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Particle-hole calculations in ^{4}He and ^{16}O with centre of mass subtracted kinetic energy

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Abstract. It is found that in light nuclei it is very important to use a relative kinetic energy operator. This kinetic energy is mass number dependent and contributes in all odd parity (J^π, T) channels. In particular it is seen to produce the spurious state exactly at zero energy in the (1^-, 0) channel in TDA both in ^{4}He and ^{16}O. The effect of the relative KE is to decrease the central force attraction and increase the relative importance of the tensor force. The latter is important in RPA. Sussex matrix elements without the hard core are used.

Keywords. CM Subtracted KE, TDA and RPA in ^{4}He, ^{16}O; transitions; realisitic force calculation.

1. Introduction

There have been several attempts to describe the excited levels of light closed shell nuclei, ^{4}He (Barrett 1967, Szydlik *et al* 1972, Singh 1974) and ^{16}O (Mavromatis *et al* 1967, Irvine *et al* 1971) using realistic interactions. The ^{4}He odd parity levels were fitted by Barrett using the Tabakin force in a TDA calculation. Szydlik *et al* (1972) used both Tabakin and Sussex matrix elements (SME in short) in a shell model calculation after renormalizing the interactions at the relative matrix element level. They found the even and odd parity levels of ^{4}He to be in general agreement with experiment though for SME the (0^+, 0) and the (0^-, 0) (J^+, T)-levels are inverted. Singh (1974) in a TDA calculation for ^{4}He, found that the (2^-, 1) level was lowest in the first order and on putting second order corrections through perturbation theory the (0^-, 0) shifted too much down. In the first two calculations the ratio of the dipole transitions from the (1^-, 1) levels to the ground state was not satisfactory while in the third calculation it was not reported.

In ^{16}O the calculations by Mavromatis *et al* (1967) and Irvine *et al* (1971) produced good $T=1$ spectrum while the $T=0$ states did not come out well. The transition from the (3^-, 0) state to the ground state fell short of the experimental value in both calculations.

In the present work we have performed a TDA and RPA calculation with the SME (without hard core) and a purely relative kinetic energy operator—i.e.

$$H = \sum_i (p_i^2/2m) - (\sum_i \mathbf{p}_i)^2/2Am + \sum_{i<j} V_{ij}$$

$$= \left(1-\frac{1}{A}\right)\sum_i \frac{p_i^2}{2m} + \sum_{i<j}\left(V_{ij} - \frac{1}{mA}\mathbf{p}_i \cdot \mathbf{p}_j\right)$$

$$= \sum_{i<j} \{V_{ij} + (\mathbf{p}_i - \mathbf{p}_j)^2/2Am\}$$

so that the relative KE enters as a two body term on the same footing as the relative potential energy.

We work with this Hamiltonian alone and hence the use of experimental single particle and hole energies is avoided. Of course, as is usual in TDA and RPA calculations, the diagonal *p–h* matrix elements contain the relevant single particle energy—the single hole energy term and for this we make use of the already available Sussex results (Dey *et al* 1969). In particular,

$$\mathscr{E}_p - \mathscr{E}_h = \sum_{n,\ \text{occupied}} [\langle \phi_p, \phi_n \,|\, H \,|\, \phi_p, \phi_n\rangle - \langle \phi_h, \phi_n \,|\, H \,|\, \phi_h, \phi_n\rangle].$$

In the above reference instead of H, KE+V was used and hence we have made the necessary changes for the centre of mass KE subtraction. It must be pointed out here that we do not satisfy the Hartree-Fock self-consistency since pure harmonic oscillator single particle and hole wave functions are used. This has a significant effect on some of our results and for ^{4}He we make an improvement. To illustrate the effect of this centre of mass KE subtraction in our Hamiltonian, we tabulate the relative matrix elements before and after the kinetic energy correction in table 1. This comparison of matrix elements of V and H, showing the dramatic difference, has direct relevance only for the off-diagonal TDA and all RPA particle hole matrix elements where the normal one body kinetic energy does not contribute. The tensor force is unaffected by the correction, so its importance is increased. The off-diagonal

