

Annual Symposium of the Hellenic Nuclear Physics Society

Τόμ. 2 (1991)

HNPS1991



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doi: [10.12681/hnps.2863](https://doi.org/10.12681/hnps.2863)

Βιβλιογραφική αναφορά:

Grypeos, M. E., Lalazissis, G. A., Massen, S. E., & Panos, C. P. (2020). DEBYE-WALLER TYPE EXPRESSIONS FOR THE NUCLEAR ELASTIC FORM FACTORS AT SMALL MOMENTUM TRANSFERS. *Annual Symposium of the Hellenic Nuclear Physics Society, 2*, 369–381. <https://doi.org/10.12681/hnps.2863>

DEBYE-WALLER TYPE EXPRESSIONS FOR THE NUCLEAR ELASTIC FORM FACTORS AT SMALL MOMENTUM TRANSFERS †

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Abstract

The problem of the estimate of the nuclear elastic form factors in Born approximation is discussed in the region of small momentum transfers q . It is shown that approximate expressions of the Debye-Waller type are suitable for estimates of these form-factors in the oscillator shell model, for sufficiently small q .

1. Introduction

It is well-known [1] that the elastic form factor in Born approximation and for a spherically symmetric density distribution $\rho(r)$:

$$F(q) = \frac{4\pi}{Zq} \int_0^\infty r \rho(r) \sin(qr) dr \quad (1.1)$$

may be estimated for small values of the momentum transfer q by using the first few terms in the power series of F around $q=0$:

$$F(q) = 1 - \frac{1}{6} \langle r^2 \rangle q^2 + \frac{1}{120} \langle r^4 \rangle q^4 - \dots = \sum_{n=0}^{\infty} \frac{(-1)^n \langle r^{2n} \rangle q^{2n}}{(2n+1)!} \quad (1.2)$$

In this "moment expansion" $\langle r^{2n} \rangle$ is the $2n$ -th moment, given by :

† Presented by M.E. Grypeos

$$\langle r^{2n} \rangle = \frac{\int_0^\infty \rho(r) r^{2n+2} dr}{\int_0^\infty \rho(r) r^2 dr} \quad (1.3)$$

Difficulties, however, may arise with this type of expansion. Thus, it may be necessary, depending on the value of q , to take into account a large number of terms in order to have a fairly accurate estimate of $F(q)$. To face this sort of difficulties it was proposed [2] to use a continued fraction expansion of series (1.2) which is truncated subsequently. In this way, considerable "acceleration of the convergence" is achieved.

The above mentioned approach was applied to the deuteron form factor in ref. 3 and in addition to it to the form factor of $^{16}_8\text{O}$ in the harmonic oscillator shell model, as well as to the form factor for a Fermi distribution, in ref. 2. In the case of $^{16}_8\text{O}$, for example, where the values obtained with the exact expression are compared with those obtained with expansion (1.2) truncated at the $n=1$ and $n=5$ terms and also with the truncated continued fraction expansion (with the same number of terms), it was easily realized (see fig. 1 of ref. 2) that the latter approach gives much better results. Not only the agreement with the exact expression is better at low q values but also at higher q the truncated continued fraction results are better behaved than those obtained with the corresponding truncated expansion (1.2).

In the present work we shall restrict ourselves to the region of low momentum transfers. Our aim is to investigate in the framework of the harmonic oscillator shell model, an alternative possibility of approximating the form factor (1.1) in this region, by using an expression, which is of the Debye-Waller type and has some attractive features. Namely: 1) It is quite simple, 2) it is applicable to spherical distributions of nuclei in a rather wide region of mass numbers and 3) its accuracy compares favorably, at least with that of the standard expression used widely in this region of low q values, that is the one obtained by truncating the moment expansion of $F(q)$ at the second term ($n=1$):

$$F(q) \simeq F_{T1}(q) = 1 - \frac{1}{6} \langle r^2 \rangle q^2 \quad (1.4)$$

The relevant formulae are given in the next section. The final section is devoted to the presentation of the numerical results obtained with the Debye-Waller type expressions for the point-proton and for the charge form factor for a number of nuclei. Comparison with other approximate expressions and with the corresponding complete harmonic oscillator one is also made.

