Investigation of the Nuclear Structure of Some Ni and Zn Isotopes with Skyrme-Hartree-Fock Interaction

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Abstract: The inelastic C2 form factors and the charge density distribution (CDD) for 58,60,62Ni and 64,66,68Zn nuclei has been investigated by employing the Skyrme-Hartree-Fock method with (Sk35-Skzs*) parametrization. The inelastic C2 form factor is calculated by using the shape of Tassie and Bohr-Mottelson models with appropriate proton and neutron effective charges to account for the core-polarization effects contribution. The comparison of the predicted theoretical values was conducted with the available measured data for C2 and CDD form factors and showed very good agreement.

Keywords: Charge density distribution (CDD), C2 form factors, Skyrme-Hartree-Fock, Shell model

Introduction: In order to know the nuclear forces and the laws that govern the interactions between elementary particles, the only possible method is that of scattering a diversity of particles by a diversity of targets. There will be three types of scattering experiments, the first one is that the incident particle has no atomic force, but interacts with the nucleus via only electromagnetic interaction, such as speedy electron scattering. The data on charge and current densities can be given. Secondly, the scattering of neutral electrical particles, for example neutrons that only contribute to nuclear fields. Lastly, the scattering of particles charged by electricity, oftentimes experiences strong nuclear contact such as proton and alpha particle. The scattering of nuclear electrons provides the most detailed knowledge about the nuclear size and distribution of charge and offers valuable information about electromagnetic currents within nuclei. Electron scattering can be a good test for calculation because it is sensitive to spatial load dependency and current densities. To explain nuclei using the nuclear shell model, one must understand the effective one- and two-body interactions. Several techniques for calculating the effective interaction for nuclei in the fp-shells have been proposed in the last 30 years. Kuo and Brown proposed the first comprehensive technique in the 1960s, using the Hamada-Johnston potential. In model space calculations, Radhi et al. showed that it is advisable to include CP effect in form-factors for nuclei in the beginning of p-shell and the end of sd-shell. F. A. Majeed et al. demonstrated that form factor calculations based on large-basis of the shell model to study the nuclei in the p, sd and fp shells considering the contribution of high-energy configurations beyond the p, sd and fp shell model space denoted as the core polarization effects. The proton and neutron matter density distribution and their related charge radii along with the ground state form factors have been investigated by Hameed BS for some selected potassium isotopes, their conducted study showed that taking into consideration the core polarization effects along with effective g-factors made remarkable enhancement in their calculations which leads to good agreement with the measured data.

The recent developments with new modern effective interactions designed for fp-shell region are still not universal and need more tuning. The nuclei at the upper limit of the fp-shell region attract attention in recent years due to their importance in
understanding the supernova explosions, therefore this study aimed to investigate the charge density distribution (CDD) and the inelastic C2 form factors for $^{58,60,62}$Ni and $^{64,66,68}$Zn nuclei by employing the Skyrme-Hartree-Fock method with (Sk35-Skzs*) parametrization and comparing he predicted theoretical calculations with the available measured data.

### Theoretical Background

#### Skyrme Effective Interaction

Skyrme presented an effective interaction for HF calculations of nuclei$^{14,15}$. In describing the ground conditions properties of nuclei with approximately ten adjustable parameters, it is the more convenient force used to fit experimental nuclei data such as binding energies and charged radii$^{16}$. The Skyrme forces are zero-range interactions that are composed of a momentum-dependent two-body term and a zero-range three-body term. A density-dependent two-body term can be replaced for the three-body term in the HF calculations. As a result, as an extended Skyrme force$^{17}$, the Skyrme forces are unified in a single form. The interaction between two bodies in Skyrme is written as follows$^{14}$:

\[ \nu_{12} = t_0 (1 + x_0 \delta) \delta(\vec{r}_1 - \vec{r}_2) + \frac{t_1}{2}(1 + x_1 \delta) \hat{\vec{k}} \delta(\vec{r}_1 - \vec{r}_2) + \frac{t_2}{6}(1 + x_2 \delta) \rho^\alpha (\vec{k}) \delta(\vec{r}_1 - \vec{r}_2) + \frac{i}{2}w_0 \hat{\vec{k}} (\hat{\delta}_1 + \hat{\delta}_2) \]

