Variation of fundamental constants and ^{229}Th

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The first excited state of the nucleus ^{229}Th has an exceptionally small excitation energy of 7.8 eV, which is expected to be very sensitive to changes in the fine structure constant α. A small difference in the Coulomb energies of the two states, which both are of the order 10^9 eV, would amplify variations in α into large variations of the transition frequency. Hartree-Fock and Hartree-Fock-Bogoliubov calculations are performed to compute the Coulomb energies of the two states. The kinetic energies are also calculated which reflect a possible variation in the nucleon or quark masses or local Lorentz invariance violation.

Keywords: Nuclear structure; ^{229}Th; Hartree–Fock; Hartree–Fock–Bogoliubov.

1. Introduction

The nucleus ^{229}Th with 90 protons and 139 neutrons occurs in nature as the daughter of the α-decaying ^{233}U and decays itself with a half life of 7880 years, again by α emission. This nucleus has attracted lot of interest as it has the lowest lying excited nuclear state known. Low lying rotational bands with $K^\pi = 5/2^+$ and $3/2^+$ can be identified, with band heads that according to recent measurements differ in energy by only about 7.8(5) eV[1]. After discussing the Hellmann–Feynman theorem for energy density functional theory two successful functionals with and without pairing are used to study ^{229}Th. For more information and details see Ref. 2 on which this contribution is based.

2. Hellmann–Feynman Theorem Revisited

As the models used are based on density-matrix functionals this section shows that the Hellmann–Feynman theorem[3] holds also for all stationary solutions in approximate schemes, provided they are variational.

Let $\mathcal{E}(\mathbf{c}, \mathbf{x})$ be the energy of a physical system that depends on external parameters $\mathbf{c}$ and on a set of variational parameters $\mathbf{x} = \{x_1, x_2, \cdots\}$ which characterize

the state of the system. $\mathbf{x}$ may also represent a set of functions in which case partial derivatives are replaced by functional derivatives.

For example, in the Hartree–Fock approximation $\mathbf{x}$ would be the set of occupied single-particle states that form a Slater determinant. In an energy density functional $\mathbf{x}$ could be the local density $\rho(\vec{r})$, and so on.

Steady state solutions $\mathbf{x}^{(n)}(\mathbf{c}),\ n = 0, 1, 2, \dots$ are obtained by the condition

$$0 = \frac{\partial \mathcal{E}}{\partial x_k}(\mathbf{c}, \mathbf{x}) \ . \tag{1}$$

At the stationary points the energy assumes the values

$$E_n(\mathbf{c}) = \mathcal{E}(\mathbf{c}, \mathbf{x}^{(n)}(\mathbf{c})), \quad n = 0, 1, 2, \dots \ . \tag{2}$$

Both, the energies and the parameters $\mathbf{x}^{(n)}(\mathbf{c})$ characterizing the stationary states depend on the constants $\mathbf{c}$. In the ground state given by $\mathbf{x}^{(0)}$ the energy $\mathcal{E}(\mathbf{c}, \mathbf{x})$ is in an absolute minimum with respect to variations in $\mathbf{x}$, while the other possible solutions $\mathbf{x}^{(n)}, n \neq 0$, represent saddle points.

The derivative w.r.t. an external parameter c_i at the stationary points leads to

$$\frac{\partial}{\partial c_i} E_n(\mathbf{c}) = \frac{\partial \mathcal{E}}{\partial c_i}\big(\mathbf{c}, \mathbf{x}^{(n)}(\mathbf{c})\big) \ + \ \sum_k \frac{\partial \mathcal{E}}{\partial x_k}\big(\mathbf{c}, \mathbf{x}^{(n)}(\mathbf{c})\big) \ \frac{\partial x_k^{(n)}}{\partial c_i}(\mathbf{c}) \ . \tag{3}$$

Due to the stationarity condition (1) the second part on the r.h.s. vanishes so that one obtains for stationary solutions the generalized Hellmann–Feynman theorem:

$$\frac{\partial}{\partial c_i} \ E_n(\mathbf{c}) = \frac{\partial \mathcal{E}}{\partial c_i}\big(\mathbf{c}, \mathbf{x}^{(n)}(\mathbf{c})\big) \ . \tag{4}$$

The derivative of the energy at the stationary solutions is just the partial derivative of the energy functional with respect to the external parameter, calculated at the solution $\mathbf{x}^{(n)}(\mathbf{c})$ for the stationary states.

