Iraqi Journal of Science

ISSN: 0067-2904

# The calculation of the charge density distributions of the 1*f*-2*p* shell nuclei using the occupation numbers of the states

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**Abstract:**

The charge density distributions (CDD) and the elastic electron scattering form factors, F(q), of the ground state for some 1*f*-2*p* shell nuclei, such as $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei have been calculated based on the use of occupation numbers of the states and the single particle wave functions of the harmonic oscillator potential with size parameters chosen to reproduce the observed root mean square charge radii for all considered nuclei. It is found that introducing additional parameters, namely $\beta_1$ and $\beta_2$ which reflect the difference of the occupation numbers of the states from the prediction of the simple shell model leads to a remarkable agreement between the calculated and experimental results of the charge density distributions throughout the whole range of $r$. The calculated elastic electron scattering form factors from $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei are very good agreement with the fitted to the experimental data throughout all values of $q$.

**Keywords:** Charge density distributions, Elastic electron scattering, Occupation numbers of the states.

# حساب توزيعات كثافة الشحنة لنوى تقع ضمن القشرة النووية 1*f*-2*p* باستخدام حالات اعداد الملئ

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**الخلاصة**

تم حساب توزيعات كثافة الشحنة ( CDD ) وعوامل التشكل F(q) للاستطارة الالكترونية المرنة للحالة الارضية لبعض النوى الواقعة ضمن القشرة النووية 1*f*-2*p* مثل النوى $^{74}$Ge، $^{76}$Ge، $^{78}$Se و $^{80}$Se بالاعتماد على كل من اعداد الملئ للحالات النووية والدوال الموجية لجهد المتذبذب التوافقي ذي اعلومات حجمية اختيرت لكي تعيد انتاج مربع متوسط انصاف اقطار الشحنة لجميع النوى تحت الدراسة. لقد وجد ان الاعلومات الاضافية ($\beta_1$ و $\beta_2$)، والتي تعكس الفرق بين اعداد الملئ للحالات النووية قيد الدراسة وبين تلك التي يتنبأ بها أنموذج القشرة البسيط، يؤدي الى توافق ممتاز بين النتائج المحسوبة والنتائج العملية لتوزيع كثافة الشحنة النووية ولكل قيم $r$. أظهرت هذه الدراسة بان النتائج النظرية لعوامل التشكل للاستطارة الالكترونية المرنة للنوى $^{74}$Ge، $^{76}$Ge، $^{78}$Se و $^{80}$Se تتفق مع النتائج العملية ولكل قيم الزخم المنتقل.

## 1. Introduction

The charge density distributions (CDD) and form factors are the most important quantities in the nuclear structure which were well studied experimentally over a wide range of nuclei. This interest in the CDD is related to the basic bulk nuclear characteristics such as the shape and size of nuclei, their binding energies, and other quantities which are connected with the CDD. Besides, the density distribution is an important object for experimental and theoretical investigations since it plays the role of a fundamental variable in nuclear theory. The CDD can be determined experimentally from the scattering of high-energy electrons by the nucleus. By measuring the elastic cross sections one obtains information about the distribution of the charges within the nucleus. Various theoretical methods [1, 2]

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are used for calculations of CDD, among them the theory of finite Fermi system, the Hartree- Fock method with skyrme effective interaction. A phenomenological method was applied that is based on the natural orbital representation to construct the ground state one body density matrix [1]. This method describes correctly both density and momentum distributions in closed shell nuclei $^{4}$He, $^{16}$O and $^{40}$Ca. Here, the parameters of the matrix are fixed by a best fit to the experimental density distribution and to the correlated nucleon momentum distribution. An analytical expression were derived for the one and two body terms in the cluster expansion of CDD and elastic form factors of 1*s* -1*p* and 2*s* -1*d* shell nuclei [3, 4]. This expression was used for the systematic study of the effect of the short-range correlations on the CDD. Their study depends on the harmonic oscillator size parameter ($b$) and the correlation parameter $\beta$, where these parameters were determined by fitting the theoretical charge form factors to the experimental one. Many particle shell model wave functions were used to calculate the form factors of the even-even nuclei with mass number $A$ = 20 - 36 that have the positive parity states [5]. Many theoretical works (with various assumptions) concerning the calculations of CDD and elastic form factors have been carried out [6-10] of 2*s* -1*d* shell nuclei. Gul'karov *et al*. [11] have calculated the *CDDs* of 2*s* -1*d* shell nuclei with the assumption that there is an inert core of filled 1*s* and 1*p* shells and the proton numbers in 2*s* and 1*d* shells are equal to 2-$\alpha$ and ($Z$-10+$\alpha$), respectively. Here, $\alpha$ represents the deviation of the shell charges from the prediction of the simple shell model and $Z$ is the proton number (total charge of the nucleus). In general, the calculated *CDD* were in good agreement with those of experimental data for all considered 2*s* -1*d* shell nuclei.