Here $\vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{2}$ and $\alpha$ is the parameters of Skyrme force. The $\vec{k} = (\vec{v}_1 - \vec{v}_2)/2\hat{i}$ and $\hat{\vec{k}} = -\left((\vec{v}_1 - \vec{v}_2)/2\hat{i}\right)$ operators are the relative momentum wave vectors of two nucleons acts to the right and to the left (i.e., the complex conjugate wavefunctions, with coordinate $\vec{r}$ respectively. The terms $t_0$, $t_1$, $t_2$, $x_1$, $x_2$, $x_3$ and $w_0$ are free parameters that describe the strengths of various interaction factors that are fitted to nuclear structure data. $\delta$ is the Pauli matrices, $\delta = \frac{1}{2} (1 + \vec{\delta}_1 \cdot \vec{\delta}_2)$ is operator of spin-exchange, and the Dirac delta function $\delta(\vec{r}_1 - \vec{r}_2)$. In the typical Skyrme–Hartree–Fock (SHF) model, the total energy density of a nucleus is expressed as$^{14}$:

\[ E = E_{\text{kin}} + E_{\text{Sky}} + E_{\text{Coul}} + E_{\text{pair}} - E_{\text{cm}} \]

$E_{\text{kin}}$ is the kinetic energy of the nucleons (proton and neutron) can be calculated using the following formula$^{15}$:

\[ E_{\text{kin}} = \sum_{i=1}^{A} \frac{\hbar^2}{2m_i} \tau_i d^3r \]

$E_{\text{sky}}$ is the energy functional of the Skyrme force and given by$^{15}$,

\[ E_{\text{sky}} = \int d^3r \left[ \frac{b_0}{2} \rho^2 - \frac{b_0}{2} \sum_q \rho_q^2 + \frac{b_3}{3} \rho^{a+2} \right. \\
- \frac{b_3}{3} \rho^a \sum_q \rho_q^2 + b_2 \tau_q \right. \\
- \frac{b_1}{2} \rho \Delta \rho - \frac{b_2}{2} \Delta \rho + b_4 \rho \nabla \cdot J \left. \right. \\
- \hat{\rho} \sum_q \rho_q \nabla \cdot J \left. \right] \]

$\rho_q$ is the local densities for protons and neutrons (depending on the value of $q$). $\rho$ is the total density, $\tau_q$ is the kinetic energy densities for protons and neutrons and $J_q$ is the spin-orbit current density. They are given by these relations$^{15}$:

\[ \rho_q(r) = \sum_{i=\sigma} \psi_i(r, \sigma, q)^* \cdot \psi_i(r, \sigma, q) \]

\[ \tau_q(r) = \sum_{i=\sigma} \left( \psi_i(r, \sigma, q)^* \nabla \psi_i(r, \sigma, q) \right)^2 \]

\[ J_q(r) = -i \sum_{i=\sigma} \psi_i(r, \sigma, q)^* \nabla \psi_i(r, \sigma, q) \]

The below are the parameters in the energy Skyrme equation$^{15,16}$:

\[ b_0 = t_0 (1 + \frac{1}{2} x_0), b_0 = t_0 (1 + \frac{1}{2} x_0) \]

\[ b_1 = \frac{1}{4} \left[ t_1 \left( 1 + \frac{1}{2} x_1 \right) + t_2 \left( 1 + \frac{1}{2} x_2 \right) \right], b_1 = \frac{1}{4} \left[ t_1 \left( 1 + \frac{1}{2} x_1 \right) - t_2 \left( 1 + \frac{1}{2} x_2 \right) \right] \]

\[ b_2 = \frac{1}{8} \left[ 3 t_1 \left( 1 + \frac{1}{2} x_1 \right) + t_2 \left( 1 + \frac{1}{2} x_2 \right) \right], b_2 = \frac{1}{8} \left[ 3 t_1 \left( 1 + \frac{1}{2} x_1 \right) + t_2 \left( 1 + \frac{1}{2} x_2 \right) \right] \]

\[ b_3 = \frac{1}{4} t_3 \left( 1 + \frac{1}{2} x_3 \right), b_3 = \frac{1}{4} t_3 \left( 1 + \frac{1}{2} x_3 \right) \]

The nucleon densities $\rho_p(r)$ and $\rho_n(r)$ may be calculated from a single particle wave function defined by the HF calculation. In the (SHF) theory using the Skyrme forces, the most general product wave functions $\psi_\beta$ consist of independently moving single particles. In this method the neutron and proton densities are given in:

\[ \rho_q(r) = \sum_{i=\sigma} |\psi_i(r)|^2 = \sum_{i=\sigma} \omega_{\beta} \cdot \frac{2 j_{\beta} + 1}{4 \pi} \left( \frac{R_{\beta}^\alpha}{r} \right)^2 \]

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where $\beta$ represents the state, $\alpha_\beta$ is the probability of the state, and $j_\beta$ the angular momentum of the state. The Coulomb energy part is the third part of the total energy equation. The exchange component contributes a modest amount of energy to the Coulomb energy. This contribution is owing to the fact that the Coulomb interaction is infinite range. The Coulomb energy is calculated as follows:

$$E_{\text{Coul}} = \frac{e^2}{2} \int \rho_0(\vec{r}) \rho_0(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|} d^3r d^3r' + E_{\text{Coul,exch}}$$

where $\rho_0$ is the total momentum operator, $A$ the nucleon number and $m$ the average nucleon mass.

