EPJ Web of Conferences **156**, 00004 (2017) DOI: 10.1051/epjconf/201715600004
RCNP 2016

Effect of exact Coulomb-exchange calculations on band-head spectra of odd-proton nuclei

Meng-Hock, Koh[1,⋆] and *Mohamad Nor,* Nurhafiza[1]

[1] *Department of Physics, Faculty of Science, Universiti Teknologi Malaysia, 81310 Skudai, Johor, Malaysia*

Abstract. Previous calculations of band-head energy spectra of odd-mass heavy nuclei in the Hartree-Fock-plus-Bardeen-Cooper-Schrieffer (HF-BCS) framework showed that the agreement with data is better for odd-neutron as compared to odd-proton nuclei. The reason for a poorer agreement with data for the latter have been ascribed to the possible usage of the Slater approximation in calculating the Coulomb-exchange term. In this work, we report the effect of exact Coulomb-exchange calculations on band-head energy spectra of two odd-proton nuclei (namely ^{237}Np and ^{241}Am) as compared to the results obtained using the Slater approximation. We performed self-consistent blocking calculations while taking the breaking of time-reversal symmetry at the mean-field level into account due to the unpaired nucleon. The SkM* and SIII parametrizations of the Skyrme interaction have been employed to approximate the effective nucleon-nucleon interaction while a seniority force is used for the pairing channel. Contrary to what was expected, our preliminary results show no improvement on the band-head spectra as compared to data when the Coulomb-exchange term is calculated exactly.

1 Introduction

Self-consistent blocking calculations of band-head energies of odd-mass nuclei have been recently performed in Ref. [1] within the Hartree-Fock-plus-Bardeen-Cooper-Schrieffer (HF+BCS) framework. Using two choice of Skyrme parametrizations namely the SIII and SkM*, the authors showed that the agreement between the calculated results and experimental data for odd-neutron nuclei (namely ^{235}U and ^{239}Pu) is better than for odd-proton nuclei (namely ^{237}Np and ^{241}Am). A possible reason for the poorer agreement with data for odd-proton nuclei is attributed to the usage of the Slater approximation [2] for the Coulomb-exchange term. As a follow-up to the previous work, we would like to investigate as to what extend the Slater approximation affects the agreement of band-head energies with data. Conversely, we want to check if exact calculations of the Coulomb-exchange term would improve the agreement of the quantity of interest with available data.

While exact calculation of the Coulomb-exchange term is possible, majority of mean-field calculations of various nuclear properties resort to using the Slater approximation due to the former being more cumbersome and requires longer computing time. Some studies on the validity of the Slater approximation have been performed starting from the work of Ref. [3] and more recently in the work of Refs. [4] and [5]. The general consensus was that the Slater approximation constitute a

⋆e-mail: kmhock@utm.my

© The Authors, published by EDP Sciences. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (http://creativecommons.org/licenses/by/4.0/).

good approximation for heavy nucleus while it is less good for light nucleus. Furthermore, the Slater approximation was found to be better in open shell nucleus as compared to nuclei in the vicinity of magic nucleus [5].

However, previous studies involved only even-even (i.e. even with respect to the proton and neutron numbers) mass nuclei whereby only the time-even densities contributes to the Hamiltonian density. In the case of odd-mass nuclei (odd-odd nuclei included), the time-odd densities does not vanish as is the case in even-even nuclei and resulting in the lifting of the Kramers degeneracy of the single-particle levels. The inclusion of the time-reversal symmetry breaking at the mean-field level (due to the time-odd densities) plays an important role in describing for e.g. the quenching of the spin gyromagnetic ratio (see Refs. [6–8]). This preliminary work is therefore, to the best of our knowlege, the first in which exact calculations of the Coulomb-exchange term is performed on top of breaking the time-reversal symmetry at the mean-field level.

