USING NIKIFOROV-UVAROV METHOD TO FIND THE SINGLE-PARTICLE NUCLEAR STATES FOR HARMONIC-OSCILLATOR POTENTIAL

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Abstract

   In this study the energy spectrum and Eigenvectors with a special type of central potential will be obtained by using Nikiforov-Uvarov method. The method covers a new algebraic technique to make an exact diagonalization to find the eigenvalues and eigenvectors of the Hamiltonian of the harmonic oscillator (HO).

Introduction

Recently, the study of the Schrödinger in the field of high energy, condensed matter, nuclear physics and related technology is therefore an important branch of physics. The quantum mechanical phenomena are also quite important in nanotechnology nowadays. There are many formalism have been used to solve the Schrödinger equation with having several type of potential, the exact solution of the Schrödinger equation with position-dependent mass using SUSY techniques is investigated (Tanaka, 2006), the Eckart Potential and its Parity-Time is solved analytically (Ping et.al, 2009), Approximate Analytical Solutions of the Klein-Gordon Equation with the Poschl-Teller Potential (Xu, et al., 2010). Among such methods, the variational methods (Flugge, et al., 1994), the algebraic method (Setare, et al, 2007), the shape invariant method (Niazian, 2010), the asymptotic iteration method(AIM) (Ozer, 2008) and the Nikiforove-Uvarove method (Nikiforov, 1988 and Sever,et al., 2008) have been introducing of the exact solution of the Schrödinger equation with several approaches.

The last method is more suitable for solving second order differential equations analytically, because Schrödinger equation is a second order differential equation, NU method today widely uses for this issue.

   The bound state Solution of radial part of Schrödinger equation gives us eigenfunctions and eigenvalues contain all necessary information to explain a quantum mechanically system. Harmonic oscillator potential solutions of the Schrodinger equation will significantly enriched our information of atomic and sub-atomic system (Ikhdair, et al., 2007) this potential plays a basic role in many branches of physics such as atomic, molecular and chemical physics. We will try to solve the Schrodinger equation with this potential using (NU) method. The paper is organized as follows. In section 1, the radial part Schrodinger equation was used to construct the Hamiltonian, in section 2, we have a review of the NU method. Finally, in Section 3, we will obtain the exact solutions of the radial part of the Schrodinger equation in spherical polar coordinate.

1. Radial Schrödinger equation for HO potential in single particle nuclear states

   Our problem that has been investigated contains a Harmonic Oscillator (HO) potential that its corresponding Hamiltonian is given by (Suhonen, 2007):

$$H = -\frac{\hbar^2}{2m}\left[\nabla_r^2 - \frac{l(l+1)}{r^2}\right] + \frac{1}{2}\, m\omega^2 r^2 \qquad (1)$$

   where m is the mass of the nucleon (proton or neutron), and ω is the angular frequency of the harmonic oscillator. Thus, from the time-independent Schrodinger equation the corresponding radial part takes the form:

$$\left[\nabla_r^2 - \frac{l(l+1)}{r^2}\right] R(r) - a^2 r^2 R(r) + f\, R(r) = 0 \qquad (2)$$

   , with,

$$a = m\omega/\hbar = 1/b^2$$
$$f = 2mE/\hbar^2$$
$$(2a)$$

Where b is the length parameter of the harmonic oscillator that differs for different nuclei, such that (Suhonen, 2007)

$$b = \sqrt{\frac{\hbar}{m\omega}} = \sqrt{\frac{c^2 \hbar^2}{mc^2(\hbar\omega)}} = \frac{\hbar c}{\sqrt{mc^2(\hbar\omega)}} = \frac{197.33}{\sqrt{940\,(\hbar\omega)}} = \frac{6.43619}{\sqrt{\hbar\omega}} \qquad (2b)$$

$$= \frac{6.43619}{\sqrt{41A^{-1/3} - 25A^{-2/3}\ MeV}} \qquad (3)$$

Knowing that $\hbar\omega$ is the energy quantized of the harmonic oscillator (Suhonen, 2007), or

$$\hbar\omega = 41A^{-1/3} - 25A^{-2/3}\ MeV \qquad (4)$$

By considering that $s = r^2$ with its first derivative $ds/dr = 2r = 2\sqrt{s}$, we can simplify eq.(2) and re-writing it in a new form such that:

$$\frac{d^2R}{ds^2} + \frac{3}{2s}\frac{dR}{ds} + \frac{1}{4s^2}[sf - l(l+1) - a^2s^2]R = 0 \qquad (5)$$

The above equation is a new form of the radial part Schrodinger equation which was prepared to be solved analytically by using UV-method and hence to find its eigenvalues and eigenvectors.

