



Eigensolution techniques, expectation values and Fisher information of Wei potential function

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Abstract

An approximate solution of the one-dimensional relativistic Klein-Gordon equation was obtained under the interaction of an improved expression for Wei potential energy function. The solution of the non-relativistic Schrödinger equation was obtained from the solution of the relativistic Klein-Gordon equation by certain mappings. We have calculated Fisher information for position space and momentum space via the computation of expectation values. The effects of some parameters of the Wei potential energy function on the Fisher information were fully examined graphically. We have also examined the effects of the quantum number n and the angular momentum quantum number ℓ on the expectation values and Fisher information respectively for some selected molecules. Our results revealed that the variation of most of the parameters of the Wei potential energy function against the Fisher information does not obey the Heisenberg uncertainty relation for Fisher information while that of the quantum number and angular momentum quantum number on Fisher information obeyed the relation.

Keywords Eigensolutions · Wave equations · Klein-Gordon equation · Fisher information · Expectation value · Potential function

Introduction

In order to find the properties of some quantum mechanical systems in the non-relativistic sector, one needs to solve the Schrödinger wave equation which in the time evolution describes either the time-dependent or time-independent solutions. Most studies carried out by uncountable number of authors focused on the solution of time-independent counterpart of the Schrödinger equation for various physical potentials of interest. Some of the potentials reported unfortunately have centrifugal term which demands the use of an approximation scheme to conveniently deal with the centrifugal term. Such potentials include the Yukawa potential, Coulomb potential, Hellmann potential and Frost-Musulin potential. The choice of the proper approximation scheme to the centrifugal term is always a constraint to the authors. However, in the atomic domain, some of these potentials cannot be used to study/

describe diatomic molecules. Thus, there is a little diversion of interest towards the empirical potential energy function for diatomic molecules [1–15]. This is because the potential function provides the most compact way to summarize our understanding of a molecule. Recently, Jia et al. [16] modified some already existing molecular potential energy functions, which are now referred to as the improved expressions for those potentials [9]. The improved expression for the molecular potential energy function for the description of diatomic molecules current motivates the authors for this study. Some of these potentials have been reported either in the relativistic or non-relativistic regime. Such reports can be found in the work of Zang et al. [17], Yahya [18], Onate and Onyeaju [19], Jia et al. [20], Adepoju and Eweh [21], Idiodi and Onate [22] and so on. However, the improved expression for Wei potential energy function has not been fully reported. This potential which is formed from the original Wei potential physically looks simple but is very complicated during calculations. This could probably be the reason why there is lack of report on the potential. The improved expression for the Wei potential energy function is of the form [16]

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$$U_W(r) = D_e \left(1 - \frac{e^{xr_e} - h e^{xr_e}}{e^{xr} - h e^{xr_e}} \right)^2, |h| < 1, \quad (1)$$

where D_e is the dissociation energy, r_e is the bond length, x is the screening parameter and h is a constant parameter of the potential. In the present study, we want to examine the relativistic Klein-Gordon equation and non-relativistic Schrödinger equation with the improved expression for Wei potential energy function using the methodology of supersymmetric approach. We also intend to calculate the position and momentum expectations as well as Fisher information for the improved expression for the Wei potential energy function. The relativistic Klein-Gordon equation provides us with a relativistic background to study spin-zero particles.

Klein-Gordon equation and the Wei potential function

For a quantum system with a rest mass M , the Klein-Gordon equation with a relativistic energy E , scalar potential $S(r)$ and vector potential $V(r)$ takes the form

$$\left[-\hbar^2 c^2 \nabla^2 - (Mc^2 + S(r))^2 + (E - V(r))^2\right] R(r) = 0. \quad (2)$$

In Eq. (2) above, ∇^2 is a Laplacian operator, \hbar is the reduced Planck constant and c is the speed of light. The Klein-Gordon equation given in Eq. (2) corresponds to the Schrödinger equation for potential $2V(r)$ in the non-relativistic limit. According to Alhaidari et al. [23], the Klein-Gordon equation whose non-relativistic limit corresponds to a potential $V(r)$ is given by [23, 24]

$$\left[\frac{d^2}{dr^2} + \left(M + \frac{S(r)}{2}\right)^2 - \left(E_{n,\ell} - \frac{V(r)}{2}\right)^2 - \frac{\ell(\ell+1)}{r^2}\right] R(r) = 0. \quad (3)$$