3. Models

This section discusses briefly the models underlying the numerical calculations: Hartee–Fock with energy density functionals and inclusion of pairing correlations.

3.1. *Hartree–Fock with density-matrix functionals*

It has turned out that an ansatz for the energy as functional of the one-body density-matrix $\hat{\rho}$, as originally proposed by Skyrme for the non-relativistic nuclear physics or by Kohn and Sham[4] for the atomic case, is very successful in describing ground state properties. However, not all of the information residing in the one-body density-matrix $\hat{\rho}$ is used. Usually one uses the local proton and neutron density $\rho_p(\vec{r}), \rho_n(\vec{r})$, kinetic energy densities $\tau_p(\vec{r}), \tau_n(\vec{r})$, current densities $\vec{j}(\vec{r})$, etc.

$$\mathcal{E}_{\mathrm{DF}}[\mathbf{c}, \hat{\rho}] = \mathcal{E}_{\mathrm{DF}}(\mathbf{c}, \rho_p(\vec{r}), \rho_n(\vec{r}), \tau_p(\vec{r}), \tau_n(\vec{r}), \vec{j}(\vec{r}), \dots) \tag{5}$$

The energy functional $\mathcal{E}_{\rm DF}[\,\mathbf{c},\hat{\rho}\,]$ contains parameters, $\mathbf{c}$, which are adjusted by fitting observables to nuclear data. In order to keep densities and currents of the fermions consistent they are expressed in terms of the single-particle states $\big|\,\phi_\nu\,\big\rangle = a^\dagger_\nu\big|\,\emptyset\,\big\rangle$ that represent the occupied states of a single Slater determinant and are eigenstates of the mean field Hamiltonian $\hat{h}_{\rm MF}[\hat{\rho}]$.

The stationarity conditions (1) lead to the self-consistent mean-field equations

$$\hat{h}_{\rm MF}[\hat{\rho}]\;\hat{\rho} = \hat{\rho}\;\hat{h}_{\rm MF}[\hat{\rho}] \quad \text{with} \quad \hat{h}_{\rm MF}[\,\hat{\rho}\,] = \frac{\delta}{\delta\hat{\rho}}\,\mathcal{E}_{\rm DF}[\,\mathbf{c},\hat{\rho}\,] \tag{6}$$

and $\hat{\rho} = \sum_{occupied}\big|\,\phi_\nu\,\big\rangle\big\langle\,\phi_\nu\,\big|$.

Because the self-consistent solution is obtained by searching for solutions of the stationarity conditions (1) the Hellmann–Feynman theorem (4) is fulfilled, even if one cannot refer to a microscopic Hamiltonian and a many-body state anymore.

One should note that it is not mandatory that the single-particle states $\big|\,\phi_\nu\,\big\rangle$ with lowest single-particle energies are occupied. Any combination of occupied states leads to a stationary solution fulfilling Eq. (6).

3.2. *Hartree–Fock–Bogoliubov*

Pairing correlations in the many-body state can be incorporated by fermonic Bogoliubov quasi-particles created by $\alpha^\dagger_\nu = v_\nu a^\dagger_\nu - u_\nu a_{\bar\nu}$ and $\alpha^\dagger_{\bar\nu} = v_\nu a^\dagger_{\bar\nu} + u_\nu a_\nu$ as linear combinations of the creation and annihilation operators, $a^\dagger_\nu, a_{\bar\nu}$, of the eigenstates of the mean-field Hamiltonian (u_ν, v_ν are real and $u^2_\nu + v^2_\nu = 1$). The pairing partner states ν and $\bar\nu$ are usually mutually time-reversed states.

