Theoretical Calculation of The Binding And Excitation Energies For $^{58}_{28}Ni_{30}$ Using Shell Model And Perturbation Theory

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Abstract

A theoretical calculation of the binding and excitation energies have been used at low – lying energies based on shell model and quantum theory. In this model, we evaluated the energies under assume $^{56}_{28}Ni_{30}$ as inert core with two nucleon extra, nucleons in the $2P_{3/2}$, $1f_{5/2}$ and $2P_{1/2}$ configuration.

Modified Surface Delta Interaction (MSDI) and Reid's Potential (RP) theory for two body matrix elements are evaluated by using a Matlab program to calculate the energies of experimental and Reid single particle energies. Our results of the theoretical calculation have been compared with the experimental results, which show no good agreement with the experiment but have a good agreement with the theoretical studies of Non Zero Pairing Shell Model (NZPSM) and Energy Spectra Method (ESM).

Key words: Modified Surface Delta Interaction, Reid's Potential, Binding and Excitation Energies, Shell Model, $^{58}_{28}Ni_{30}$, Perturbation Theory.

Introduction

The nuclear shell model is based on the analogous model for the orbital structure of atomic electrons in atoms. In some areas, it gives more detailed predictions than the other model. In principle, the shell models energy level structure can be used to predict nuclear excited state [1].

The concept of symmetry in physics is a very powerful tool for the understanding of the behavior of nature. Symmetries are intimately related to conservation laws and to conserved quantities which, in quantum mechanics, is translated into good quantum numbers. In nuclear physics, several symmetries have been identified. In particular, isospin quantum number *t*, with symmetry is related to the identical behavior of protons *tz* = −1/2 and neutrons *tz* = 1/2 in the nuclear field [2].

In the study of nuclear structure properties, nuclear masses or binding energies (*BE*) and, more in particular, two-neutron separation energies (*S*2n), are interesting probes to find out about specific nuclear structure correlations that are present in the nuclear ground state[3]. In most cases, non-relativistic kinematics is used. The bare nucleon-nucleon (or nucleon-nucleon-nucleon) interactions are inspired by meson exchange theories or more recently by chiral perturbation theory, and must reproduce the nucleon-nucleon phase shifts, and the properties of the deuteron and other few body systems [4]. Maria G. Mayer's discussion of the magic numbers in nuclei has clearly demonstrated the nuclear shell structure is associated with the independent-particle model for nuclei. In this model, each closed-shell configuration provides a convenient first approximation. In this approximation, one can assume that the system under consideration consists of a closed-shell core plus valence particles in a valence shell. This approach very successfully explains the ground state properties of nuclei [5].

Theory

To calculate the properties of nuclear ground and excited state depending on quantum mechanical and perturbation theories, one must have the available wave functions of these states. The wave function can satisfy of the schrodinger equation that is given by [6]:

$$H\,|\varphi(r)\rangle = E|\varphi(r)\rangle \ldots\ldots\ldots\ldots (1)$$

Where H: is the non relativistic Hamiltonian operator can be formally by [6]:

$$H = H_0 + H_{res} \ldots\ldots\ldots\ldots (2)$$

Where H_0: is the Hamiltonian of one body potential, and H_{res} is the residual interaction

substitute of Eq. (2) in Eq. (1) results.

$$(H_0 + H_{res})\,|\varphi(r)\rangle = H_0|\varphi(r)\rangle + H_{res}|\varphi(r)\rangle \ldots\ldots\ldots\ldots (3)$$

The wave function for the first order perturbation theory is given by [6]:

$$|\varphi(r)\rangle = |\varphi^0(r)\rangle + |\dot{\varphi}(r)\rangle \ldots\ldots\ldots\ldots (4)$$

And energies

$$E = E^0 + \acute{E} \ldots\ldots\ldots\ldots (5)$$

Inserting Eq. (4) in Eq.(3) we can find the zeros order quantity [7]:

$$H_\circ\,|\varphi^\circ(r)\rangle = E^\circ|\varphi^\circ(r)\rangle \ldots\ldots\ldots\ldots (6)$$

And the first order quantity is given by [7]:

$$H_0|\dot{\varphi}(r)\rangle + H_{res}|\varphi^0(r)\rangle = E^0|\dot{\varphi}(r)\rangle + \acute{E}\,|\acute{\varphi^0}(r)\rangle \ldots\ldots\ldots\ldots(7)$$

Multiply Eq.(7) by $|\varphi^0(r)\rangle$on the left, results.