In Eq. (3) above, we have taken $c = \hbar = 1$ and introduced the term $\frac{\ell(\ell+1)}{r^2}$ which allows the approximate solutions for one-dimensional system with ℓ as the angular momentum quantum number. The centrifugal term can be approximated using the formula

$$\frac{1}{r^2} \approx \frac{(\rho_0 + \rho_1 + \rho_2)}{r_e^2}, \quad (4)$$

where ρ_0 , ρ_1 and ρ_2 are parameters of the approximation scheme whose values will be defined later. Substituting Eqs. (1) and (4) into Eq. (3), we have

$$\frac{d^2 R_{n,\ell}(r)}{dr^2} = \left[V_N + \frac{V_T e^{-xr}}{1 - h e^{xr} e^{-xr}} + \frac{V_R e^{-2xr}}{(1 - h e^{xr} e^{-xr})^2} \right] R_{n,\ell}(r), \quad (5)$$

where we have used the following for mathematical simplicity

$$V_N = (M + E_{n,\ell})(M - E_{n,\ell} + D_e) + \frac{\ell(\ell+1)\rho_0}{r_e^2}, \quad (6)$$

$$V_T = \frac{\ell(\ell+1)\rho_1}{r_e^2} - 2(M + E_{n,\ell})bD_e, \quad (7)$$

$$V_R = \frac{\ell(\ell+1)\rho_2}{r_e^2} + (M + E_{n,\ell})b^2D_e, \quad (8)$$

$$\rho_0 = 1 + \frac{3(1-xr_e) + 2h(3-xr_e)e^{-xr_e} + h^2(3h+xr_e)e^{-2xr_e}}{x^2 r_e^2}, \quad (9)$$

$$\rho_1 = \frac{6h(xr_e-3) - 18h^2 e^{-xr_e} + 2(2xr_e-3)e^{xr_e} - 2h^2(3+hxr_e)e^{-2xr_e}}{x^2 r_e^2}, \quad (10)$$

$$\rho_2 = \frac{18h^2 + 2h^3(6+xr_e)e^{-xr_e} + 2h(6-xr_e)e^{xr_e} + h^4(3+xr_e)e^{-2xr_e} + (3-xr_e)e^{2xr_e}}{x^2 r_e^2}. \quad (11)$$

$$b = e^{xr_e}(1-h). \quad (12)$$

To adopt the use of the supersymmetric approach and formalism to solve Eq. (5), first we write the ground state wave function as

$$R_{0,\ell}(r) = \exp(-\int W(r) dr), \quad (13)$$

where $W(r)$ is a supersymmetric superpotential function, which is a solution to Eq. (5). Taking Eq. (5) as a Riccati differential equation, we propose a superpotential function of the form

$$W(r) = V_C + \frac{V_L e^{-xr}}{1 - h e^{xr} e^{-xr}}, \quad (14)$$

where, V_C and V_L are superpotential constants whose values can be determined by simple manipulation of Eqs. (14) and (15). Relating the superpotential function to the Riccati equation, we have

$$W^2(r) - \frac{dW(r)}{dr} = V_N + \frac{V_T e^{-xr}}{1 - h e^{xr} e^{-xr}} + \frac{V_R e^{-2xr}}{(1 - h e^{xr} e^{-xr})^2}. \quad (15)$$

In the present study, we only consider the bound state solutions for the wave function which satisfy the boundary conditions $\frac{R_{n,\ell}(r)}{r} = \{0, r \rightarrow \infty, \infty, r \rightarrow 0\}$. These regularity conditions make us have a restriction condition that $V_C > V_L$. Substituting Eq. (14) into Eq. (15) and with some reasonable mathematical manipulations, we can now deduce the two superpotential constants in Eq. (14) as follows:

$$V_C^2 = V_N, \quad (16)$$

$$V_L = \frac{b}{2} \left(-1 \pm \sqrt{1 + \frac{4\ell(\ell+1)\rho_2}{x^2 r_e^2} + \frac{4(M + E_{n,\ell})D_e r_e^2}{x^2}} \right), \quad (17)$$

$$V_C = \frac{(M + E_{n,\ell})D_e b(2+b) + \frac{\ell(\ell+1)(\rho_2 - \rho_1)}{r_e^2}}{2V_L} - \frac{V_L}{2}. \quad (18)$$

Table 1 Spectroscopic parameters of the molecules studied in this work [28]