The aim of the present work is to extend the calculations of Gul'karov *et al*. [11] to higher shells (such as the 1f-2p shell nuclei) and to derive an analytical expression for the CDD based on the use of the single particle harmonic oscillator wave functions and the occupation numbers of the states.

## 2. Theory

The charge density distribution (CDD) of one body operator can be written as [12]:

$$\rho_{ch}(r) = \frac{1}{4\pi}\sum_{n\ell}\xi_{n\ell}\, 2(2\ell+1)\left|R_{n\ell}\right|^2 \tag{1}$$

Where $\xi_{n\ell}$ is the proton occupation probability of the state $n\ell$ ($\xi_{n\ell}=0$ or 1 for closed shell nuclei and $0<\xi_{n\ell}<1$ for open shell nuclei) and $R_{n\ell}$ is the radial part of the single particle harmonic oscillator wave function. In the simple shell model, the 1*f*-2*p* shell nuclei are considered as an inert core of filled *1s, 1p, 1d,* and *2s* while the *1f* orbit is occupied by (Z-20) protons. According to the assumption of the simple shell model of Eq. (1), an analytical expression for the *CDD* of 1*f*-2*p* shell nuclei is obtained as:

$$\rho_{ch}(r) = \frac{e^{-r^2/b^2}}{\pi^{3/2}b^3}\left[5+4\left(\frac{r}{b}\right)^4+\frac{8}{105}(Z-20)\left(\frac{r}{b}\right)^6\right] \tag{2}$$

where $Z$ is the atomic number of nuclei, $b$ is the harmonic oscillator size parameter.
The normalization condition of the $\rho_{ch}(r)$ is given by [13]

$$Z = 4\pi\int_0^\infty \rho_{ch}(r)r^2dr \tag{3}$$

and the mean square radius (MSR) of the nuclei is given by [13]

$$\langle r^2\rangle = \frac{4\pi}{Z}\int_0^\infty \rho_{ch}(r)r^4dr \tag{4}$$

Introducing Eq. (2) into Eq. (4) and integrating, the MSR of 1*f* -2*p* shell nuclei is obtained as

$$\langle r^2\rangle = \frac{b^2}{Z}\left(\frac{9Z-60}{2}\right) \tag{5}$$

The calculated results obtained by Eq. (2) have a poor agreement with experimental data. To derive an explicit form for the *CDD* of 1*f*- 2*p* shell nuclei, we assume that there is a core of filled 1*s*, 1*p* and 1*d* orbitals and the proton occupation numbers in 2*s*, 1*f* and 2*p* orbitals are equal to, respectively, (2-$\beta_1$), (Z-20-$\beta_2$) and ($\beta_1$+ $\beta_2$) and not to 2, (Z-20) and 0 as in the simple shell model, where the parameters $\beta_1$ and $\beta_2$ are the occupation number of higher shells. Using this assumption, with the help of Eq. (1), the ground state charge density distribution can be written as:

$$\rho_{ch}(r)=\frac{e^{-r^2/b^2}}{\pi^{3/2}b^3}\left\{5-\frac{3}{2}\beta_1+\left(\frac{11}{3}\beta_1+\frac{5}{3}\beta_2\right)\left(\frac{r}{b}\right)^2+\left(4-2\beta_1-\frac{4}{3}\beta_2\right)\left(\frac{r}{b}\right)^4\right.$$
$$\left.+\left(\frac{4}{21}\beta_2+\frac{8}{105}(Z-20)+\frac{4}{15}\beta_1\right)\left(\frac{r}{b}\right)^6\right\} \tag{6}$$

and the corresponding MSR is

$$\langle r^2\rangle=\frac{b^2}{Z}\left(\frac{9Z-60}{2}+\beta_1\right) \tag{7}$$

The central CDD, $\rho_{ch}\ (r=0)$ is obtained from Eq. (6) as

$$\rho_{ch}(0)=\frac{1}{\pi^{3/2}b^3}\left[5-\frac{3}{2}\beta_1\right] \tag{8}$$

then $\beta_1$ is obtained from Eq. (8) as

$$\beta_1=\frac{2}{3}\left[5-\rho_{ch}(0)\pi^{3/2}b^3\right] \tag{9}$$

In eq's (7) and (9), the values of the central density $\rho_{ch}(0)$ and $\langle r^2\rangle$ are taken from the experiments while the parameter $b$ is chosen in such a way as to reproduce the experimental root mean square radii of nuclei.

Next we use the plane wave born approximation (PWBA) to study the elastic electron scattering form factors from considered nuclei. In the PWBA, the incident and scattered electron waves are represented by plane waves. The elastic electron scattering form factor is simply given by the Fourier-Bessel transform of the ground state charge density distribution (CDD) [1], *i.e.*

$$F(q)=\frac{4\pi}{Z}\int_0^\infty \rho_{ch}(r)\,j_0(qr)\,r^2dr, \tag{10}$$

where

$$j_0(qr)=\frac{\sin(qr)}{qr} \tag{11}$$

Is the zeroth order spherical Bessel function, q is the momentum transfer from the incident electron to the target nucleus and the $\rho_{ch}(r)$ is the CDD of the ground state.

An analytical expression for elastic electron scattering form factor F(q) can be obtained by introducing the form of the CDD of Eq. (6) into Eq. (10), and performing the integration, *i.e.*,

$$F(q)=\frac{1}{Z}\left\{Z+\left[\frac{(10-Z)}{2}-\frac{\beta_1}{6}\right](qb)^2+\left[\frac{\beta_1}{20}+\frac{\beta_2}{24}+\frac{(Z-15)}{20}\right](qb)^4\right.$$
$$\left.-\left[\frac{\beta_1}{240}+\frac{\beta_2}{336}+\frac{(Z-20)}{840}\right](qb)^6\right\}e^{-q^2b^2/4} \tag{12}$$

Several corrections must be applied to the form factor given in equation (12) to convert it into a representation appropriate for a comparison with the experimental form factor. One of these corrections is the center of mass $F_{cm}(q)$ . The $F_{cm}(q)$ removes the spurious state arising from the motion of the center of mass when shell model wave function is used and given by [5]:

$$F_{cm}(q)=e^{\left(\frac{b^2q^2}{4A}\right)} \tag{13}$$

where $A$ is the nuclear mass number and $b$ is the harmonic-oscillator size parameter.

In the shell-model the nucleon is assumed to be a point, but nucleons are actually of finite size, then the calculated form factors have to be corrected by another correction which takes into account the finite size of the nucleon. The finite nucleon size correction $F_{fs}(q)$ takes the form [5]:

$$F_{fs}(q) = e^{\left(\frac{-0.43q^2}{4}\right)} \quad \textbf{(14)}$$

In this study, we compare the calculated CDD of considered nuclei with those of two parameter Fermi model 2*PF*, which are extracted from the analysis of elastic electron-nuclei scattering experiments, and is given by [13]

$$\rho_{ch}(r) = \frac{\rho_0}{1+e^{(r-c)/z}} \quad \textbf{(15)}$$

where the constant $\rho_0$ is obtained from the normalization condition of the charge density distribution of Eq. (3).