2. Theory of the UV-method

In the Nikiforove-Uvarove (UN) method, the Schrödinger equation which is a second order linear differential equation, can be reduced to a generalized equation of hypergeometric type:

$$\Psi''(s) + \frac{\tilde{\tau}(s)}{\sigma(s)}\Psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\Psi(s) = 0 \qquad (6)$$

where both $\sigma(s)$ and $\tilde{\sigma}(s)$ can be described as polynomial of second degree, and $\tilde{\tau}(s)$ is a first degree polynomial. In such a way that $\Psi(s)$ is a separable function given by (Ikhdair, 2010):

$$\Psi(s) = \phi(s)\ y(s) \qquad (7)$$

, knowing that $\phi(s)$ is obtained from the solution of the differential equation:

$$\left.\begin{array}{c} \dfrac{1}{\phi(s)}\dfrac{d\phi(s)}{ds} = \dfrac{\pi(s)}{\sigma(s)} \\ with \\ \pi(s) = \dfrac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\dfrac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma}(s) + k(s)\,\sigma(s)} \end{array}\right\} \qquad (8)$$

While the function $y(s)$ satisfies the following hyper-geometric differential equation:

$$\sigma(s)y''(s) + \tau(s)y'(s) + \lambda y(s) = 0 \qquad (9)$$

Here, the function $k(s)$ can be found from the relation (Zhang, 2010):

$$\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma}(s) + k(s)\,\sigma(s) = As^2 + Bs + C = 0 \qquad (10)$$

Where A, B, and C are some coefficients independent on variable (s).

Now by defining a new function $\tau(s)$ and $\pi(s)$ to be a polynomial of degree at most one such that

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \qquad (11)$$

under the condition $\tau'(s) < 0$, the eigenvalues of the Hamiltonian can be obtained from the equation

$$\lambda_n = k(s) + \pi'(s) = -n\,\tau'(s) - \frac{n(n-1)}{2}\sigma'(s)\ , \qquad (n = 0,1,2,3,\dots) \qquad (12)$$

Now to find the eigenvectors $\Psi(s)$ that consists of $\phi(s)$ and $y(s)$, we must solve the first part of eq.(8) to find $\phi(s)$, and then $y(s)$,that satisfies eq.(9), can be determined from the polynomials which are given by the Rodrigues relation (Berkdemir, 2006):

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n}[\sigma^n(s) \; \rho(s)] \tag{13}$$

, with the weight function $\rho(s)$ to be found from the solution of

$$\frac{d}{ds}(\sigma \; \rho) = \tau \; \rho \tag{14}$$

In eq.(13) B_n represents the normalization constant which can be whose determined from:

$$\int_{-\infty}^{\infty} y_n^2(s) \, \rho(s) \; ds = 1 \tag{15}$$

3. Eigenvalues and eigenvectors of the Hamiltonian

Now we wish to emphasis a comparison between eqs.(5 & 6) , we will clearly get

$$\left. \begin{aligned} \tilde{\tau}(s) &= 3 \; , \quad \sigma(s) = 2\,s \; , \quad \sigma'(s) = 2 \\ \tilde{\sigma}(s) &= sf - l(l+1) - a^2 s^2 \end{aligned} \right\} \tag{16}$$

Then by using the functions $\sigma(s), \sigma'(s)$,and $\tilde{\tau}(s)$ in eq.(16) to substitute in the second part of eq.(8), the function $\pi(s)$ can be obtained to be:

$$\pi(s) = -\frac{1}{2} \mp \begin{cases} a\,s + A_l & , \quad k_+ = \dfrac{f}{2} + aA_l \\ \\ a\,s - A_l & , \quad k_- = \dfrac{f}{2} - aA_l \end{cases} \;,\; A_l^2 = \frac{1 + 4l(l+1)}{4} \tag{17}$$

And hence, by putting both the functions $\tilde{\tau}(s)$ and $\pi(s)$ in eq.(11) and by taking into consideration the condition $\tau'(s)$, we get:

$$\left. \begin{aligned} \tau(s) &= 2 + 2A_l - 2a\,s \\ \\ k &= k_- = \frac{f}{2} - aA_l \end{aligned} \right\} \;,\; \tau'(s) = -a \; < 0 \tag{18}$$