Molecule	$D_e(\text{eV})$	$r_e(\text{\AA})$	$\mu = m(\text{a. m. u})$
CuLi	1.74	2.310	6.259494
ScN	4.56	1.768	10.682771
NiC	2.76	1.621	9.974265
CrH	2.13	1.694	0.988976
TiH	2.05	1.781	0.987371
ScH	2.25	1.776	0.986040
LiH	2.5152672118	1.5956	0.8801221
HCl	4.619030905	1.2746	0.9801045
TiC	2.66	1.790	9.606079
ScF	5.85	1.794	13.358942

Using Eq. (14), we can easily construct a pair of supersymmetric partner potentials as

$$V_+(r) = W^2(r) - \frac{dW(r)}{dr} = V_C^2 + \frac{2V_C V_L e^{-xr}}{1 - h e^{x r_e} e^{-xr}} + \frac{V_L(V_L - x)e^{-2xr}}{(1 - h e^{x r_e} e^{-xr})^2}, \tag{19}$$

$$V_-(r) = W^2(r) + \frac{dW(r)}{dr} = V_C^2 + \frac{2V_C V_L e^{-xr}}{1 - h e^{x r_e} e^{-xr}} + \frac{V_L(V_L + x)e^{-2xr}}{(1 - h e^{x r_e} e^{-xr})^2}. \tag{20}$$

The partner potentials in Eq. (19) and Eq. (20) satisfied the following relationship

$$V_+(r, a_0) = V_-(r, a_1) + R(a_1), \tag{21}$$

where $a_0 = V_L$, is an old set of parameters and a_1 which is a function of a_0 , is a new set of parameters which fully indicates

that $a_1 = f(a_0) + x$, and $R(a_1)$ called the residual or remainder term. The remainder term is independent of the variable r . Thus, $V_L \rightarrow V_L + x$. This mapping and Eq. (21) lead to the establishment of the following relationship:

$$R(a_1) = a_0(2V_L + a_0) - a_1(2V_L + a_1), \tag{22}$$

$$R(a_2) = a_1(2V_L + a_1) - a_2(2V_L + a_2), \tag{23}$$

$$R(a_3) = a_2(2V_L + a_2) - a_3(2V_L + a_3), \tag{24}$$

$$R(a_n) = a_{n-1}(2V_L + a_{n-1}) - a_n(2V_L + a_n). \tag{25}$$

Therefore, the energy eigenvalues can be determined by using the shape invariance approach [20, 25] via

$$E_0^{(-)} = 0, \tag{26}$$

$$E_n^{(-)} = \sum_{\kappa=1}^n R(a_\kappa) = R(a_1) + R(a_2) + R(a_3) + \dots + R(a_n), \tag{27}$$

$$\begin{aligned} \bar{E} &= E_0^{(-)} + E_n^{(-)} \\ &= \frac{(M + E_{n,\ell})D_e b(2 + b) + \frac{\ell(\ell + 1)(\rho_2 - \rho_1)}{r_e^2}}{2a_0} - \frac{a_0}{2}, \end{aligned} \tag{28}$$

This gives full energy eigenvalue equation as

$$(M + E_{n,\ell})(M - E_{n,\ell} - D_e) - \frac{\ell(\ell + 1)\rho_0}{r_e^2} = \left[\frac{bD_e(M + E_{n,\ell})(b + 2) + \frac{\ell(\ell + 1)(\rho_2 - \rho_1)}{r_e^2} - \left(1 + 2n + \sqrt{1 + \frac{4\ell(\ell + 1)\rho_2}{x^2 r_e^2} + \frac{4(M + E_{n,\ell})D_e r_e^2}{x^2}}\right)^2}{1 + 2n + \sqrt{1 + \frac{4\ell(\ell + 1)\rho_2}{x^2 r_e^2} + \frac{4(M + E_{n,\ell})D_e r_e^2}{x^2}}} \right]^2 \tag{29}$$

$$\psi_n(y) = N_n y^{\Upsilon_T} (1 - y)^{0.5(1 + \Upsilon_R)} P_n^{(2\Upsilon_T, \Upsilon_R)}(1 - 2y), \tag{30}$$

$$\Upsilon_P = \frac{2(M + E_{n,\ell})bD_e}{x^2} - \frac{\rho_1 \ell(\ell + 1)}{x^2 r_e^2}, \tag{31}$$