In terms of the canonical single-particle states the many-body trial state is expressed as

$$\big|\,\Psi_{\rm HFB}\,\big\rangle = a^\dagger_\mu \prod_\nu \Big(\sqrt{1-v^2_\nu} + v_\nu\; a^\dagger_\nu a^\dagger_{\bar\nu}\Big)\;\big|\,\emptyset\,\big\rangle\;, \tag{7}$$

where μ denotes the unpaired (blocked) state and ν runs over all other paired states. Besides the variational parameters residing in the operators $a^\dagger_\nu$ that create eigenstates of the mean-field Hamiltonian the energy depends now also on the variational parameters v_ν.

As the trial state (7) has no sharp particle number the energy functional has to be augmented by a constraint on the mean proton number $\mathcal{Z}$ and the mean neutron number $\mathcal{N}$.

$$\mathcal{E}_{\rm HFB} = \mathcal{E} - \lambda_p\mathcal{Z} - \lambda_n\mathcal{N}\;. \tag{8}$$

The proton and neutron chemical potentials, λ_p and λ_n, which determine the mean proton and neutron number, have to be regarded as members of the set $\boldsymbol{c}$ of external parameters. The additional constraints do not alter the arguments leading to the Hellmann–Feynman theorem, thus it is also valid in the HFB case.

Introducing a generalized density matrix $\widehat{\mathcal{R}}$, which contains the normal one-body density, $\hat{\rho}$, and the abnormal one, $\hat{\kappa}$, the stationarity condition leads to

$$\widehat{\mathcal{H}}_{\rm MF}[\widehat{\mathcal{R}}]\;\widehat{\mathcal{R}} = \widehat{\mathcal{R}}\,\widehat{\mathcal{H}}_{\rm MF}[\widehat{\mathcal{R}}] \quad \text{with} \quad \widehat{\mathcal{H}}_{\rm MF}[\widehat{\mathcal{R}}] = \frac{\delta}{\delta\widehat{\mathcal{R}}}\,\mathcal{E}_{\rm HFB}\big[\boldsymbol{c},\widehat{\mathcal{R}}\big] \tag{9}$$

quite in analogy to the mean-field equations (6) without pairing correlations. The pseudo-Hamiltonian $\widehat{\mathcal{H}}_{\rm MF}[\widehat{\mathcal{R}}]$ results again from a variation of the HFB energy functional given in Eq.(8). It contains the mean-field Hamiltonian $\hat{h}_{\rm MF}$ and a pairing part $\hat{\Delta}$. For details and further reading see Refs. 2, 5, 6.

4. Amplification

According to the Hellmann–Feynman theorem a small variation $\delta\alpha$ of the fine structure constant results in a variation of the energy given by

$$\frac{\partial E_n}{\partial\alpha}\delta\alpha = \left(\big\langle\, V_C\,\big\rangle - \big\langle\, T_p\,\big\rangle\frac{\alpha\frac{dm_p}{d\alpha}}{m_p} - \big\langle\, T_n\,\big\rangle\frac{\alpha\frac{dm_n}{d\alpha}}{m_n}\right)\frac{\delta\alpha}{\alpha} \tag{10}$$

with V_c, T_p, T_n denoting the Coulomb, proton kinetic, and neutron kinetic energy, respectively. The possible dependence of the nuclear interaction, e.g. through meson masses, on α is neglected here.