We would like to point out that the approximate treatment for the form factor is analogous to the one for the relative probability P for the recoilless Λ production in nuclei, described recently [4]. Such a process has a similarity with the Mössbauer effect for which a Debye-Waller factor expression for P and for the corresponding quantities of other similar processes, including scattering, has been given or discussed in the past [5].

Finally we should recall that knowledge of the form factor for small values of momentum transfer -though not always sufficiently small- is needed in physical problems and thus it appears desirable to have, if possible, simple expressions in making easily estimates.

Simple expressions for $F(q)$ may also arise by using phenomenological densities for which the form factor can be obtained analytically and their parameters have been suitably determined. These parameters may then be related to the harmonic oscillator size parameter b , e.g. by equating the expression of the m.s. radius of the assumed density of the nucleus with the expression of the m.s. radius in the oscillator shell model.

As an example in which nuclear form factors at rather small values of q are used, we mention the exotic (μ^-, e^-) conversion in nuclei, in which the bound muon of a muonic atom is converted into an electron :



Such a process aroused special experimental and theoretical interest in recent years (see ref. 6 and references therein). In the coherent process of (1.5), that is when the nucleus (A, Z) remains in its ground state, the dependence of the rate on the nuclear parameters was obtained [6] by using oscillator shell model nuclear form factors.

2. The approximate expression for $F(q)$

An alternative possibility to that mentioned in the introduction in obtaining an approximate expression for $F(q)$ at low q values is, instead of keeping only the two first terms of the expansion and omitting completely the higher ones, to take into account exactly these two terms and also approximately the higher ones. This may be done, for example, by expressing $F(q)$, in the form:

$$F(q) = \exp\left(-\frac{1}{6} \langle r^2 \rangle q^2\right) + \Delta F(q) \quad (2.1)$$

and write approximately [5]:

$$F(q) \simeq F_{DW}(q) = \exp\left(-\frac{1}{6} \langle r^2 \rangle q^2\right) \quad (2.2)$$

This amounts to omitting the series of the correction terms:

$$\Delta F(q) = \sum_{n=2}^{\infty} (-1)^n q^{2n} \left[\frac{\langle r^{2n} \rangle}{(2n+1)!} - \frac{\langle r^2 \rangle^n}{6^n n!} \right] \quad (2.3)$$

It should be noted that this series starts from $n=2$. Thus, there are no omitted correction terms with $n=0$ and $n=1$ by using approximate expression (2.2). The omission of the correction terms in expression (2.1) is equivalent to the replacement in expansion (1.2) of $\langle r^{2n} \rangle / (2n+1)!$ by $\langle r^2 \rangle^n / 6^n n!$ ($n=2,3,\dots$). In order to have an idea of the consequence of this replacement we may estimate both terms by using the equivalent uniform density distribution :

$$\rho(r) = \rho_0 [1 - \Theta(r - R)] \quad (2.4)$$

where Θ is the unit step function and the radius R is given by $R = \sqrt{\frac{5}{3} \langle r^2 \rangle}$. In this way we find

$$\Delta F = \sum_{n=2}^{\infty} (-1)^n (Rq)^{2n} \left[\frac{3}{(2n+1)!(2n+3)} - \frac{1}{10^n n!} \right] \quad (2.5a)$$

From the above result it is suggested that if we wish expression (2.2) to be a fairly good approximation to the form factor (1.2), the quantity (Rq) should be sufficiently small, so that the omitted terms (ΔF) to be negligible. Thus, not only the value of the momentum transfer should be quite small but also the nucleus should not be heavy. For the heavier nuclei one should restrict the values of q to a smaller region from the origin in order to obtain reasonable results.