$$\acute{E}\langle\varphi^{\circ}(r)|\varphi^{\circ}(r)\rangle = \langle\varphi^{\circ}(r)|H_{res}|\varphi^{\circ}(r)\rangle + \langle\varphi^{\circ}(r)|H_{\circ} - E_{\circ}|\dot{\varphi}(r)\rangle \ldots\ldots\ldots\ldots(8)$$

According to Eq.(6) the second term of Eq.(8) vanishes:

When H_0 is Hermition operator, then

$$\acute{E} = \langle\varphi^{\circ}(r)|H_{res}|\varphi^{\circ}(r)\rangle \ldots\ldots\ldots\ldots(9)$$

The energy of state in Eq. (5)

$$E = E^0 + \acute{E} = \langle\varphi^{\circ}(r)|H_o|\varphi^{\circ}(r)\rangle + \langle\varphi^{\circ}(r)|H_{res}|\varphi^{\circ}(r)\rangle \ldots\ldots\ldots\ldots(10)$$

$$= \sum_{k=1}^{A} \mathcal{C}_{ak} + \langle\varphi^{\circ}(r)|H_{res}|\varphi^{\circ}(r)\rangle \ldots\ldots\ldots\ldots(11)$$

Where $\sum_{k=1}^{A} \mathcal{C}_{ak}$: is the contribution of the single particle energies and $\langle\varphi^{\circ}(r)|H_{res}|\varphi^{\circ}(r)\rangle$ is the residual interaction.

For shell model calculation one assume that a meaning full description of a nucleus can be made in term of an inert core of closed shell and extra nucleons in the orbit **S** which can not be occupied by core nucleus. Then the total binding energies are given by[8].

$$E^b \text{ (core } +\lambda^2) = 2\,\mathcal{C}_\lambda + \acute{E_\lambda}(\lambda^2) + E^{B.E}(core) \ldots\ldots\ldots\ldots (12)$$

Where $\mathcal{C}_\lambda$ is the single particle energies, $\acute{E_\lambda}$ is the residual interaction energies and $E^{B.E}(core)$ is the energy of the core that assume.

When we assume the modified surface delta interaction, (MSDI) is the best potential interaction of the two bodies, the residual interaction Energy $\acute{E}_\lambda$ is given by [8].

$$\acute{E_\lambda} = \langle \mathrm{j_a j_b}|V_{1,2}^{MSDI}|\mathrm{j_a j_b}\rangle_{JT=1} = -A\,\frac{(2\mathrm{j_a}+1)(2\mathrm{j_b}+1)}{2(2J+1)(1+\delta_{ab})}\langle \mathrm{j_b} - \tfrac{1}{2}\mathrm{j_a}\ \tfrac{1}{2}|J0\rangle^2[1 + (-1)^{l_a+l_b+J+T}] + B + C \ldots\ldots\ldots\ldots(13)$$

And the two bodies, the residual interaction energy with Reid potential is given by [9].

$$\acute{E_\lambda} = \langle \mathrm{j_a j_b}|V_{1,2}^{MSDI}|\mathrm{j_a j_b}\rangle_{JT=1} \times (\frac{18}{A})^{\frac{1}{3}} \ldots\ldots\ldots\ldots (14)$$

The excitation energy $E_{Ext\ (k)}$ of k^{th} excited state is followed from the binding energy of the nucleus in k state which took the results in respect to the ground state k_0 binding energy given by[6]:

$$E_{Ext\ (k)} = E^{B.E}\,(k) - E^{B.E}\ (k_0) \ldots\ldots\ldots\ldots (15)$$

Results

Shell model developments have been applied to evaluate the binding and excitation energies for $^{58}_{28}Ni_{30}$ nuclei that are assumed to be describes by an inert closed shell core and two nucleons. The two neutrons occupy in the $2P_{3/2}$ $1f_{5/2}$ configuration orbit. The model space $\langle 2p_{3/2}1f_{5/2}\rangle$ describe in the representation (J^{π} ,T) combination (0^{+},1) and ($2,1^{+}$) for $\left|2p_{3/2}\right\rangle$, ($4^{+}$,1) and ($2^{+}$,1) for $\left|2p_{3/2}\ 1f5/2\right\rangle$ and (0^{+},1) , (2^{+},1) and(4^{+},1) for $\left|1f_{5/2}\right\rangle$ and allowed for the two neutrons in configuration space.

The matrix element of two particles interaction are calculated by using Modified Surface Delta Interaction (MSDI) Eq.(13) with Matlab version (6.5), on the other hand, we calculated the matrix element depending on Reid potential with same program using expression and result of our calculation are listed in table(1) and table(2) respectively.

The core binding energy can be calculated from Eq.(12) with mass number are : $M(^{58}_{28}Ni_{30}) = (57.942116)$amu ,$M(_0n^1)$=(1.008665) amu and $M(_1p^1)$=(1.007276) amu [10].

