Theoretical Evaluation of Neutron-nucleus Scattering Parameters from Experimental Data in the $6 \leq A < 60$ Mass Region

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Systematic calculations of the neutron-nucleus scattering parameters at several neutron energies $E_i < 2$ keV have been performed for 37 isotopes (^{6}Li, ... ^{59}Co) in the mass region of $6 \leq A < 60$, using the large compilation of experimental neutron-nucleus scattering data obtained in Garching. In the first stage of these calculations, the s-wave potential scattering radius R', the scattering lengths b_{coh}, $b_{\pm}$, and the bound state parameters (E_{b}, $\Gamma_{\gamma\mathrm{r}}$, $g\Gamma_{\mathrm{n}}^0$) have been calculated for each isotope, employing the general least squares fit (GLSQF) for the experimental and the corresponding theoretical values of the total neutron-nucleus cross sections $\sigma_{\mathrm{tot}}^{\mathrm{exp}}(E_i)$ at several energies E_i, absorption cross sections $\sigma_{\mathrm{abs}}(E_0)$ and of the coherent scattering lengths b_{coh}. The theoretical expressions for these parameters were deduced on the basis of the usual S-matrix formalism with no assumption about the particular shape of the optical model potential. In the second stage of our calculations, the spherical Fiedeldey-Frahn optical potential was employed for the pure theoretical description or the above mentioned neutron-nucleus scattering characteristics. The results obtained have been analyzed and compared with the values deduced from measurements.

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1. Introduction

Neutron-nucleus potential scattering radii, scattering lengths, and total and absorption cross sections are important quantities for the interpretation of slow neutron scattering experiments, which are common methods for fundamental research in physics and other disciplines, for instance, for the investigation of structure and dynamics of condensed matter. The scattering length is the basic quantity to describe the strength of neutron-nucleus interaction at low energies. The values of scattering lengths vary irregularly from one nucleus to another. This effect is due to a strong dependence on specific features of the nuclear structure. – On the other hand, free potential scattering radii being of fundamental interest for the theory of optical nuclear model can be deduced from coherent scattering lengths by subtracting resonance contributions. The values of potential scattering radii increase with the nuclear mass number. The size and systematics are predictions for the optical model.

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Directly measurable quantities are the bound coherent scattering length $b_{\mathrm{coh}}(E_{00})$ near to zero neutron energy $E_{00} = 0.00053$ eV and the neutron total transmission cross section $\sigma_{\mathrm{tot}}^{\mathrm{exp}}(E_i)$. These quantities were systematically determined with high precision during nearly two decades at the FRM research reactor in Garching. Data were obtained for elements and isotopes with $3 \leq Z \leq 90$ and were compiled together with available scattering lengths data given by other authors and using other methods in [1]. The scattering lengths were measured by small angle scattering with Christiansen filter technique, and more accurately with the gravity refractometer. The total cross sections were determined from transmission measurements of quasi-monoenergetic neutron beams with energies $E_i \leq 2$ keV, where resonance absorption [2], resonance scattering [3] and resonance filter techniques [4] were used. In some cases, the absorption cross sections $\sigma_{\mathrm{abs}}^{\mathrm{exp}}(E_0)$ ($E_0 = 0.0253$ eV) were deduced from transmission measurements with cold neutrons [5].

The obtained $\sigma_{\mathrm{tot}}^{\mathrm{exp}}(E_i)$, $\sigma_{\mathrm{abs}}^{\mathrm{exp}}(E_0)$ and b_{coh} values, together with the compiled resonance parameters from [6], form a complete set of input parameters neces-

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sary for the neutron-nucleus strong interaction scattering radii $R'(j)$ evaluation. Moreover, the precise experimental data obtained in [1] allow to check the completeness of the resonance data given in [6] and fully describe the neutron-nucleus interaction over a wide neutron energy range. In many cases new bound level parameters must be fitted to obtain a consistent data set.

In most cases, accurate and reliable values are needed as input data not just for elements but also for separated isotopes. Using fitted neutron-nucleus scattering parameters for 38 isotopes with $6 \leq A < 60$ and completed resonance data and cross sections for natural targets given in [1, 6], total and absorption cross sections have been calculated for corresponding energies E_i for each stable isotope j of the targets considered. These results are given in Section 2.

In the second stage of our calculations, described in Section 3, we have used the optical potential model suggested by Fiedeldey and Frahn [7]. The model parameters were determined from the fit of obtained theoretical total cross sections to the isotopic total cross sections calculated in Section 2. Then, the obtained optical model parameters were used for the evaluation of the scattering radii $R'(j)$.

2. Evaluation of Neutron-nucleus Scattering Parameters in the Frame-work of *S*-matrix Formalism

In order to evaluate the neutron-nucleus strong interaction scattering radii $R'(j)$ and the corresponding bound level parameters, i. e. negative resonance energy $E_b(j)$, gamma and neutron widths $\Gamma_{\gamma b}$ and $\Gamma_{\gamma b}(j)$, the directly measured values of the total cross sections $\sigma_{tot}^{exp}(E_i)$ for natural targets, absorption cross sections $\sigma_{abs}^{exp}(E_0)$ and the bound coherent scattering lengths $b_{coh}(E_{00})$ must be connected to those parameters.