Table 2 Momentum expectation value $\langle p^2 \rangle$ for CuLi, ScN, NiC, TiC and ScF molecules with $x = 1.05$ and $h = 0.9$

n	ℓ	CuLi	ScN	NiC	TiC	ScF
0	0	-23,852.26472	-145,485.7231	-38,189.94113	-46,482.85557	-373,472.2371
1	0	-42,643.85423	-263,935.0685	-91,641.21111	-96,145.35235	-604,181.0134
	1	-67,128.13874	-503,180.0626	-348,696.1641	-244,672.8886	-924,118.9816
2	0	-69,267.08396	-413,720.4745	-167,379.2627	-165,121.5364	-879,707.5049
	1	-103,331.1345	-722,289.8427	-526,407.6306	-369,996.3902	-1,271,710.857
	2	-185,451.8651	-1,505,142.828	-1,629,813.450	-939,056.1072	-2,191,146.409
3	0	-106,176.8816	-604,937.9378	-274,973.5159	-260,643.1966	-1,212,403.371
	1	-152,275.1721	-998,037.7650	-763,131.6392	-536,396.8541	-1,690,133.816
	2	-259,906.8941	-1,966,634.974	-2,163,425.463	-1,263,342.538	-2,794,659.931
	3	-458,412.4234	-3,860,668.839	-5,242,966.795	-2,766,055.920	-4,821,310.259

Table 3 Position expectation value $\langle r^2 \rangle$ for CuLi, ScN, NiC, TiC and ScF molecules with $x = 1.05$ and $h = 0.9$

n	ℓ	CuLi	ScN	NiC	TiC	ScF
0	0	507.1527428	3276.808566	1578.462481	1379.367544	5276.688800
1	0	519.3542100	3279.196355	1580.280978	1388.465888	5270.925631
	1	566.4176231	3593.097768	1999.210083	1630.237930	5551.014095
2	0	535.5716866	3315.349723	1611.755680	1417.634082	5302.825094
	1	586.5310635	3663.031760	2070.135880	1682.706895	5614.075970
	2	674.1967993	4269.374387	2728.018942	2097.068278	6198.571848
3	0	553.1016240	3371.230462	1656.004751	1455.985133	5359.739849
	1	607.4716820	3745.773069	2146.615947	1740.084468	5695.992760
	2	698.8264775	4376.601372	2819.914181	2167.250603	6309.559238
	3	811.5090679	5154.053617	3560.106138	2657.723152	7119.462248

$$\Upsilon_R = \sqrt{1 + \frac{4\rho_2\ell(\ell+1)}{x^2r_e^2} + \frac{4(M+E_{n,\ell})D_e b^2}{x^2}}, \quad (32)$$

$$\Upsilon_T = \sqrt{\frac{(M+E_{n,\ell})(M-E_{n,\ell}-D_e)}{x^2} - \frac{\ell(\ell+1)\rho_0}{x^2r_e^2}}, \quad (33)$$

Non-relativistic limit

The solution of the Schrödinger equation can be obtained directly from the solution of relativistic Klein-Gordon equation by making some certain transformations. Thus, when we make the following transformation: $M + E_{n,\ell} \rightarrow \frac{2mE_{n,\ell}}{\hbar^2}$, and $M - E_{n,\ell} \rightarrow -E_{n,\ell}$, where m is equivalent to the reduced mass. Equation (29) becomes a solution of Schrödinger equation with energy equation as

$$E_{n,\ell} = \Upsilon_Q \frac{x^2 \hbar^2}{2m} \left[\frac{\Upsilon_1 \frac{2mbD_e(b+2)}{x^2 \hbar^2} + \frac{\ell(\ell+1)(\rho_2 - \rho_1)}{r_e^2} - \left(1 + 2n + \sqrt{1 + \frac{\ell(\ell+1)\rho_2}{x^2 r_e^2} + \frac{8mD_e b^2}{x^2 \hbar^2}}\right)^2}{2 \left(1 + 2n + \sqrt{1 + \frac{\ell(\ell+1)\rho_2}{x^2 r_e^2} + \frac{8mD_e b^2}{x^2 \hbar^2}}\right)} \right]. \quad (34)$$

$$\Upsilon_Q = D_e + \frac{\ell(\ell+1)\rho_0 \hbar^2}{2mr_e^2}. \quad (35)$$

Table 4 Fisher information for position for CrH, TiH, ScH, LiH and HCl molecules with $x = 1.05$ and $h = 0.9$