Table 1. Relative matrix elements (in MeV) with and without KE correction (b=1·5 fm)

Channel	n	n'	Bare	With KE corrections		Used in
				A=4	A=16	
$^1S_0$	0	0	−8·45	−1·50	−6·71	TDA
	0	1	−6.90	−1·22	−5·49	RPA
$^1P_1$	0	0	3·02	14·59	5·91	TDA
$^3S_1$	0	0	−9·97	−3·02	− 8·23	TDA
	0	1	−6·82	−1·14	−5·41	RPA
$^3P_0$	0	0	−2·57	9·00	0·32	TDA
$^3P_1$	0	0	3·14	14·71	6·03	TDA
$^3P_2$	0	0	−1·85	9·72	1.04	TDA
$^3S_1$–$^3D_1$	0	0	−7·72	−7·72	−7·72	RPA
(tensor)	0	1	−0·66	−0·66	−0·66	TDA

Table 2. Centre of mass correction for two-particle matrix elements used in ^{4}He TDA calculation (in units of $\hbar\omega/A$)

Matrix elements	J	T	$\hat{O}_{12}=(p_1^2+p_2^2)/2Am$	$\hat{O}_{12}=\mathbf{p}_1\cdot\mathbf{p}_2/Am$
$\langle Os_{1/2}, Op_{1/2}\|\hat{O}_{12}\|Os_{1/2}.Op_{1/2}\rangle_{JT}$	0	0	2	−1/2
	0	1	2	+1/2
	1	0	2	−1/6
	1	1	2	+1/6
$\langle Os_{1/2}, Op_{3/2}\|\hat{O}_{12}\|Os_{1/2}, Op_{3/2}\rangle_{JT}$	1	0	2	+1/6
	1	1	2	−1/6
	2	0	2	−1/2
	2	1	2	+1/2
$\langle Os_{1/2}, Op_{3/2}\|\hat{O}_{12}\|Os_{1/2}, Op_{1/2}\rangle_{JT}$	1	0	0	2/3
	1	1	0	−2/3

tensor matrix elements are large and their coefficients in the Moshinsky expansion of RPA matrix elements are also large. We avoided separate tables for the two b regions suitable for helium and oxygen and used an oscillator length corresponding to the former as an illustration. For a larger b value the trend shown in table 1 persists.

In diagonal TDA matrix elements, in addition to relative corrected matrix elements of table 1, the particle-hole energy difference contains the one and two body kinetic energies. The one body term is partly included in the matrix elements of table 1 and the two body part gives a constant shift. The breakdown of the one body and the two body terms is shown, as an illustration, in some two-particle matrix elements relevant for ^{4}He, in table 2. These two-particle matrix elements summed with some Racah recoupling coefficients over J, T give the particle-hole matrix to be diagonalized in TDA or RPA. The formalism and phase convention is given in the references and several modern texts and will not be repeated here. It is seen in table 2 that the two body kinetic energy term is J, T dependent.

In ^{16}O an extra interesting feature appears. The $\mathbf{p}_i\cdot\mathbf{p}_j$ term has zero two-particle matrix element when the direct as well as the exchange term contains a $p_{1/2}$ state connecting a $d_{5/2}$ state, i.e. of the type $\langle p_{1/2}\|\mathbf{p}\|d_{5/2}\rangle$. After the particle-hole transformation and diagonalization this enchances the effect of the lowest $p_{\frac{1}{2}}^{-1}\, d_{5/2}$-configuration. This is the factor responsible for the large octupole transition obtained by us compared with the earlier calculations without the centre of mass correction. On using the centre of mass subtracted kinetic energy, the spurious state in (1^-, 0) channel automatically comes out at zero energy in TDA.