The total cross section for a target $\sigma_{tot}^{calc}(E_i)$ can be calculated by adding up the total cross section $\sigma_{tot}^{calc}(j, E_i)$ for a particular isotope j weighted by the abundance p_j of isotopes in the target:

$$\sigma_{tot}^{calc}(E_i) = \sum_j p_j \sigma_{tot}^{calc}(j, E_i). \tag{1}$$

The total cross section for the separated isotope can be composed as

$$\begin{aligned}\sigma_{tot}^{calc}(j, E_i) = \sigma_s^{calc}(j, E_i) + \sigma_{abs}^{calc}(j, E_i) \\ + \sigma_{LS}^{calc}(j, E_i) + \sigma_{sol}^{calc}(j, E_i),\end{aligned} \tag{2}$$

where $\sigma_s^{calc}(j, E_i)$ is the elastic scattering cross section calculated from the S-matrix formalism, $\sigma_{abs}^{calc}(j, E_i)$ is the absorption term and $\sigma_{LS}^{calc}(j, E_i)$, $\sigma_{sol}^{calc}(j, E_i)$ are small contributions from spin orbital (Schwinger) scattering and solid-state effect cross sections, calculated according to [8].

In the low energy region it is sufficient to perform calculations only for s-partial wave total cross sections, so $\sigma_s^{calc}(j, E_i)$ were taken from [8, 9] as

$$\begin{aligned}\sigma_s^{calc}(j, E_i) = \frac{\pi}{k_i^2}\Big(4\sin^2\delta(j, E_i) - 2\Sigma_1 \sin^2\delta(j, E_i) \\ - 4\Sigma_2 \sin^2\delta(j, E_i) + \Sigma_3 + \Sigma_4\Big),\end{aligned} \tag{3}$$

where k_i is the neutron wave number at energy E_i and $\delta(j, E_i)$ is the total s-wave scattering phase shift, consisting here of strong and neutron-electron terms:

$$\begin{aligned}\delta(j, E_i) = -k_i\Big(R'(j) + Z(j) b_{ne} \frac{A(j)}{A(j) + M_n} \\ \cdot \big(F(j, E_i) - H(j, E_i)\big)\Big),\end{aligned} \tag{4}$$

where $Z(j)$ and $A(j)$ denote the nucleus charge and the atomic mass number of isotope j, respectively. The angular averaged atomic form factor $F(j, E_i)$ and the nuclear charge form factor $H(j, E_i)$ were taken from [10]. For the neutron-electron scattering length the numerical value $b_{ne} = -1.32 \cdot 10^{-3}$ fm (obtained in Garching) was assumed, having the best experimental confirmation (see e. g. [10]). The Garching b_{ne} value also gives a neutron mean square charge radius which agrees better with the majority of the theoretical predictions (see [8]).

The statistically weighted resonance sums $\sum_1$, $\sum_2$ and $\sum_3$, $\sum_4$ are given as

$$\begin{aligned}\sum_{1,2} &= g_+(j)\sum_{1,2}^{+} + g_-(j)\sum_{1,2}^{-}, \\ \sum_{3,4} &= g_+(j)\Big(\sum_{1,2}^{+}\Big)^2 + g_-(j)\Big(\sum_{1,2}^{+}\Big)^2,\end{aligned} \tag{5}$$

where $g_\pm(j)$ denotes the spin statistical factors of the j-th isotope with the nuclear spin $I(j)$:

$$g_+(j) = \frac{I(j) + 1}{2I(j) + 1}, \quad g_-(j) = \frac{I(j)}{2I(j) + 1}. \tag{6}$$

In the low energy region, where resonances are usually well-resolved, the sums $\sum_1^{\pm}$ and $\sum_2^{\pm}$ can be expressed as

$$\sum_1^{\pm} = \sum_{r=m+1}^{\pm} \frac{k_i}{k_r} \frac{\Gamma_{nr}(E_i - E_r)}{(E_i - E_r)^2 + \frac{\Gamma_r^2}{4}} + \sum_{r=1}^{m\pm} \frac{k_i}{k_b} \frac{\Gamma_{nb}(E_i - E_b)}{(E_i - E_b)^2 + \frac{\Gamma_b^2}{4}}, \tag{7}$$

$$\sum_2^{\pm} = \sum_{r=m+1}^{\pm} \frac{k_i}{k_r} \frac{\Gamma_{nr}\Gamma_{\gamma r}/2}{(E_i - E_r)^2 + \frac{\Gamma_r^2}{4}} + \sum_{r=1}^{m\pm} \frac{k_i}{k_b} \frac{\Gamma_{nb}\Gamma_{\gamma b}/2}{(E_i - E_b)^2 + \frac{\Gamma_b^2}{4}}, \tag{8}$$

where m is the number of bound levels (at negative energy E_b), $\Gamma_r = \Gamma_{nr} + \Gamma_{\gamma r}$ is the width for a resolved resonance, and $\Gamma_b = \Gamma_{nb} + \Gamma_{\gamma b}$ is the width for a bound level. The summation must be carried out over all resolved resonance states of the compound nucleus with defined spin value ($\sum^+$ for $J = I + {}^1/_2$ and $\sum^-$ for $J = I - {}^1/_2$) for each isotope j.

