectral functions and spectroscopic factors

As a first example for the effects of the restoration of the Galilei invariance we want to evaluate the spectral functions and spectroscopic factors for the uncorrelated oscillator A-nucleon ground states of the doubly closed shell nuclei listed in (2.21). For single Slater-determinant states the usual hole spectral functions are trivial. We obtain for all occupied (hole) states Hh

$$f^{\rm nor}_{Hh}(\vec{k}) \equiv \langle\,|c^\dagger_{\vec{k}\,h} b_{Hh}|\,\rangle = \langle H|\vec{k}\rangle\,. \quad (3.1)$$

The hole spectral functions are thus the complex conjugates of the momentum space representation all the occupied states. They measure the "momentum dependence of the hole states".

The states (2.19) occuring in (3.1) form a complete set. Therefore the spectroscopic factors are

$$S^{\rm nor}_{Hh} \equiv \int {\rm d}^3\vec{k}\,|f^{\rm nor}_{Hh}(\vec{k})|^2 = \left\{\begin{matrix} 1 & \text{for } Hh \text{ occupied} \\ 0 & \text{else} \end{matrix}\right\} \quad (3.2)$$

and, obviously

$$\sum_{Hh} S^{\rm nor}_{Hh}\, d(H) = A\,, \quad (3.3)$$

where $d(H)$ is the degeneracy ($2l_H+1$, l_H being the orbital angular momentum) of the state H.

Similarly, the particle spectral functions are just given by

$$f^{\rm nor}_{Pp}(\vec{k}) \equiv \langle\,|c_{\vec{k}\,p} b^\dagger_p|\,\rangle = \langle\vec{k}|\,P\rangle\,. \quad (3.4)$$

Again the spectroscopic factors are trivial. We obtain

$$S^{\rm nor}_{Pp} \equiv \int {\rm d}^3\vec{k}\,|f^{\rm nor}_{Pp}(\vec{k})|^2 = \left\{\begin{matrix} 0 & \text{for } Pp \text{ occupied} \\ 1 & \text{else} \end{matrix}\right\}. \quad (3.5)$$

This is the "normal" description of an uncorrelated state as indicated by the superscript "nor" in the above equations. The deviations from this simple picture usually are interpreted as a measure for correlations.

However, this description does not conserve Galilei invariance. In order to restore the latter we have first to ensure that the initial as well as the final bound systems are in their respective COM rest frames and second the plane wave nucleon has to be described by a relative motion wave function with respect to the $(A-1)$-nucleon system. For the (not yet normalized) hole spectral function thus we have to calculate

$$\begin{aligned} &\langle\,|c^\dagger_{\vec{k}\,h}\exp\{-i\vec{k}\cdot\vec{R}_{A-1}\}\hat{C}_{A-1}(0)b_{Hh}|\,\rangle = \\ &\int {\rm d}^3\vec{a}\langle\,|c^\dagger_{\vec{k}\,h}\exp\{-i\vec{k}\cdot\vec{R}_{A-1}\}\exp\{i\vec{a}\cdot\hat{P}_{A-1}\}b_{Hh}|\,\rangle = \\ &\left(\frac{4}{A-1}\right)^{3/2} b^3\pi\sqrt{\pi}\left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\exp\left\{-\frac{1}{2}\frac{A}{A-1}\kappa^2\right\} \\ &\times\frac{1}{\pi\sqrt{\pi}}\int {\rm d}^3\vec{y}\exp\{-y^2\}\tilde{r}_H(\vec{\beta}\,',\vec{\beta}_1)\,, \end{aligned} \quad (3.6)$$

where use has been made of the operator (2.27) with $\vec{q}_1 = -\vec{\kappa}/(A-1)$ and $\vec{q}_2 = 0$. The functions $\tilde{r}_H$ are given in eqs. (2.47), (2.49) and (2.51) for the three considered nuclei, respectively, and

$$\vec{\beta}\,' \equiv \sqrt{\frac{2}{A-1}}\,\vec{y}\,,$$

while

$$\vec{\beta}_1 \equiv \sqrt{\frac{2}{A-1}}\,\vec{y} + i\sqrt{2}\frac{A}{A-1}\,\vec{\kappa}\,. \tag{3.7}$$

