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Nuclear distributions, rms radii and form factors with the harmonic oscillator shell model*

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ABSTRACT : General expressions for calculating nuclear distributions (proton, charge, matter and momentum), mean radii and nuclear form factors are derived by extending recent related works. They are based either on the simple harmonic oscillator shell model or on its modification in which fractional occupation probabilities of the surface orbits are used to fit the experimental elastic electron scattering data. The method is applied to the spherical nucleus ^{40}Ca and the values of the partial occupation probabilities are compared with those determined from experimental reaction data.

1. INTRODUCTION

The distributions of the nuclear charge, momentum and nuclear matter are among the most important nuclear properties. The radial charge distribution is now quite well known [1-3] from model independent analysis of electron-nucleus scattering data (via the nuclear form factors) and very precise measurements of muonic x-ray transitions. Also the most accurately known nuclear-size parameter, the root mean square radius (rms) of the charge distribution along the valley of maximum stability, is extracted from these data. Theoretically, the considered properties are extensively studied [4-15] (the weakness of the interaction and the knowledge of the interaction mechanism being the most significant reason) by using single-particle potential models [4-7] and other self-consistent methods [8-10]. During the last decade the momentum distribution has received much attention on the theoretical side [9,16].

Recently [6,9], the corrections to the single-particle results of the above properties in the nuclear ground state, which come from different sorts of correlations, have been taken into account by assuming fractional occupation probabilities for the valence orbitals in light nuclei [4-6,9] or by including ground state correlations in the closed shell configuration of the ground state [11,12].

In this work, first we derive expressions for the nuclear distributions and the mean square radii similar to those found in ref. [15] for the form factor by using the simple harmonic oscillator shell model. Second we generalize the method of ref. [6] and calculate the nuclear densities and form factors in the framework of this model by assuming however that the surface nucleons of a nucleus are distributed in the valence orbitals (j-levels) with probabilities described by adjustable parameters. With this method we can choose more than two j-levels. The number of the parameters (in this

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work we use three) depends on the assumed model space and can be determined by those bound states for which the experimental data show significant occupancy. Their exact values are determined by fitting to the experimental data of the elastic electron scattering form factor. The method is applied to the double magic nucleus ^{40}Ca and the resulting occupation probabilities are compared with those of ref. [4,5].

2. INDEPENDENT PARTICLE FORMALISM

2.1 Radial charge, matter and momentum distributions

In the framework of the single particle shell model the density distribution $\rho(\vec{r})$ is spherically symmetric for closed (sub)shell nuclei. If we assume that the ground state of such a nucleus (A, Z), is adequately described by a Slater determinant constructed from single particle wave functions, the proton (neutron) distribution is simply the sum of the squares of the point-proton (neutron) wavefunctions. The more interesting radial proton distribution $\rho(r)$ is simply obtained by

$$\rho(r) = \frac{1}{4\pi} \sum_{\substack{(n, l) \\ \text{occupied}}} (2j + 1) |R_{nl}(r)|^2 \quad (1)$$

where $R_{nl}(r)$ is the radial part of the single particle wavefunction with quantum numbers n, l and j . Using the fact that $|R_{nl}(r)|^2$ can be written as the product of $e^{-(r/b)^2}$ times a polynomial of even powers in the quantity (r/b) [13,14], where b is the h.o. parameter, after some further elaboration eq. (1) can be written in the simple form

$$\rho(r) = \frac{1}{\pi^{3/2} b^3} e^{-(r/b)^2} \Pi(Z) \quad (2)$$

with $\Pi(Z)$ being the polynomial

$$\Pi(Z) = \sum_{\lambda=0}^{N_{\max}} f_{\lambda} \chi^{2\lambda}, \quad \chi = r/b \quad (3)$$

In eq. (3) $N_{\max}$ is the number of quanta of the highest occupied proton (neutron) level in the j - j scheme and the coefficients f_{λ} are defined by

$$f_{\lambda} = \sum_{(n, l) \text{ occ.}, \lambda \geq l} \frac{\pi^{1/2} (2j + 1) n! C_{nl}^{\lambda-1}}{2 \Gamma(n+l+3/2)} \quad (3a)$$

where the coefficients $C_{nl}^{\lambda-1}$ are given in appendix A of ref. [15]. The usefulness of eq. (2) becomes more clear by looking at table 1, which gives the exact values of f_λ for all closed (sub)shell nuclei. They are all rational numbers and in the majority they are