**Tassie and Bohr-Mottelson**

The Tassie model (TM) used in NushellX@MSU\(^{16}\) for core polarization is a more elastomeric and modified modeling that allows for a non-uniform mass and charge density distribution. In the TM model, the CP charge density is determined by the nucleus ground state charge density. The two-body charge density for all occupied shells, including the core, has been used to obtain the ground state charge density. The Tassie shape core polarization transition density, which is based on the collective modes of the nuclei is given by:

$$\rho_{jz}^{\text{core}}(i, f, r) = \frac{1}{2} C(1 + \tau_z) r^{-1} \frac{d \rho_0(i, f, r)}{dr}$$

where $C$ is a constant of the proportionality and $\rho_0$ is the charge density distribution for the ground state two-body, which is given as:

$$\rho_0 = \left\{ \psi | \hat{\rho}_{\text{eff}}^{(2)}(\vec{r}) | \psi \right\} = \sum_{i<j} \left( \langle ij | \hat{\rho}_{\text{eff}}^{(2)}(\vec{r}) | ij \rangle - \langle ij | \hat{\rho}_{\text{eff}}^{(2)}(\vec{r}) | ji \rangle \right)$$

where,

$$\hat{\rho}_{\text{eff}}^{(2)}(\vec{r}) = \frac{1}{2(A-1)} f(r_{ij}) \sum_{i \neq j} \left( \delta(\vec{r} - \vec{r}_i) + \delta(\vec{r} - \vec{r}_j) \right) f(r_{ij})$$

where $i$ and $j$ are all the required quantum numbers, i.e., the functions $f(r_{ij})$ are the two-body short range correlation (SRC). In this work, a simple model form of short-range correlation has been adopted\(^{20}\), i.e.,

$$f(r_{ij}) = 1 - \exp \left(-\beta(r_{ij} - r_c)^2\right)$$

where $r_c$ is the suitable hard core radius and $\beta$ is a parameter of the correlation. For this model the Coulomb form factor becomes:

$$F_j^2(q) = \frac{4\pi}{2J_i + 1 Z} \left\{ \int_0^\infty r^2 f_j(qr) \rho_0^{ms}(i,f,r) dr + C \int_0^\infty f_j(qr) r^{J+1} \frac{d \rho_0(i,f,r)}{dr} dr \right\} F_m(q) F_f(q)$$

but,

$$\int_0^\infty f_j(qr) r^{J+1} \frac{d \rho_0(i,f,r)}{dr} dr = \int_0^\infty \frac{d}{dr} \left[ f_j(qr) r^{J+1} \rho_0(i,f,r) \right] dr$$

where the first term gives zero contribution, the second and the third term can be combined together as:

$$-q \int_0^\infty r^{J+1} \rho_0(i,f,r) \left[ \frac{d}{d(qr)} + \frac{J+1}{qr} \right] f_j(qr) dr$$

from the recursion of the spherical Bessel function\(^{17}\):

$$\left[ \frac{d}{d(qr)} + \frac{J+1}{qr} \right] f_j(qr) = f_{J-1}(qr)$$

$$\int_0^\infty f_j(qr) r^{J+1} \frac{d \rho_0(i,f,r)}{dr} dr = -q \int_0^\infty r^{J+1} \rho_0(i,f,r) f_{J-1}(qr) dr$$

Therefore, the form factor of eq.(14) takes the form:

$$F_j^2(q) = \frac{4\pi}{2J_i + 1 Z} \left\{ \int_0^\infty r^2 f_j(qr) \rho_0^{ms}(i,f,r) dr \right\}$$
\[-qC \int_0^\infty r^{j+1} \rho_0(i,f,r) j_{j-1}(qr) \, dr \} F_m(q) F_r(q) \ldots \] 21

The constant of the proportionality $C$ can be determined from the form factor evaluated at $q = k$, i.e. substituting $q = k$ in above equation we obtained:\n\[ C = \frac{\int_0^\infty r^2 j_k(kr) \rho_{jz}^m(i,f,r) \, dr - ZF_j(k)}{\int_0^\infty r^{j+1} \rho_0(i,f,r) j_{j-1}(kr) \, dr} \ldots \] 22

