

PRESENT STATUS OF REALISTIC SHELL-MODEL CALCULATIONS *

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The present paper is comprised of two parts. First, we give a brief survey of the theoretical framework for microscopic nuclear structure calculations starting from a free nucleon–nucleon potential. Then, we present some selected results of a comprehensive study of nuclei near doubly closed shells. In all these shell-model calculations we have made use of realistic effective interactions derived from the Bonn-A nucleon–nucleon potential by means of a G -matrix folded-diagram method. We show that this kind of calculation yields a very good agreement with experiment for all the nuclei considered. This leads to the conclusion that realistic effective interactions are now able to describe with quantitative accuracy the properties of complex nuclei.

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1. Introduction

A basic input to nuclear shell-model calculations is the model-space effective interaction V_{eff} . Over the past fifty years a variety of empirical effective interactions have been constructed, several of them leading to a very successful description of nuclear structure properties. While this approach has proved to be of great practical value in the interpretation of a large number of experimental data, it is not satisfactory from a first-principle point of view. In fact, a fundamental goal of nuclear structure theory is to understand the properties of complex nuclei in terms of the nucleon–nucleon (NN) interaction. This implies the derivation of V_{eff} from the free NN potential. As is well known, a first step in this direction was taken by Kuo and Brown [1], who in the mid 1960s derived an s - d shell effective interaction

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from the Hamada–Johnston potential [2]. A few years later, an effective interaction for the lead region was derived by Kuo and Herling [3] from the same potential. This was then used in an extensive shell-model study [4] of several nuclei around doubly magic ^{208}Pb .

Although the results of these early works were more than encouraging, in the following two decades there was much skepticism [5] about the reliability of what had become known as “realistic” shell-model calculations. As a consequence, this kind of calculation was practically no longer pursued.

From the late 1970s on, however, there has been substantial progress towards a microscopic approach to nuclear structure calculations starting from a free NN potential. This has concerned both the two basic ingredients which come into play in this approach, namely the NN potential and the many-body methods for deriving the model-space effective interaction.

As regards the first point, several NN potentials have been constructed, which give a quite good, or even excellent, description of the NN scattering data and are suitable for application in nuclear structure. Regarding the theoretical basis of these potentials, they can be divided into two categories, according to whether they are based on the meson theory of nuclear forces or are purely phenomenological in nature (except for the one-pion-exchange tail which is included in all potentials). We shall discuss this subject in some detail in subsection 2.1.

As for the second point, an accurate calculation of the Brueckner G -matrix has become feasible while the so-called $\hat{Q}$ -box folded-diagram series for the effective interaction V_{eff} can be summed up to all orders using iterative methods. An outline of the essentials of this derivation will be given in subsection 2.2.

Based on these improvements, in recent years there has been a revival of interest in shell-model calculations employing effective interactions derived from the free NN potential. In this context, a key issue is how accurate description of nuclear structure properties can be provided by realistic effective interactions. We have concentrated our efforts during the past five years on this problem, trying to assess systematically the role of these interactions in nuclear structure theory. To this end, we have studied a number of nuclei around doubly magic ^{100}Sn , ^{132}Sn , and ^{208}Pb [6–14]. In particular, we have focused attention on nuclei with few valence particles or holes, since they provide the best testing ground for the basic ingredients of shell-model calculations, especially as regards the matrix elements of the effective NN interaction. It is our aim here to give a brief survey of the present status of realistic shell-model calculations. While it should be mentioned that calculations similar to ours have been performed for the Sn isotopes and the $N = 82$ isotones [15, 16], the content and conclusions of this paper are based exclusively on our own comprehensive study.

Although we have studied some nuclei with both neutrons and protons in valence shells [12], we shall only consider here nuclei with identical valence nucleons, for which we feel we have now a well defined scenario. In several cases we have also performed calculations using various effective interactions derived from different NN potentials [11]. All the results summarized in this paper, however, have been obtained by making use of effective interactions derived from the Bonn-A free NN potential. We will come back to this point in the following Section.

Our presentation is organized as follows. In Sec. 2 we give an outline of the theoretical framework in which our realistic shell-model calculations have been performed. Some selected results are presented in Sec. 3, where we also comment on the whole of our calculations. Sec. 4 presents a summary of our conclusions.