**3. Results and Discussion**

The analytical expression of Eq. (6) has been used to study the CDD's for some even- *A* of 1*f*-2*p* shell nuclei, such as $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei. The harmonic oscillator size parameter *b* is chosen such that to reproduce the measured root mean square radii (*rms*) of nuclei under study and the parameter $\beta_1$ is determined by introducing the chosen value of *b* and the experimental central density $\rho_{exp}(0)$ into Eq. (9), while the parameter $\beta_2$ is assumed as a free parameter to be adjusted to obtain agreement with the experimental CDD. It is important to remark that when $\beta_1=\beta_2=0$, Eq. (6) is reduced to that of the simple shell model prediction.

In Table-1, we present the values of the parameters (*c* and *z*) used to extract 2*PF* CDD's together with central charge densities $\rho_{exp}(0)$ for $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei. Table-2 displays all parameters needed for calculating $\rho_{ch}(r)$ of Eq. (6), such as the harmonic oscillator size parameter *b* and the calculated parameters of $\beta_1$ and $\beta_2$ for considered nuclei. Table-3 demonstrates the calculated occupation numbers for 2*s*, 1*f*, and 2*p* shells and the calculated root mean square charge radii $\langle r^2\rangle_{cal}^{1/2}$ obtained by Eqs. (5) and (7).

**Table 1**- Values of the parameters (*c* and *z*) required by the *CDD* of 2*PF* model together with $\rho_{exp}(0)$.

| *Nuclei* | 2*PF* [14] | | $\rho_{exp}(0)$ ( $fm^{-3}$) [14] |
|---|---|---|---|
| | *c* (*fm*) | *z* (*fm*) | |
| $^{74}$Ge | 4.454 | 0.608 | 0.0730171 |
| $^{76}$Ge | 4.54 | 0.578 | 0.0703697 |
| $^{78}$Se | 4.581 | 0.5729 | 0.0730977 |
| $^{80}$Se | 4.667 | 0.5339 | 0.0706811 |

**Table 2-** Calculated parameters used in Eq. (6) for the calculations of the *CDD*.

| *Nuclei* | Z | *b* (*fm*) | $\beta_1$ | $\beta_2$ |
|---|---|---|---|---|
| $^{74}$Ge | 32 | 2.154 | 0.62278 | 1.11502 |
| $^{76}$Ge | 32 | 2.181 | 0.62158 | 1.12498 |
| $^{78}$Se | 34 | 2.171 | 0.55503 | 1.35812 |
| $^{80}$Se | 34 | 2.181 | 0.60958 | 1.19241 |

**Table 3**- Calculated occupation numbers of 2*s*, 1*f*, and 2*p* shells together with $\langle r^2\rangle_{cal}^{1/2}$ and $\langle r^2\rangle_{\exp}^{1/2}$.

| *Nuclei* | Occupation No. of 2*s* (2-$\beta_1$) | Occupation No. of *1f* (Z-20- $\beta_2$) | Occupation No. of 2*p* ($\beta_1$+ $\beta_2$) | $\langle r^2\rangle_{cal}^{1/2}$ obtained Eq (5) | $\langle r^2\rangle_{cal}^{1/2}$ obtained Eq (7) | $\langle r^2\rangle_{\exp}^{1/2}$ [13, 14] |
|---|---|---|---|---|---|---|
| $^{74}$Ge | 1.3772 | 10.8849 | 1.7378 | 4.065 | 4.076 | 4.075 |
| $^{76}$Ge | 1.3784 | 10.8750 | 1.7465 | 4.116 | 4.127 | 4.127 |
| $^{78}$Se | 1.4449 | 12.6418 | 1.9131 | 4.129 | 4.138 | 4.138 |
| $^{80}$Se | 1.3904 | 12.8075 | 1.8020 | 4.14 | 4.15 | 4.137 |