2. Results

A. The nucleus ^{4}He:

In table 3 the results of TDA and RPA calculations are given. The agreement with experiment is fairly good. The second column (TDA) gives odd parity levels with

Table 3. Energy Levels of ^{4}He (in Mev)

$J^\pi T$	$b=1{\cdot}4$ fm			$b=1{\cdot}5$ fm			Experiment	
	Approx A	Approx B		Approx A	Approx B			
	TDA	TDA	RPA	TDA	TDA	RPA		
$0^-, 0$	28·9	28·4	26·9	24·5	23·3	21·9	21.4	
$0^-, 1$	32·9	32·0	30·9	28·2	26·1	25·4	27·4	(29·5)
$1^-, 0$	38·7	37·8	37·6	33·1	30·9	30·8	31·0	
$1^-, 1$	36·4	35·7	35·5	31·4	29·6	29·4	30·5	
$1^-, 1$	32·0	31.4	31·3	28·2	26·7	26·6	27·8	(27·4)
$2^-, 0$	29·2	28·7	28·7	25·6	24·3	24·2	22·9	
$2^-, 1$	28·3	27·9	27·9	25·2	23·9	23·9	26·8	(26·4)
$0^+, 0$	—	23·6	23·2	—	18·3	17·3	20·3	
$2^+, 0$	—	29·1	29·0	—	24·7	24·6	29·0	

Approx. A means that hole and particle s-states are restricted to one oscillator state only.
Approx. B corresponds to the particle and hole states obtained through a mini HF calculation (see the text).

holes in helium taken to be pure oscillators as in Barrett (1967). In a strict sense, without the use of Hartree-Fock single particle and hole states, the Tamm Dancoff or the Random phase approximations are not valid. So, we perform a mini HF calculation taking the hole s-state to be

$$|hs\rangle = C_0|0s\rangle + C_1|1s\rangle$$

while the particle s-state is

$$|ps\rangle = -C_1|0s\rangle + C_0|1s\rangle.$$

With these TDA and RPA calculations can now be made for odd as well as even parity states and the results are presented in columns three and four marked B in table 3. Although it is well known that the C_0, which decouples the ground state from the even parity one particle-hole state, is close to unity for helium, we still find that the use of this can cause a change of one to two MeV in the odd parity levels.

It appears from table 3 that one needs a larger b value of 1·5 fm for the odd parity states as compared to the even parity states. This is as expected since in our odd parity calculation the unoccupied p-states occur and single oscillators have been used for them. Oscillators with a larger b value have better overlap with Hartree-Fock valence state wavefunctions.

Higher order corrections within the shell model framework are $3\hbar w$ above and this corresponds to about 60 MeV. Such excitations take one into the continuum and could be forgotten in the present context. The ratio of dipole transitions from the upper and lower $(1^-, 1)$ states to the ground state is 0·7 which is to be compared to the experimental lower limit of 0·5 (Barrett *et al* 1966).

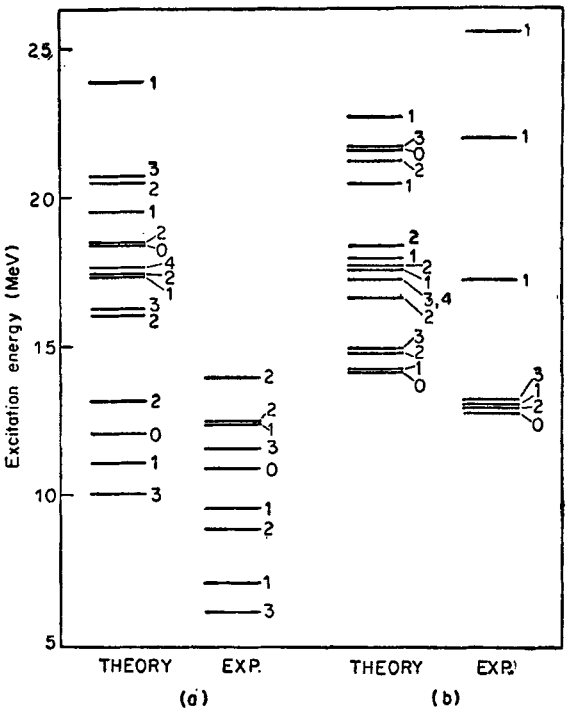

Figure 1. Odd parity energy levels of ^{16}O. The calculated levels are the RPA ones with $b=1{\cdot}9$ fm. (a) $T=0$ and (b) $T=1$ levels.

