Shell model and Hartree-Fock calculations of electron scattering form factors for ^{25}Mg nucleus

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Abstract

Shell model and Hartree-Fock calculations have been adopted to study the elastic and inelastic electron scattering form factors for ^{25}Mg nucleus. The wave functions for this nucleus have been utilized from the shell model using USDA two-body effective interaction for this nucleus with the *sd* shell model space. On the other hand, the SkXcsb Skyrme parameterization has been used within the Hartree-Fock method to get the single-particle potential which is used to calculate the single-particle matrix elements. The calculated form factors have been compared with available experimental data.

Key words

Skyrme Hartree-Fock, shell model, electron scattering, ^{25}Mg nucleus.

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حسابات نموذج القشرة و هارتري- فوك لعوامل تشكل للاستطارة الالكترونية لنواة ^{25}Mg

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الخلاصة

حسابات نموذج القشرة وهارتري - فوك اعتمدت لدراسة عوامل التشكل المرنة والغير المرنة لنواة ^{25}Mg. تم الحصول على الدوال الموجية لهذه النواة باستخدام نموذج القشرة والتفاعل المؤثر للجسيمين نوع USDA مع فضاء نموذج القشرة *sd*. من جهة اخرى، سكريم باراميتر من نوع SkXcsb استخدم مع طريقة هاريتري-فوك للحصول على جهد الجسيم الواحد والذي يستخدم لحساب عناصر مصفوفة الجسيم الواحد. حسابات عوامل التشكل قورنت مع النتائج العملية المتاحة.

Introduction

The Hartree-Fock (HF) method has provided the most reliable and least arbitrary tool for studying the nuclear structure. In a harmonic oscillator (HO) shell-model basis the HF method takes into account the smearing of the orbit occupation probabilities far from the Fermi surface. The diffuseness problem of the orbit occupation probabilities near the Fermi surface when using large-basis shell-model calculations leads to develop an effective approach. In this approach, the aspects HF method combine with the complex configuration mixing encountered in the shell-model calculations.

The interaction between nucleons and accurate treatment of the many-body problem in atomic nuclei gives enough information on the residual interactions as well as an average potential for the shell model. The residual interaction, interaction between the valence nucleons, plays an

important role in accounting for many nuclear properties such as nuclear densities and form factors (longitudinal and transverse). It is usually represented by a set of two-body matrix elements, either directly determined from a best fit to experimental energy levels, or derived from a phenomenological potential. The best-studied regions and a comprehensive review of shell model interactions in different model spaces is given by Brown et al. [1].

The HF method can be used to obtain the single-particle wave functions and the average density. The quantitative success of HF calculations is, however, limited by the lack of knowledge of the exact nucleon-nucleon interaction and its renormalisation in finite nuclei. The actual nuclear interactions are approximated by an average one-particle potential. The evolution of this one-body potential is more accurately and fundamentally taken into account with the self-consistent mean-field (SCMF), which is usually treated separately from the valence interaction. The SCMF can be achieved by using HF approach with Skyrme-type interactions [2].

Vautherin and Brink [3] have proposed the Skyrme interaction, which has been the most popular interaction used within the HF calculations of nuclear landscape. With a proper parameterization, Skyrme interaction gives satisfactory results both for the saturation properties of nuclear matter and the properties of the giant resonances. The advantage provided by this interactions over other interactions that have an explicit finite range, is that the computations for the HF potentials and two-body matrix elements can be carried out relatively fast.

The *sd* model space includes the $1s_{1/2}$, $0d_{5/2}$ and $0d_{3/2}$ valence orbits. The renormalized G matrix for the *sd*-shell was developed in the mid 1960's by Kuo and Brown [4, 5, 6]. These G matrix interactions give reasonable agreement with the experimental A = 18and A = 38 spectra. When the G matrix is used to calculate the spectra for the *sd*-shell nuclei with more than two particles or holes, the agreement with the experimental energy spectra deteriorates rapidly as the number of particles or holes is increased [7]. The USDA effective two body matrix elements (ETBME) [8] has been used in this model space to evaluate the one body density matrix element (OBDM).