A fundamental remark as to bound levels concerns their number: there is no doubt that several bound levels exist but normally they lie far away below zero energy so that their individual energy influence cannot be resolved even by very precise cross section measurements in the eV-region. Therefore it is usual to summarize all bound levels to a fictive single level which describes well the interaction properties in the low energy range. Only in a few cases (for instance Th), two bound levels are resolved because of their close distance to zero energy.

For the mass region of $6 \leq A < 60$ it is not necessary to take into account the small contribution of unresolved resonances in the high energy region. The resonance energy E_r, reduced neutron width $\Gamma_{nr}^0 = \Gamma_{nr}/\sqrt{E_r}$, gamma-absorption width $\Gamma_{\gamma r}$, and compound spin J were inserted in (7) and (8) as they are listed in [6]. The bound level parameters E_b, Γ_{nb} and $\Gamma_{\gamma b}$ were fitted in order to achieve better agreement with new experimental data.

According to [9], the absorption cross section is written as

$$\sigma_{abs}^{calc}(j, E_0) = g_+(j)\sigma_{abs}^{calc}(j, E_0)^+ + g_-(j)\sigma_{abs}^{calc}(j, E_0)^-, \tag{9}$$

where

$$\sigma_{abs}^{calc}(j, E_0)^{\pm} = \pi \sum_{r=m+1}^{\pm} \frac{1}{k_r k_0} \frac{\Gamma_{nr}\Gamma_{\gamma r}}{(E_0 - E_r)^2 + \frac{\Gamma_r^2}{4}} + \pi \sum_{r=1}^{m\pm} \frac{1}{k_b k_0} \frac{\Gamma_{nb}\Gamma_{\gamma b}/2}{(E_0 - E_b)^2 + \frac{\Gamma_b^2}{4}}. \tag{10}$$

k_r, k_b and k_0 are the neutron wave numbers at energies E_r, E_b and E_0, respectively.

Since bound coherent scattering lengths were measured very close to zero energy ($E_{00} = 0.00053$ eV), it is possible to express them via the real part of the total scattering amplitude at the same energy in the following way:

$$b_{coh}^{calc}(j, E_{00}) = -\mathrm{Re}\, f(j, E_{00}) \frac{A(j)}{A(j) + M_n}, \tag{11}$$

where

$$\mathrm{Re}\, f(j, E_{00}) = g_+ \mathrm{Re}\, f^+(j, E_{00}) + g_- \mathrm{Re}\, f^-(j, E_{00}) \tag{12}$$

and $\mathrm{Re}\, f^{\pm}(j, E_{00})$ according to [9, 10] is given as

$$\mathrm{Re}\, f^{\pm}(j, E_{00}) = \frac{1}{2k_{00}} \left((1 - \Sigma_2^{\pm}) \sin 2\delta(j, E_{00}) - \Sigma_1^{\pm} \cos 2\delta(j, E_{00}) \right). \tag{13}$$

In addition, the spin state scattering lengths can be calculated as

$$b_{\pm}(j, E_{00}) = -g_{\pm} \mathrm{Re}\, f^{\pm}(j, E_{00}) \frac{A(j)}{A(j) + M_n}, \tag{14}$$

The approach used in the present work in order to evaluate the neutron-nucleus strong interaction scattering radii $R'(j)$ and the corresponding bound level parameters (resonance energy $E_b(j)$, gamma and neutron widths $\Gamma_{\gamma b}$ and Γ_{nb}), is based on the simultaneous minimization of the following equations for theoretical and the experimental neutron transmission characteristics:

$$\sum_i \left[\sigma_{tot}^{calc}(E_i) - \sigma_{tot}^{exp}(E_i) \right]^2 = \min, \tag{15}$$

$$\sum_j \left[\sigma_{abs}^{calc}(j, E_0) - \sigma_{abs}^{exp}(j, E_0) \right]^2 = \min, \tag{16}$$

Table 1. Experimental and calculated values of total and absorption cross sections (in barns).