In addition, it is seen from expression (2.5a) that the first term ($n=2$) is $(qR)^4 (\frac{1}{280} - \frac{1}{200})$. Thus, the third term in the approximate expression (2.2) is larger than the corresponding one in expression (1.2) and therefore, in view also of the form of the higher terms, F_{DW} should give somehow larger values than those of the exact expression in the region we are interested.

We also mention that similar conclusions could be drawn if the harmonic oscillator model is used. In this case, the expression of $\langle r^2 \rangle^n$ is given analytically in a simple way (see below), but a general expression of $\langle r^{2n} \rangle$ is not easily obtained, although for specific light nuclei the $2n$ -th moment is easily calculated too. In the case of the harmonic oscillator model, the main difference in the expression of ΔF , apart from the change in

the coefficients in (2.5a), is the replacement of R by the harmonic oscillator parameter b which determines the size of the nucleus. If we consider, for example, nuclei with atomic numbers in the region $2 \leq Z \leq 8$, the expression of ΔF becomes

$$\Delta F = \sum_{n=2}^{\infty} (-1)^n (bq)^{2n} \left[\frac{1}{2^{2n} n!} \left(\frac{(2n+3)Z - 4n}{3Z} - \left(\frac{5Z-4}{3Z} \right)^n \right) \right] \quad (2.5b)$$

By considering, more specifically, the case of $^{16}_8\text{O}$ and the first terms of (2.5b) we may easily check that the coefficients of $(-1)^n (bq)^{2n}$ are negative and therefore the previously made conclusion about the values of F_{DW} is verified in this case too. In addition it may be seen, by expressing b^2 in terms of R^2 , that the resulting coefficient of the $n=2$ term of ΔF in (2.5b) and the corresponding one in (2.5a) are of the same order of magnitude.

We consider the point-proton form factor obtained with a nuclear model. The corresponding density distribution $\rho(r)$ and from this the mean square radius $\langle r^2 \rangle$ in expression (2.2) will be calculated on the basis of the assumed nuclear model. We assume, as previously, for simplicity the harmonic oscillator shell model (without spin-orbit part). The mean square radius may then be given analytically by quite a simple expression [7]. For closed shell nuclei the result is:

$$\langle r^2 \rangle_{N_m} = \frac{1}{Z} \sum_{n_s=0}^{N_m} (n_s + \frac{3}{2}) Z_{n_s} = \frac{3}{4} \frac{\hbar}{m\omega} (N_m + 2) \quad (2.6)$$

In these expressions Z is the atomic number of the nucleus, n_s the harmonic oscillator quantum number for each shell ($n_s=0,1,2,\dots$) and N_m its value for the highest filled shell. Z_{n_s} is the number of protons in each shell.

The above expression can be extended to the case of open shell nuclei in which the highest shell is partly filled, under the assumption that the protons in the open shell contribute on the average, the same amount as if this shell were completely filled. The corresponding expression for the m.s. radius of the protons is

$$\langle r^2 \rangle_{N_m} = \frac{\hbar}{M\omega} \frac{(N_m + 2)(3Z + v) + 2v}{4Z} \quad (2.7)$$

where N_m is the oscillator quantum number of the highest completely filled shell and v the number of protons in the valence shell. It is seen immediately that for $v=0$ this expression goes over to (2.6).

We may therefore write the approximate expression of the form-factor (2.2) in the case of the simple harmonic oscillator shell model we are discussing in the following form

$$F_{DW}(q) = \exp\left(-\left(\frac{\hbar^2}{M}\right) \left[\frac{(N_m + 2)(3Z + v) + 2v}{24Z}\right] \frac{q^2}{\hbar\omega}\right) \quad (2.8)$$

This expression is of the Debye-Waller type and can be easily used in practice to estimate the point-proton form factor for a variety of nuclei at sufficiently small values of q . The corresponding expression for neutrons is quite analogous.