The single-particle matrix elements, calculations may be done using different types of single particle potential such as the HO, Wood-Saxon (WS) and the Skyrme potentials. In order to determine the sensitivity of transverse form factor to the nuclear potential, the results of the spherical HF calculation can be carried out for a given nucleus using Skyrme potential with different parameterizations for the ground and excited states of its occupied orbit. The HF method does not include the deformation correlations since they will be part of the SM aspect [9]. The next step is to constructing the resultant diagonalized Hamiltonian matrices of all possible Slater determinants for the chosen energy operator in the chosen closely spaced valence orbitals to obtain the wave functions and correlation energies.

In the present work, elastic and inelastic electron scattering form factors for ^{25}Mg nucleus will be calculated using the *sd*-model space and SkXcsb [10] Skyrme parameterization within HF method. This parameterization gives the rms charge radius equal to 3.0059 fm for ^{25}Mg which is in agreement with the experimental value 3.0284 fm [11]. Also, the calculated binding energy is

199.225 MeV which is in good agreement with the experimental value 205.6 MeV [12]. The measured dipole moment equal to -0.914 nm which is reasonably close to the experimental value -0.85545 (8) nm [13].

Theory

Skyrme interaction V_{Skyrme} can be written as the sum of two- and three-body parts [13]. The Skyrme forces with the three-body term replaced by a density-dependent two-body term, which are unified in a single form as an extended Skyrme force [14]:

$$\hat{V}_{Skyrme} = \hat{V}^m + \hat{V}^{LS} + \hat{V}^t, \quad (1)$$

where,

$$\hat{V}^m = t_0\left(1 + x_0\hat{P}_\sigma\right)\delta_{12} + \frac{t_3}{6}\left(1 + x_3\hat{P}_\sigma\right)\rho^\alpha(r_1)\delta_{12}$$
$$+\frac{t_1}{2}\left(1 + x_1\hat{P}_\sigma\right)\left(\delta_{12}\hat{k}^2 + \hat{k}'^2\delta_{12}\right) + t_2\left(1 + x_2\hat{P}_\sigma\right)\hat{k}'\delta_{12}\hat{k}$$

$$\hat{V}^{LS} = it_4(\hat{\sigma}_1 + \hat{\sigma}_1).\hat{k}' \times \delta_{12}\hat{k}$$
$$\hat{V}^t = \frac{t_0}{2}\{\left(3\left(\hat{\sigma}_1.\hat{k}'\right)\left(\hat{\sigma}_2.\hat{k}'\right) - (\hat{\sigma}_1.\hat{\sigma}_2)\hat{k}'^2\right)\delta_{12}$$
$$+\delta_{12}\left(3\left(\hat{\sigma}_1.\hat{k}\right)\left(\hat{\sigma}_2.\hat{k}\right) - (\hat{\sigma}_1.\hat{\sigma}_2)\hat{k}^2\right)\}$$
$$+t_0\left(3\left(\hat{\sigma}_1.\hat{k}'\right)\delta_{12}\left(\hat{\sigma}_2.\hat{k}\right) - (\hat{\sigma}_1.\hat{\sigma}_2)\hat{k}'.\delta_{12}\hat{k}\right)$$

where $\delta_{12} = \delta(r_1 - r_2)$, and the three-body part by

$$V_{123}^{(3)} = t_3\delta_{12}\delta_{13} \quad (2)$$

The $\hat{k}$ and $\hat{k}'$ are relative momentum operators which are defined as

$$\hat{k} = \frac{1}{2i}\left(\vec{\nabla}_1 - \vec{\nabla}_2\right), \qquad \hat{k}' = -\frac{1}{2i}\left(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2\right) \quad (3)$$

with the $\hat{k}'$ acting to the left. The tensor force $\hat{V}^t$ is usually neglected.The Skyrme parameterizations are usually determine by fitting the experimental ground state properties of finite nuclei within HF calculation.

The total binding energy of a nucleus, according to the Skyrme-Hartree-Fock (SHF) method is obtained self-consistently from the energy functional [2]

$$E = E_{kin}(\tau) + E_{Skyrme}(\rho, \tau, J) + E_{Coul}\left(\rho_p\right) + E_{pair} - E_{cm}\ , \quad (4)$$

where the kinetic energy is given by:

$$E_{kin} = \int d^3r \left[\frac{\hbar^2}{2m_p}\tau_p + \frac{\hbar^2}{2m_n}\tau_n\right] \quad (5)$$