, and clearly the second part of eq.(18) makes the function $\pi(s)$ to be rewrites as:

$$\left. \begin{aligned} \pi(s) &= -\frac{1}{2} + A_l - a\,s \\ &\quad and \\ \pi'(s) &= -a \end{aligned} \right\} \tag{19}$$

To find the eigenvalues we must use the functions $k(s)$, $\pi'(s)$, and $\sigma''(s)$ in eq.(12) and the definitions of (a) and (f) in eq.(2a),i.e.,

$$\left. \begin{aligned} (2n + A_l + 1)a &= \frac{f}{2} \\ &\quad or \\ E_{nl} &= (2n + A_l + 1)\hbar\omega \end{aligned} \right\} \;,\; A_l^2 = \frac{1 + 4l(l+1)}{4} \tag{20}$$

The second part of eq.(20) represents the exact analytical eigenvalues of the Hamiltonian of the harmonic oscillator.

Now, determination of the eigenfuctions $\Psi(s)$ requires to solve the differential equations in the first part of eq.(8) and eq.(14) which give :

$$\phi(s) = s^{\frac{2A_l - 1}{4}} e^{-a\,s/2} \tag{21}$$

, and

$$\rho(s) = s^{A_l} e^{-as} \tag{22}$$

Return to the Rodrigues relation in eq.(13), and using $\sigma(s)$ in eq.(11) and $\rho(s)$ in eq.(22) , the function $y_n(s)$ becomes:

$$y_n(s) = \frac{B_n}{s^{A_l} e^{-as}} \frac{d^n}{ds^n}[(2s)^n s^{A_l} e^{-as}] = \frac{B_n 2^n}{s^{A_l} e^{-as}} \frac{d^n}{ds^n}[s^{n+A_l} e^{-as}] \tag{23}$$

, which can be expressed in terms of the Laguerre functions [15] ,or

$$y_n(s) = B_n 2^n \, n! \; L_n^{A_l}(a\,s) \qquad\qquad (24)$$

, with the normalization constant B_n that is determined in eq.(15) and takes the from:

$$B_n = \sqrt{\frac{2\,a^{A_l+1}}{2^{2n}\,n!\,\Gamma(n+A_l+1)}} \qquad\qquad (25)$$

Finally, by putting B_n in eq.(24) and then using eq.(24) and eq.(21) in eq.(7), the exact eigenvectors will be determined to be:

$$\Psi(s) = R(s) = s^{\frac{2A_l-1}{4}} e^{-a\,s/2} y(s) = \sqrt{\frac{2\,n!a^{A_l+1}}{\Gamma(n+A_l+1)}}\, s^{\frac{2A_l-1}{4}} e^{-a\,s/2} L_n^{A_l}(a\,s) \qquad (26)$$

, equivalently, the relations $s = r^2$ and $a = 1/b^2$ makes eq.(26) to give

$$R_{nl}(r) = \sqrt{\frac{2\,n!}{b^3\,\Gamma(n+A_l+1)}}\left(\frac{r}{b}\right)^{A_l-\frac{1}{2}} e^{-r^2/(2b^2)} L_n^{A_l}(r^2/b^2) \qquad\qquad (27)$$

3- Results and discussion

The full diagonalization methods play important roles for dealing with the quantum systems such as atomic and nuclear physics. One of the most famous potentials that can be used widely in the Hamiltonian of such systems is the harmonic oscillator potential.

In section (2), the Hamiltonian was constructed for the harmonic oscillator potential. Then the Nikiforov-Uvarov method was proposed to solve the Schrödinger equation with harmonic potential then we have obtained an analytical expression for the energy spectrum and the eigenfunctions; so it was found that the energy eigenvalues are degenerate and depending on the allowed quantum numbers.

These results may have many interesting applications in the different quantum mechanical systems and nuclear physics. Therefore, in this study, after proposing the nucleus $_{19}K^{37}$ to be used for testing the process of diagonalization, the harmonic oscillator energy $(\hbar\omega)$ and the quantity (A_l) were calculated, and hence, the eigenvalues E_{nl} were obtained for the orbital quantum numbers $6 \geq l \geq 0$ and the main quantum numbers $5 \geq n \geq 0$. Table (3-1) shows the tabulated values for the calculated eigenvalues for the nucleus $_{19}K^{37}$.