The oscillator spacing may be found from the "experimental" value of the oscillator parameter $b = (\hbar/M\omega)^{1/2}$, determined either from the experimental m. s. charge radius or from the fitting of the charge form factor to the experimental data of the elastic electron scattering experiments. Alternatively semi-empirical formulae for $\hbar\omega$ may be used for rough estimates, as for example [8]

$$\hbar\omega = 37.48A^{-1/3} - 7.71A^{-1} \quad (2.9)$$

Other possibilities in determining $\hbar\omega$ may be also considered.

Given the point-proton form factor $F(q)$, the charge form factor F_{ch} may be obtained by means of the proton charge form factor f_p and the Tassie-Barker correction [1] $f_{TB} = \exp(b^2 q^2 / 4A)$ for the centre of mass-motion :

$$F_{ch}^{DW}(q) = f_p(q) f_{TB} F_{DW}(q) \quad (2.10)$$

Other corrections should have a small effect to our results and are omitted here. For the proton charge form factor a double-Gaussian parametrization was used [9]

$$f_p(q) = A_{p_1} \exp(-a_{p_1}^2 q^2 / 4) - (A_{p_1} - 1) \exp(-a_{p_2}^2 q^2 / 4) \quad (2.11)$$

where $a_{p_1} = 0.72199$ fm, $a_{p_2} = 0.35246$ fm and $A_{p_1} = 0.63387$. This form factor gives a good fit to the experimental e-p scattering data in a wide range of values of q ($0 < q^2 < 62 \text{ fm}^{-2}$). The value of the m. s. radius of the proton charge distribution, corresponding to this form factor is 0.564 fm^2 .

The approximate expressions F_{DW} and F_{ch}^{DW} given above will be used in the next section for our numerical estimates of the form factors.

3. Numerical results and discussion

In this section we shall obtain the numerical values of the Debye-Waller type form factor for a number of nuclei and we shall compare them with those, obtained with other approximate expressions, as well as with the complete harmonic oscillator expressions.

We consider mainly the nuclei $^{16}_8\text{O}$, $^{28}_{14}\text{Si}$, $^{40}_{20}\text{Ca}$, $^{90}_{40}\text{Zr}$ and calculate the values of point-proton form factor with the expressions (1.4) and (2.8) and also with the approximate expression

$$F_{TCF1} = \frac{1}{1 + \frac{1}{6} \langle r^2 \rangle q^2} \quad (3.1)$$

which is the one-term truncated continuous fraction expansion [2,3]. For the complete harmonic oscillator expression, we use the following one for nuclei with $8 \leq Z \leq 20$

$$F(q) = \left[1 - \frac{8(Z-5)}{3Z}y + \frac{4(Z-8)}{3Z}y^2 \right] e^{-2y} \quad (3.2)$$

where

$$y = \frac{b^2 q^2}{8} \quad (3.3)$$

For heavier nuclei the expression for $F(q)$ becomes more complicated.

It should be noted that expression (3.2), for the open shell nuclei, has been derived with the same simplifying assumption used in the derivation of expression (2.7) for the m.s. radius. The expression resulting by filling first the 1d states [1] differs in the third term in the parenthesis. The difference in the coefficient of q^4 is, however, rather small and it does not have any significant effect in the region of small q values, in which we are interested. The results obtained with expression (2.9) for $\hbar\omega$ are given in tables 1-5 for values of q between 0 and 1 fm^{-1} . Similar are the results if the "experimental" values for the oscillator parameter are used (see table 6 for $^{16}_8\text{O}$ where we used the value $b = 1.687 \text{ fm}$ for the harmonic oscillator parameter [10]).

It is seen from these tables that as long as q is sufficiently small the approximate expressions give reasonable results. It is also seen that among the three expressions that of F_{DW} gives the best results. This is encouraging. The less satisfactory results are obtained with the truncated expression (1.4). The values obtained with this expression begin to deteriorate at smaller values of q , in comparison with the corresponding values pertaining to the other approximate expressions. For sufficiently small values of q , expression (1.4) underestimates the form factor, while (2.8) and (3.1) overestimate. The overestimate of (2.8) is, however, smaller than that of (3.1).