The Coulomb interaction is a well-known piece of the nuclear interaction. However, its infinite range makes it very time consuming to evaluate the exchange part exactly and it is unwise to spend most of the computing time on a small contribution. Therefore the Coulomb-exchange part is treated in the so-called Slater approximation and one can obtain for the Coulomb energy E_{Coul} [14]

$$E_{kin} = \frac{e^2}{2}\int_0^\infty \int_0^\infty \frac{\rho_p(r)\rho_p(r')}{|r - r'|} d^3r d^3r'$$
$$+ E_{Coul,Exch} \quad (6)$$

$$E_{Coul,Exch} = -\frac{3}{4}e^2\left[\frac{3}{\pi}\right]^{1/3}\int_0^{\infty}\rho_p(r)^{3/4}d^3r \quad (7)$$

The Coulomb part of the energy functional depends only on the charge density of the nucleus; however in many cases an approximation is made that replaces the charge density with the proton density. The E_{Skyrme} is the energy functional of the Skyrme force and given by:

$$E_{Skyrme} = \int d^3r\left[\frac{b_0}{2}\rho^2 - \frac{b_0'}{2}\sum_q\rho_q^2 + \frac{b_3}{3}\rho^{\alpha+2} - \frac{b_3'}{3}\rho^{\alpha}\sum_q\rho_q^2 + b_1\rho\tau - b_1'\sum_q\rho_q\tau_q - \frac{b_2}{2}\rho\Delta\rho + \frac{b_2'}{2}\sum_q\rho_q\Delta\rho_q - b_4\rho\nabla.J - b_4'\sum_q\rho_q\nabla.J_q\right] \quad (8)$$

The value of $q \in \{\mathrm{p},\mathrm{n}\}$, ρ is the total density. Depending on the value of q the ρ_q, τ_q and J_q are the local densities, the kinetic energy densities and the spin-orbit current densities respectively for the protons and the neutrons they are given by

$$\rho_q = \sum_{k\in\Omega_q} v_k^2\,|\psi_k|^2, \quad \tau_q = \sum_{k\in\Omega_q} v_k^2\,\left|\vec{\nabla}\psi_k\right|^2,$$
$$J_q = -\frac{i}{2}\sum_{k\in\Omega_q} v_k^2\left[\psi_k^{\dagger}\vec{\nabla}\times\hat{\sigma}\psi_k - \left(\vec{\nabla}\times\hat{\sigma}\psi_k\right)^{\dagger}\psi_k\right]. \quad (9)$$

where ψ_k is the single-particle wave function and υ_k^2 is the occupation probability calculated taking the residual pairing interaction into account. The parameters b_i and b_i' used in E_{Skyrme} equation were chosen to give a compact formulation of the energy functional, the corresponding mean-field Hamiltonian and the residual interaction [2]. The term E_{pair} is the pairing energy functional of the form:

$$E_{pair} = \sum_{q\in p,n}\frac{V_q}{4}\int_0^{\infty}\left[1 - \left(\frac{\rho(r)}{\rho_c}\right)^{\gamma}\right]\bar{\rho}_q(r)^2dr \quad (10)$$

where $\bar{\rho}_q$ is the pairing density V_q, γ and ρ_c are parameters that are phenomenologically adjusted. The kinetic part of the total energy E is not exactly equal to $\frac{\sum_i^A \hat{p}_i^2}{2m}$ because the kinetic energy of the center of mass E_{cm} must be subtracted:

$$T = \sum_i^A\frac{\hat{p}_i^2}{2m} - \frac{\left(\sum_i^A\hat{p}_i\right)^2}{2mA} = \frac{1}{2m}\left(1-\frac{1}{A}\right)\sum_i^A\hat{p}_i^2 - \frac{1}{2mA}\sum_{i\neq j}^A\hat{p}_i\cdot\hat{p}_j \quad (11)$$

The first term on the second line is again a one-body kinetic term with a corrected mass$' = m\frac{A}{A-1}$.

The electron scattering form factor involving angular momentum J and momentum transfer q, between initial and final nuclear shell model states of spin $J_{i,f}$ are [15]

$$\left|F_J^{\eta}(q)\right|^2 = \frac{4\pi}{Z^2(2J_i+1)}\left|\sum_{T=0,1}\begin{pmatrix} T_f & T & T_i \\ -T_Z & 0 & T_Z\end{pmatrix}\langle J_f T_f\|\|\hat{T}^{\eta}_{JT}\|\|J_i T_i\rangle\right|^2 \times \left|F_{f.s}(q)\right|^2 \times \left|F_{f.s}(q)\right|^2 \quad (12)$$

where η selecting the longitudinal (L), transverse electric (E) and transverse magmatic (M) form factors, respectively $F_{c.m}(q) = e^{q^2b^2/4A}$ is the correction for the lack of translational invariance in the shell model (center-of-mass correction) and $F_{f.s}(q) = e^{-0.43q^2/A}$is the nucleon finite size (fs) form factor while $T_Z$is the z-component of the isospin for the initial andfinal states and is given by $T_Z = (Z-N)/2$.