2 Details of the approach

This work is based on the HF+BCS framework assuming axial and parity symmetric nuclear shape. The effective nucleon-nucleon interaction is approximated with the phenomenological Skyrme interaction. More specifically, we have make use of the SIII Skyrme parametrization [10]. For the BCS pairing treatment, the seniority force is used whereby the pairing strengths, G_q entering the pairing matrix element, g_q

$$g_q = \frac{G_q}{N_q + 11} \tag{1}$$

has been fitted to the odd-even mass staggering of some actinide nuclei (refer Ref. [1] for details of the fitting procedure). The parameter N_q above refers to the number of nucleons for a given charge q. The retained values are $G_n = 17.15$ MeV and $G_p = 14.00$ MeV for the neutron and proton pairing strengths, respectively. All single-particle states up to 6 MeV above the chemical potential with a smooth cut-off of $\mu = 0.2$ MeV has been considered for the BCS calculations.

In the case of odd-mass nucleus, the lowest-energy solution for a particular blocked K^π configuration is obtained by blocking one single-particle state k nearest to the Fermi level. The third component of the total angular momentum of the blocked state Ω_k is assumed to correspond to the nuclear spin of the whole nucleus (i.e. $K = \Omega_k$). The blocking procedure was implemented in the code by setting the occupation number v_k^2 of the single-particle state k to 1.

A consequence of blocking a single-particle state is that now the time-odd local densities entering the Hamiltonian densities (defined in terms of the action of the time-reversal symmetry operator) does not vanish as is the case for the ground-state of even-even nucleus. Discussions on these local densities as well as the Hartree-Fock equations can be found for e.g. in Appendix A of Ref. [9].

When performing calculations using the Slater approximation, the contribution from the Coulomb-exchange term to the total binding energy of the nucleus is given by

$$E_{exch.Coul.}^{(Slater)} = -\frac{3}{4}e^2\Big(\frac{3}{\pi}\Big)^{1/3} \int \mathbf{d^3r}\, \rho_p^{4/3}(\mathbf{r}) \tag{2}$$

The negative sign in the equation (2) reflects the fact that this term provides additional binding energy to the nucleus. On the other hand, the matrix elements of the Coulomb exchange term can be calculated exactly. The details of such procedure are rather lengthy and we would rather refer the readers to the literatures for e.g. Refs. [5, 11, 12]

The HF+BCS solution serves as an intrinsic state solution $\langle\Phi^{\alpha}_{K\pi}|\hat{H}_{eff}|\Phi^{\alpha}_{K\pi}\rangle$ in the Bohr unified model description whereby the total energy of the nucleus $E_{K\pi\alpha}$ is given by [1]

$$E_{K\pi\alpha} = \langle\Phi^{\alpha}_{K\pi}|\hat{H}_{eff}|\Phi^{\alpha}_{K\pi}\rangle - \frac{\langle\hat{\mathbf{J}}^2_{core}\rangle}{2\mathcal{J}} + \frac{\hbar^2}{2\mathcal{J}}\Big[I(I+1) - K(K-1) + \delta_{K,\frac{1}{2}}a(-1)^{I+\frac{1}{2}}\Big(I+\frac{1}{2}\Big)\Big] \tag{3}$$

The Coriolis coupling effect has been neglected except for $K = 1/2$ which is taken care by the decoupling parameter a. The decoupling parameter and the rotational energy $\frac{\langle\hat{\mathbf{J}}^2_{core}\rangle}{2\mathcal{J}}$ have been computed from the microscopic polarized even-even core solution.

Setting the nuclear spin, I, to $I = K$ for band-head, we obtained

$$E_{K\pi\alpha} = \langle\Phi^{\alpha}_{K\pi}|\hat{H}_{eff}|\Phi^{\alpha}_{K\pi}\rangle - \frac{\langle\hat{\mathbf{J}}^2_{core}\rangle}{2\mathcal{J}} + \frac{\hbar^2}{2\mathcal{J}}\Big[2K + \delta_{K,\frac{1}{2}}a(-1)^{I+\frac{1}{2}}\Big(I+\frac{1}{2}\Big)\Big] \tag{4}$$

Using equation (4), the excitation energy $E^{*}_{K\pi\alpha}$ is calculated with respect to the energy of the ground-state band. The moment of inertia $\mathcal{J}$ has been calculated by using the Inglis-Belyaev formula (see e.g. Ref. [14]) omitting the blocked single-particle state and its conjugate state.