2. Theoretical framework

2.1. The nucleon-nucleon potential

As regards the field of NN potentials, we only give here a brief survey of the main aspects relevant to nuclear structure. An historical review and a detailed description of the most recent developments are to be found in Refs. [17–22].

From the theoretical viewpoint, the only quantitative models for the NN interaction are based on meson theory. Indeed, the early sound theoretical models were the one-boson-exchange (OBE) potentials first developed in the 1960s. Later on, sustained efforts were made to take into account multi-meson exchanges, in particular the 2π -exchange contribution. These efforts have been essentially based on two approaches: dispersion relations and field theory. The work along these two lines, which went on for about a decade, resulted eventually in the Paris potential [23] and in the so called “Bonn full model” [24], the latter including also contributions beyond 2π . These potentials fit the world NN data below 300 MeV laboratory energy with a $\chi^2/\text{datum} = 3.71$ and 1.90, respectively [18]. The Bonn full model is, however, an energy-dependent potential, which makes it inconvenient for application in nuclear structure calculations. Therefore, an energy-independent one-boson-parametrization of this potential has been developed [17,24], which has become known as “Bonn A potential”. The phase-shift predictions by this potential are very similar to the ones by the Bonn full model with a χ^2/datum of about 2. Bonn-A, like full Bonn, includes nonlocalities leading to a weak tensor force, as measured by the predicted D -state probability of the deuteron, $P_D=4.4\%$, to be compared [18] with 5.8% for the Paris potential.

Over the last ten years or so both the Paris and Bonn-A potentials have been used in nuclear structure calculations. In some cases [6, 8, 11, 25, 26] comparisons between the results given by these two potentials have been made, which speak in favor of the Bonn-A potential. In particular, from our own calculations for several medium-heavy nuclei [6, 8, 11], it turns out that this potential leads to the best agreement with experiment for all of the nuclei considered.

During the last few years, new high-quality NN potentials have been constructed which fit the 1992 Nijmegen database [27] (this contains 1787 pp and 2514 np data below 350 MeV) with a $\chi^2/\text{datum} \approx 1$. These are the potentials constructed by the Nijmegen group, Nijm-I, NijmII and Reid93 [28], the Argonne V_{18} potential [29], and the CD-Bonn potential [22, 30]. The first four potentials are purely phenomenological in nature (except for the correct OPE tail) while CD-Bonn is essentially a new version of the OBE Bonn potential with an additional fit freedom obtained by adjusting the parameters of the σ boson in each partial wave [22]. A comparison between the predictions of these potentials is made in Refs. [20, 21]. In this context, it may be mentioned that in Ref. [22] the χ^2/datum produced by these potentials in regard to the 1999 NN database is considered and the conclusion is drawn that the CD-Bonn potential gives the most accurate reproduction of the presently available NN data.

All the high-precision NN potentials mentioned above use about 45 parameters. The price one has to pay to achieve a very accurate fit of the NN data is well brought out by noting that while Bonn-A has only 13 parameters, which are coupling constants and cutoff masses (see Table A.1 of Ref. [17]), CD-Bonn uses 43 free parameters [22]. This makes it clear that, to date, high-quality potentials with an excellent $\chi^2/\text{datum} \approx 1$ can only be obtained within the framework of a substantially phenomenological approach.

Since the high-precision NN potentials fit almost equally well the NN data up to the inelastic threshold, they are essentially identical on-shell. They may largely differ, however, in their off-shell behavior. These off-shell differences may show up in nuclear matter [31] and nuclear structure calculations. As mentioned in the Introduction, we are currently studying to which extent nuclear structure calculations depend on the NN potential used as input. From the results obtained so far [11] it turns out that Bonn-A and CD-Bonn give similar results. These two potentials have essentially the same off-shell behavior [30], but show large differences on-shell in terms of the χ^2 . The findings of our nuclear structure calculations are quite in agreement with those of Refs. [18, 21] which are based on calculations of the binding energy of the triton. In this connection, it is worth noting that still to date the experimental value (8.48 MeV) of this quantity is best reproduced

by the Bonn-A potential, which predicts 8.35 MeV [32]. The prediction of the CD-Bonn potential (8.0 MeV) comes rather close to this value while all the other high-precision potentials underbind the triton by about 800 keV. This may be traced to differences in the strength of the tensor force. While Bonn-A and CD-Bonn predict $P_D = 4.4\%$ and 4.8% , respectively, the other potentials yield $P_D \approx 5.7\%$ [21]. These facts suggest that potentials with a weak tensor force may lead to a better description of nuclear structure properties. This is quite an interesting point since differences in P_D may in turn be traced to off-shell differences. We shall not go further into this subject here, but would like to emphasize that it certainly demands a more quantitative understanding.