The reduced matrix element of the electron scattering operator $\hat{T}_{J,t_z}$expressed as the sum of the product of OBDM $X^J_{J_fJ_i}(t_z, j_i, j_f)$ and the single-particle matrix elements, and is given by

$$\langle J_f\|\hat{T}_{J,t_z}\|J_i\rangle = \sum_{j_i j_f} X^J_{J_fJ_i}(t_z, j_i, j_f)\langle j_f\|\hat{T}_{J,t_z}\|j_i\rangle \quad (13)$$

where j_i and j_f label single-particle states for the shell model space, and $t_z = 1/2$ for a proton and $t_z = -1/2$ for a neutron. The multipolemagnetic operator in terms of single nucleon Pauli-isospint_z is

$$\hat{T}^M_{JM,t_z}(q) = \int d\vec{r}\left\{\vec{M}_{JLM}(q,\vec{r})\cdot\vec{J}_c(\vec{r},t_z) + q\left[\frac{1}{q}\vec{\nabla}\times\vec{M}_{JLM}(q,\vec{r})\cdot\vec{\mu}(\vec{r},t_z)\right]\right\} \quad (14)$$

where$\vec{J}_c(\vec{r},t_z)$ is the convection current coming from the intrinsic magnetic moments of target nucleus, and$\vec{\mu}(\vec{r},t_z)$ is the magnetization density operator. The vector function $\vec{M}_{JLM}(q.\vec{r})$ is expressed as,

$$\vec{M}_{JLM}(q.\vec{r}) = j_L(qr)\vec{Y}_{JLM}(\Omega_r) \quad (15)$$

where $\vec{Y}_{JLM}(\Omega_r)$ is the vector spherical harmonics, defined as:

$$\vec{Y}_{JLM}(\Omega_r) = \sum_{M_L q}\langle LM_L 1q|JM\rangle\,\vec{Y}_{JLM}(\theta,\varphi)\hat{e}_k \quad (16)$$

with $\hat{e}_{\pm1} = \frac{1}{\sqrt{2}}(\hat{x}\pm i\hat{y})$ and $\hat{e}_0 = \hat{z}$ are the basis vector.

The transition probability is defined at the photon point; with momentum transfer $q = k = E_x/\hbar c$ (E_x is the excitation energy). Since the center of mass and finite nucleon size correction factors are nearly equal to one for this value of q, the reduced transition probability $B(\eta J)$ is written in terms of the form factor in this limit as [16]:

$$B(\eta J) = \frac{[(2J+1)!!]^2Z^2e^2}{4\pi k^{2J}}\left|F_J^{\eta}(k)\right|^2 \quad (17)$$

Results and discussion

In the present work, the SM and HF method have been applied to investigate elastic and inelastic of ^{25}Mg nucleus. The *sd* shell model space has been used for this purpose with suitable Hamiltonian to provide the realistic wave functions. The single-particle matrix elements have been calculated with SHF potential with different parameterizations. The OBDM elements have been calculated using the NuShellX@MSU [17] shell model code which uses proton-neutron formalism. The OBDMs are then used to calculate the magnetic matrix element MJ operator.

According to the *sd* shell model space, ^{25}Mg nucleus is considered as an inert ^{16}O core $(1s)^4$ $(1p)^{12}$ and nine valence nucleons distributed over the active

shells $1d_{5/2}$, $2s_{1/2}$ and $1d_{3/2}$. The USDA Hamiltonian [7] has been used to provided realistic *sd*-shell ($1d_{5/2}$, $1d_{3/2}$, $2s_{1/2}$) wave functions for the states $5/2^+$ ground state (GS), $7/2_1^+$ 1.612 MeV and $9/2_1^+$ 3.405 MeV.