Table 4. Transition rates (in WU) to the ground state for ^{16}O

(J^π, T)	TDA		RPA		Mavromatis *et al* (1967)	
	E(MeV)	B(En)	E(MeV)	B(En)	E(MeV)	B(En)
$(1^-, 1)$	22·9	0·38	22·68	0·55	25·43	0·77
	20·61	3·74	20·49	3·90	23·75	2·18
	18·02	0·02	17·97	0·02	20·87	0·0
	17·76	0·04	17·70	0·03	17·73	0·03
	14·31	0·03	14·29	0·03	13·52	0·04
$(3^-, 0)$	20·81	0·46	20·74	0·57	22·55	0·43
	16·39	0·66	16·34	0·66	16·66	1·39
	10·96	8·58	10·11	13·28	7·14	9·7
$(3^-, 1)$	21·76	4·57	21·72	4·88	25·22	2·76
	17·42	3·64	17·38	3·88	18·91	1·51
	15·05	1·48	15·03	1·60	13·66	1·10

Obviously, n is 1 for 1^- states and 3 for 3^- states

B. The nucleus ^{16}O

The ^{16}O negative parity RPA results are displayed in figure 1. As expected the $T=1$ levels are in good agreement with experimental ones but the $T=0$ states, particularly

the (1^-, 0) and (2^-, 0) are not. Many explanations have been attempted, including a 1^- rotational band by Kelson and others. We do not go into details of these but instead refer the reader to the excellent review by Irvine *et al* (1971).

The dipole and octupole transitions to the ground state are given in table 4. Established experimental results exist only for the lowest (1^-, 1) level (0·033 WU) and the lowest (3^-, 0) level (Stroetzel (1968) gets the value of about 12 whereas Alexander and Allen (1965) quote it to be 14 WU) Calculated values in table 4 are in good agreement with these. We have also compared our transitions with those of Mavromatis *et al* (1967) in which Hamada-Johnston potential was used in the 1 $\hbar w$ subspace.

Not tabulated are the transitions from our zero spuriosity (1^-, 0) states all of which show very little dipole strength (order of 10^{-3} WU) in agreement with experiment (Swann 1970). RPA always enhances the transition rates strongly. It is to be noted that in our calculations only the theoretical lowest order single particle energies have been used. The use of experimental or HF single particle energies often tends to push down the $T=0$ levels more than the $T=1$ levels. We use a slightly high b value (1·9 fm) and this is justified by its better overlap with HF wave-functions of Ellis and Mavromatis (1971).

3. Conclusions

A notable feature of our calculation is that the (1^-, 0) centre of mass state is numerically at zero energy both in ^{4}He and ^{16}O in TDA. The RPA, however, gives a small imaginary eigenvalue (0·55i for helium and 1·4i in oxygen). It is understood that this is due to the lack of HF self-consistency. The magnitude of the imaginary eigenvalue for ^{4}He decreases when the HF self-consistency is partially restored. We again emphasize that our results are obtained without the use of experimental single particle energies or without adjusting the particle-hole gap as suggested by Irvine *et al* (1971). It is concluded that fairly good agreement with experiment can be obtained with a parameter free lowest order RPA calculation with the centre of mass subtracted kinetic energy operator. Of course, there are many other known methods to handle the centre of mass motion in TDA and RPA calculations. Provided that the harmonic oscillator is a good approximation to the HF potential, our method and the one of adding $\frac{1}{2}mA\omega^2R^2$ (Singh 1974) are equivalent. However, in some of the existing TDA calculations with the latter prescription (Mavromatis and Singh 1973), the exchange contribution to the TDA off diagonal matrix elements has not been properly corrected. In general terms, the subtraction of the centre of mass KE and thus dealing with the relative KE is straightforward both conceptually and operationally, but by no means it is a unique one.

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