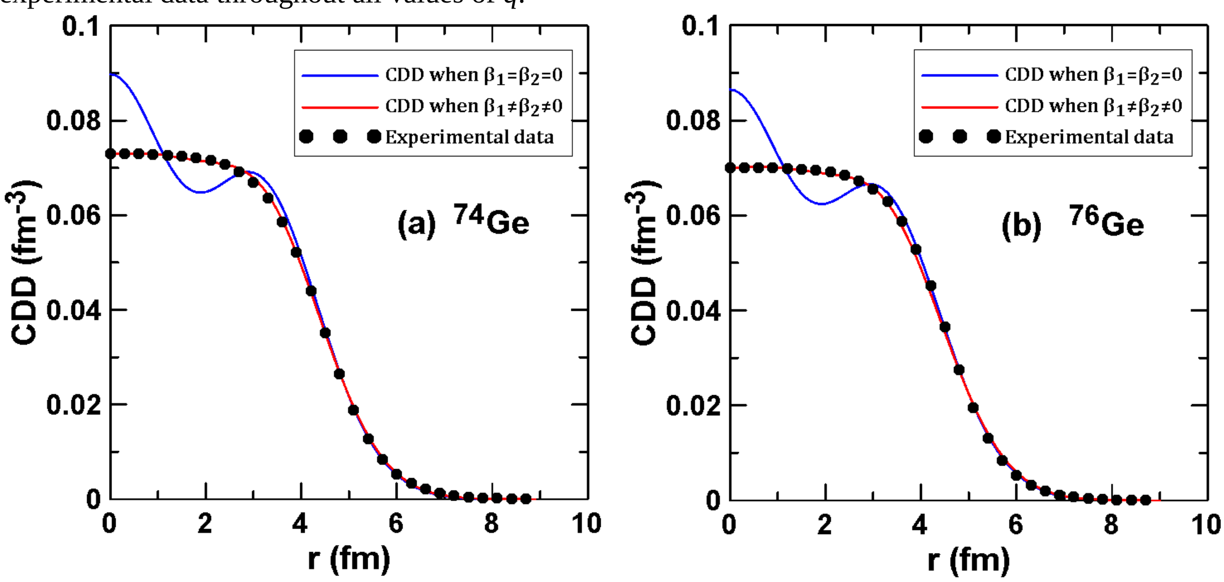
The dependence of the CDD's (in fm$^{-3}$) on $r$ (in fm) for $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei is shown in Figure-1. The blue and red curves are the calculated results using Eq. (6) with $\beta_1= \beta_2=0$ and $\beta_1\neq \beta_2\neq 0$, respectively whereas the filled circle symbols correspond to the experimental data [14]. This figure shows that the blue curves are in poor agreement with the experimental data, especially for small *r*. Inclusion of the parameters $\beta_1$ and $\beta_2$ (i.e., considering the higher orbitals) in the calculation leads to a very good agreement with the experimental data as demonstrated by the red curves. It is obvious that the form of the *CDD's* represented by (6) behaves as an exponentially decreasing function as seen by red distributions for all considered nuclei of figure 1. This figure shows that the probability of finding a proton near the central region ($0 \le r \le 2$ *fm*) of $\rho_{ch}(r)$ is larger than the tail region ($r > 2$ *fm*). Besides, including the higher shells through introducing the values of $\beta_1$ and $\beta_2$ presented in Table-2, into Eq. (6) leads to reducing significantly the central region of $\rho_{ch}(r)$ and increasing slightly the tail region of $\rho_{ch}(r)$ as seen by the red distributions. This means that the effect of inclusion of higher shells in our calculations tends to increase the probability of transferring the protons from the central region of the nucleus towards its surface and tends to increase the root mean square charge radius $\langle r^2 \rangle^{1/2}$ of the nucleus see Table-3 and then makes the nucleus to be less rigid than the case when there is no such effect. Figure-1 also illustrates that the blue distributions in all considered nuclei are not in good accordance with those of 2*PF* model especially at the central region of $\rho_{ch}(r)$ but once the higher shells are considered in the calculations due to the introduction the calculated values of $\beta_1$ and $\beta_2$ given in Table-2 into Eq. (6), the results for the *CDD* become in astonishing accordance with those of 2*PF* throughout the whole values of *r*.