Fig. 1a shows the calculated total contribution of M1, M3, and M5 multipoles for the USDA effective interaction for the $5/2^+$ GS of ^{25}Mg nucleus using SkXcsb parameterization along with experimental data [18]. It is clear that the total transverse form factor is in good agreement with the experimental data. The contribution to the total form factor for M1 is dominant at momentum transfer below q=1.5 fm^{-1}. For high momentum transfer up to q=1.5 fm^{-1} the contribution of M5 is very large. Therefore one can see that the M5 is more sensitive to the experimental data and describes it very well in the momentum transfer range from 1 to 3fm^{-1}. The total transverse magnetic form factor is also calculated with different Skyrme parameterizations and plotted together with the conventional HO potential in comparison with experimental data in Fig.1b. Additionally one can see that the total transverse magnetic form factor curve calculated with SkXcsb parameterization is the nearest curve to the experimental data than the other parameterizations and HO potential curves.

The total (a) elastic longitudinal form factor and its contributions C0, C2 and C4 for the ^{25}Mg are calculated using SkXcsb parameterization and illustrated in Fig. 2a. It is noticeable that the C0 have two diffraction minima with approximately the location within q=1.4 fm^{-1} and q=2.4 fm^{-1} respectively. The C2 contribution is dominated at low and high momentum transfer, while the C4 has a small contribution to the total at the medium q around 2 fm^{-1}. The transvers electric form factors E2 and E4 with their summation are shown in Fig. 2b. The main contribution to the E2+E4 curve is belonging to E2 multipoles.

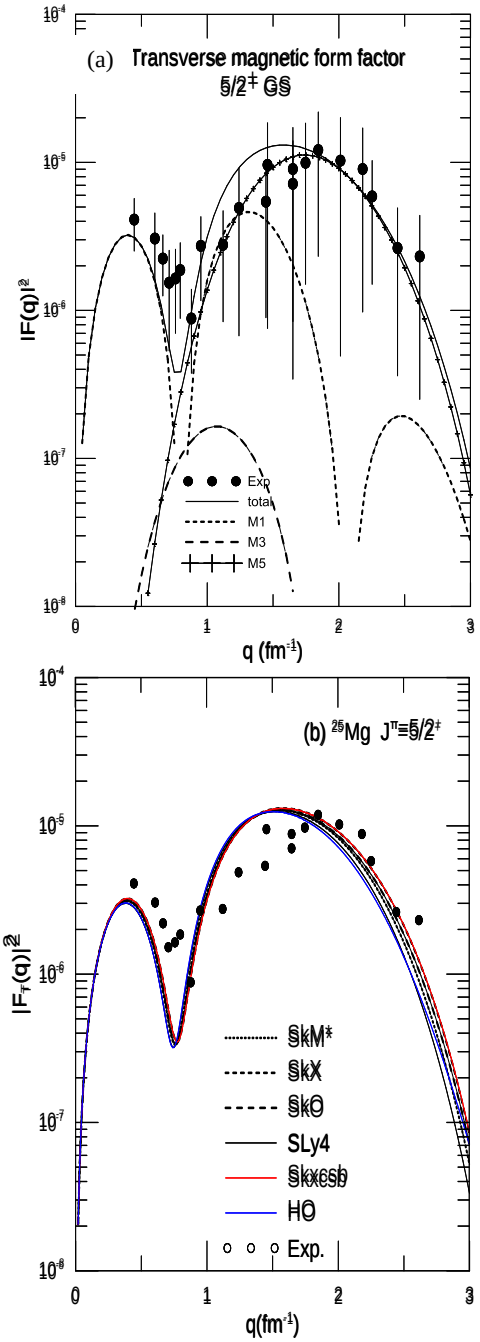

Fig. 1: The total theoretical magnetic form factor for GS of ^{25}Mg $J^\pi=5/2^+$ nuclei compared with experimental data [18] (a) using SkXcsb parameterization (b) using different Skyrme parameterizations and HO.