Table (3-1):The calculated eigenvalues for the harmonic oscillator Hamiltonian for the values $6 \geq l \geq 0$ and $5 \geq n \geq 0$.

	n					n			
1	0	0	1.5	16.8795	21	2	6	11.5	129.41
2	0	1	2.5	28.1325	22	3	0	7.5	84.3975
3	0	2	3.5	39.3855	23	3	1	8.5	95.6505
4	0	3	4.5	50.6385	24	3	2	9.5	106.904
5	0	4	5.5	61.8915	25	3	3	10.5	118.157
6	0	5	6.5	73.1445	26	3	4	11.5	129.41
7	0	6	7.5	84.3975	27	3	5	12.5	140.663
8	1	0	3.5	39.3855	28	3	6	13.5	151.916
9	1	1	4.5	50.6385	29	4	0	9.5	106.904
10	1	2	5.5	61.8915	30	4	1	10.5	118.157
11	1	3	6.5	73.1445	31	4	2	11.5	129.41
12	1	4	7.5	84.3975	32	4	3	12.5	140.663
13	1	5	8.5	95.6505	33	4	4	13.5	151.916
14	1	6	9.5	106.904	34	4	5	14.5	163.169
15	2	0	5.5	61.8915	35	4	6	15.5	174.422
16	2	1	6.5	73.1445	36	5	0	11.5	129.41
17	2	2	7.5	84.3975	37	5	1	12.5	140.663
18	2	3	8.5	95.6505	38	5	2	13.5	151.916
19	2	4	9.5	106.904	39	5	3	14.5	163.169
20	2	5	10.5	118.157	40	5	4	15.5	174.422

In Table(3-1), the fourth column represents the listed eigenvalues with the units of $\hbar\omega$; while in the fifths column the eigenvalues were listed in the units of MeV.

To study the nature of the eigenvectors, i.e., the harmonic oscillator wave functions $R_{nl}(r)$ in eq.(27), we must take into consideration its quantum numbers (n & l) and the mass number of the nucleus A.

In Fig.(1) the eigenvectors were plotted in the plot-range $0 \leq r \leq 12$ Fermi and for the quantum numbers $n = 3$ and $0 \leq l \leq 5$. As shown in the figure, the number of the nodes can be obtained by the quantum number (n) and thus it shows that all curves have the same nodes because the principal quantum number (n=3); but increasing the orbital quantum number (l)

leads to decrease the first amplitude and the position of the peak shifts toward wright side, it means that at l=0 the amplitude is maximum while for the case of l=5 the amplitude is minimum.

Now by remaining the orbital quantum number invariant and changing (n) we observe that increasing (n) causes to appear new nodes in the curve and also increases the peak-amplitudes, see Fig(2).