Z	Highest occupied j-level	$\lambda=0$	$\lambda=1$	$\lambda=2$	$\lambda=3$	$\lambda=4$	$\lambda=5$
2	0s ^{1/2}	2					
6	0p ^{3/2}	2	8/3				
8	0p ^{1/2}	2	4				
14	0d ^{5/2}	2	4	8/5			
16	1s ^{1/2}	5	0	44/15			
20	0d ^{3/2}	5	0	4			
28	0f ^{7/2}	5	0	4	64/105		
32	1p ^{3/2}	5	20/3	-4/3	176/105		
38	0f ^{5/2}	5	20/3	-4/3	64/3		
40	1p ^{1/2}	5	10	-4	8/3		
50	0g ^{9/2}	5	10	-4	8/3	32/189	
58	0g ^{7/2}	5	10	-4	8/3	32/105	
64	1d ^{5/2}	5	10	8/5	-8/15	16/21	
68	1d ^{3/2}	5	10	16/3	-8/3	16/15	
70	2s ^{1/2}	35/4	0	14	-16/3	4/3	
82	0h ^{11/2}	35/4	0	14	-16/3	4/3	128/3465
92	0h ^{9/2}	35/4	0	14	-16/3	4/3	64/945

Table 1. The exact coefficients f_λ , which give the proton (neutron) density and momentum distributions for all closed (sub)shell nuclei up to ²⁰⁸Pb by using expressions (2), (3), (3a) and (4), are listed in the form of rational numbers.

simple numbers. The sequence of the single particle j-levels assumed (second column in table 1) is that of ref. [13].

It is evident that the determination of the polynomial $\Pi(Z)$ is essential since its knowledge is sufficient in order to find the density distribution (1). Up to now $\Pi(Z)$ have been explicitly calculated [6,7,16] only for light nuclei. The knowledge of coefficients $f_\lambda(Z)$ (table1) enables us to write explicit expressions of the form of eq. (2) for all closed

(sub)shell nuclei of the periodic table. Thus, in the case of ^{90}Zr , for example, we can write simply

$$\rho(r) = \frac{1}{\pi^{3/2} b^3} \left\{ 5 + 10 \left(\frac{r}{b}\right)^2 - 4 \left(\frac{r}{b}\right)^4 + \frac{8}{3} \left(\frac{r}{b}\right)^6 \right\} e^{-(r/b)^2} \quad (3b)$$

The same coefficients f_λ of table 1 can be also used for the calculation of the proton (neutron) momentum distribution which is given by the expression (see ref. [17])

$$\eta(k) = 8 \pi^{3/2} b^3 e^{-(kb)^2} \Pi(Z) \quad (4)$$

(where k is the momentum transfer). For example, the proton (neutron) momentum distribution of ^{16}O , is written as

$$\eta(k) = 8 \pi^{3/2} b^3 e^{-(kb)^2} \left\{ 2 + 4 (kb)^2 \right\} \quad (4a),$$

result compatible with that of ref. [16a] p. 50. (We use the normalization relations of ref. [16a] p. 50 separately for protons and neutrons in $\rho(r)$ and $\eta(k)$. See also ref. [9]).

We should mention that $f_\lambda(Z)$ have been derived under the assumption that the filling numbers of the states for closed (sub)shell nuclei are those predicted by the simple oscillator shell model, namely, $2j+1$ for occupied states and zero for unoccupied ones. In the present work we shall also see how these coefficients can be helpful in order to describe approximately the proton density distribution of all (closed (sub)shell or open (sub)shell) nuclei with fractional occupation numbers of the surface orbits (see section 3 below).