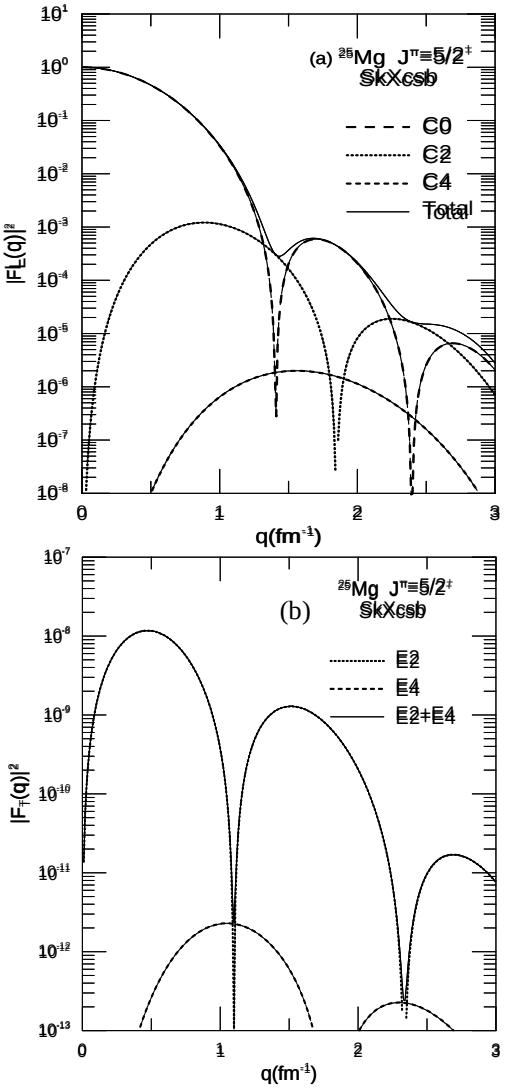

Fig. 2: Theoretical longitudinal (a) and transverse (b) form factors for ^{25}Mg in $5/2^{+}$ state using SkXcsb parameterization.

The total transvers form factor and its contributions M1, E2, M3, E4 and M5 for the first $7/2_1^{+}$excited state 1.612 MeV of ^{25}Mg nucleus are calculated and presented in Fig. 3. The results of the total transverse form factor calculated using SkXcsb parameterization are in reasonable agreement comparing with the experimental data [19]. The main contribution in most of the regions of momentum transfer comes from M1 and M5, where M1 has the dominant contribution in the region between 0 and 1.2 fm^{-1} and M5 has the main contribution in the range of momentum transfer from 0.5 to 3 fm^{-1}. M1 and E4 have small contribution to the total transverse form factor in the range 1.2 to 2 fm^{-1} of momentum transfer.

The calculation of the total contribution of E2, M3, E4 and M5 multipoles for the exited $9/2_1^{+}$ state with an excitation energy of 3.405 MeV in the ^{25}Mg nucleus using the SkXcsb parameterization was shown Fig. 4. The total form factor was compared with the available experimental data [19]. Inspection of the total transverse curve reveals that the shape of the calculated form factors is in qualitative agreement with the experimental data. The M5 component of the transverse scattering dominates at high momentum transfer for 1.5 to 3 fm^{-1}. For low momentum transfer below 0.5 fm^{-1} the E2 component is dominant. While M3 component dominant in the medium momentum transfer from 1.75 to 1.5 fm^{-1}.

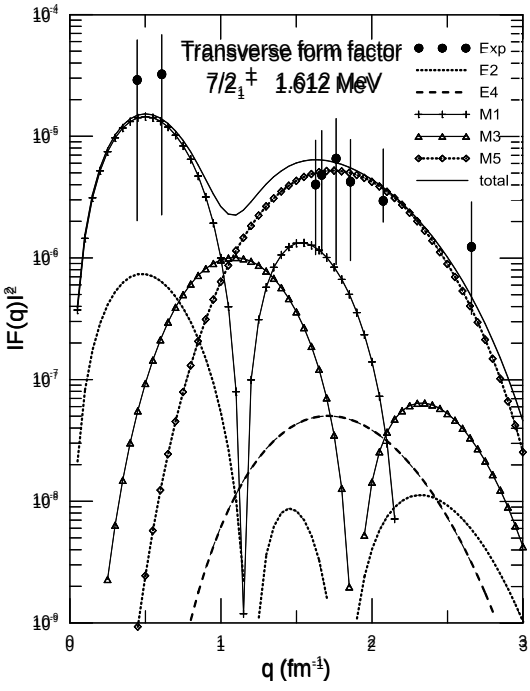

Fig. 3: Theoretical longitudinal and transverse form factors for $7/2_1^{+}$, 1.612 MeV using SkXcsb parameterization compared with experimental data [19].