n	ℓ	CrH	TiH	ScH	LiH	HCl
0	0	-3184.299535	-3174.910673	-3568.996162	-3233.685465	-6428.319575
1	0	-15,910.51257	-14,910.35557	-16,276.91363	-17,304.50607	-36,981.98441
	1	-399,497.1340	-282,255.8325	-292,098.4626	-609,645.1462	-3,272,510.437
2	0	-48,663.97710	-44,292.69428	-47,450.60665	-54,605.31854	-114,295.6524
	1	-684,586.0871	-494,091.2044	-509,568.4564	-1,016,964.139	-4,886,788.319
	2	-3,123,316.740	-2,152,356.025	-2,210,004.624	-4,881,860.944	-27,175,795.96
3	0	-117,281.8705	-104,837.7809	-110,956.9614	-134,127.8827	-276,132.6828
	1	-1,104,085.562	-810,204.2109	-833,364.8791	-1,605,727.546	-7,051,916.945
	2	-4,352,280.250	-3,047,050.572	-3,124,131.833	-6,674,446.238	-34,593,529.98
	3	-12,034,672.01	-8,235,554.850	-8,437,125.297	-18,935,433.31	-106,445,225.4

Table 5 Fisher information for momentum for CrH, TiH, ScH, LiH and HCl molecules with $x = 1.05$ and $h = 0.9$

n	ℓ	CrH	TiH	ScH	LiH	HCl
0	0	1328.919338	1219.443793	1395.635935	1654.983713	4654.928758
1	0	1498.747137	1369.696262	1560.297986	1879.320373	5192.835038
	1	3777.059118	3171.348794	3525.534509	5226.617760	17,374.96882
2	0	1630.358633	1489.883277	1697.032454	2044.669199	5636.800475
	1	4085.250732	3436.142790	3817.330501	5644.381494	18,574.42746
	2	6217.990312	5189.781128	5752.290615	8627.508749	28,250.94484
3	0	1674.981967	1538.091762	1759.430534	2087.936868	5817.499453
	1	4378.911662	3686.879177	4093.955819	6043.618126	19,725.20060
	2	6546.031836	5471.169007	6063.002021	9076.679412	29,620.44092
	3	8612.051406	7188.345359	7960.282101	11,910.07087	38,057.70061

Fisher information and expectation value

The Fisher information entropy measures the narrowness and the oscillation nature of the probability distribution [26]. The Fisher information has been used as a measure of uncertainty in various fields of science. In this work, we are going to calculate Fisher information using the radial expectation values of an improved expression for Wei molecular potential energy function. The Fisher information for position space and momentum space respectively are given by

$$I(\rho) = \int \frac{[\nabla \rho(r)]^2}{\rho(r)} dr, \tag{36}$$

$$I(\gamma) = \int \frac{[\nabla \gamma(r)]^2}{\gamma(r)} dr, \tag{37}$$

where $\gamma(r)$ and $\rho(r)$ respectively denote the position and momentum densities. Thus, the Fisher information with any

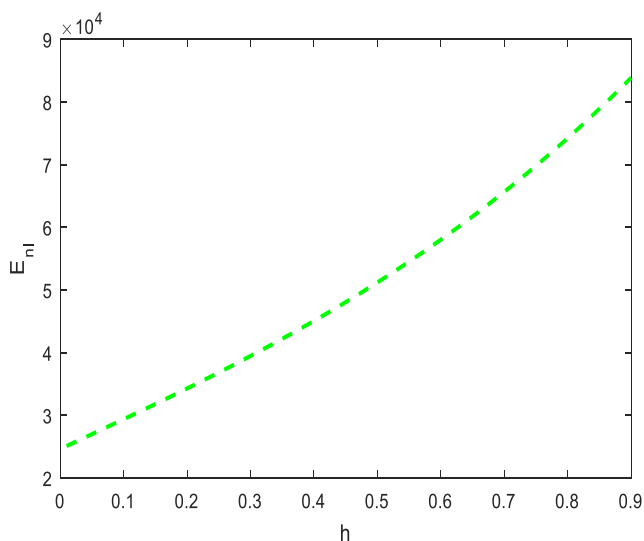


Fig. 1 Variation of energy $E_{n, \ell}$ against the potential parameter h with $x = 1.05$, $m = \hbar = n = \ell = 1$, $r_e = 0.1$ and $D_e = 5$

ℓ -state for the physical state of the system is defined by the expectation value of the squared of logarithmic gradient of associated density $\rho_{E_{n,\ell}}(\vec{r})$ and $\gamma_{E_{n,\ell}}(\vec{r})$, given by Dehesa et al. [27] and Romera et al. [26] as

$$I(\rho) = 4 \langle p^2 \rangle_{n,\ell} - 2(2\ell + 1) |m_0| \langle r^{-2} \rangle_{n,\ell}, \tag{38}$$

$$I(\gamma) = 4 \langle r^2 \rangle_{n,\ell} - 2(2\ell + 1) |m_0| \langle p^{-2} \rangle_{n,\ell}. \tag{39}$$