2.2 Mean radii and root mean square radius

The mean radial moment of order m for a nucleus is defined as follows

$$\langle r^m \rangle = \frac{\int_0^\infty \rho(r) r^{m+2} dr}{\int_0^\infty \rho(r) r^2 dr} \quad (5)$$

The simplified form for the radial distribution $\rho(r)$, eq. (2), enables us to write eq. (5) after integration as

$$\langle r^m \rangle = \frac{b^m}{Z} \sum_{\lambda=0}^{N_{\max}} f_\lambda q_\lambda \quad (5a)$$

where

$$q_\lambda = \frac{(2\lambda + 2\mu + 1)!!}{2^{\lambda+\mu}}, \quad m=2\mu \quad \text{and} \quad q_\lambda = 2(\lambda + \mu + 1)!, \quad m=2\mu+1 \quad (5b)$$

(μ is a positive integer). In the case of the mean square radius ($m=2$ and $\mu=1$), which is one of the more interesting radial moments, eq. (5a) takes the simple form

$$\langle r^2 \rangle = \frac{b^2}{Z} \sum_{\lambda=0}^{N_{\max}} f_\lambda \frac{(2\lambda + 3)!!}{2^{\lambda+1}} = b^2 \frac{S}{Z} \quad (5c)$$

where the sum S for all the closed (sub)shell nuclei is an integer number (see table 2).

Z	2	6	8	14	16	20	28	32	38	40	50	58	64	68	70	82	92
S	3	13	18	39	46	60	96	114	141	150	205	249	282	304	315	393	458

Table 2. The integer numbers S of eq. (5) determining the mean square radii for all closed (sub)shell nuclei.

As examples we find using table 2, the root mean square radius of ^{40}Ca , which is $\langle r^2 \rangle^{1/2} = b\sqrt{3}$, and that of ^{90}Zr , which is $\langle r^2 \rangle^{1/2} = b\sqrt{3.75}$.

2.3 Form factors

In the independent particle model the proton and neutron nuclear form factors, which are functions of the square of the momentum (k^2), can be obtained from the radial density (1) by using the relation

$$F(k^2) = 4\pi \int_0^\infty \rho(r) j_0(kr) r^2 dr \quad (6)$$

($j_0(x)$ is the zero order Bessel function). It has been found [15] that for closed (sub)shell nuclei these form factors are given by a simple expression of the form

$$F(k^2) = \frac{1}{Z} e^{-\alpha^2/4} \sum_{\lambda=0}^{N_{\max}} \theta_\lambda \alpha^{2\lambda}, \quad \alpha=kb \quad (7)$$

where the dependence on the momentum k is contained in the parameter α . The coefficients θ_λ are defined in ref. [15] and their exact values are given in table 3. We see that they are also rational numbers as the respective coefficients for $\rho(r)$. Equation (7) can also be written in the form of eq. (2) as

$$F(k^2) = \frac{1}{Z} e^{-\alpha^2/4} \Phi(Z), \quad \Phi(Z) = \sum_{\lambda=0}^{N_{\max}} \theta_{\lambda} \alpha^{2\lambda} \quad (7a)$$

where again the knowlegde of $\Phi(Z)$ is sufficient for the calculation of the form factors $F(k^2)$.

Z	Highest occupied j-level	$\lambda=0$	$\lambda=1$	$\lambda=2$	$\lambda=3$	$\lambda=4$	$\lambda=5$
2	0s ^{1/2}	2					
6	0p ^{3/2}	6	-2/3				
8	0p ^{1/2}	8	-1				
14	0d ^{5/2}	14	-3	1/10			
16	1s ^{1/2}	16	-11/3	11/60			
20	0d ^{3/2}	20	-5	1/4			
28	0f ^{7/2}	28	-9	13/20	-1/105		
32	1p ^{3/2}	32	-11	61/60	-11/420		
38	0f ^{5/2}	38	-14	79/60	-1/30		
40	1p ^{1/2}	40	-15	3/2	-1/24		
50	0g ^{9/2}	50	-65/3	5/2	-5/56	1/1512	
58	0g ^{7/2}	58	-27	33/10	-107/840	1/840	
64	1d ^{5/2}	64	-31	17/4	-173/840	1/336	
68	1d ^{3/2}	68	-101/3	293/60	-31/120	1/240	
70	2s ^{1/2}	70	-35	21/4	-7/24	1/192	
82	0h ^{11/2}	82	-45	29/4	-73/168	37/4032	-1/27720
92	0h ^{9/2}	92	-160/3	107/12	-31/56	151/12096	-1/15120

Table 3. The exact coefficients θ_{λ} , which determine the proton and neutron form factors for all closed (sub)shell nuclei up to ²⁰⁸Pb by using eq. (7).