The binding energies of the nucleus of each case for configuration (J^{π} ,T)values have been calculated with Eq.(13) with single particle energies $e_{2P3/2}$ =-10.2549, $e_{1f5/2}$ =-9.4356 and $e_{2P1/2}$ =-9.1562 MeV [11], he tresults are tabulated in table(3) for MSDI and table (4) for RP respectively .

Therefore, the excitation energies follow directly from the different values and evaluated with Eq.(15), the results are summarized in tables(5) and(6) for MSDI and RP alternatively .

Briefly the single particle energies were taken from the observed spectrum for A=57-56 with a least squares fit for $2P_{3/2}$, $1f_{5/2}$ and $2P_{1/2}$ orbits which are equal to (-10.254, -9.4356,and -9.1562)Mev respectively[12] .

Discussion

It is shown that the sequence of the lower levels is well, but the level spacing is somewhat tool the effect of variation of the strength parameter for calculation.

It clear that for the MSDI or RP theory will agree quite well for the excitation energy comparing with experimental.

These work quite for first or second excited state but for higher spectral, they become very complicated because several nucleons can be excited simultaneously into super position of many different configurations to produce a given nuclear spin and parity.

Figure (1), shows the low- lying state that MSDI has an agreement with the experimental than RP and the variance with experimental that similar with NZPSM, but at lower.

While figure (2), shows a good agreement with ESM method while not good with NZPSM.

The ground state configuration indicates that all the proton sub shell filled, and all the neutrons are in filled sub shell except for the last two, which are in sub shell on there own. There are many possibilities to consider for the excited state.

One neutron of the $2P_{3/2}$ promote to $1f_{5/2}$ or $2P_{1/2}$ gives a configuration $2P_{3/2}$, $1f_{5/2}$ or $1P_{3/2}$, $2P_{1/2}$ promote one of $1P_{3/2}$ to others.

All these possibilities would correspond to the smallest energy shift, so it should be founded over the others, the next excited state might involves moving the last neutron up to a farther level to($1f_{5/2}$)or putting it back where it was and adapting configuration option ($2P_{3/2}$, $1f_{5/2}$) which is favored over ($1P_{3/2}$, $2P_{1/2}$)because it keeps the excited neutrons paired with another. This should have a slightly lower energy than creating two unpaired protons when comparing these predictions, with the observed excited levels, it is found that the expected excited do exist.

The influence of the single particles energies are viewed by comparing the calculated values from the NZPSM, ESM model with those obtained from calculations. This shows that

the binding and excitation energies of the low –lying level for A››30 are hardly affected by the inclusion of $f_{5/2}$ orbit that the MSDI, RP, NZPSM and ESM which describes less than for $1p_{3/2}$ orbital and $2p_{3/2}$ orbital.

Our results of the spectra that's obtained from RP potential in figures (1-2), show that it is not good with experimental data but with a good agreement for the results that are obtained by using MSDI especially for low lying level. On the other hand, the expected spectra that gate from result is constructed from mixing state configuration.

Conclusion

The present contribution addresses the role of shell model calculation in low lying energy .We show that both the MSDI and RP are not present in experimental values exactly that lead to conclude MSDI and RP which are limited successfully describing for light nuclei ,and poor describe that mediate nucleus and heavy .Also the energies for binding and excitation spectra are produced from the cooperation of mixing state configuration ,and we expected that mixing calculation gave good results to describe these nucleus .On the other hand, the shell model calculation results depend on the single particles energies effect.
Summarizing, we may conclude that for correlating the available experimental data, the present calculation with MSDI interaction is rather successful than RP.

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Table No.(1): The calculated matrix element for modified surface delta interaction (MSDI)

J_a	J_b	J_c	J_d	J	T	$\langle J_a J_b \mid V^{MSDI} \mid J_a J_b \rangle$
5/2	5/2	5/2	5/2	0	1	-3.0000
5/2	5/2	5/2	5/2	2	1	-0.6857
5/2	5/2	5/2	5/2	4	1	-0.2857
3/2	3/2	3/2	3/2	0	1	-2.0000
3/2	3/2	3/2	3/2	2	1	-0.4000
3/2	5/2	3/2	5/2	4	1	1.1429
3/2	5/2	3/2	5/2	2	1	0.3429

Table No. (2): The calculated matrix element for two bodies' matrix element using Raid potential (RP)