3 Results

Calculations of band-head energies have been performed for ^{237}Np and ^{241}Am using both the Slater approximation and exact calculations of the Coulomb-exchange term. The results are plotted in Fig. 1 and Fig. 2 and compared to experimental data. The excitation energies are tabulated in Table 1 together with the calculated values for the moment of inertia. The latter is given in terms of energy parameter $A = \frac{\hbar^2}{2a\mathcal{J}}$ and was obtained after multiplying the moment of inertia by a factor of 1.32 as proposed by Ref. [13]

From the figures, it appears that spectra obtained from exact Coulomb-exchange calculations and Slater approximation are almost similar. Only some blocked configurations obtained from exact calculations are pushed further apart, resulting in a less compress spectra. However, the root-mean-square energy deviations of 562 keV and 521 keV for exact calculations and Slater approximation, respectively, show that the exact calculations do not improve the agreement with data as was initially thought.

4 Conclusion

We have performed exact Coulomb-exchange calculations for band-head energies of two odd-proton nuclei and to compare the results with those obtained using the usual Slater approximation. The SIII Skyrme parametrization and the seniority force were employed for this study. It was found that the energy spectra obtained from both sets of calculations to be rather similar with no significant improvement in the agreement to data when exact calculations were performed. Nevertheless, it is still premature to conclude that exact Coulomb-exchange calculations has no meaningful impact when band-head energies are concerned. Further work is needed especially by focusing on regions whereby more experimental data are available for comparison.

5 Acknowledgement

M.H.K would like to acknowledge Dr. Yap Yung Szen for the financial support rendered to him through the Universiti Teknologi Malaysia Encouragement Grants (Vot. No. 11J23). The author would also like to extend his gratitude to Prof. Philippe Quentin (CENBG) for a fruitful discussion on this particular work.

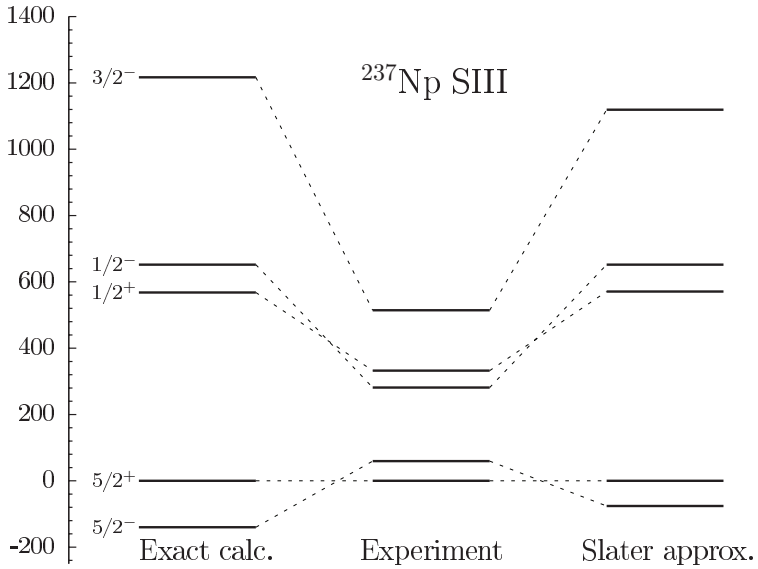

Figure 1: Comparison of the band-head energy spectra of ^{237}Np obtained using the two different approaches for the calculations of the Coulomb-exchange term as compared to experimental data [17]. The results pertaining to Slater approximation and exact calculations are explicitly indicated.