At this point we should mention several corrections that have to be made to the simple formalism described in this section. They are the corrections inserted if we take into account: (i) the nucleon finite size, (ii) the center of mass motion and (iii) relativistic

effects. As it was shown in ref. [6,18] these corrections significantly improve the results obtained with eqs. (2) and (7). We shall not discuss this point any further here (see ref. [17]). However, we must stress that, if we take into account the finite size of the nucleon and the centre of mass motion by using the folding method, we can obtain similar expressions to those of eqs. (2) and (7a) for $\rho(r)$ and $F(k^2)$, respectively, but in this case we need more coefficients f_λ and θ_λ in order to describe the polynomials $\Pi(Z)$ and $\Phi(Z)$. Also the definitions of f_λ and θ_λ are more complicated [15,17].

3. STUDY WITH PARTIAL OCCUPATION PROBABILITIES

In the previous section we assumed that the occupation probabilities of the states are unity ($a_{nlij} = 1$) for states below the Fermi level and zero above it (mean field approximation). It is well known that even the spherical nuclei ^{16}O and ^{40}Ca do not have good closed shells. In this section we will exploit the form of eqs. (2), (4) and (7a) in order to construct general expressions for calculating the nuclear (proton and neutron) distributions (charge density and momentum), form factors and rms charge radii in the case when the filling numbers of the states are not integers.

In this way we include to some extent configuration mixing and various sorts of correlations by inserting a number of parameters describing the occupation numbers of the surface levels.

This method generalizes the approach, which has been developed [6] in the framework of shell model with harmonic oscillator potential by introducing fractional occupation probabilities to the surface orbits for light nuclei up to ^{48}Ca . The parameters are chosen, as usually, so that some observed nuclear properties are reproduced. This is done here by first taking occupation probabilities from one-nucleon transfer reactions (see ref. [4-7]) and then making any necessary adjustments in order to obtain agreement with the experimental data for the charge form factor.

In the general case, even when there are not closed (sub)shells, we can make the following approximation for the average total density (see e.g. ref. [9])

$$\rho(r) = \frac{1}{4\pi} \sum_{\text{all } (n,l,j)} (2j+1) a_{nlij} |R_{nlij}|^2 \quad (8)$$

where a_{nlij} are the proton (neutron) occupation probabilities for the orbit characterized by the quantum numbers n, l, j . The sum in eq. (8) runs over all the quantum numbers (n, l, j) of the single particle states. For the orbits below the Fermi level of the nucleus, the "core-orbits", $a_{nlij} = 1$ i.e. they are equal to the simple shell model predictions, but for the active (surface) orbits $a_{nlij} < 1$. Also $a_{nlij} \neq 0$ for some orbits above the Fermi level. The following sum-rules hold:

$$\sum_{(n,l) \text{ j closed.}} (2j+1) = \sum_{\text{all } (n,l) \text{ j}} (2j+1) a_{nlj} = Z \quad (8a)$$

The differences of a_{nlj} from 0 or 1 is an indication of how realistic is the used single particle potential model. The fractional filling numbers $(2j+1) a_{nlj}$, of each state are known from experimental data.

From the data of tables 1 and 2 and from the eqs. (2), (4), (5c) and (7a) we shall derive now simple parametric expressions with one, two or three parameters, describing the deviation of filling numbers from those of the simple shell model ones.

For simplicity we consider as a first example the case where only two filling numbers of the states are not integers i.e. 1) the highest occupied near the Fermi surface j -level, which according to the simple shell model is fully occupied and 2) the first above it, which according to the simple shell model is empty. In order to find the one-parameter formula for every closed (sub)shell nucleus (A,Z) , which contains as special cases the results of ref. [6] for light nuclei, we must use the polynomials $\Pi(Z)$ giving the density of three adjacent closed (sub)shell nuclei i.e. the considered nucleus and two more with:

a) $Z_1 < Z$ (which has as upper occupied level the one lying just below the Fermi level of the nucleus in question) and

b) $Z' > Z$ (which has as upper occupied level the one lying just above the Fermi level of the nucleus in question).