As the temporal variation of the fundamental constant α is at most tiny, it has been proposed to consider transition frequencies $\omega = E_1(\alpha) - E_0(\alpha)$ that can be measured with high precision. The relative variation $\delta\omega/\omega$ is given as

$$\frac{\delta\omega}{\omega} = \frac{1}{\omega}\left(\frac{\partial E_1}{\partial\alpha} - \frac{\partial E_0}{\partial\alpha}\right)\delta\alpha = \frac{1}{\omega}\left(\Delta V_C - \Delta T_p\frac{\alpha\frac{dm_p}{d\alpha}}{m_p} - \Delta T_n\frac{\alpha\frac{dm_n}{d\alpha}}{m_n}\right)\frac{\delta\alpha}{\alpha} = A\;\frac{\delta\alpha}{\alpha}\;, \tag{11}$$

where $\Delta X = \big\langle\, X\,\big\rangle_1 - \big\langle\, X\,\big\rangle_0$ denotes the difference of the expectation values of the operators $X = \{V_C, T_p, T_n\}$ calculated with the two stationary states.

The results discussed in Sec. 5 show that ΔT_n and ΔT_p are of the same order as ΔV_C so that the terms with the proton and neutron mass variations (see Meissner et al.[7]) can be neglected.

Instead of measuring the nuclear transition frequency Berengut et al.[8] proposed to look at atomic transitions that feel the isomeric field shift, which depends on the charge radii and quadruple moments of the two nuclear states.

The theoretical task is to investigate these states carefully in order to get a reliable estimate for their Coulomb and kinetic energies. For the calculation of these quantities in the following section state-of-the-art mean-field models are employed and also the effects of pairing correlations are included.

5. Results for ^{229}Th

Flambaum[9] proposed the transition $3/2^+ \to 5/2^+$ in the nucleus ^{229}Th for a measurement of $\delta\alpha/\alpha$ because the resulting amplification $A = \Delta V_C/\omega$ with $\omega = 7.8$ eV and a possible difference between the Coulomb energies of the two states of order

Table 1. Total, Coulomb, neutron and proton kinetic energies of the ^{229}Th $5/2^+$ ground state calculated with different energy functionals. Differences of these energies between $3/2^+$ first excited state and $5/2^+$ ground state.

	Exp.	SkM*		SIII	
$5/2^+$	Ref. [10]	HF	HFB	HF	HFB
E^{tot} [MeV]	-1748.334	-1739.454	-1747.546	-1741.885	-1748.016
V_C [MeV]		923.927	924.854	912.204	912.216
T_n [MeV]		2785.404	2800.225	2783.593	2794.909
T_p [MeV]		1458.103	1512.705	1442.018	1477.485
$3/2^+ - 5/2^+$	Ref. [1]				
ΔE^{tot}[MeV]	0.000 008	0.619	-0.046	0.141	-0.074
ΔV_C [MeV]		0.451	-0.307	-0.098	0.001
ΔT_n [MeV]		2.570	0.954	-0.728	0.087
ΔT_p [MeV]		0.688	0.233	-0.163	-0.022

MeV could be rather large. As the Coulomb energy cannot be measured it has to be calculated. For that two successful energy functionals, SIII[11] and SkM*[12], are employed.

As can be seen from Table 1, for the energetically lowest Slater determinant with $K^\pi = 5/2^+$ the total HF binding energy agrees with the measured one up to about 9 MeV for the SkM* and up to about 6 MeV for the SIII energy functional. Keeping in mind that no parameters have been adjusted to the specific nucleus considered here it is surprising that these mean-field models can predict the experimental binding energy of 1748.334 MeV with an uncertainty of only about 0.5 %.

By rearranging the occupation of the single-particle states such that the last neutron sits in a $K^\pi = 3/2^+$ state one obtains after minimization of the total energy an excited HF state that is to be regarded as the intrinsic state of the experimentally observed $K^\pi = 3/2^+$ band.