Z	Isotope	p	— Total cross sections $\sigma_{tot}(E_i)$ —										Absorption cross section $\sigma_{abs}(E_i)$	
			E_i = 1.26 [eV]		E_i = 5.19 [eV]		E_i = 18.6 [eV]		E_i = 128 [eV]		E_i = 1970 [eV]		E_0 = 0.025 [eV]	
			σ_{tot}^{exp}	σ_{tot}^{calc}	σ_{tot}^{exp}	σ_{tot}^{calc}	σ_{tot}^{exp}	σ_{tot}^{calc}	σ_{tot}^{exp}	σ_{tot}^{calc}	σ_{tot}^{exp}	σ_{tot}^{calc}	σ_{tot}^{WW}	σ_{tot}^{calc}
3	^{nat}Li		8.1(7)	8.1	4.6(4)	4.6							71(2)	35.77
	^{6}Li	7.50		95.98		48.51							940(4)	481.56
	^{7}Li	92.50	1.07(4)	1.09	1.10(4)	1.08							0.0454(30)	0.0436
7	^{nat}N		10.05(5)	10.04	10.02(9)	10.03							0.0747(7)	0.0750
	^{14}N	99.63		10.059		10.051							0.0750(8)	0.0750
	^{15}N	0.37		4.608		4.608							0.024(8)	0.024
9	^{19}F	100	3.63(2)	3.63	3.65(1)	3.64							0.0096(5)	0.0096
11	^{11}Na	100	3.10(4)	3.10	3.06(3)	3.06							0.530(5)	0.530
12	^{nat}Mg		3.421(4)	3.420	3.417(4)	3.420							0.063(3)	0.018
	^{24}Mg	78.99		3.700		3.703								0.003
	^{25}Mg	10.00		1.841		1.832								0.159
	^{26}Mg	11.01		2.823		2.826								–
13	^{27}Al	100	1.445(1)	1.432	1.429(1)	1.425							0.321(3)	0.114
14	^{nat}Si		2.065(2)	2.067	2.058(2)	2.056							0.171(3)	0.168
	^{28}Si	92.23		2.024		2.013							0.177(5)	0.117
	^{29}Si	4.67		2.485		2.487							0.101(14)	0.101
	^{30}Si	3.10		2.625		2.620							0.107(2)	–
15	^{31}P	100	3.267(16)	3.267	3.239(11)	3.239							0.172(2)	0.172
16	^{nat}S		1.052(2)	1.050	1.021(2)	1.014							0.52(1)	0.52
	^{32}S	95.02		1.020		0.983							0.53(4)	0.53
	^{33}S	0.75		2.472		2.447							0.35(4)	0.35
	^{34}S	4.21		1.483		1.468							0.224(5)	0.227
17	^{nat}Cl		20.24(3)	20.14	16.90(8)	16.99							33.1(3)	33.0
	^{35}Cl	75.77		26.24		22.10							43.6(4)	43.61
	^{37}Cl	24.23		1.29		1.26							0.433(6)	0.437
21	^{45}Sc	100	25.04(3)	25.04	22.83(5)	22.83	64.5(3)	20.83	13.53(2)	13.53	0.413(8)	0.206	27.2(2)	24.9
22	^{nat}Ti		4.746(6)	4.735	4.273(6)	4.294	4.081(6)	4.095	4.021(6)	3.996	5.167(17)	5.095	6.09(13)	6.08
	^{46}Ti	7.93		2.922		2.883		2.861		2.814		2.321	0.6(2)	0.6
	^{47}Ti	7.28		3.341		3.221		3.156		3.032		2.654	1.7(2)	1.7
	^{48}Ti	73.94		5.379		4.811		4.556		4.446		5.972	7.8(3)	7.94
	^{49}Ti	5.51		0.873		0.715		0.638		0.574		1.468	2.2(3)	2.2
	^{50}Ti	5.34		4.404		4.396		4.390		4.372		4.145	0.179(3)	0.179
23	^{nat}V		5.527(7)	5.519	5.168(6)	5.174	4.992(5)	5.019	4.997(5)	4.969	7.609(12)	7.610	5.08(4)	4.76
	^{50}V	0.25		7.359		2.742		1.122		5.829		10.701	60(40)	58
	^{51}V	99.75		5.515		5.180		5.029		4.968		7.602	4.9(1)	4.635
24	^{nat}Cr		3.817(10)	3.817	3.59(1)	3.604							3.07(8)	3.069
	^{50}Cr	4.35		5.005		3.881							15.9(2)	15.9
	^{52}Cr	83.79		3.151		3.101							0.76(6)	0.76
	^{53}Cr	9.50		9.430		8.153							18.2(15)	18.2
	^{54}Cr	2.36		2.679		2.659							0.36(4)	0.36
25	^{55}Mn	100	3.929(20)	3.907	3.001(30)	3.056	2.985(31)	2.931	6.80(15)	6.81	120(5)	113.3	12.5(4)	12.9
27	^{59}Co	100	11.23(4)	11.24	8.68(5)	8.73							37.18(6)	36.01

$$\sum_j \left[\frac{A(j) + M_n}{A(j)} \mathrm{Re}\, f(j, E_{00}) + b_{coh}^{exp}(j, E_{00}) \right]^2 = \min, \tag{17}$$

where the index i assumes the values i = 1,...,5 for the monochromatic neutron energies E_i = 1.26, 5.19, 18.6, 128, and 1970 eV used in the Garching experiments. The minimization procedure was performed according to Levenberg-Marcardt method of iterations. The measured $\sigma_{tot}^{exp}(E_i)$, $\sigma_{abs}^{exp}(j, E_0)$, $b_{coh}^{exp}(j, E_{00})$ taken from [1, 11], and some additional data of the nucleus resonance parameters compiled in [6] form the set of input data used in our fit according to (15) - (17). The evaluations were carried out for each target separately.

The results of the neutron-nucleus scattering parameter calculations for 38 isotopes (^{6}Li,... ^{59}Co) in

Table 2. Experimental and calculated bound coherent scattering lengths (in fm), at neutron energy E_{00} = 0.00053 [eV].