For a given quantum number n and angular momentum quantum number ℓ , $I(\rho)$ and $I(\gamma)$ provide maximum and minimum values when $m_0 = 0$, therefore, Eqs. (38) and (39) respectively become

$$I(\rho) = 4 \langle p^2 \rangle_{n,\ell}, \tag{40}$$

$$I(\gamma) = 4 \langle r^2 \rangle_{n,\ell}. \tag{41}$$

The expectation values $\langle r^2 \rangle_{n, \ell}$ and $\langle p^2 \rangle_{n, \ell}$ will be calculated using the Hellmann-Feynman theorem. According to the theorem,

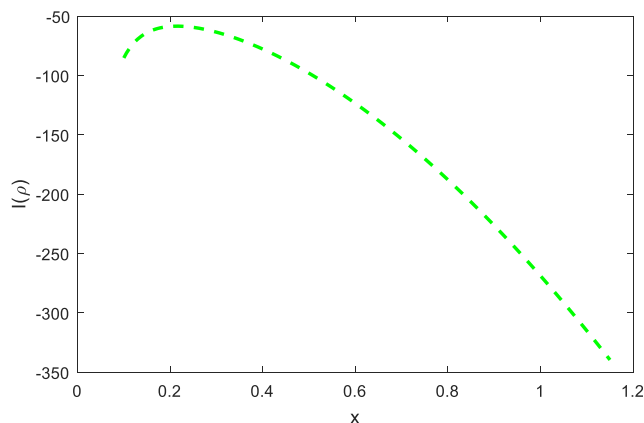


Fig. 2 Fisher information for position space $I(\rho)$ at the ground state against the screening parameter x with $m = D_e = 1$, $h = 0.9$, $r_e = 0.1$ and $\ell = 0$

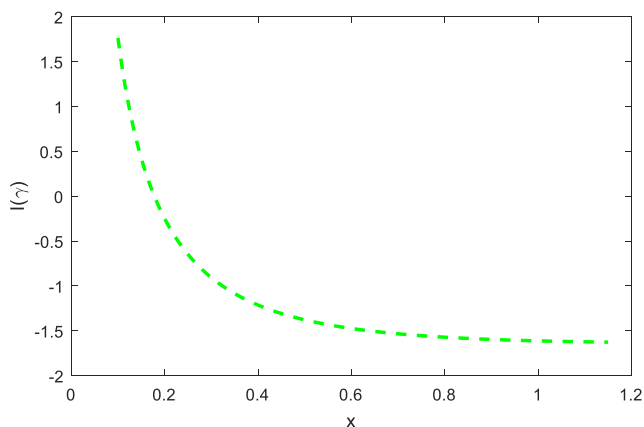


Fig. 3 Fisher information for momentum space $I(\gamma)$ at the ground state against the screening parameter x with $m = D_e = 1$, $h = 0.9$, $r_e = 0.1$ and $\ell = 0$

$$\frac{\partial E_v(v)}{\partial v} = \left\langle \psi_v(v) \left| \frac{\partial H(v)}{\partial v} \right| \psi_v(v) \right\rangle, \quad (42)$$

provided that the associated normalized eigenfunction $\psi_v(v)$ is continuous with respect to the parameter v . The effective Hamiltonian of the improved expression for Wei potential energy function radial wave function is given as

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2} + D_e \frac{2D_e b(1-h)e^{-xr}}{1-h e^{x r_e} e^{-xr}} + \frac{D_e b^2(1-h)^2 e^{-2xr}}{(1-h e^{x r_e} e^{-xr})^2}. \quad (43)$$

To obtain the expectation value for $\langle r^2 \rangle$, we set $q = m$ to have

$$\langle r^2 \rangle_{n,\ell} = D_e \frac{x^2 \hbar^2 D_e}{2mb^2} \left[\frac{\frac{2mb(b+2)}{x^2 \hbar^2 (\gamma_0 - 1 - 2n)} \gamma_0^4 + \gamma_1^2 - \frac{2mb(b+2)}{x^2 \hbar^2} [\gamma_0^2 + \gamma_1] \gamma_0}{\gamma_0^2} \right]. \quad (44)$$