**Results and Discussion:**

There are many theoretical tools available to describe the properties of fp-shell nuclei that are available. Such calculations vary with the completion of the space of the shell model, the mass dependent of the involved parameters and the two-matrix elements is appropriate in terms of experimental results, in the present work $^{58,60,62}$Ni and $^{64,66,68}$Zn. The jun45 interaction has been used to give the 1f5/2p1/2g9/2-shell model wave functions. The core is taken as $^{58}$Ni for all the nuclei under study with different valence neutrons for Ni isotopes and two valence protons with different values of valence neutrons for Zn isotopes. The Bohr-Mottelson and Tassie models were employed to perform the present calculations. The curve with red dots displays the results of the calculations Tassie in any of the following diagrams (see Fig.1). The Bohr-Mottelson calculations are shown by the solid blue curve.

The parameters used with Sk35-Skzs* used to perform the calculations are listed in Table 1.

**Table 1. The Skyrme parameterization which is adopted in the calculations**

| Force  | Sk35-Skzs* |
|--------|------------|
| $t_0$  | -1446.759  |
| $t_1$  | 250.852    |
| $t_2$  | -132.993   |
| $t_3$  | 12127.649  |
| $W_0$  | 153.054    |
| $x_0$  | 0.329      |
| $x_1$  | 0.518      |
| $x_2$  | 0.139      |
| $x_3$  | 0.018      |
| $\alpha$ | 1/2       |

$^{58,60,62}$Ni Isotopes

The shell model calculations have been performed by adopting the model space jj44 with core at $^{56}$Ni, therefore we have 2, 4 and 6 valence neutrons for $^{58}$Ni, $^{60}$Ni, and $^{62}$Ni, respectively. The longitudinal form factor $C2$ for the state $(J^nT = 2^+_1)$ of $^{58}$Ni nucleus in fp-shell is presented in Fig. 1. The effective interaction jun45 is utilized as effective interaction for the calculations of the shell model and the (Sk35-Skzs*) residual interaction to calculate the matrix element for the interactions from initial to final states. The first maxima are very well reproduced by both Tassie Model and Bohr-Mottelson calculations. The second maxima did not agree in comparison with the calculations. The experimental data for this state is taken from Ref. 21. The effective proton and neutron charges used in these calculations are 0.5 and 1.5, respectively. Figure 2 shows the CDD obtained with the investigated Skyrme parameterization Sk35-Skzs* used in this work as well as the experimental charge distributions for $^{58}$Ni nucleus. Theoretically the calculated CDD is quite consistent with the experimental calculations with the Skyrme parameterization.

**Figure 1. C2 form factor for the 2^+_1 state in $^{58}$Ni. Measured data from 21.**

**Figure 2. Charge density distribution for $^{58}$Ni using Skyrme parameterization “Sk35-Skzs*”. Measured data from 21.**
The C2 longitudinal form factor for the state \((J^\pi T = 2_1^+ 2)\) of \(^{60}\text{Ni}\) nucleus has been calculated by Tassie model and Bohr-Mottelson models. The calculations according to standard shell model the core is taken at \(^{56}\text{Ni}\) with four neutrons as valence particles outside the core, as shown in Fig. 3. The core polarization is considered by using the effective proton and neutron charges. Figure 4 shows the CDD obtained with the investigated Skyrme parameterization Sk35-Skzs\(^*\) used in this work as well as the experimental charge distributions for \(^{60}\text{Ni}\) nucleus. The comparison of the predicted theoretical values was compared with the available measured data for CDD and C2 form factors and showed good agreement.

The nucleus \(^{62}\text{Ni}\) excites in this transition from ground state \((J^\pi T = 0_1^+ 3)\) to the excited state \((J^\pi T = 2_1^+ 3)\) with the corresponding energy 1.172 MeV. The C2 longitudinal form factor of \(^{62}\text{Ni}\) nucleus in \(1f_{5/2} 2p_{1/2} 1g_{9/2}\)-shell is presented in Fig. 5. The j\(u\)n43 is utilized as an effective residual interaction for the calculations of the shell model. The third maxima are very well reproduced by both Tassie and Bohr-Mottelson calculations. The experimental data for this state are taken from Ref\(^{23}\). Figure 6 shows the CDD obtained with the investigated Skyrme parameterization Sk35-Skzs\(^*\) used in this work as well as the experimental charge distributions for \(^{62}\text{Ni}\) nucleus. The comparison of the predicted theoretical values was compared with the available measured data for CDD and C2 form factors and showed good agreement.