Inspection of the CDD of the $^{76}$Ge and $^{80}$Se nuclei which are shown in Figures-1(b) and 1(d), indicate that the additional neutrons to the $^{76}$Ge and $^{80}$Se nuclei, lead to change slightly the distribution of the protons in the shells because of the nuclear interactions between these additional neutrons and the protons. This interactions leads to some decrease in the CDD especially at the central regions of these nuclei. By the additional neutrons to these nuclei, the charges are removed from the interior and from the tail of the distributions and transferred into the surface regions.

The dependence of elastic electron scattering form factors on the momentum transfer (q) (in fm$^{-1}$) for considered nuclei is shown in Figure-2. As there is no data available for $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei, we have compared the calculated form factors (solid curves) of these nuclei with those obtained by the Fourier transform of the 2PF density (filled circle symbols). This figure shows that the solid curves are very good agreement with the fitted to the experimental data. All the first and second diffraction minima are reproduced in the correct places.

**4. Conclusions**

This study leads to the conclusion that the introduction of additional parameters $\beta_1$ and $\beta_2$ that reflect the difference of the occupation numbers of the states from the prediction of the simple shell model gives very good agreement between the calculated and experimental results of the charge density distributions throughout the whole range of *r*. The calculated elastic electron scattering form factors from $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei are very good agreement with the fitted to the experimental data throughout all values of *q*.



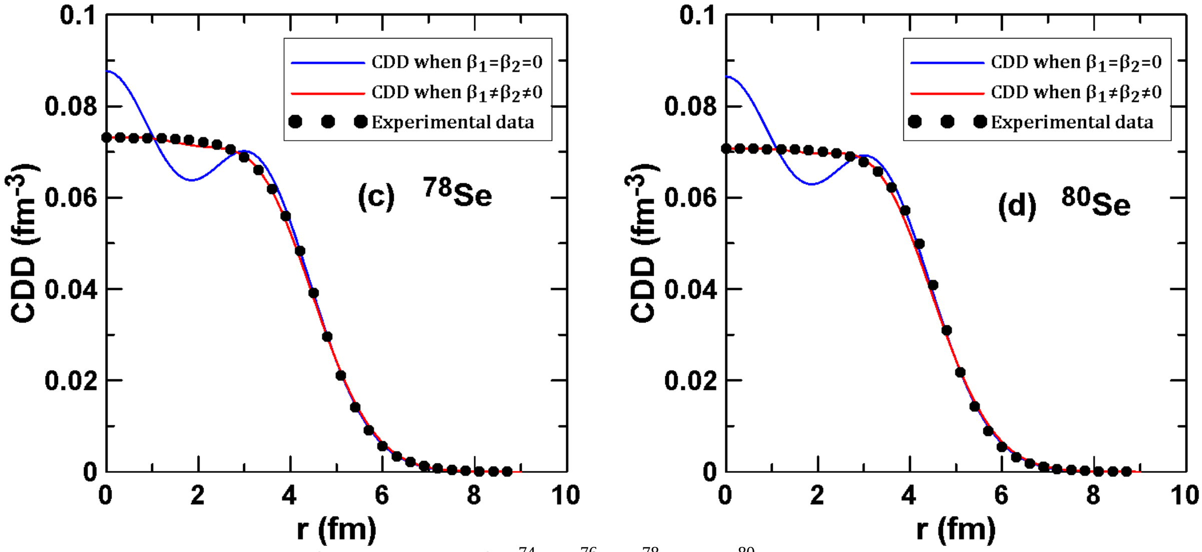



**Figure 1-** The dependence of the CDD on $r$ for $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei. The blue and red curves are the calculated CDD of Eq. (6) when $\beta_1 = \beta_2 = 0$ and $\beta_1 \neq \beta_2 \neq 0$, respectively. The filled circle symbols are the experimental data taken from ref. [14].