Using the normalisation of the A-nucleon determinants (2.54) and the corresponding 1-hole states (2.63) and (2.64) one obtains

$$f^{\rm pro}_{Hh}(\vec{k}) \,=\, \langle H|\vec{k}\rangle_{\rm rel}\sqrt{S^{\rm pro}_{Hh}}\,, \tag{3.8}$$

where the superscript "pro" refers here to the translationally invariant "projected" description and the subscript "rel" indicates that in the Fourier transform of the oscillator function H the nucleon mass M (occuring in the oscillator length) has to be replaced by the reduced mass $MA/(A-1)$. In Cartesian representation of momentum space we have (see eq. (2.5))

$$\langle\vec{n}\,|\vec{k}\,\rangle_{\rm rel} = \left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\left(\frac{A}{A-1}\right)^{3/4} \times\exp\left\{-\frac{1}{2}\frac{A}{A-1}\kappa^2\right\}\prod_{i=1}^{3}\left(n_i|\sqrt{\frac{A}{A-1}}\kappa_i\right). \tag{3.9}$$

The projected spectroscopic factors in eq. (3.8) are given by

$$S^{\rm pro}_H \,=\, \left\{\begin{array}{ll} 1 & \text{for } H=0s \text{ in } {}^4\text{He}\\ \frac{4}{5} & \text{for } H=0s \text{ in } {}^{16}\text{O}\\ \frac{16}{15} & \text{for } H=0p \text{ in } {}^{16}\text{O}\\ \frac{1410}{1521} & \text{for } H=0\tilde{s} \text{ in } {}^{40}\text{Ca}\\ \frac{1400}{1521} & \text{for } H=0p \text{ in } {}^{40}\text{Ca}\\ \frac{1600}{1521} & \text{for } H=1s \text{ in } {}^{40}\text{Ca}\\ \frac{1600}{1521} & \text{for } H=0d \text{ in } {}^{40}\text{Ca}\end{array}\right\}, \tag{3.10}$$

respectively. The subscript h has been supressed here, since the spectroscopic factors are the same for each spin-isospin combination. The tilde on the $0\tilde{s}$ state for ^{40}Ca indicates that here the orthonormalized state (2.64) is meant. The results (3.10) are identical to those derived by Dieperink and de Forest already in 1974 [13]. Their method to obtain (3.10), however, is confined to harmonic-oscillator configurations, while the projection method used here can be also used for general configurations.

It is easily checked that as in the unprojected case

$$\sum_{Hh} S^{\rm pro}_{Hh} d(H) \,=\, A\,. \tag{3.11}$$

The spectroscopic factors for the hole states out of eq. (3.10) are displayed in fig. 1. The general feature (except for the trivial case of ^{4}He) is that the occupation of the low-lying shells (with excitation energies $\geq 1\hbar\omega$) is depleted while that of the (non-spurious) hole states in the last shell is enhanced. On first sight spectroscopic factors with values larger than one may be hard to understand. However, consider the simple example of two spinless fermions living in one dimension and occupying the oscillator states ($b = 1$ fm, for simplicity)

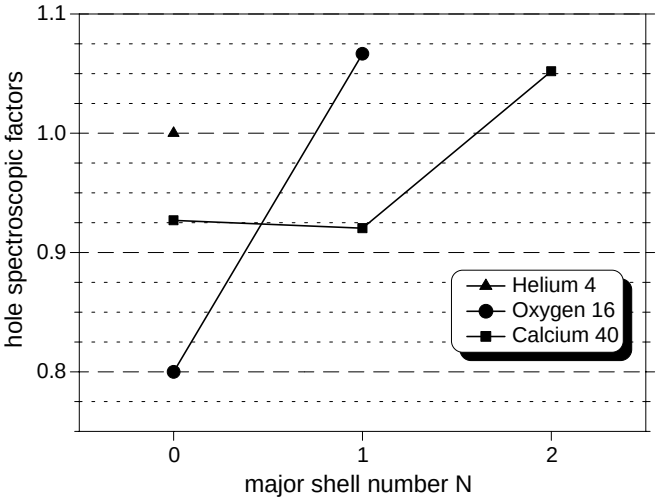

Fig. 1. The projected hole spectroscopic factors (3.10) are plotted for the three nuclei ^{4}He, ^{16}O and ^{40}Ca. They have to be compared with the conventional description (3.2) of an uncorrelated system which gives one for all the occupied states.

$$\begin{aligned} &\langle x|1\rangle = (\sqrt{\pi})^{-1/2}\exp\{-x^2/2\}\\ \text{and}\qquad &\langle x|2\rangle = (2\sqrt{\pi})^{-1/2}\exp\{-x^2/2\}x\,. \end{aligned} \tag{3.12}$$

