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RESEARCH ARTICLE

A new simple method for hydrogen atom and molecule ion in momentum space with using dirac delta functions

Binesh, A., Arabshahi, H and Sadremomtaz, A

[1]Physics Department, Payam Nour University, Fariman, Iran
[2]Physics Department, Ferdowsi University of Mashhad, Mashhad, Iran
[3]Physics Department, University of Guilan., Rasht, Iran

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We introduce a new simple method with using delta function interactions to compute the exact momentum representation wave function for Hydrogen atom as well as the Hydrogen molecule. Finally, we use Maple R.8 to plot the curves and discuss about the results with some interesting points, which we find in the limits.

Key words: Delta function; Hydrogen atom; Maple; Momentum

INTRODUCTION

The exact computational of the momentum space wave functions for bound states of quantum mechanical systems is usually not possible, and one must obtain the momentum representation in terms of an integral equation. A system of particular is the Hydrogen atom. For this system the momentum space wave function for the bound states in three dimensions have been obtained [1]. However, they are quite complicated. In the paper the bound state momentum space wave function of the one dimensional Hydrogen atom with δ function interaction is obtained. The exact momentum representation function for one the one dimensional Hydrogen molecule ion with δ function interactions is also obtained. Because these calculations can be carried out quit simply this problem, may be useful in discussing the momentum representation in quantum mechanics course.

***Corresponding author:** arabshahi@um.ac.ir

Hydrogen Atom

The Schordinger equation for the one dimensional Hydrogen atom with δ function is given by [2,3]

$$\left(\frac{-\hbar^2}{2m}\right)\psi'' - e^2\delta(x)\psi = E\psi \tag{1}$$

equation (1) has a bound solution

$$\psi(x) = a_0^{-1/2}\exp\left(-\left|x/a_0\right|\right) \tag{2}$$

where $a_0 = \hbar^2/me^2$. The energy eigen value for this state is

$$E = E_0 = -me^4/2\hbar^2 \tag{3}$$

the momentum space wave function maybe obtained most easily by Fourier transforming equation (1). One obtains

$$(p^2/2m - E)\phi(p) = e^2(2\pi\hbar)^{-1/2}\int \exp(-ipx/\hbar)\delta(x)\psi(x)dx = e^2(2\pi\hbar a_0)^{-1/2}$$

……………..... (4)

thus

$$\phi(p) = \frac{(2a_0/\pi\hbar)^{1/2}}{[1+(pa_0/\hbar)^2]} \quad \text{…………...(5)}$$

this result was obtained by Lieber using a different method. Plots of $|\psi(x)|^2$ as a function of x and $|\phi(p)|^2$ as a function of p are shown in fig. 1, the widths of distribution for *x* and *p*, yield the uncertainly relation. Using equation 2,

$$(\Delta x)^2 = \langle x^2 \rangle = \int x^2\psi^2(x)dx = a_0^2/2 \quad \text{….. (6)}$$

using equation (1),

$$(\Delta p^2) = \langle p^2 \rangle = 2m\langle E \rangle + 2me^2\langle \delta(x) \rangle = (\hbar/a_0)^2 \quad \text{…..(7)}$$

thus

$$\Delta x \Delta p = (\hbar/2)\sqrt{2} \quad \text{……………………… (8)}$$

which is greater the minimum value possible (Gaussian wave function) by a factor of $\sqrt{2}$.

III. Hydrogen Molecular Ion

The Schordinger equation for one-dimensional Hydrogen molecular ion with d function interaction is given by

$$\left(\frac{-\hbar^2}{2m}\right)\psi'' - e^2\delta(x-a)\psi - e^2\delta(x+a)\psi = E\psi \quad \text{…… (9)}$$

where the nuclei are located at the position $x = \pm a$. Equation (9) has one symmetric bound state solution ,

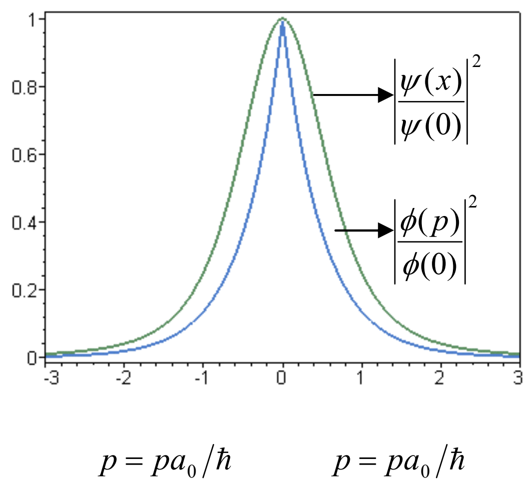

Fig.1. Variation probability amplitudes in position and momentum spaces versus *x* and *p*