Table 1. Values of the $^{16}_8\text{O}$ point-proton form factor obtained with the complete and approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9892	0.9892	0.9893	0.9893
0.2	0.9576	0.9568	0.9586	0.9577
0.3	0.9068	0.9028	0.9114	0.9073
0.4	0.8398	0.8271	0.8526	0.8412
0.5	0.7600	0.7299	0.7873	0.7633
0.6	0.6715	0.6110	0.7200	0.6778
0.7	0.5786	0.4706	0.6358	0.5889
0.8	0.4853	0.3085	0.5912	0.5008
0.9	0.3952	0.1248	0.5333	0.4168
1.0	0.3113	-0.0805	0.4807	0.3394

Table 2. Values of the $^{28}_{14}\text{Si}$ point-proton form factor obtained with the complete and approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9842	0.9840	0.9843	0.9842
0.2	0.9379	0.9362	0.9400	0.9382
0.3	0.8650	0.8564	0.8744	0.8662
0.4	0.7712	0.7447	0.7966	0.7747
0.5	0.6635	0.6011	0.7149	0.6711
0.6	0.5494	0.4257	0.6352	0.5631
0.7	0.4362	0.2182	0.5612	0.4576
0.8	0.3300	-0.0211	0.4948	0.3602
0.9	0.2357	-0.2923	0.4362	0.2746
1.0	0.1563	-0.5954	0.3853	0.2028

Table 3. Values of the ${}^{40}_{20}\text{Ca}$ point-proton form factor obtained with the complete and approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9809	0.9807	0.9811	0.9809
0.2	0.9254	0.9230	0.9285	0.9259
0.3	0.8389	0.8267	0.8523	0.8409
0.4	0.7292	0.6919	0.7645	0.7348
0.5	0.6060	0.5186	0.6750	0.6179
0.6	0.4790	0.3067	0.5906	0.4999
0.7	0.3573	0.0564	0.5145	0.3892
0.8	0.2482	-0.2325	0.4479	0.2916
0.9	0.1567	-0.5599	0.3906	0.2102
1.0	0.0850	-0.9257	0.3418	0.1458

Table 4. Values of the ${}^{90}_{40}\text{Zr}$ point-proton form factor obtained with the complete and approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9691	0.9687	0.9696	0.9692
0.2	0.8811	0.8748	0.8887	0.8823
0.3	0.7491	0.7182	0.7802	0.7544
0.4	0.5917	0.4991	0.6662	0.6060
0.5	0.4293	0.2173	0.5609	0.4572
0.6	0.2800	-0.1271	0.4701	0.3240
0.7	0.1570	-0.5341	0.3946	0.2156
0.8	0.0668	-1.0038	0.3329	0.1348
0.9	0.0095	-1.5360	0.2828	0.0792
1.0	-0.0196	-2.1309	0.2421	0.0437

Table 5. Values of the $^{208}_{82}\text{Pb}$ point-proton form factor obtained with the approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000
0.1	0.9473	0.9500	0.9487
0.2	0.7893	0.8260	0.8100
0.3	0.5260	0.6784	0.6225
0.4	0.1573	0.5427	0.4305
0.5	-0.3168	0.4316	0.2680
0.6	-0.8962	0.3453	0.1501
0.7	-1.5809	0.2793	0.0757
0.8	-2.3709	0.2288	0.0344
0.9	-3.2663	0.1899	0.0140
1.0	-4.2671	0.1596	0.0052