**Figure 3.** C2 form factor for the \(2_1^+ 2\) state in \(^{60}\text{Ni}\). Measured data from\(^{21}\).

**Figure 4.** Charge density distribution for \(^{60}\text{Ni}\) using Skyrme parameterization “Sk35-Skzs\(^*\)”. Measured data from\(^{21}\).

**Figure 5.** C2 form factor for the \(2_1^+ 3\) state in \(^{62}\text{Ni}\). Measured data from\(^{22}\).

**Figure 6.** Charge density distribution for \(^{62}\text{Ni}\) using Skyrme parameterization “Sk35-Skzs\(^*\)”. Measured data from\(^{23}\).
The shell model calculations for Zn isotopes have been performed by considering the jj44 model space which assumes $^{56}\text{Ni}$ as core with 2 protons and 6, 8 and 10 neutrons outside the core for $^{64}\text{Zn}$, $^{66}\text{Zn}$, and $^{68}\text{Zn}$, respectively. The C2 longitudinal form factor for $^{64,66,68}\text{Zn}$ isotopes have been calculated in Figs.7,8,9 respectively by Tassie model and Bohr-Mottelson models. The effective interaction jun45 is utilized as effective interaction for the calculations of the shell model and the (Sk35-Skzs*) residual interaction to calculate the matrix element for the interactions from initial to final states. The experimental data was reproduced by both Tassie Model and Bohr-Mottelson calculations for the $^{64,66,68}\text{Zn}$ isotopes. The experimental data for this state was aken from Ref.22. The effective proton and neutron charges used in these calculations are 0.5 and 1.0, respectively. Figures 10,11,12. show the CDD obtained with the investigated Skyrme parameterization Sk35-Skzs used in this work as well as the experimental charge distributions for $^{64,66,68}\text{Zn}$ isotope. The comparison of the predicted theoretical values was compared with the available measured data for CDD and C2 form factors and showed good agreement.

Figure 7. C2 form factor for the $2^+_2$ state in $^{64}\text{Zn}$. Measured data from23.

Figure 8. C2 form factor for the $2^+_3$ state in $^{66}\text{Zn}$. Measured data from22.

Figure 9. C2 form factor for the $2^+_4$ state in $^{68}\text{Zn}$. Measured data from22.

Figure 10. Charge density distribution for $^{64}\text{Zn}$ using Skyrme parameterization “Sk35-Skzs”. Measured data from23.
Figure 11. Charge density distribution for $^{66}$Zn using Skyrme parameterization **“Sk35-Skzs*”**. Measured data from 22.

Figure 12. Charge density distribution for $^{68}$Zn using Skyrme parameterization **“Sk35-Skzs*”**. Measured data from 23.

Conclusion:
The present study detailed theoretical investigation to study the form factors and charge density distribution (CDD) of inelastic electron scattering for some selected fp-shell nuclei. The theoretical calculations were employed the Skyrme-Hartree-Fock method with (Sk35-Skzs*) parametrization. The comparison of the predicted theoretical values was compared with the available measured data for CDD and C2 form factors and showed good agreement.

Authors' declaration:
- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Besides, the Figures and images, which are not ours, have been given the permission for re-publication attached with the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee in University of Baghdad.

Authors' contributions:
S.A.A and S.A.E. motivated the idea of the present study. S.A.A. had performed the calculations and both S.A.A. and S.A.E. collaborate to get the experimental data and plot the graphs.

S.H.S and H.M.T wrote the introduction section and the goal of the study.

All the authors participated in discussing and writing the introduction and discussion sections and the conclusions came out from the study.

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استقصاء التركيب النووي لبعض نظائر النيكل والزئبق بواسطة تفاعل سكيرم هارتري فوك

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الخلاصة:
تم التقصي عن عوامل التشكل C2 غير مرن ووزع كثافة الشحنة (CDD) لـ 58,60,62Ni و 64,66,68Zn من خلال استخدام طريقة Sk35-Skzs مع مكثفات Skyrme-Hartree-Fock. تم حساب عوامل التشكل C2 غير مرن باستخدام شكل نماذج Tassie و Bohr-Mottelson المتوقعة مع البيانات المسبقة المتاحة لعواميم الشكل 2 و CDD وأظهرت توافقًا جيدًا.

الكلمات المفتاحية: توزيع كثافة الشحنة (CDD)، عوامل التشكل C2، سكيرم هارتري فوك، نموذج القشرة