As already mentioned in the Introduction, the results presented in this paper have all been obtained by using the Bonn-A potential. The brief survey given above should serve mainly the purpose of showing that this potential provides a sound basis not only to test the accuracy of realistic shell-model calculations, but also the meson theory in which it is rooted.

2.2. The shell-model effective interaction

In our calculations we make use of two-body effective interactions derived from the free NN potential by way of a G -matrix folded diagram method. Here, we only outline the essentials of the method and give the references relevant to this short presentation. A detailed description of the derivation of V_{eff} including a more complete list of references can be found in Refs. [33,34].

As usual, the effective interaction V_{eff} is defined by

$$H_{\text{eff}}P\psi_\mu = (H_0 + V_{\text{eff}})P\psi_\mu = E_\mu P\psi_\mu, \quad (1)$$

where the eigenvalues E_μ are a subset of the eigenvalues of the original Hamiltonian in the full space, $\mu = 1, 2 \dots d$ with d denoting the dimension of the model space. $H_0 = T + U$ is the unperturbed Hamiltonian, T being the kinetic energy and U an auxiliary potential introduced to define a convenient single-particle basis. U is usually chosen to be the harmonic oscillator potential. Here P denotes the projection operator onto the chosen model space, which generally consists of a major shell above the doubly closed core.

The first problem one is confronted with in the derivation of V_{eff} is that all modern NN potentials have a strong repulsive core, which makes perturbation calculations meaningless. This difficulty can be overcome by introducing the G -matrix defined by the integral equation [35]

$$G(\omega) = V + VQ_2 \frac{1}{\omega - Q_2 T Q_2} Q_2 G(\omega), \quad (2)$$

where V represents the NN potential, T is the two-nucleon kinetic energy, and ω , commonly referred to as starting-energy, is the unperturbed energy of the interacting nucleons. The operator Q_2 is the Pauli exclusion operator for two interacting nucleons, to make sure that the intermediate states of G must not only be above the filled Fermi sea but also outside the model space within which equation (2) is to be solved. Thus the Pauli operator Q_2 is dependent on the model space chosen, and so is the corresponding G -matrix. Note that the operator Q_2 is defined in terms of harmonic oscillator wave functions while plane-wave functions are employed for the intermediate states of the G -matrix. As regards the harmonic oscillator parameter $\hbar\omega$ we have used the values given by the formula $\hbar\omega = (45A^{-1/3} - 25A^{-2/3})$ MeV, where A is the mass number of the core.

The operator Q_2 is specified, as discussed in [35], by three numbers n_1 , n_2 , and n_3 , each representing a single-particle orbital (the orbits are numbered starting from the bottom of the oscillator well). In particular, n_1 is the number of orbitals below the Fermi surface of the doubly magic core, n_2 fixes the orbital above which the passive single-particle states start, and n_3 denotes the number of orbitals of the full space. In principle, this last number should be infinite. In practice, as we shall see in the following, it is chosen to be a large but finite number.

It should be noted that in the calculation of G the space of active single-particle states, which is defined as the number of levels between n_1 and n_2 , may be different from the model space within which V_{eff} is defined. Several arguments for choosing the former larger than the latter are given in [35]. Generally, n_2 is fixed so as to include two major shells above the Fermi surface. In our calculation for the lead region, however, we have found that a substantially better agreement with experiment is obtained when n_2 is increased from two to three shells above the n_1 -th orbit [13].

An accurate calculation of the plane-wave G -matrix (2) is feasible by using the Tsai-Kuo method [36]. This method gives the exact solution of G as

$$G = G_F + \Delta G. \quad (3)$$

The free G -matrix is

$$G_F = V + V \frac{1}{\omega - T} G_F, \quad (4)$$

and the Pauli correction term ΔG is given by

$$\Delta G = -G_F \frac{1}{e} P_2 \frac{1}{P_2(\frac{1}{e} + \frac{1}{e} G_F \frac{1}{e}) P_2} P_2 \frac{1}{e} G_F, \quad (5)$$

with $e \equiv (\omega - T)$ and $P_2 = 1 - Q_2$.