Constructing a Slater determinant out of these two states and calculating the hole spectroscopic factors in the *normal* way, one obtains by construction $S^{\rm nor}_1 = S^{\rm nor}_2 = 1$. Using the Galilei-invariant prescription, however, one realises immediately that a relative state of the form $\sim \exp\{-(x(1)-x(2))^2/4\}$ cannot be formed with this two wave functions. Thus the projected spectroscopic factors are here $S^{\rm pro}_1 = 0$ and $S^{\rm pro}_2 = 2$. Now nucleons have spin and isospin and live in three instead of one dimensions. Nevertheless, looking at the results for ^{16}O one still sees the "remainder" of what is obtained in the simple one-dimensional example. The physical reason is quite simple: the hole states with excitation energies larger or equal $1\hbar\omega$ contain spurious admixtures due to the motion of the nucleus as a whole. Eliminating these via projection into the COM rest frame leads to a depletion of the corresponding hole strenth. On the other hand, the sum rule (3.11) has to be fulfilled. Consequently the eliminated strength reappears in the last (non-spurious) shell. A similar argument is also given in ref. [13].

For the particle states the situation is a little more complicated. Since the projection operator into the COM rest frame mixes the various radial excitations with the same angular-momentum quantum numbers, the direct analog to (3.6) is difficult to normalize. Thus, we use here a sligthly different prescription. We start by computing

the (normalized) particle-particle overlap kernels

$$n_{12}(\vec{k},\,\vec{k}\,') \equiv \frac{\langle\,|\exp\{i\vec{k}\cdot\vec{R}_A\}c_{\vec{k}\,1}\hat{C}_{A+1}(0)c^{\dagger}_{\vec{k}\,'\,2}\exp\{-i\vec{k}\,'\cdot\vec{R}_A\}|\,\rangle}{\langle\,|\hat{C}_A(0)|\,\rangle} =$$
$$\Delta_{12}\Big\{\delta^{(3)}(\vec{k}\,'-\vec{k}) - \frac{b^3}{\pi\sqrt{\pi}}\left(\frac{A}{A-1}\right)^{3/2}$$
$$\times\exp\left\{-\frac{A^2+1}{2A(A-1)}(\kappa^2+\kappa'^2) - \frac{2}{A-1}\vec{\kappa}\cdot\vec{\kappa}\,'\right\}$$
$$\times\frac{1}{\pi\sqrt{\pi}}\int \mathrm{d}^3\vec{y}\exp\{-y^2\}x(\vec{\beta}\,'_2,\,\vec{\beta}_1)\Big\}, \qquad (3.13)$$

where use has been made of the operator (2.27) with $\vec{q}_1 = \vec{\kappa}/A$ and $\vec{q}_2 = \vec{\kappa}\,'/A$ and the function x is defined by eqs. (2.47), (2.50) and (2.53). For (2.46) we obtain here

$$\vec{\beta}\,'_2 \equiv \sqrt{\tfrac{2}{A-1}}\left(\vec{y} + \tfrac{iA}{\sqrt{A-1}}(\vec{\kappa} + \tfrac{1}{A}\vec{\kappa}\,')\right),$$
$$\vec{\beta}_1 \equiv \sqrt{\tfrac{2}{A-1}}\left(\vec{y} + \tfrac{iA}{\sqrt{A-1}}(\vec{\kappa}\,' + \tfrac{1}{A}\vec{\kappa})\right). \qquad (3.14)$$

Again we introduce "relative" oscillator wave functions by replacing the nucleon mass M now by the reduced mass $MA/(A+1)$. In Cartesian representation of momentum space these have the form

$$\langle\vec{k}\,'|\vec{n}\rangle_{\rm rel} = \left(\frac{b}{\sqrt{\pi}}\right)^{3/2}\left(\frac{A+1}{A}\right)^{3/4}$$
$$\times\exp\left\{-\frac{1}{2}\frac{A+1}{A}\kappa'^{\,2}\right\}\prod_{i=1}^{3}\left(\sqrt{\frac{A+1}{A}}\kappa'_i|n_i\right). \qquad (3.15)$$

The projected particle-spectral functions are then defined by

$$f^{\rm pro}_{\vec{n}\,p}(\vec{k}) \equiv \int \mathrm{d}^3\vec{k}\,'n_{pp}(\vec{k},\,\vec{k}\,')\langle\vec{k}\,'|\vec{n}\,\rangle_{\rm rel}\,. \qquad (3.16)$$