For nuclei with $20 \leq Z \leq 28$, for example, we must use the polynomials $\Pi(Z_1=16)$, $\Pi(Z_c=20)$ and $\Pi(Z'=28)$ for the density $\rho(r)$ (and momentum distribution $\eta(k)$), the polynomials $\Phi(Z_1=16)$, $\Phi(Z_c=20)$ and $\Phi(Z'=28)$ for the form factor and the sums $S(Z_1=16)$, $S(Z_c=20)$ and $S(Z'=28)$ for the mean square radius of the (point) proton distribution. The result for the density can be written as

$$\Pi(Z, \alpha_1) = \Pi(Z_1) + [\Pi(Z_c) - \Pi(Z_1)] \frac{Z_c - Z_1 - \alpha_1}{Z_c - Z_1} + [\Pi(Z') - \Pi(Z_c)] \frac{Z - Z_c + \alpha_1}{Z' - Z_c} \quad (9)$$

where the two last terms in eq. (9) give the contribution of the active (surface) levels with occupation numbers $Z_c - Z_1 - \alpha_1$ and $Z - Z_c + \alpha_1$ respectively. We give here as an example, the relevant expressions for ^{40}Ca . For the density $\rho(r)$ the polynomial $\Pi(Z)$ is

$$\Pi(Z=20, \alpha_1) = 5 + \frac{60 - 4\alpha_1}{15} \left(\frac{r}{b}\right)^4 + \frac{8\alpha_1}{105} \left(\frac{r}{b}\right)^6 \quad (10.a)$$

For the form factor the polynomial $\Phi(Z)$ is

$$\Phi(Z=20, \alpha_1) = 20 - \frac{30 + \alpha_1}{6} (kb)^2 + \frac{15 + 2\alpha_1}{60} (kb)^4 - \frac{\alpha_1}{840} (kb)^6 \quad (10.b)$$

Eqs. (3)-(11) of ref. [6] can be derived from our general eqs. (2), (5c), (7a) and the parametric eq. (9) if we use the sequence of the j-levels used in ref. [6]. For example, for the derivation of eq. (3) of ref. [6] for the density of ^{16}O , we must use the polynomials $\Pi(Z_1=6)$, $\Pi(Z_c=8)$ and $\Pi(Z'=10)$, which correspond to the sequence of j-levels: $0s^{1/2}$, $0p^{3/2}$, $0p^{1/2}$, $1s^{1/2}$, $0d^{5/2}$, of the work of Gul'karov et al. [6]. From eqs. (3) and (3a) above we find [17]: $\Pi(Z'=10) = 5 + (4/3) \chi^4$, which, by using eq. (9), gives the eq. (3) of ref. [6].

The important possibility offered by eqs. (2), (5), (7) and (9) is the construction of two, three et.c. parametric equations describing the properties discussed in section 2 for a closed (sub)shell nucleus by means of the fractional occupation probabilities of the j-orbitals. We assume now that the surface nucleons of such a nucleus are spread in four partially occupied j-levels: two below the Fermi surface and two above it. Then the three-parametric expression which describes the proton density of the nucleus is given by eq. (2) with $\Pi(Z)$ given by

$$\begin{aligned} \Pi(Z, \alpha_1, \alpha_2, \alpha_3) = & \Pi(Z_2) \frac{\alpha_1}{Z_1 - Z_2} + \Pi(Z_1) \left[\frac{\alpha_2}{Z_c - Z_1} - \frac{\alpha_1}{Z_1 - Z_2} \right] + \Pi(Z_c) \left[\frac{Z' - Z}{Z' - Z_c} - \frac{\alpha_2}{Z_c - Z_1} - \frac{\alpha_3}{Z' - Z_c} \right] + \\ & + \Pi(Z') \left[\frac{Z - Z_c}{Z' - Z_c} + \frac{\alpha_3}{Z' - Z_c} - \frac{\lambda}{Z' - Z'} \right] + \Pi(Z'') \frac{\lambda}{Z'' - Z'} \end{aligned} \quad (11)$$

($\lambda = \alpha_1 + \alpha_2 - \alpha_3$) where the parameters α_i give the depletion of states below the Fermi surface ($(2j+1) - \alpha_i = (2j+1)a_{nlij}$) and the occupation numbers above it ($\alpha_i = (2j+1)a_{nlij}$). Also $Z_2 < Z_1 < Z_c < Z' < Z''$ for the adjacent Z-closed levels ($Z_c < Z < Z'$). The same expressions hold for the $\Phi(Z)$ giving the form factors and $S(Z)$ giving the mean square radii.