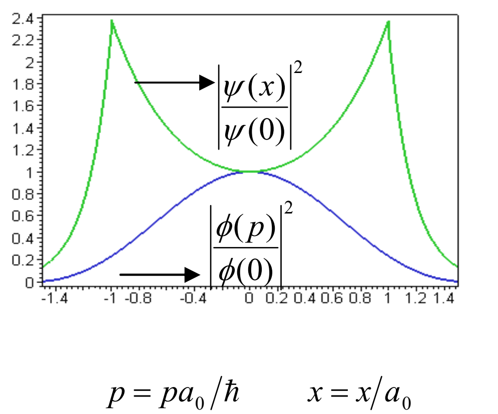

Fig. 2. Variation probability amplitudes in position and momentum spaces versus *x* and *p*
(assumed a= a_0 & β=2)

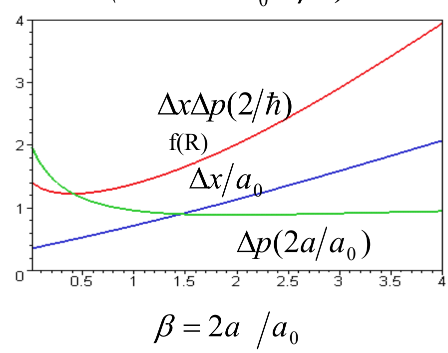

Fig.3. Variation uncertainty in position, momentum and uncertainty relation versus *β when R=2a*

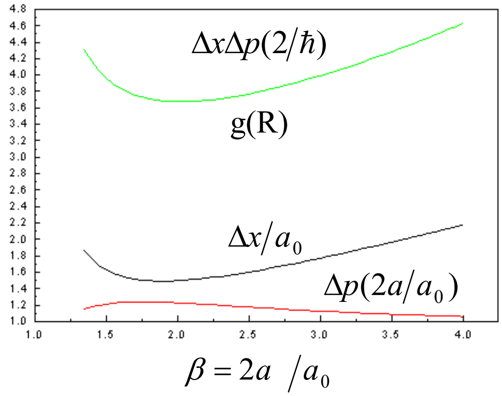

Fig.4. Variation uncertainty in position, momentum and uncertainty relation versus *β when R=2a*

$p = pa_0/\hbar \qquad x = x/a_0$

Fig.1 Variation probability amplitudes in position and momentum spaces versus *x* and *p*

$$\psi(x) = A\cosh(\gamma x/a) \qquad |x| < a \qquad \text{(10-a)}$$

$$B\exp(-\gamma|x|/a) \qquad |x| > a \qquad \text{(10-b)}$$

with $A = (2/a_0)^{1/2}(1+2\gamma-\beta)^{-1/2}\exp(-\gamma)$ and $B = (2/a_0)(1+2\gamma-\beta)^{-1/2}\cosh(\gamma)$, where $\beta = 2a/a_0 = \gamma[1+\tanh(\gamma)]$. The energy eigenvalue for this state is

$$R = E_0(2\gamma/\beta)^2 \qquad (11)$$

the momentum space wave function is obtained most easily by Fourier transforming

equation (9). One obtains

$$\left[(p^2/2m - E)\phi(p) = e^2(2\pi\hbar)^{-1/2}\int \exp(-ipx/\hbar)[\delta(x-a)+\delta(x+a)]\psi(x)dx\right]$$

$$= e^2(2\pi\hbar)^{-1/2}\psi(a)\cos(pa/\hbar) \qquad (12)$$

$$= 2e^2(\pi\hbar a_0)^{-1/2}(1+2\gamma-\beta)^{-1/2}\exp(-\gamma)\cosh(\gamma)\cos(pa/\hbar)$$

thus

$$\phi(p) = \frac{4^2(a_0/\pi\hbar)^{-1/2}(1+2\gamma-\beta)^{-1/2}\exp(-\gamma)\cosh(\gamma)\cos(pa/\hbar)}{(pa_0/\hbar)^2 + (2\gamma/\beta)^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots(13)$$

plots of $|\psi(x)/\psi(0)|^2$ as a function of *x* and $|\phi(p)/\phi(0)|^2$ as a function of *p* are shown in figure 2. One my again compute the widths of the distribution for *x* and *p* to evaluate the uncertainty relation. Using equation (10),