Z	Isotope	I	b_{coh}^{exp}	b_{coh}^{calc}	b_{+}^{calc}	b_{-}^{calc}	b_{coh}^{Mugh}	b_{+}^{Mugh}	b_{-}^{Mugh}
3	^{nat}Li		−1.90(3)				−1.95(3)		
	^{6}Li	1	2.0(1)	2.00	1.095	2.563	2.2	0.87	4.7
	^{7}Li	3/2	−2.22(2)	1.69[a]	0.961	2.326	−2.29	−3.98	0.52
6	^{nat}C		6.648(4)				6.6484(13)		
	^{12}C	0	6.6535(14)	6.653	6.142	–	6.6535(14)		
	^{13}C	1/2	6.19(9)	6.19	5.602	6.173	6.19(9)	5.47(9)[b]	6.59(36)[b]
7	^{nat}N		9.36(3)				9.36(2)		
	^{14}N	1	9.37	9.37	10.67	6.20	9.37(2)	10.1(2)[b]	6.2(3)[b]
	^{15}N	1/2	6.44	6.44	6.77	6.21	6.44(3)	6.32	6.73
8	^{nat}O		5.805(4)				5.805(4)		
	^{16}O	0	5.805(5)	5.805	5.466	–	5.805(5)		
	^{17}O	5/2	5.62(45)	5.69	5.524	5.169	5.66(5)	5.54(7)[b]	5.11(17)[b]
	^{18}O	0	5.84(7)	5.84	5.533	–	5.87(7)		
9	^{19}F	1/2	5.654(12)	5.64	5.32	5.5	5.654(10)	5.35(2)[b]	5.48(2)[b]
11	^{11}Na	3/2	3.63(2)	3.63	5.87	−0.57	3.63(2)	6.18(4)[b]	−0.930(60)[b]
12	^{nat}Mg		5.376(20)				5.376(20)		
	^{24}Mg	0	5.67(3)[c]	5.640	5.413	–	5.67(3)		
	^{25}Mg	5/2	3.64(14)[c]	3.644	4.730	1.764	3.64(14)	3.72	3.48
	^{26}Mg	0	4.91(15)[c]	4.913	4.720	–	4.91(15)		
13	^{27}Al	5/2	3.449(9)	3.46	3.21	3.51	3.449(1)	3.58(2)[b]	3.01(2)[b]
14	^{nat}Si		4.152(15)				4.1491(10)		
	^{28}Si	0	4.106(6)	4.106	3.961	–	4.106(6)		
	^{29}Si	1/2	4.70(10)	4.718	4.500	4.670	4.70(10)	3.98(15)[b]	6.41(37)[b]
	^{30}Si	0	4.58(8)	4.582	4.450	–	4.58(8)		
15	^{31}P	1/2	5.13(1)	5.13	4.43	5.023	5.13(1)		
16	^{nat}S		2.847(1)				2.85(1)		
	^{32}S	0	2.804(2)	2.81	2.72	–	2.804(2)		
	^{33}S	3/2	4.47(19)	4.47	3.91	5.05	4.76(19)		
	^{34}S	0	3.48(3)	3.48	3.38	–	3.48(3)		
17	^{nat}Cl		9.5792(8)				9.5792(8)		
	^{35}Cl	3/2	11.70(9)	11.72	14.96	5.23	11.70(9)	15.9[b]	3.9(3)[b]
	^{37}Cl	3/2	3.08(6)	3.08	2.61	2.94	3.08(6)	2.93[b]	3.10[b]
21	^{45}Sc	7/2	12.24(13)[c]	12.24	4.66	13.51	12.24(13)	7.0(5)	19.0(5)
22	^{nat}Ti		−3.370(13)				−3.363(13)		
	^{46}Ti	0	4.72(5)	4.72	4.61	–	4.7(2)		
	^{47}Ti	5/2	3.53(7)	3.53	0.59	7.46	3.2(2)		
	^{48}Ti	0	−5.86(2)	−5.46	−5.34	–	−5.85(3)		
	^{49}Ti	7/2	0.98(5)	0.98	2.58	−1.12	0.7(2)		
	^{50}Ti	0	5.88(10)	5.88	5.76	–	5.4(2)		
23	^{nat}V		−0.443				−0.41(1)		
	^{50}V	6		−0.495	0.631	−1.977			
	^{51}V	7/2		−0.546	4.616	−7.158			
24	^{nat}Cr		3.635(7)				3.635(7)		
	^{50}Cr	0	−4.50(5)	−4.50	−4.41	–	−4.50(5)		
	^{52}Cr	0	4.914(15)	4.90	4.81	–	4.914(15)		
	^{53}Cr	3/2	−4.20(3)	−4.20	0.298	−11.491	−4.20(3)	1.12(25)	−12.78(27)
	^{54}Cr	0	4.55(10)	4.55	4.46	–	4.55(10)		
25	^{55}Mn	5/2	−3.750(18)	−3.394	−5.180	−0.820	−3.73(2)		
27	^{59}Co	7/2	2.487(11)	2.491	−3.107	9.684	2.78(4)		

[a] Fit not possible because there are too few resonance data. [b] These are $a^{\pm}$ values, related with $b^{\pm}$ via $b = a(A+1)/A + Zb_{ne}$. c) Data taken from [6].

the mass region $6 \leq A < 60$ can be found in Tables 1 - 3. The simultaneous minimization of (15) - (17) allows to obtain a unique set of $\sigma_{tot}^{calc}(E_i)$, $\sigma_{abs}^{calc}(j, E_0)$ and $b_{coh}^{calc}(j, E_{00})$ values which is in very good agreement with corresponding measured values for the isotopes and natural elements, too (see Tables 1 and 2).