The final figure, Fig.(3), shows the plot of the eigenvectors for three different nuclei ($A = 4,27,60$) for the quantum numbers $n = 2$ and $l = 3$. Fig(3) have the same characteristic of Fig.(1) so as increasing in A means the decreasing the amplitude and shifting the posit n toward wright side.
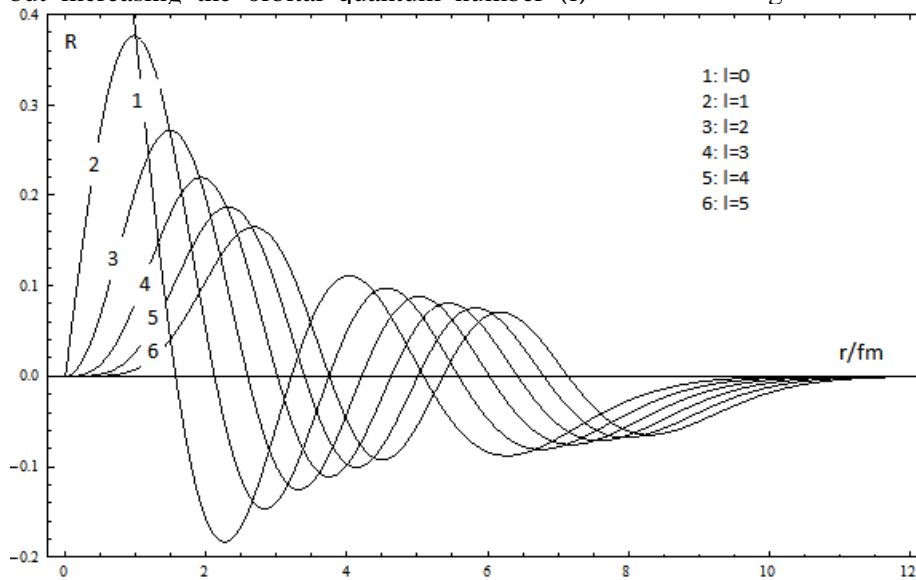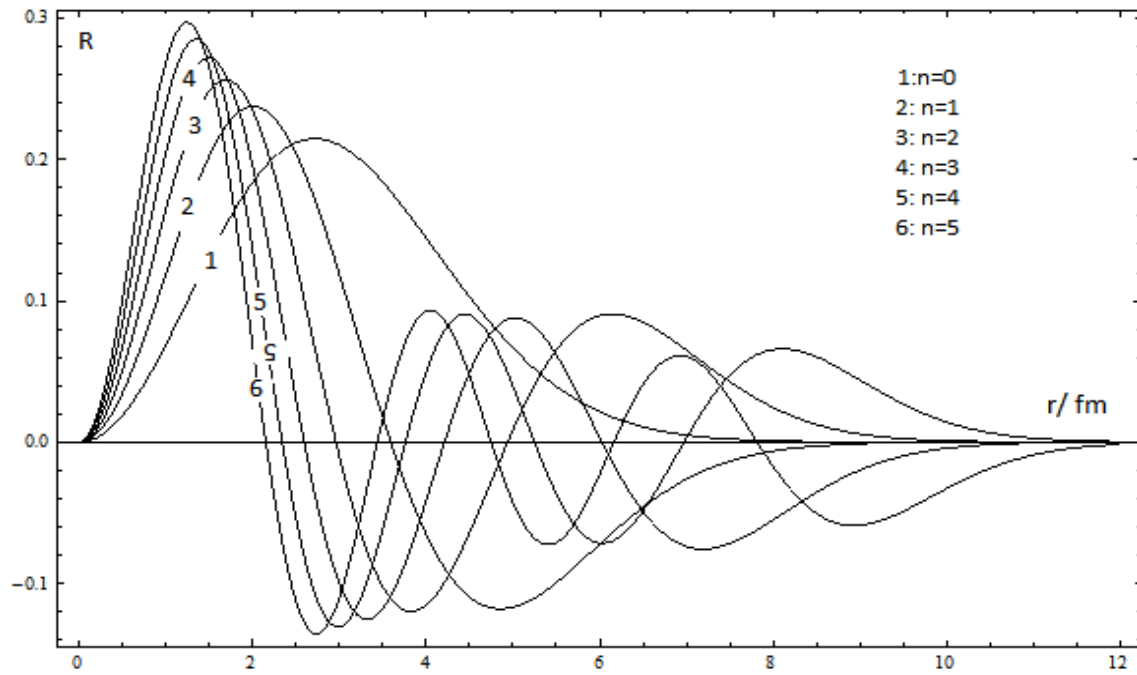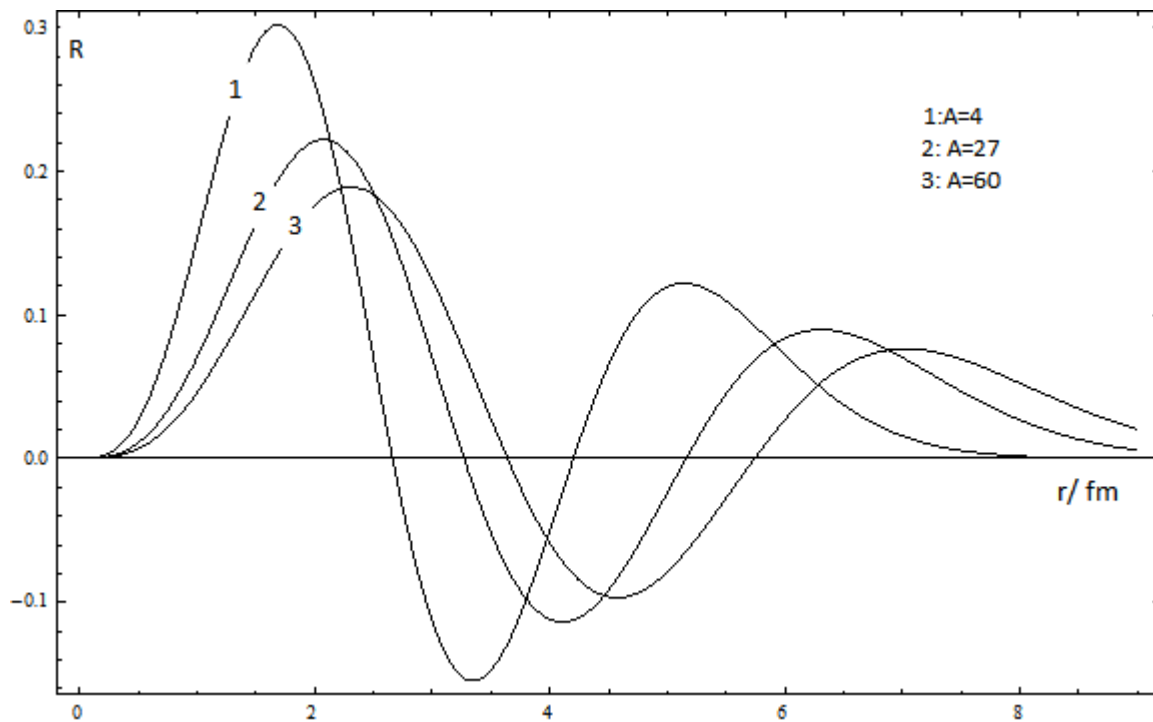