Table 6 Values of the $^{16}_8\text{O}$ point-proton form factor obtained with the complete and approximate expressions (see text) for various values of q using the "experimental" value for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9881	0.9880	0.9882	0.9881
0.2	0.9532	0.9522	0.9543	0.9533
0.3	0.8973	0.8923	0.9028	0.8979
0.4	0.8241	0.8086	0.8394	0.8258
0.5	0.7376	0.7010	0.7698	0.7415
0.6	0.6427	0.5694	0.6990	0.6501
0.7	0.5444	0.4139	0.6305	0.5565
0.8	0.4471	0.2344	0.5664	0.4651
0.9	0.3549	0.0311	0.5079	0.3795
1.0	0.2709	-0.1962	0.4553	0.3023

Table 7. Values of the $^{16}_8\text{O}$ charge form factor obtained with the complete and approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9888	0.9887	0.9888	0.9888
0.2	0.9557	0.9549	0.9567	0.9558
0.3	0.9029	0.8988	0.9074	0.9034
0.4	0.8333	0.8207	0.8460	0.8347
0.5	0.7508	0.7211	0.7778	0.7541
0.6	0.6599	0.6004	0.7075	0.6660
0.7	0.5651	0.4595	0.6385	0.5751
0.8	0.4705	0.2991	0.5732	0.4856
0.9	0.3801	0.1201	0.5129	0.4009
1.0	0.2968	-0.0767	0.4582	0.3236

Table 8. Values of the $^{40}_{20}\text{Ca}$ charge form factor obtained with the complete and approximate expressions (see text) for various values of q using expression (2.9) for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9802	0.9801	0.9804	0.9802
0.2	0.9229	0.9204	0.9259	0.9233
0.3	0.8336	0.8215	0.8469	0.8356
0.4	0.7211	0.6842	0.7560	0.7267
0.5	0.5955	0.5096	0.6634	0.6072
0.6	0.4671	0.2992	0.5760	0.4876
0.7	0.3454	0.0545	0.4973	0.3762
0.8	0.2375	-0.2224	0.4285	0.2789
0.9	0.1482	-0.5294	0.3694	0.1987
1.0	0.0793	-0.8642	0.3191	0.1361

It is further seen from the numerical results that when the nucleus becomes heavier the region of validity of the approximate expressions has to be restricted to smaller values of q . This, as well as the above mentioned overestimate regarding F_{DW} , are expected on the basis of the remarks made in section 2.

Table 9. Values of the $^{16}_8\text{O}$ charge form factor obtained with the complete and approximate expressions (see text) for various values of q using the "experimental" value for $\hbar\omega$

$q \text{ fm}^{-1}$	$F(q)$	F_{T1}	F_{TCF1}	F_{DW}
0.0	1.0000	1.0000	1.0000	1.0000
0.1	0.9877	0.9876	0.9877	0.9877
0.2	0.9515	0.9505	0.9527	0.9516
0.3	0.8938	0.8888	0.8992	0.8944
0.4	0.8183	0.8029	0.8335	0.8200
0.5	0.7295	0.6933	0.7614	0.7334
0.6	0.6327	0.5605	0.6881	0.6400
0.7	0.5329	0.4051	0.6172	0.5447
0.8	0.4348	0.2280	0.5509	0.4523
0.9	0.3427	0.0300	0.4904	0.3665
1.0	0.2595	-0.1879	0.4362	0.2896

The behaviour of the charge form factors is similar. We give only the results for $^{16}_8\text{O}$ and $^{40}_{20}\text{Ca}$ using expression (2.9) for $\hbar\omega$ (see tables 7,8) and for $^{16}_8\text{O}$ using $b=1.687 \text{ fm}$ (table 9). Expression (2.11) for the proton form factor was used. The Gaussian form factor or the Chandra and Sauer one [11] gave similar results.

We may conclude that Debye-Waller type expressions for the point proton or charge form factors (based on expression (1.1)) are suitable in estimating these form factors in the harmonic oscillator shell model for a variety of nuclei, as long as the momentum transfer is sufficiently small. Their main advantage is their remarkable simplicity.

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