Table 3. Bound states parameters and potential scattering radii R'.

Z	Isotope	I	— Bound states parameters —							R'	
			J	E_b [keV]	E_b^{Mugh} [keV]	$\Gamma_{\gamma b}$ [eV]	$\Gamma_{\gamma b}^{Mugh}$ [eV]	h	$hg\Gamma_{nb}^{0}$ [eV]	$hg\Gamma_{nb}^{0\,Mugh}$ [eV]	R'_{calc} [fm]	R'_{Mugh} [fm]
3	^{6}Li	1	1/2	–483.22	–808	$3.152\cdot10^{6}$	$3.152\cdot10^{6}$	1	67951	295	2.52	–
	^{7}Li	3/2	1	–925.02	–	850	–	2	10.65	–	2.50	3.7(2)
6	^{12}C	0	1/2	–1531		3		1	608		5.29	6.3(10)
	^{13}C	1/2	1	–1957		0.546		1	409.2		5.30	6.6(20)
			0	–220		0.546		1	87.7			
7	^{14}N	1	3/2	–6615.34	–3534	0	–	1	11.1	880	5.82	5.8(3)
			3/2	–149.56	–144	2.400	1.7(3)	1	285	276		
			1/2	–2487.89	–2524	0	–	1	3187	1010		
	^{15}N	1/2	0	–2369.41	–2369	0.034	(0.034)	2	209	209	5.22	5.93(10)
			1	–2039.29	–2093	0.034	(0.034)	2	1421	707.8		
8	^{16}O	0	0	–3635		0.441		1	1391		4.73	4.8(1)
			2	–3786		1.02		1	129		4.68	4.7(2)
	^{17}O	5/2	3	–2612		1.02		1	628			
			2	–2428		1.02		1	137			
	^{18}O	0	1/2	–2604		0.23		1	1168		4.63	4.64(11)
9	^{19}F	1/2	1/2	–	–	–	–	2	–	–	5.50	5.7(2)
11	^{11}Na	3/2	2	–21.3	–100	0.3	(0.3)	2	6.830	6.325	5.36	5.7(1)
12	^{24}Mg	0	–	–	–	–	–	1	–	–	5.57	5.4(1)
	^{25}Mg	5/2	–	–	–	–	–	2	–	–	4.73	4.9(3)
	^{26}Mg	0	–	–	–	–	–	1	–	–	4.72	4.3(2)
13	^{27}Al	5/2	–	–	–	–	–	2	–	–	5.00	5.0(1)
14	^{28}Si	0	1/2	–96.78	–210	6.800	(5.8)	1	25.324	120	5.31	4.8(2)
	^{29}Si	1/2	0	–6.84	–35	9.000	(3)	2	0.256	18.84	4.54	4.0(2)
	^{30}Si	0	–	–	–	–	–	1	–	–	4.45	4.3(2)
15	^{31}P	1/2	0	–455.8	–5.9	103.7	(2)	2	167.56	1.32	5.01	4.7(2)
16	^{32}S	0	1/2	–2.21	–10	1.900	(1.9)	1	0.2436	4.57	3.65	3.92(2)
	^{33}S	3/2	2	–7.10	–7.102	0.680	(0.68)	2	0.966	5.77	3.70	3.85(10)
			1	–1.92	–3.658	0.680	(0.68)	2	0.856	1.53		
	^{34}S	0	1/2	–1.58	–10	1.900	(1.9)	1	0.0728	2.69	3.42	3.6(1)
17	^{35}Cl	3/2	2	–0.217	–0.18	0.567	(0.556(20))	2	1.272	1.174	2.91	3.9(3)
			1	0.023	–	0.010	–	2	0.020	–		
	^{37}Cl	3/2	1	–5.023	–	4.400	–	2	0.940	–	3.19	3.4(1)
			2	–11.456	–	4.200	–	2	0.0006	–		
21	^{45}Sc	7/2	3	–0.67	–0.702	1.035	(1.035)	2	5.242	5.522	4.04	4.4(10)
			4	–0.37	–0.485	–	–	2	1.662	1.710		
22	^{46}Ti	0	1/2	–15.10	–16.5	1.350	(1.35)	1	21.036	23.8	3.40	3.5(3)
	^{47}Ti	5/2	2	–5.96	–5.96	1.200	(1.2)	2	10.805	11.6	3.60	3.6(3)
			3	–2.00	–	0.300	–	2	0.560	–		
	^{48}Ti	0	1/2	–95.55	–	35.800	–	1	28.570	–	3.71	3.9(3)
	^{49}Ti	7/2	4	–0.31	–0.314	0.780	(0.78)	2	0.0789	0.104	4.02	4.0(3)
			3	–0.10	–	0.150	–	2	0.014	–		
	^{50}Ti	0	1/2	–20.45	–16.8	1.100	(1.1)	1	15.522	10.3	4.55	4.5(3)
23	^{50}V	6	11/2	–0.014	–0.016	0.600	(0.6)	2	0.00739	0.01006	4.51	–
	^{51}V	7/2	4	–27.88	–17.6	1.470	(1.49)	2	76.244	43.24	6.03	6.9(2)
			3	–9.05	–6	2.410	(1.49)	2	7.653	5.94		
24	^{50}Cr	0	1/2	–0.65	–0.509	1.000	(1)	1	0.5953	0.348	4.54	5.0(3)
	^{52}Cr	0	1/2	–5.37	–6.87	5.070	(1.75)	1	2.677	4.38	5.41	5.2(4)
	^{53}Cr	3/2	2	–1.58	–1.6	2.270	2.27	2	0.461	1.37	5.58	5.4(3)
			1	–0.75	–0.91	2.270	2.27	2	0.734	0.749		
	^{54}Cr	0	1/2	–10.23	–10.23	2.900	(2.9)	1	2.786	2.7	5.21	5.3(3)
25	^{55}Mn	5/2	3	–0.06	–5.1	0.132	(0.75)	2	0.037	4.36	6.15	–
			2	–0.14	–2.4	0.100	(0.75)	2	0.220	4		
27	^{59}Co	7/2	3	–0.48	–0.500	0.447	0.447	2	1.701	1.8684	6.10	6.80(70)
			4	–0.39	–0.475	0.447	0.447	2	0.1061	0.1303		