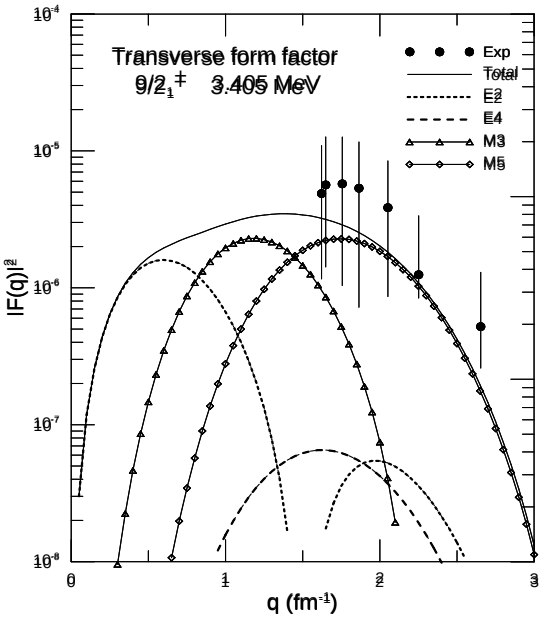

Fig. 4: Theoretical longitudinal and transverse form factors for $9/2_1^+$, 3.405 MeV using SkXcsb parameterization compared with experimental data [19].

The energy levels and reduced transition probabilities for low-lying positive parity states have been calculated in the *sd* model space with USDA effective interaction and SkXcsb parameterization and were shown in Fig.5 compares the calculated energy levels with the experimental energy spectrum. Although precise agreement between the theoretical and experimental schemes is not carry out very successfully, it is clear that the shell model calculations with SkXcsb parameterization are able to predict for the high density of positive parity states. The calculated values for all transitions in ^{25}Mg, which are considered in the present work have been tabulated in Table 1.

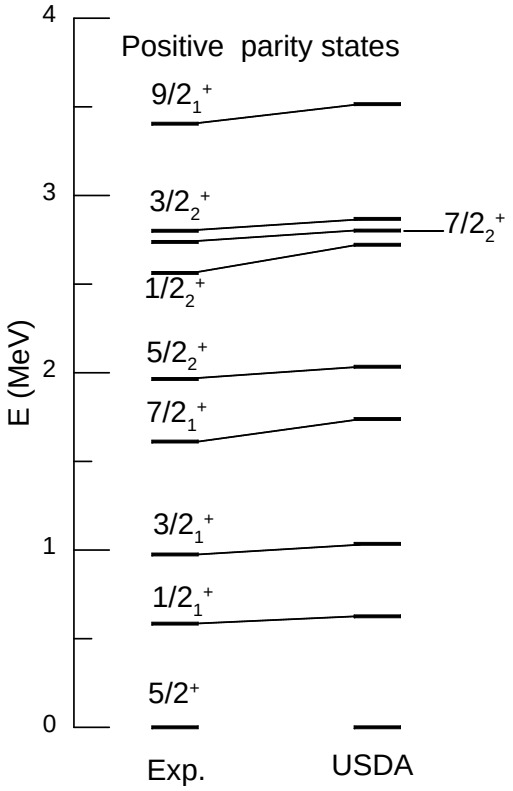

Fig. 5: Energy levels for the positive parity states of ^{25}Mg nucleus compared with experimental data taken from [20].

Table 1: Excitation energies, reduced transition probabilities for the positive parity states of ^{25}Mg nucleus.

	E_x (MeV)			$B(EJ)$ (e^2 fm^4)	
$J_i^\pi \rightarrow J_f^\pi$	Exp.[18]	Theory	*wL*	Exp.[18]	Theory
5/2+ → 7/2+	0.0	0.0	E2	104.21(6)	122.3
1/2+ → 3/2+	1.5540	1.675	E2	52.11(6)	41.86

Conclusions

In studying the extent of applicability of the selected Skyrme parameterizations to the ^{25}Mg nucleus, it can be noticed a good general agreement, which was found in extensive comparisons of measured transverse magnetic form factors with the calculated results using the Skyrme parameterization. The results of this

study serve to provide a better understanding of the nuclear structures of the investigated target nucleus and may be considered as an indication to the validity of the SM+HF model in this nucleus. The extent of the agreement is, in most cases, significantly further improved by constraining the HF calculations to use shell-model occupancies. The agreement observed revealed the adequacy of the HF mean-field approximation for this nucleus.

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