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Variational Analysis of Quantum Uncertainty Principle

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Abstract: *It is well known that the cornerstone of quantum mechanics is the famous Heisenberg uncertainty principle. This principle, which states that the product of the uncertainties in position and momentum must be greater than or equal to a very small number proportional to Planck's constant, is typically taught in quantum mechanics courses as a consequence of the Schwartz inequality applied to the non-commutation of the quantum position and momentum operators. In the following, we present a more pedagogically appealing approach to derive the uncertainty principle through a variational analysis. Using this extremum approach, it is first shown that the Gaussian spatial wave function is the optimal solution for the minimum of the product of the uncertainties in position and wavenumber associated with the Fourier transformed Gaussian wave function. Ultimately, as a consequence of this Fourier transform pair analysis, and the de Broglie connection between the momentum and the wavenumber representation of a general quantum particle, the Heisenberg uncertainty principle is derived.*

Keywords: *Quantum Heisenberg Uncertainty Principle, Quantum Pedagogy, Fourier Transform Pairs, Variational Analysis, Schwarz Inequality.*

1. INTRODUCTION

The cornerstone of quantum mechanics is the famous Heisenberg uncertainty principle. This principle gives a non-negative lower bound on the product of the uncertainty in the position of a quantum particle and its momentum. The quantum uncertainty principle is also directly connected to the more fundamental inequality relationship of the product of the uncertainty in position of a general wave function and the uncertainty in wavenumber associated with the Fourier transform of the wave function. However, the derivation of the Fourier transform inequality relation between the uncertainty in position and the uncertainty in wavenumber is typically derived using the Schwartz inequality [1-5]. This approach is intimately tied to the uncertainties associated with two non-commuting operators: the quantum position and momentum operators and vast generalizations of this idea have been developed. As a pedagogically better approach to understanding the quantum uncertainty principle, instead of first introducing the quantum mechanics student to abstract mathematical approaches, the fundamental uncertainty principle can instead be derived using a much more appealing optimization approach, using the calculus of variation.

First, in the remainder of this section, a Gaussian wave function is described as providing an optimal extremum of the product of the uncertainty in position and the uncertainty in wavenumber, where the details of the Gaussian wave function in position and the Fourier transformed wave function are provided. In section 2, the variational analysis derivation of the optimal product is shown to be solved using a Gaussian wave function, for the simplest case of a wave function in position space which is real and centered about the origin, resulting in the simplest version of the uncertainty principle. In section 3, the variational analysis is extended to the general case of a complex wave function which is centered about a general coordinate location, which is solved by a general Gaussian wave function, thus providing the general uncertainty relation for the product of the uncertainty in position and the uncertainty in wavenumber. In section 4, as a counter example to the optimal Gaussian wave function, a two sided exponential wave function is explored in order to demonstrate that it does not lead to the optimal minimum product of the uncertainties in position and wavenumber. Finally, in section 5, results are provided which lead to the important quantum mechanics discussion associated with the application of the variationally derived general Fourier transform pair inequality. Specifically, using the de Broglie connection of the wavenumber to the momentum of the quantum particle, the famous Heisenberg uncertainty principle is derived. This ultimately provides a much more appealing understanding for quantum physics students.

The following is a calculus of variation calculation of the uncertainty principle, which relates the uncertainty in position, Δx, of a wave function, $\psi(x)$, to the uncertainty in wavenumber, Δk, of the Fourier transform, $\varphi(k)$, of the wave function. It will be shown that the extremum (minimum) solution of the product of the two uncertainties, $\Delta x\Delta k$, is achieved using a Gaussian wave function in position, x, space,

$$\psi(x)=\frac{1}{(2\pi)^{1/4}\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right], \tag{1}$$

and its Fourier transform in wavenumber, k, space,

$$\varphi(k)=\frac{1}{(2\pi)^{1/4}\sqrt{\Delta k}}\exp\left[-(k/\Delta k)^2/4\right]. \tag{2}$$