J_a	J_b	J_c	J_d	J	T	$\langle J_a J_b \mid V^{MSDI} \mid J_a J_b \rangle$
5/2	5/2	5/2	5/2	0	1	-0.388
5/2	5/2	5/2	5/2	2	1	-0.0846
5/2	5/2	5/2	5/2	4	1	-1.307
3/2	3/2	3/2	3/2	0	1	-0.510
3/2	3/2	3/2	3/2	2	1	-0.136
3/2	5/2	3/2	5/2	4	1	1.123
3/2	5/2	3/2	5/2	2	1	0.0822

Table No.(3): The binding energy B.E (MeV) for $(^{58}_{28}Ni_{30})$ that is calculated with (MSDI)

Configuration	J^{π} T	Binding Energy (B.E)(MeV)
$2P_{3/2}$	0+ 1	-504.9516345
	2+ 1	-504.2621793
$2P_{3/2}$ $1f_{5/2}$	4+ 1	-502.7778362
	2+ 1	-503.1226638
$1f_{5/2}$	0+ 1	-503.744269
	2+ 1	-502.7467259
	4+ 1	-502.5743121

Table No. (4): The binding energy B.E(MeV) for ($^{58}_{28}Ni_{30}$) that is calculated with Raid potential (RP)

Configuration	**J^{π} T**	**Binding Energy (B.E)(MeV)**
$2P_{3/2}$	0+ 1	-504.9088
	2+ 1	-504.6054
$2P_{3/2}$ $1f_{5/2}$	4+ 1	-502.5785
	2+ 1	-503.6193
$1f_{5/2}$	0+ 1	-504.1892
	2+ 1	-503.3922
	4+ 1	-503.0182

Table No.(5): Results of the excitation energies $E_{Ext.}$ (MeV) for $^{58}_{28}Ni_{30}$ that are calculated with (MSDI)

Configuration	J^{π} T	Excitation Energies (Ex.E)(MeV)
$2P_{3/2}$	0+ 1	0
	2+ 1	-0.6896552
$2P_{3/2}$ $1f_{5/2}$	4+ 1	-2.1739983
	2+ 1	-1.88291707
$1f_{5/2}$	0+ 1	-1.2075655
	2+ 1	-2.2051086
	4+ 1	-2.377522431

Table No. (6): Results of the excitation energies $E_{Ext.}$(MeV) for $^{58}_{28}Ni_{30}$ that are calculated by using Raid potential (RP)

Configuration	J^{π} T	Excitation Energies (Ex.E)(MeV)
$2P_{3/2}$	0+ 1	0
	2+ 1	-0.3034
$2P_{3/2}$ $1f_{5/2}$	4+ 1	-2.3303
	2+ 1	-1.2895
$1f_{5/2}$	0+ 1	-0.7196
	2+ 1	-1.5166
	4+ 1	-1.8906