The G_F matrix does not contain the Pauli exclusion operator and hence its calculation is relatively convenient. To compute ΔG , we have to perform some matrix operations within the model space P_2 . The only necessary approximation in the Tsai-Kuo method is to make n_3 a finite number. It was shown [35], however, that a sufficiently large value of n_3 ensures the accuracy of this approximation.

As a last point, it is worth noting that for asymmetric doubly closed cores the Q_2 operators for protons and neutrons are different, as the valence-proton and -neutron orbits outside the core are different. In this case, the calculation of G is more complicated [8]. In fact, one has first to calculate G_F in a proton-neutron representation. Then ΔG , which depends on the P_2 operator, has to be calculated for protons and neutrons separately.

Using the above G -matrix we can now calculate V_{eff} in the model space. This interaction, which is energy independent, can be written schematically in operator form as [37]

$$V_{\text{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} + \dots, \quad (6)$$

where $\hat{Q}$ (referred to as $\hat{Q}$ -box) is a vertex function composed of irreducible linked diagrams in G , and the integral sign represents a generalized folding operation. $\hat{Q}'$ is obtained from $\hat{Q}$ by removing terms of first order in the reaction matrix G . In our calculations we take the $\hat{Q}$ -box to be composed of G -diagrams through second order. They are precisely the seven first- and second-order diagrams considered by Shurpin *et al.* [38]. Note that for nuclei with valence holes the calculation of the $\hat{Q}$ -box is somewhat different. In fact, in this case the external valence-particle lines appearing in the diagrams of [38] have to be replaced with valence-hole lines [14].

After the $\hat{Q}$ -box is calculated, V_{eff} is obtained by summing up the folded-diagram series (6) to all orders by means of the Lee-Suzuki iteration method [39]. This last step can be performed in an essentially exact way for a given $\hat{Q}$ -box.

It is worth mentioning that the V_{eff} obtained with the procedure described above represents the effective interaction only between two-valence particles or holes. This effective interaction contains one- and two-body terms. It is customary, however, to use a subtraction procedure [38] so that only the two-body terms are retained. As far as the one-body terms are concerned, it is assumed that they modify the unperturbed part of the Hamiltonian, which justifies the use of experimental single-particle energies.

As regards the electromagnetic observables, we have calculated them by making use of effective operators [40, 41] which take into account core-polarization effects. More precisely, by using a diagrammatic description as in Ref. [40], we have only included first-order diagrams in G . This implies that folded-diagram renormalizations are not necessary [41].

3. Review of selected results

To illustrate the quantitative accuracy of realistic shell-model calculations in describing the spectroscopic properties of nuclei near closed shells, we report here some results of the study we have performed over the past few years. These are to be viewed as samples of the whole body of results we have obtained for medium- and heavy-mass nuclei having or lacking few identical particles with respect to double shell closures.

As already pointed out in the preceding Sections, all the results presented here have been obtained by making use of effective interactions derived from the Bonn-A free NN potential. Regarding the single-particle or -hole energies, we have taken them from the experimental spectra of the corresponding single-particle or -hole valence nuclei, wherever available. This is indeed the case of the four nuclei ^{130}Sn , ^{134}Te , ^{206}Pb , and ^{210}Po , for which we report here the calculated spectra. Actually, only for the $N = 50$ isotones and the light Sn isotopes we had to use a different procedure to fix the single-hole and single-particle spectrum, respectively. As regards the electromagnetic observables, no use has been made of empirical effective charges since, as mentioned in subsection 2.1, the effective operators needed for their calculation have been derived in a microscopic way.

TABLE I

Experimental and calculated low-energy levels in ^{130}Sn .