In most cases the achieved agreement between the calculated and experimental values was within 0.1%. However, in some cases the fit was not possible, even when some of parameters were fixed at their values given in [6], e. g. ^{7}Li.

In general, the strong interaction s-wave scattering radii $R'_{\mathrm{calc}}(j)$ and the bound level parameters $E_{\mathrm{b}}(j)$, $\Gamma_{\mathrm{nb}}(j)$, and $\Gamma_{\gamma\mathrm{b}}(j)$ evaluated from this input set (see Table 3) can be considered as rather reliable. In Table 3 the obtained bound state parameters are compiled and compared with the values in [6].

3. Neutron-nucleus Scattering Characteristics in the Framework of the Optical Model

For the theoretical description of low-energy neutron scattering in the mass region $6 \leq A < 60$ we have chosen the optical potential suggested by Fiedeldey and Frahn in [7]. This potential is everywhere continuously differentiable, permits closed-form solutions of the Schrödinger equation, and its imaginary part consists of both volume and surface absorption terms. It is given by

$$V(r) = -V_0 \cdot \begin{cases} (1 + i\zeta_1)[1 - \rho_1(r)] + i\zeta_2\rho_1(r), \\ \qquad\qquad r \leq R_0, \\ i\zeta_2\rho_2(r), \qquad r \geq R_0, \end{cases} \tag{18}$$

where

$$\rho_n(r) = \{\cosh[R_0 - r)/d_n]\}^{-2}, \; n = 1, 2, \tag{19}$$

$R_0 = 1.35\, A(j)^{1/3}$ and V_0, d_1, d_2, ζ_1, ζ_2 are variable model parameters.

From the solution of the s-wave Schrödinger equation with potential (18), the average reflection coefficient for the j-th isotope is obtained as (see [7])

$$\overline{\eta_j} = \overline{\eta_j}(k_i, R_0, V_0, d_1, d_2, \zeta_1, \zeta_2). \tag{20}$$

In case of zero target spin the average total cross section $\overline{\sigma_{\mathrm{tot}}}$ and the compound nucleus formation cross section σ_{com} can be expressed via $\overline{\eta_j}$ in the form

$$\begin{aligned} \overline{\sigma_{\mathrm{tot}}} &= (2\pi/k_i^2)\mathrm{Re}\,(1 - \overline{\eta_j}) \\ &\approx 4\pi R'^2 + (2\pi^2/k_i^2)(\overline{\Gamma_n}/D), \end{aligned} \tag{21}$$

$$\begin{aligned} \overline{\sigma_{\mathrm{com}}} &= (\pi/k_i^2)(1 - |\overline{\eta_j}|^2) \\ &\approx (2\pi^2/k_i^2)(\overline{\Gamma_n}/D)\left[1 - \frac{1}{2}\pi(\overline{\Gamma_n}/D)\right], \end{aligned} \tag{22}$$

where $(\overline{\Gamma_n}/D)$ is the average strength function for s-scattering.