Table 1 shows that the excited states occur at 0.619 MeV for the SkM* and at 0.141 MeV for the SIII density functional. The difference in Coulomb energies ΔV_C amounts to 0.451 MeV for SkM* and to -0.098 MeV for SIII. Without selfconsistently minimizing the energy for the two sets of neutron occupation numbers the Coulomb energies of the two states would be identical because the occupied proton single-particle states were not changed. The Coulomb energy difference comes from the fact that the different occupied last neutron orbits polarize the protons in a slightly different way.

The deviations between the two energy functionals reflect the differences in the structure of the intrinsic states as also seen from the difference in the single-particle states discussed in Ref. 2.

The next step is to include pairing correlations with the Bogoliubov ansatz (7) and do self-consistent HFB calculations based on the SkM* and SIII density-matrix functionals. The two states are generated by self-consistently blocking either the $5/2^+$ or the $3/2^+$ quasiparticle state for pairing and putting in one neutron only.

The agreement of total energy with the experimental one is improved for both functionals with an amazingly small deviation of less than 0.05%. But the Coulomb

energy differences shrink, see Table 1. For the SIII energy functional, only 1 keV remains for ΔV_C. This reduces the amplification factor of Eq. (11) to about 100. For SkM* a larger value of ΔV_C of about 300 keV is obtained due to a larger splitting of the corresponding single-particle orbitals. From this one must conclude that pairing correlations result in states with even more similar charge distributions than in the HF calculation. Therefore, such correlations not only decrease the anticipated amplification factors but also make their determination very uncertain, due to dependence on very detailed properties of the mean-field and pairing effects. As even the sign of the amplification factor is uncertain, much more refined calculations are needed that include coupling to low-lying core excitations and projection on eigenstates with good total angular momentum and particle number. Before being able to provide reasonably trustable numbers how the transition energy varies as function of the fine structure constant α one has to make sure that the model reproduces the three low lying rotational $K^\pi = 5/2^+, 3/2^+, 5/2^-$ bands up to $J \approx 9/2$ and the known transitions within the bands and between them. This would provide more confidence in the quality of the many-body states and their Coulomb energy.

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References

1. B. R. Beck, *et al.*, Phys. Rev. Lett. **98** 142501 (2007) and LLNL-PROC-415170 (2009). Xinxin Zhao, *et al.*, Phys. Rev. Lett. 109, 160801 (2012). E. Peik, K. Zimmermann, Phys. Rev. Lett. **111**, 018901 (2013). J. Jeet, *et al.*, Phys. Rev. Lett. **114**, 253001.
2. E. Litvinova, H. Feldmeier, J. Dobaczewski, and V. V. Flambaum, Phys. Rev. C **79**, 064303 (2009).
3. H. Hellmann, Z. Physik **85**, 180 (1933).
   R. P. Feynman, Phys. Rev. **56**, 340 (1933).
4. W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
5. J. Dobaczewski, W. Nazarewicz, T. R. Werner, J. F. Berger, C. R. Chinn, and J. Dechargé, Phys. Rev. C **53**, 2809 (2006).
6. S. Krewald, V. B. Soubbotin, V. I. Tselyaev, and X. Viñas, Phys. Rev. C **74**, 064310 (2006).
7. U.-G. Meißner, A. M. Rakhimov, A. Wirzba, and U. T. Yakhshiev, Eur. Phys. J. A **31**, 357 (2007).
8. J. C. Berengut, V. A. Dzuba, V. V. Flambaum, and S. G. Porsev, Phys. Rev. Lett **102**, 210801 (2009).
9. V. V. Flambaum, Phys. Rev. Lett. **97**, 092502 (2006).
10. G. Audi, A. H. Wapstra, and C. Thibault, Nuc. Phys. **A 729**, 337 (2003).
11. M. Beiner, H. Flocard, N. Van Giai, P. Quentin, Nucl. Phys. **A238**, 29 (1975).
12. J. Bartel, P. Quentin, M. Brack, C. Guet, and H.-B. Håkansson, Nucl. Phys. **A386**, 79 (1982).