J^π	E (MeV)	
	Exp.	Calc.
0^+	0.000	0.000
2^+	1.221	1.353
7^-	1.947	1.814
4^+	1.996	2.063
5^-	2.085	1.937
4^-	2.215	1.990
6^+	2.257	2.244
8^+	2.338	2.324
10^+	2.435	2.402

In Tables I–IV we compare the experimental [42,43] and calculated low-energy spectra of ^{130}Sn , ^{134}Te , ^{206}Pb , and ^{210}Po . An example of the kind of agreement between theory and experiment [42,44] for the electromagnetic properties is given in Table V, where the moments and the $E2$ transition rates for ^{210}Po are reported. We see that the observed excitation energies in all the four nuclei are very well reproduced by our calculations, the discrepancy being less than 100 keV for most of the states. The agreement

TABLE II

Experimental and calculated low-energy levels in ^{134}Te .

J^π	E (MeV)	
	Exp.	Calc.
0^+	0.000	0.000
2^+	1.279	1.299
4^+	1.576	1.583
6^+	1.691	1.721
6^+	2.398	2.371
2^+	2.462	2.553
4^+	2.554	2.584
1^+	2.631	2.515
5^+	2.727	2.671

TABLE III

Experimental and calculated low-energy levels in ^{206}Pb .

J^π	E (MeV)	
	Exp.	Calc.
0^+	0.000	0.000
2^+	0.803	0.804
0^+	1.165	1.036
3^+	1.340	1.259
2^+	1.467	1.273
4^+	1.684	1.693
1^+	1.704	1.546
2^+	1.784	1.697
4^+	1.998	1.934
2^+	2.148	2.124
$^a 3^+$	2.197	2.142
7^-	2.200	2.156
$^a 1^+$	2.236	2.101
0^+	2.315	2.135
6^-	2.384	2.312
2^+	2.423	2.280

^aThis spin-parity assignment is suggested by our calculations (see Ref. [9]).

between experiment and theory is also very good for the electromagnetic properties of ^{210}Po , with the only exception of $B(E2; 2_1^+ \rightarrow 0_1^+)$. It should be mentioned, however, that our value is consistent with that of a previous calculation [45], while the experimental one has been derived in a way [46] which makes it rather unreliable [13].

TABLE IV

Experimental and calculated low-energy levels in ^{210}Po .

J^π	E (MeV)	
	Exp.	Calc.
0^+	0.000	0.000
2^+	1.181	1.130
4^+	1.427	1.395
6^+	1.473	1.493
8^+	1.557	1.555
8^+	2.188	2.179
2^+	2.290	2.292
6^+	2.326	2.367
4^+	2.382	2.394
1^+	2.394	2.220
5^+	2.403	2.422
3^+	2.414	2.380
7^+	2.438	2.437

TABLE V

Experimental and calculated $B(E2)$ values (W.u.), Q moments (eb), and μ moments (nm) in ^{210}Po .

Quantity	Exp.	Calc.
$B(E2; 2_1^+ \rightarrow 0_1^+)$	0.56 ± 0.12	3.55
$B(E2; 4_1^+ \rightarrow 2_1^+)$	4.53 ± 0.15	4.46
$B(E2; 6_1^+ \rightarrow 4_1^+)$	3.00 ± 0.12	3.07
$B(E2; 8_1^+ \rightarrow 6_1^+)$	1.10 ± 0.05	1.25
$\mu(6_1^+)$	$\pm 5.48 \pm 0.05$	+5.29
$\mu(8_1^+)$	$+7.35 \pm 0.05$	+7.06
$\mu(11_1^-)$	$+12.20 \pm 0.09$	+13.12
$Q(8_1^+)$	-0.552 ± 0.020	-0.588
$Q(11_1^-)$	-0.86 ± 0.11	-0.92

More complete spectra of the four nuclei considered here may be found in Refs. [7, 9–11, 13], while the results obtained for all other nuclei included in our study are given in Refs. [6–9, 11, 13, 14]. We also refer the reader to these papers for a detailed analysis of the spectroscopic properties of the various nuclei. It seems appropriate, however, to show here the overall agreement between our results and the experimental data, at least as regards the energy levels. A quantity which provides such an information is the *rms*

TABLE VI

Root mean square deviation σ . See text for details.