To obtain the expectation value for $\langle p^2 \rangle$, we set $q = D_e$ to have

$$\langle p^2 \rangle_{n,\ell} = \gamma_2^2 - \frac{x^2 \hbar^2}{b^2} [\gamma_0^2 + \gamma_1] \left[(\gamma_0^2 + \gamma_1) - \frac{2mD_e b(b+2)}{x^2 \hbar^2 \gamma_0} \left(1 + \frac{[\gamma_0(1-\gamma_0) + \gamma_1]}{\gamma_0} \right) \right], \quad (45)$$

where

$$\gamma_0 = 1 + 2n + \sqrt{1 + \frac{4\ell(\ell+1)\rho_2}{x^2 r_e^2} + \frac{8mD_e b^2}{x^2 \hbar^2}}, \quad (46)$$

$$\gamma_1 = \frac{2mbD_e(b+2)}{x^2 \hbar^2} + \frac{\ell(\ell+1)(\rho_2 - \rho_1)}{r_e^2}, \quad (47)$$

$$\gamma_2^2 = \frac{\ell(\ell+1)\hbar^2(\rho_0 + 2\rho_2 - 2\rho_1)}{2r_e^2}. \quad (48)$$

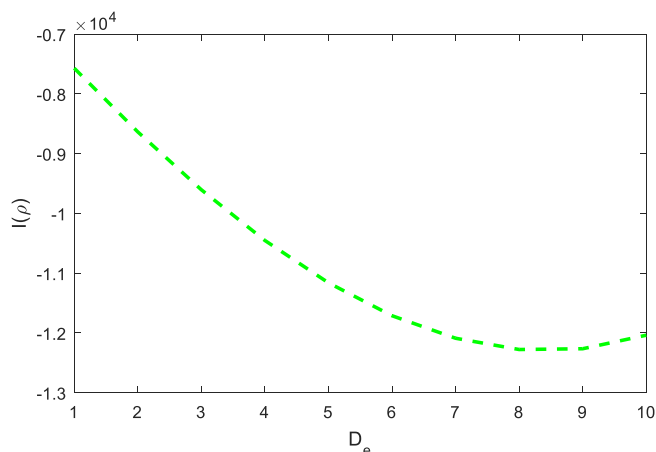


Fig. 4 Fisher information for position space $I(\rho)$ at the ground state against the screening parameter x with $m = 1$, $x = 1.05$, $h = 0.1$, $r_e = 0.1$ and $\ell = 0$

Results and discussion

In Table 1, we presented the spectroscopic parameters for the selected diatomic molecules used in this study. In Table 2 and Table 3, respectively, we presented the numerical values for momentum expectation value and position expectation value. It is observed from Table 2 that the momentum expectation value decreases as both the quantum number n and angular momentum quantum number ℓ increase respectively and collectively for all the selected molecules. The revised is observed in the position space as shown in Table 3. In Table 4 and Table 5, respectively, we numerically presented Fisher information for position space and momentum space for the same set of molecules. In the position space, Fisher information decreases as the quantum number n and angular momentum quantum number ℓ increase respectively and collectively. This trend is found to be opposite in Table 5 where Fisher information for momentum space is observed for different

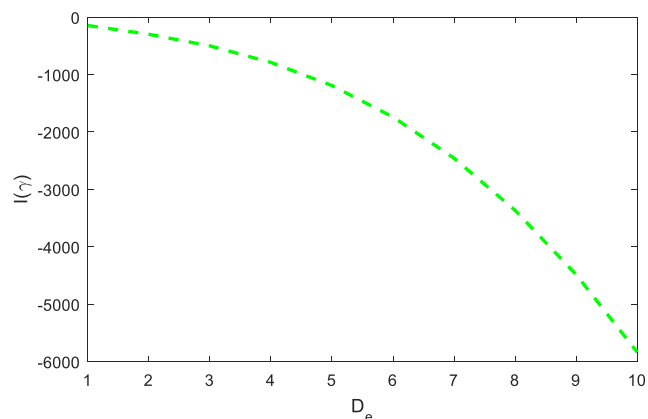


Fig. 5 Fisher information for position space $I(\gamma)$ at the ground state against the screening parameter x with $m = 1$, $x = 1.05$, $h = 0.9$, $r_e = 0.1$ and $\ell = 0$