Expressions (2), (5), (7), (9) and (11) can be used approximately even for nearly closed (sub)shell nuclei. Also the nucleon momentum distribution $\eta(k)$ for spherically symmetric systems is given by means of expressions similar to (9) and (11).

4. RESULTS AND DISCUSSION

The method described above was applied to the core nucleus ^{40}Ca . We assume that the surface protons for ^{40}Ca are distributed on the $1s^{1/2}$, $0d^{3/2}$, $0f^{7/2}$, and $1p^{3/2}$, (sub)shells which are partially occupied. We use eq. (11) in order to obtain the polynomials $\Pi(Z)$ containing the parameters α_1 , α_2 , α_3 which describe the fractional occupation probabilities of these four levels and we determine the parameters by fitting to the charge form factor $F(k^2)$. The result for the charge density distribution of ^{40}Ca as a function of r is shown and compared with the available experimental data on the nuclear charge density in fig. 1. The agreement is very good with the values of the occupation numbers for the active levels shown in table 4. The rms radius, which

essentially determines the h.o. parameter b ($b = 1.998 \text{ fm}^{-1}$), is equal to $\langle r^2 \rangle^{1/2} = 3.4803 \text{ fm}$ i.e. equal to the experimental value [10].

Fig. 1. Plot of the proton density distribution in ^{40}Ca as calculated with the simple harmonic oscillator shell model (dashed-line) and with eq. (11) by assuming fractional occupation probabilities (solid line). The experimental data (circles) of ref. [10] are also shown.

The occupation numbers found together with the experimental ones are listed in table 4. We can see that the values of the parameters α_2 and α_3 are in good agreement with the experimental values [4,5], but the value of α_1 we found is larger than the corresponding experimental one. This also affects the occupation probability of the $1p_{3/2}$ shell for which our results show that it is 15% occupied while in ref. [4,5] it was found to be 4.3% occupied.

Orbital	$(2j+1)a_{nll}$ Exp.	$(2j+1)a_{nll}$ Th.
$1p_{3/2}$	0.15	0.60
$0f_{7/2}$	0.56	0.75
$0d_{3/2}$	3.59	3.75
$1s_{1/2}$	1.70	1.35

Table 4. Experimental and theoretical occupation numbers for the active levels of ^{40}Ca .

In ref. [6] only one parameter was used and it was determined from the value of $\rho(r)$ in the centre of the nucleus although in this region the experimental uncertainty of $\rho(r)$

is large. As it is obvious from eqs. (10a) and (10b) none of α_i can be determined in this way.

In fig. 2 the calculated elastic charge form factor for ^{40}Ca as a function of the momentum transfer k is shown. For comparison the results obtained by putting $\alpha_i=0$ i.e. the simple shell model results (dashed line) are also shown. The improvement because of the fractional occupation probabilities is obvious. Beyond $k \approx 3.0 \text{ fm}^{-1}$ our results predict another diffraction minimum, not predicted by the simple shell model but existing in the experimental data though in a different position. The elastic electron scattering experimental data shown are from ref. [10].

Fig. 2. Plot of the elastic charge form factor for ^{40}Ca as calculated from the simple shell model (dashed-line) and assuming fractional occupation probabilities (solid line). The prediction of the third minimum by our method is evident. The experimental data shown (circles) are from ref. [10].

We note that in calculating the quantities $\rho(r)$ and $F(k^2)$, the finite proton size and centre of mass corrections have not been taken into account.

5. CONCLUSIONS

In the present work we have calculated the coefficients f_λ (eq. (3) and (3a)) and θ_λ (eq.(7)), which give the proton and neutron nuclear densities, rms radii and form factors

for all closed (sub)shell nuclei in the harmonic oscillator shell model. With the aid of them we generalized the method of calculating nuclear densities and form factors of ref. [6]. This method takes into account approximately the different sorts of correlations and configuration mixing found in many nuclei, by assuming fractional occupation probabilities of the states.

The calculation of the charge density distribution and charge form factor of the ^{40}Ca , gives good results for low and medium momentum transfers, but for $k \geq 3.0 \text{ fm}^{-1}$ various sorts of correlations must be explicitly introduced [9,12,16].

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