Evaluating this expression with the help of the recursion relations (2.4), we obtain after a lengthy but straightforward calculation

$$f^{\rm pro}_N(\vec{k}) = \langle\vec{k}|\vec{n}\rangle_{\rm rel}\sqrt{S^{\rm pro}_N}\,, \qquad (3.17)$$

where $N = n_1+n_2+n_3$ is the major shell quantum number and the irrelevant spin-isospin quantum numbers have been supressed. For the projected particle spectroscopic factors one gets in the three considered nuclei

$$S^{\rm pro}_N(A=4) = \left(1-(-)^N\frac{1}{A^N}\right)^2,$$
$$S^{\rm pro}_N(A=16) = \left(1-(-)^N\frac{1}{A^N}\left[1-N(A+1)\right]\right)^2,$$
$$S^{\rm pro}_N(A=40) = \Big(1-(-)^N\frac{1}{A^N}\Big[1-\frac{1}{2}(A+1)(A+3)$$
$$\times N+\frac{1}{2}(A+1)^2N^2\Big]\Big)^2. \qquad (3.18)$$

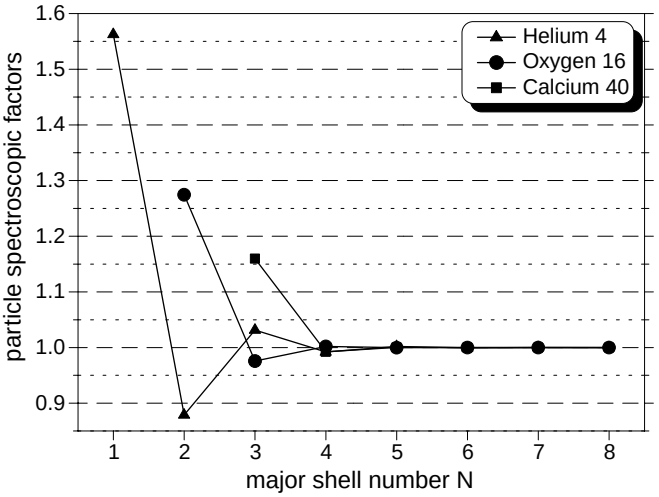

Fig. 2. The projected particle spectroscopic factors (3.18) are plotted for the three nuclei ^{4}He, ^{16}O and ^{40}Ca. They have to be compared with the conventional description (3.5) of an uncorrelated system which gives one for all the unoccupied states.

One can verify easily that the expressions (3.18) give zero for all major shells which are occupied in the corresponding reference determinants $|\,\rangle$. The results for the particle states are plotted in fig. 2. Here one observes an oscillating behaviour. The spectroscopic factors are larger than one for the first unoccupied shell (non-spurious particle states), smaller than one for the next shell ($1\hbar\omega$ excitations), again enhanced for $2\hbar\omega$ excitations and so on. The deviations from the normal result decrease, however, with increasing N.

4 Conclusions

In the first of the present series of papers it was demonstrated how with the help of projection techniques the Galilei invariance of simple bound states can be restored. The mathematical tools to perform such projections for simple oscillator configurations have been developed so that now the effects of the restoration of Galilei invariance can be studied for arbitrary observables. It should be stressed, however, that the projection method is not restricted to harmonic-oscillator configurations but can be used also for general determinants.

As a first example the spectral functions and spectroscopic factors for simple oscillator ground states of ^{4}He, ^{16}O and ^{40}Ca have been computed. For the one-hole states complete agreement with the results of Dieperink and de Forest [13] was obtained. It turned out that the restoration of Galilei invariance has considerable effects on our notion of an "uncorrelated system". Even in the simple oscillator case treated here, the hole and particle spectroscopic factors (3.10) and (3.18) are rather different from the usual ones (3.2) and (3.5). Using them (and this one should do) as reference instead of the normal description thus leads to a rather different interpretation for the amount of correlations seen in a physical experiment.

It should be stressed furthermore that while the functional dependence of the COM-projected spectral functions in this simple example could be easily reproduced by the "normal" approach if modified oscillator length parameters are used, the spectroscopic factors are independent of the choice of the oscillator length. We shall see some consequences of this fact in the analysis of quasi-elastic electron scattering in paper four of the present series of papers. For the case of ^{16}O such effects have also been analysed in a recent paper [14].

The author is grateful to Prof. Akito Arima who suggested the present investigation many years ago.

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