Hence, for the potential scattering radius $R'(j)$ we have approximately

$$R'(j) \approx (1/k_i)\left[\frac{1}{2}|\overline{\eta_j}| - \frac{1}{2}\mathrm{Re}\,\overline{\eta_j}\right]^{1/2}. \tag{23}$$

Now, the total cross section of a separate isotope can be calculated according to (2), replacing on the right side the first term $\sigma_{\mathrm{s}}^{\mathrm{calc}}(j, E_i)$ by the shape elastic cross section

$$\sigma_{\mathrm{s}}^{\mathrm{calc}}(j, E_i) = (\pi/k_i^2)|1 - \overline{\eta_j}|^2 \tag{24}$$

and adding the neutron-electron scattering cross section term, evaluated by means of (3) and (4), i. e.

$$\begin{aligned} \sigma_{\mathrm{tot}}^{\mathrm{calc}}(j, E_i) &= \sigma_{\mathrm{el}}^{\mathrm{calc}}(j, E_i) + \sigma_{\mathrm{ne}}^{\mathrm{calc}}(j, E_i) + \sigma_{\mathrm{abs}}^{\mathrm{calc}}(j, E_i) \\ &\quad + \sigma_{\mathrm{LS}}^{\mathrm{calc}}(j, E_i) + \sigma_{\mathrm{sol}}^{\mathrm{calc}}(j, E_i). \end{aligned} \tag{25}$$

The optical model parameters V_0, d_1, d_2, ζ_1, ζ_2 can be deduced from the fit of expression (15), where $\sigma_{\mathrm{tot}}^{\mathrm{calc}}(E_i)$ is defined by (1) and (25). These five parameters have been evaluated for the ^{46,48,50}Ti isotopes, because in the considered mass region only these isotopes have zero nuclear spin, and the cross sections were measured in Garching at five energy points.

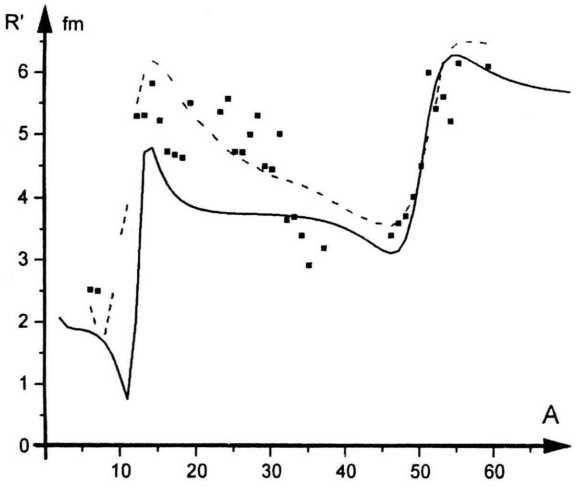

Fig. 1. The dependence of s-wave potential scattering radii $R'(j)$ on the isotope mass number A. (Solid line: this work; dashed line: Saxon-Woods model [6]; black squares: from experimental values, Table 3).

The minimization of total cross sections at E_i = 1.26, 5.19, 18.6, 128 and 1970 eV for ^{46,48,50}Ti isotopes gave the following set of Fiedeldey-Frahn optical potential parameters:

$$V_0 = 58.46 \text{ [MeV]},$$
$$d_1 = 0.32 \text{ [fm]}, \ \zeta_1 = 0.0351,$$
$$d_2 = 0.134 \text{ [fm]}, \ \zeta_2 = 0.0983.$$

The values of the parameters $V_0, d_1, d_2, \zeta_1, \zeta_2$ evaluated in this way have been used for the calculation of $R'_{\text{optic}}(j)$ values for all 38 isotopes considered in this work, employing the approximation (23). The results of $R'_{\text{optic}}(j)$ calculations with the above given parameters are shown in Fig. 1 by the solid line. The dashed line is taken from [6] and corresponds to Saxon-Woods model results, given here for comparison. The data for $R'_{\text{calc}}(j)$, evaluated in Sect. 2 (see last column in Table 3), are denoted by black squares.

4. Conclusion

In this work, a theoretical study of low-energy neutron-nucleus interaction has been performed on the basis of precise measurements of cross sections and coherent scattering lengths in Garching. The evaluated set of bound level parameters fits very well the energy dependence of absorption and scattering cross sections for isotopes and consequently also for natural elements. The data set is completely consistent and reproduces measured spin incoherence in a correct way. In many cases the bound levels given in [6] are obtained only from the evaluation of the energy dependence of the absorption cross section. Consequently the resonance contributions could not be completely included in the determination of R'. The fit of bound levels presented in this work is suitable to fill this gap.

The obtained s-wave potential scattering radii complete and provide additional data being necessary for optical model calculations. The fact that the isobars ^{50}Ti, ^{50}V, and ^{50}Cr have the same scattering radii, is an indication for a good fit and for a complete description of resonances. The s-wave scattering radii obtained by calculations with a complex Fiedeldey-Frahn potential differ from the Saxon-Woods model significantly, especially at masses lower then $A = 30$. The peaks in the curve $R'(A)$ at $A = 14$ and $A = 55$ and the shallow minimum at $A \approx 40$ agree in both models. In the mass range $A = 45$ to 55 (in the vicinity of a double magic number) both models give congruent data.

For more precise optical model evaluations and other potential adaptions experimental cross sections are needed at more than five energy points. Very helpful are even/even-nuclei with nuclear spin zero.

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