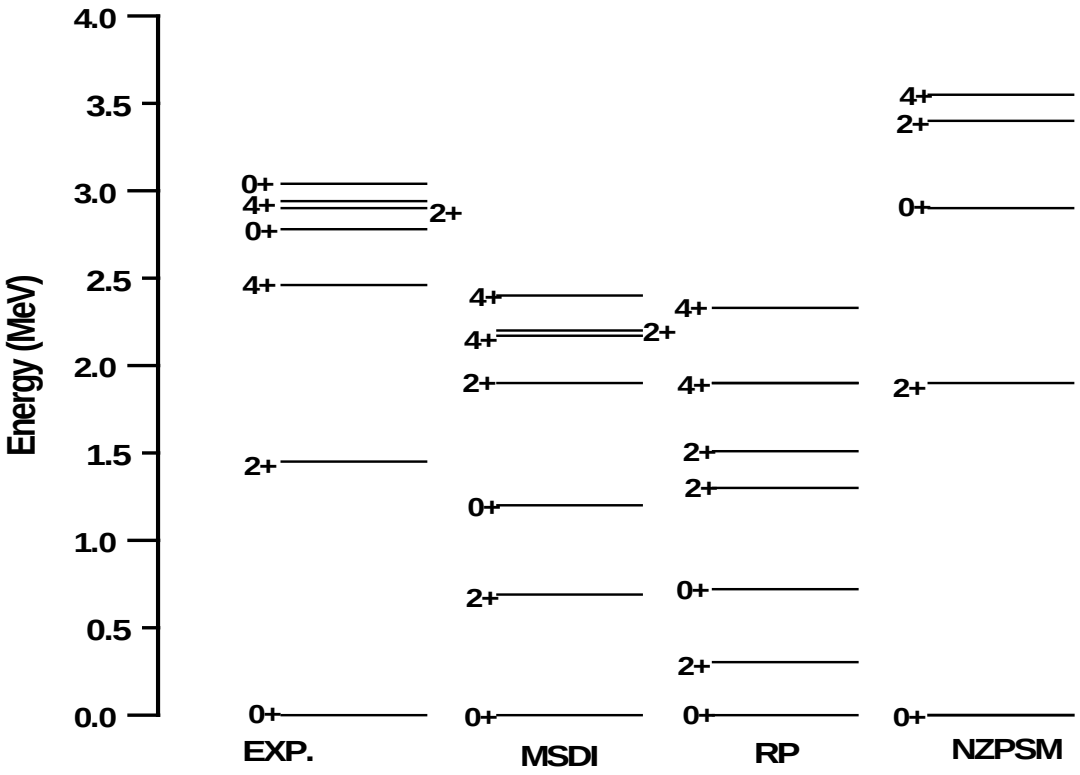

Fig.(1):Our results for spectra level energy for Ni-58 using MSDI and Rp. compared with experimental and NZPSM method.

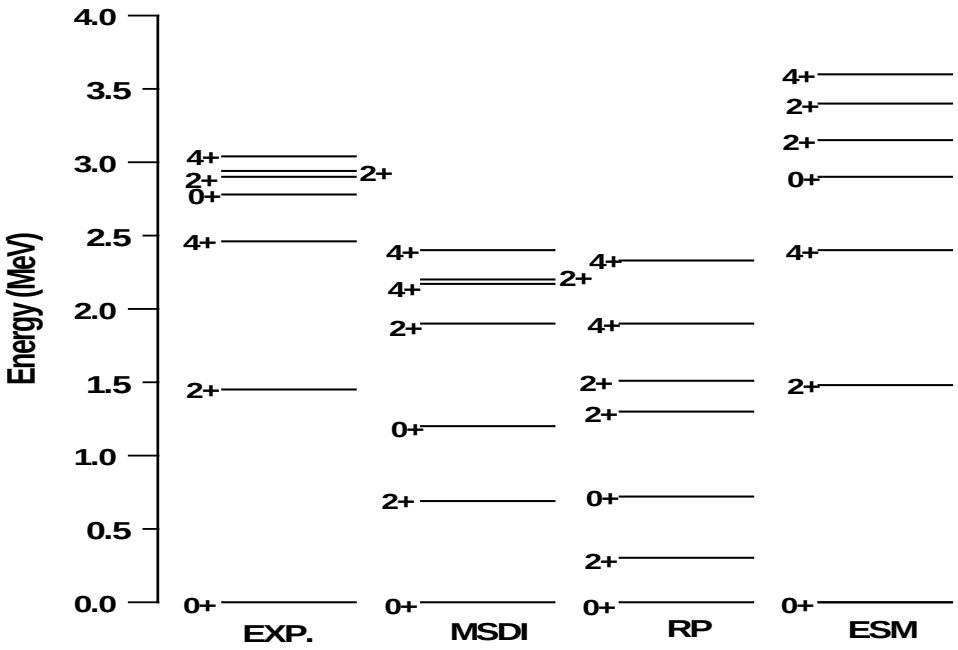

Fig.(2):The calculation of spectra energy level for Ni-58 compared with experimental and ESM method.

الحسابات النظرية لطاقات الربط والاثارة لنواة $(^{58}_{28}Ni_{30})$ باستعمال انموذج القشرة ونظرية الاضطراب

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الخلاصة

أستعملت الحسابات النظرية لطاقات الربط والاثارة للمستويات الدنيا للطاقات بأعتماد انموذج القشرة النووي ونظرية الكم. في هذا الأنموذج قيمت الطاقات على أفتراض نواة $(^{58}_{28}Ni_{30})$ قلب داخلي مع أثنين من النيوكليونات الخارجية ، وهذه النيوكليونات هي ضمن تشكيل $2P_{3/2}$, $1f_{5/2}$ and $2P_{1/2}$.
تم أستعمال برنامج الماتلاب لحساب قيم مصفوفة تفاعل سطح دالتا المطور(MSDI) وجهد ريد (RP) لجسيمتيين من عناصر المصفوفة وذلك لحساب الطاقات العملية وطاقة جسيمة ريد المنفردة. قورنت الحسابات النظرية مع النتائج العملية، التي تبين توافقاً ضعيفاً معها، ولكن التوافق كان جيداً مع الدراسات النظرية لأنموذج القشرة المزدوج اللاصفري(NZPSM)، وطريقة طيف الطاقة(ESM).

الكلمات المفتاحية: تفاعل سطح دالتا المطور،جهد ريد، طاقات الربط والاثارة، أنموذج القشرة، $^{58}_{28}Ni_{30}$ ،نظرية الاضطراب.