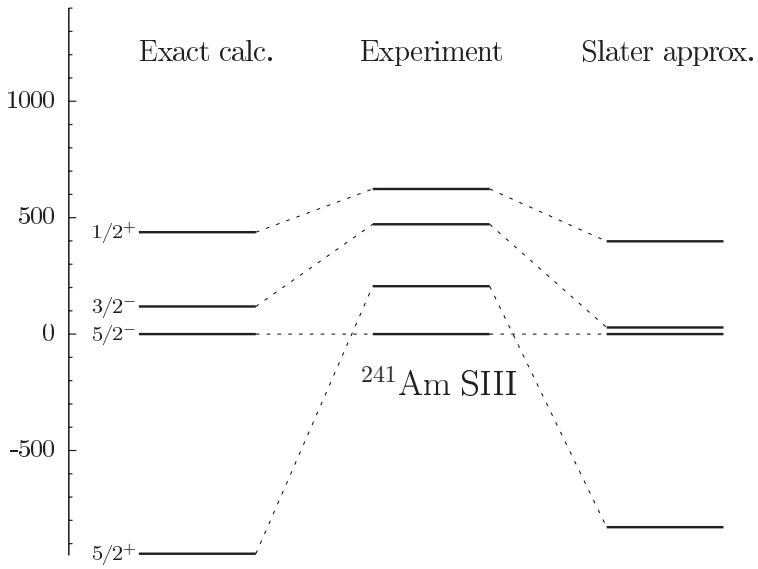

Figure 2: Similar to Fig. 1 but for ^{241}Am nucleus.

Table 1: Excitation energies of band-head states $E^*_{K\pi\alpha}$ and energy parameter ($A = \frac{\hbar^2}{2\beta\mathcal{J}}$) obtained from exact Coulomb-exchange calculations as compared to when Slater approximation is being used. The constant $\beta = 1.32$ of Ref. [13] is to account for the Thouless-Valatin correction term. Experimental data taken from Ref. [17] are included for comparison.

Nucleus	K^π	$E^*_{K\pi}$ [MeV]			A [keV]		
		Exact	Slater	Exp.	Exact	Slater	Exp.
^{237}Np	$5/2^+$	0	0	0	10.62	10.85	4.7
	$5/2^-$	-140	-76	59.5	8.56	9.27	6.2
	$1/2^-$	652	652	281.35	9.08	9.90	6.9
	$1/2^+$	568	571	332	8.16	8.82	6.2
	$3/2^-$	1218	1120	514.2	9.65	10.19	6.3
^{241}Am	$5/2^-$	0	0	0	8.32	9.02	5.9
	$5/2^+$	-943	-829	205.9	10.32	10.59	4.2
	$3/2^-$	119	28	471.8	8.90	9.52	6.5
	$1/2^+$	437	398	623.1	7.76	8.44	6.0

References

[1] Meng-Hock Koh, Dao Duy Duc, T.V. Nhan Hao, Ha Thuy Long, P. Quentin and L. Bonneau, Eur. Phys. J. A **52**, 3 (2016)
[2] J. C. Slater, Phys. Rev. **81**, 385 (1951)
[3] C. Titin-Schnaider and P. Quentin, Phys. Lett. B **49**, 397 (1974).
[4] J. Skalski, Phys. Rev. C **63**, 024312 (2001)
[5] J. Le Bloas, Meng-Hock Koh, P. Quentin, L. Bonneau, and J. I. A. Ithnin, Phys. Rev. C **84**, 014310 (2011)
[6] P. Quentin, L. Bonneau, N. Minkov and D. Samsœn, Int. J. Mod. Phys. E **19**, 611 (2010)
[7] L. Bonneau, J. L. Bloas and P. Quentin, Int. J. Mod. Phys. E **20**, 252 (2011)
[8] L. Bonneau, N. Minkov, Dao Duy Duc, P. Quentin, and J. Bartel, Phys. Rev. C **91**, 054307 (2015)
[9] Meng-Hock Koh, L. Bonneau, P. Quentin, T. V. Nhan Hao, and H. Wagiran, Phys. Rev. C **95**, 014315 (2017)
[10] M. Beiner, H. Flocard, Nguyen Van Giai and P. Quentin, Nucl. Phys. A **238**, 29 (1975)
[11] D. Vautherin, Phys. Rev. C **7**, 296 (1973)
[12] P. Quentin, J. Phys. (France) **33**, 457 (1972)
[13] J. Libert and M. Girod, J.-P. Delaroche, Phys. Rev. C **60**, 054301 (1999)
[14] D. W. L. Sprung, S. G. Lie, M. Vallieres and P. Quentin, Nucl. Phys. A **236**, 37 (1979)
[15] K. J. Pototzky, J. Erler, P.-G. Reinhard and V. O. Nesterenko, Eur. Phys. J. A **46**, 299 (2010)
[16] H. Flocard, P. Quentin, A. K. Kerman and D. Vautherin, Nucl. Phys. A **2013**, 433 (1973)
[17] A. K. Jain, R. K. Sheline, P. C. Sood and Kiran Jain, Rev. Mod. Phys. **62**, 2 (1990)