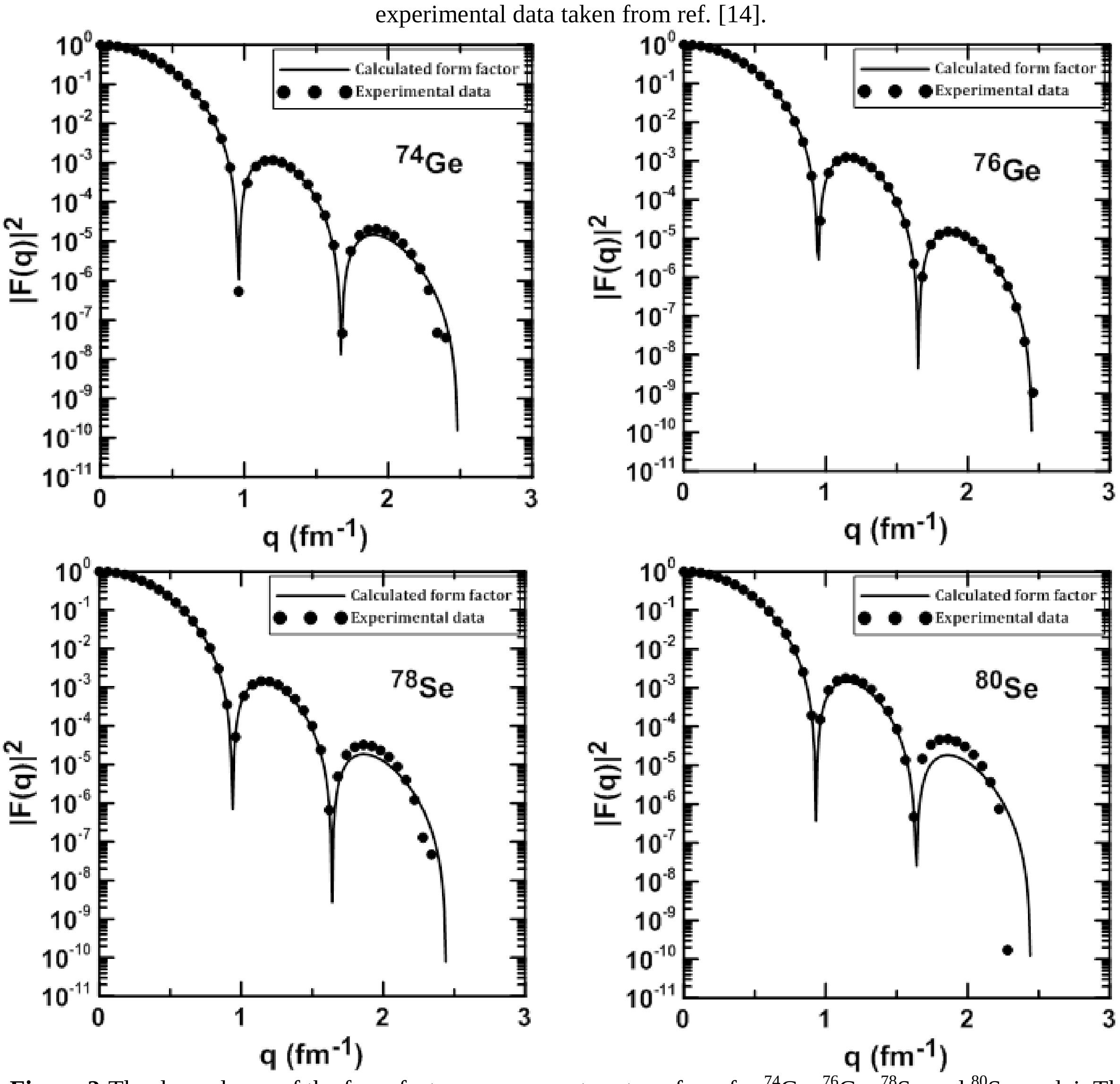



**Figure 2-**The dependence of the form factors on momentum transfer $q$ for $^{74}$Ge, $^{76}$Ge, $^{78}$Se and $^{80}$Se nuclei. The solid curves are the form factors calculated using Eq. (12). The filled circle symbols are the form factors obtained by the Fourier transform of the 2*PF* [14].

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