$$(\Delta x)^2 = \langle x^2\rangle = \frac{a_0^2}{2}(1+2\gamma-\beta)^{-1}\exp(-2\gamma)(\beta/2\gamma)^3 \times \left[\exp(2\gamma)(2\gamma^2+1)+(4\gamma^3/3+2\gamma^2+2\gamma+1)\right] \quad \ldots\ldots\ldots(14)$$

using equation (9),

$$(\Delta p)^2 = \langle p^2\rangle = 8(\hbar/a_0)^2\left[(1+2\gamma-\beta)^{-1}\exp(-2\gamma)\cosh^2(\gamma) - \gamma^2/2\beta^2\right] \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(15)$$

thus

$$\Delta x\Delta p = (\hbar/2)f(R) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(16)$$

where $f(R)$ is a function of the distance, *R=2a*, between the nuclei which is obtained by taking the square root of the product of equations (14) and (15). The uncertainty in the values of *x* and *p* and the uncertainty relation are plotted as a function of *R* in fig. 3. As may be seen in fig.3 the uncertainty in the position increases without limit as the distance between the nuclei increase, but the uncertainty in the momentum decreases by factor of 2. In the limit that $R \to 0$, Δx, as obtained from equation (14), is decreased by factor of 2 compared to that obtained from equation (16), and is the same as for one dimensional helium atom $(a \to a_0/2)$. The uncertainty in the momentum, as obtained from equation (15), is increased by a factor of 2 compared to that obtained from equation (7). Hence, the uncertainty relation, given in equation (8), remains unchanged.

It is of interest to that the antisymmetric state of the Hydrogen molecule ion also has negative energy for $a = a_0/2$. However, the energy *E(R)* is always greater than $E(\infty) = E_0$, the energy of a Hydrogen atom and a Hydrogen atom ion. The antisymmetric solution of equation (9) is,

$$\psi(x) = A' \sinh(\gamma x/a) \qquad |x| < a$$

(17-a)

$$B' \exp(-\gamma|x|/a) \qquad |x| > a$$

(17-b)

with $A' = (2/a_0)(1+2\gamma-\beta)^{-1}\exp(-\gamma)$ and $B' = (2/a_0)(1+2\gamma-\beta)^{-1}\sinh(\gamma)$, where now $\beta = 2a/a_0 = \gamma[1+\coth(\gamma)]$. The momentum space wave function obtained by Fourier transforming equation (9) is,

$$\phi(p) = \frac{-4i^2(a_0/\pi\hbar)^{1/2}\exp(-\gamma)\sinh(pa_0/\hbar)}{(pa_0/\hbar)^2 + (2\gamma/\beta)^2} \qquad \ldots\ldots(18)$$

the widths of distribution are

$$(\Delta x)^2 = \langle x^2 \rangle = \frac{a_0^2}{2}(1+2\gamma-\beta)^{-1}\exp(-2\gamma)(\beta/2\gamma)^3 \times \left[\exp(2\gamma)(2\gamma^2+1) + (4\gamma^3/3 + 2\gamma^2 + 2\gamma + 1)\right] \quad \ldots\ldots(19)$$

and

$$(\Delta p)^2 = \langle p^2 \rangle = 8(\hbar/a_0)^2\left[(1+2\gamma-\beta)^{-1}\exp(-2\gamma)\sinh^2(\gamma) - \gamma^2/2\beta^2\right] \quad \ldots\ldots\ldots\ldots(20)$$

thus

$$\Delta x \Delta p = (\hbar/2)g(R) \qquad \ldots\ldots\ldots\ldots\ldots (21)$$

where *g(R)* is again a function of *R* obtained from equation 19 and 20. The uncertainty in the values of *x* and *p,* and the uncertainty relation plotted as a function of *R* in fig.5. For the negative parity state the energy is negative only for $a > a_0/2$, $\beta = 1$ and $\gamma = 0$. Then $\Delta x = a_0/2\sqrt{2}\gamma \to \infty$, $\Delta p = 2\sqrt{2}\hbar\gamma^{1/2}/a_0 \to 0$ and $\Delta x\Delta p \to (\hbar/2)g(0) = \hbar/\gamma^{1/2} \to \infty$. The momentum representation of the one dimensional Hydrogen atom with a δ function interaction is a useful example to discuss in a quantum mechanics course because of the ease of carrying out computations. We have also shown that one easily obtain the momentum space wave function for one-dimensional Hydrogen molecule ion with δ function interactions.

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