Nucleus	Number of levels	σ (keV)
^{96}Pd	7	122
^{97}Ag	4	108
^{98}Cd	4	107
^{102}Sn	3	92
^{104}Sn	5	165
^{130}Sn	8	119
^{134}Te	15	127
^{135}I	10	59
^{136}Xe	14	90
^{204}Pb	32	122
^{205}Pb	17	64
^{206}Pb	24	94
^{210}Po	37	87
^{211}At	19	64
^{212}Rn	13	85

deviation σ [47]. In Table VI we report the σ values for all the nuclei we have studied with at most four identical valence particles or holes in the region of doubly magic ^{100}Sn , ^{132}Sn , and ^{208}Pb . The number of levels included in the calculation of σ is also reported. It should be noted that the very limited number of data for the lighter nuclei reflects the experimental situation. In fact, these nuclei lie well away from the valley of stability and only recently some experimental information on their spectroscopic properties has become available. In any case, we see that the σ values are all very small, 7 out of 15 being less than 100 keV and only one reaching 165 keV.

Finally, for ^{98}Cd , ^{102}Sn , ^{130}Sn , ^{134}Te , ^{206}Pb , and ^{210}Po we show in Table VII the comparison between the observed [48,49] and calculated ground-state binding energies relative to the closest doubly closed core. For the absolute scaling of the six sets of single-particle or single-hole energies, the mass excess values for nuclei with one particle or one hole with respect to ^{100}Sn , ^{132}Sn , and ^{208}Pb are needed. These have been taken from Refs. [48,49]. As regards the Coulomb interaction between the valence protons in ^{98}Cd , ^{134}Te , and ^{210}Po , we assume that its contribution is equal to the matrix element of the Coulomb force between the two-proton states $(g_{9/2})^2_{J=0+}$, $(g_{7/2})^2_{J=0+}$, and $(h_{9/2})^2_{J=0+}$, respectively. From Table VII we see that an excellent agreement with experiment is obtained, the calculated values falling within the error bars for all the nuclei considered.

TABLE VII

Experimental and calculated ground-state binding energies (MeV). See text for comments.

Nucleus	B	
	Exp.	Calc.
^{98}Cd	-3.98 ± 0.48	-4.56 ± 1.33
^{102}Sn	24.03 ± 0.59	23.60 ± 1.33
^{130}Sn	-12.52 ± 0.04	-12.82 ± 0.06
^{134}Te	20.56 ± 0.04	20.62 ± 0.07
^{206}Pb	-14.12 ± 0.00	-14.12 ± 0.01
^{210}Po	8.78 ± 0.00	8.79 ± 0.01

4. Summary and outlook

In this paper, we have tried to give a self-contained review of the present status of realistic shell-model calculations, as it appears to us through the work we have carried out in this field during the past five years. The main aim of this work has been to give an answer to the crucial question of whether this kind of calculation is able to provide a quantitative description of nuclear structure properties. We think we can now definitely answer this question in the affirmative with a word of caution. As already mentioned in the Introduction, the main body of our calculations has until now concerned nuclei with identical valence nucleons. As a consequence, we may only claim to have a stringent test of the isospin $T = 1$ matrix elements of the effective interaction. A careful test of the $T = 0$ matrix elements is of course equally important. We should point out, however, that in a recent study [12] of the doubly odd nucleus ^{132}Sb we have obtained results which are as good as those regarding like nucleon systems. Along the same lines we are currently studying other nuclei with both neutrons and protons outside closed shells.

Another main question relevant to microscopic nuclear structure calculations is the extent to which they depend on the NN potential used as input. As briefly discussed in subsection 2.1, we are also trying to explore this problem. We only emphasize here that the Bonn-A potential, which we have used as initial input in all the calculations reported in Sec. 3, yields results which are similar to (in some cases even somewhat better than) those produced by its modern, high-precision, version CD-Bonn. This indicates that, as far as nuclear structure is concerned, the χ^2 produced by an NN potential is not, within reasonable limits, the most important aspect. In other words, on-shell differences have little influence on nuclear structure results.

To conclude, we may say that the stage for realistic shell-model calculations is by now well set, that is to say the way is finally open to a more fundamental approach to the nuclear shell model than the traditional, empirical one. From a first-principle point of view, however, we should be aware that a substantial theoretical progress in the field of NN interaction is still in demand. This may not be necessarily achieved within the framework of the traditional meson theory. Suffice here to mention a promising alternative approach, the chiral effective theory, which is actively being pursued [50].

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