Fig.(1): Harmonic oscillator wave functions for nucleus $A = 37$ and corresponding to the quantum numbers $n = 3$ and $0 \leq l \leq 5$

Fig.(2): Harmonic oscillator wave functions for nucleus $A = 37$ and corresponding to the quantum numbers $l = 3$ and $0 \leq n \leq 5$

Fig.(3): Harmonic oscillator wave functions for the nuclei $A = 4, 27, 60$ and corresponding to the quantum numbers $n = 2$ and $n = 3$

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Conclusion

We have applied the NU method to solve the Schrödinger equation for the most-known harmonic oscillator Hamiltonian that has many interesting applications in the quantum mechanical systems and nuclear physics. We obtain analytical expression for the energy spectrum and the eigenfunctions.

After diagonalizing the Hamiltonian for the single-particle states in nuclei, we have found the energy eigenvalues are their eigenfunctions. It was found that the eigenvalues and eigenfunctions were the same with those of the other methods.

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خلاصة

في هذه الدراسة استخدمنا طريقة نيكيفوروف–يافروف لحل معادلة شرودنجر المذبذب التوافقي لبناء هاميلتون الحركة وتطبيقه لدول جسيم واحد من النويات في نوى.

باستخدام الأسلوب المذكور للنويات ، تم تحديد القيم الذاتية والمتجهات الذاتية، ثم قمنا بمقارنة القيم الذاتية مع نتائج الأساليب الأخرى التي كانت في الاتفاق التام. وقد قمنا بحساب المتجهات الذاتية ورسمها لنوى مختلفة ولنفس أعداد الكم وأيضا لأعداد الكم مختلفة ونفس النواة.

پوخته

له م توێژینەوەدا هەستاوین به به کارهێنانی رێگەیەکی تازه که بریتیه له میتۆدی نیکیڤۆرۆڤ یاڤەرۆڤ بۆ شیکارکردنی هاوکێشەی شرۆدینگەر بۆ ماته ووزەی لەرەلەری هارمونی ، بۆ ئەو مەبەستەش لەو ماتەووزەیه هامیلتۆنی جوولەکه دروست کراوەو جێبەجیّ کراوه بەسەرئاسته ووزەی نیوکلۆنەکانی ناو ناوکی ئەتۆمدا.

به پشتبەستن به رێگەی ناو براو بۆ دۆزینوەی برە خۆییەکان بۆ ئاسته کانی نیوکلۆنەکانی نا و ئەتۆم و ئەنجامەکانیش بەتەواوەتی چوونیەك بوون لەگەل ئەو رێگانەی که پێشتر بەکارهێنراوون . له دواییشدا ئاراسته خوییەکان بەکارهێنراوونه نەخشەیان کێشراوه بۆ چەند ناوکه ئەتۆمیّکی جیاواز و هەمان ژمارەی کوانتەمی ، بۆ یەك ناوکه ئەتۆم و گۆڕینی ژماره کوانتەمیەکان.