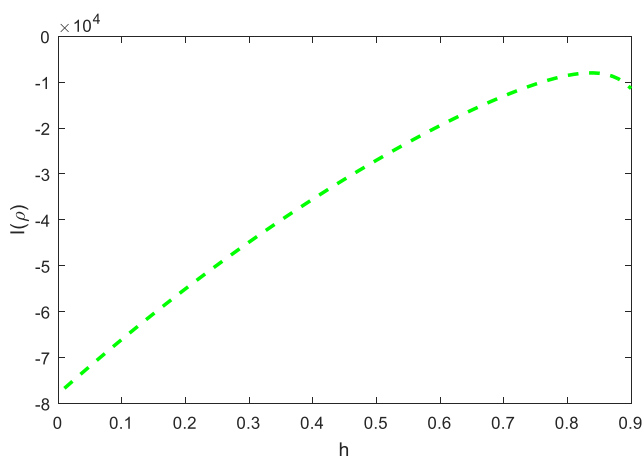


Fig. 6 Fisher information for position space $I(\rho)$ at the ground state against the screening parameter x with $m = D_e = 1$, $x = 1.05$, $r_e = 0.1$ and $\ell = 0$

values of the quantum number and angular momentum quantum number. The selected diatomic molecules are due to the purpose they served in some areas such as chemical synthesis, electronic transport properties in the areas of chemical physics, nature of bonding and stability of temperature.

The variation of energy eigenvalue against the potential parameter h is shown in Fig. 1. The energy of the system increases monotonically as the potential parameter goes up from 0. It is observed that the energy of the system can never be zero even at the zero value of the potential parameter h . In Fig. 2 and Fig. 3, we examined the variation of Fisher information against the screening parameter x . In both cases, as the screening parameter increases steadily, the Fisher information decreases. It is noted that an increase in the screening parameter results in an increase in Fisher information for both position space and momentum space. Figures 2 and 3 revealed that the variation of the Fisher information with the screening parameter does not satisfy the Heisenberg uncertainty relation. In Fig. 4 and Fig. 5, we plotted Fisher information for position space and for momentum space respectively with the

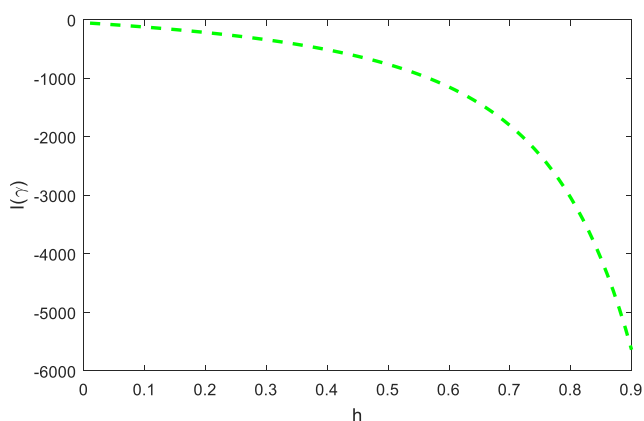


Fig. 7 Fisher information for momentum space $I(\gamma)$ at the ground state against the screening parameter x with $m = D_e = 1$, $x = 1.05$, $r_e = 0.1$ and $\ell = 0$

dissociation energy. We noticed that as the dissociation energy increases steadily, the Fisher information for both the position space and momentum space respectively decreases. Thus, the dissociation energy and the screening parameter for the Wei potential have the same effect on the Fisher information. In both cases, a squeezing effect is highly observed. In Fig. 6 and Fig. 7, we examined the behaviour of Fisher information for position space and for momentum space respectively against the potential parameter h . In the position space, Fisher information increases as the potential parameter increases while in the momentum space, Fisher information decreases monotonically as the potential parameter increases steadily. Thus, for the position space, there is an increase in the uncertainty of the system which brings about a decrease in the accuracy for predicting the localization of a particle, while in the momentum space, the uncertainty decreases and thus results in a high degree of accuracy for predicting the localization of a particle. The Heisenberg uncertainty relation for Fisher information is satisfied in Fig. 6 and Fig. 7. It is interesting to note that this potential function, though similar to other potential functions, exhibits some different features. The variation of the Fisher information with each of the potential parameters showed a squeezing effect.

Conclusions

We studied the approximate analytical solutions of the Schrödinger equation for an improved expression for Wei potential energy function with a suitable approximation scheme to the centrifugal term using the methodology of supersymmetric approach. The explicit bound state energy equation for this potential in the relativistic and non-relativistic equations was obtained. Furthermore, we applied the Hellmann-Feynman theorem on the solution of the non-relativistic equation and obtained the formula for the expectation values of $\langle r^2 \rangle$ and $\langle p^2 \rangle$. The solutions obtained have been used to calculate the Fisher information for position space and momentum space. Numerically, the expectation values and Fisher information for some selected molecules were studied. We noted that the variation of some parameters of the Wei potential energy function has the same trend for Fisher information for both position space and momentum space, respectively, which do not obey the Heisenberg uncertainty relation for Fisher information.

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