Here, it should be noted that the probability density in position, $|\psi(x)|^2$, and the probability density in wavenumber, $|\varphi(k)|^2$, are both properly normalized such that the integrals of each are one. For this Gaussian wave function situation, it is found that the product of these uncertainties is the optimal minimum product,

$$\Delta x\Delta k = 1/2. \tag{3}$$

Preliminary to the variational analysis provided below, it is useful to first review some of the well-known aspects of the Gaussian wave function, $\psi(x)$, given in equation (1). The Fourier transform, $\varphi(k)$, of the Gaussian wave function can be obtained by contour integration, where

$$\begin{aligned}\varphi(k)&=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dx\psi(x)e^{-ikx}=\frac{1}{(2\pi)^{1/4}\sqrt{2\Delta x}}\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}dx\exp\left[-(x/\Delta x)^2/4-ikx\right]\\&=\frac{\sqrt{2\Delta x}}{(2\pi)^{1/4}}\exp\left[-(\Delta xk)^2\right]\left\{\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty}dz\,\mathrm{e}^{-(z+i\Delta xk)^2}\right\}=\frac{\sqrt{2\Delta x}}{(2\pi)^{1/4}}\exp\left[-(\Delta xk)^2\right]\end{aligned}. \tag{4}$$

Here, it should be noted that the Gaussian integral, equation (4), is achieved using the standard technique of completing the square in the exponent, and deforming the complex contour integral to the real axis, as the integrand is entire, and the integral along the real axis is $\sqrt{\pi}$. For convenience in the following, it will be assumed that all integrals are over the R^3 infinite domain, [- infinity, + infinity], as is shown explicitly in equation (4). The probability density in x space,

$$|\psi(x)|^2=\frac{1}{\Delta x\sqrt{2\pi}}\exp\left[-(x/\Delta x)^2/2\right], \tag{5}$$

is properly normalized, with a unity integral over all space, as

$$\int dx|\psi(x)|^2=\frac{1}{\Delta x\sqrt{2\pi}}\int dx\exp\left[-(x/\Delta x)^2/2\right]=\frac{1}{\sqrt{\pi}}\int dte^{-t^2}=1\cdot \tag{6}$$

In addition, since the Gaussian wave function is centered about the origin, $x=0$, then the first moment of the probability density (the expectation value of position) is zero, $\langle x\rangle=0$, and the variance of the probability density in x space is given by the second moment of the probability density, where

$$\int dxx^2|\psi(x)|^2=\frac{1}{\Delta x\sqrt{2\pi}}\int dxx^2\exp\left[-(x/\Delta x)^2/2\right]=\frac{2(\Delta x)^2}{\sqrt{\pi}}\int dtt^2e^{-t^2}=(\Delta x)^2. \tag{7}$$

Similarly, but alternatively associated with the Fourier transform of the Gaussian wave function, $\varphi(k)$, and the associated probability density in k space, $|\varphi(k)|^2$, it is useful to consider a different parameterization, instead of using Δx, it is useful to write

$$\Delta x = 1/2\Delta k, \tag{8}$$

and as a result, the Fourier transformed wave function, equation (4), is the same as equation (2), where

$$\varphi(k) = \frac{1}{(2\pi)^{1/4}\sqrt{\Delta k}} \exp\left[-(k/\Delta k)^2/4\right], \tag{9}$$

and the probability density is

$$|\varphi(k)|^2 = \frac{1}{\Delta k\sqrt{2\pi}} \exp\left[-(k/\Delta k)^2/2\right]. \tag{10}$$

Consequently, it should be clear that the wave function, equation (1), and its Fourier transform, equation (2), have the same Gaussian structure; in addition, the probability density in x space, equation (5), and the probability density in k space, equation (10), also have the same Gaussian structure, with the replacement of Δx by Δk. Thus, it is also true that the probability density in k space is centered about the origin, $k=0$, such that the first moment of the probability density (the expectation value of wavenumber) is zero, $\langle k\rangle = 0$, and the variance of the probability density in k space is given by the second moment of the probability density, where

$$\int dk k^2 |\varphi(k)|^2 = \frac{1}{\Delta k\sqrt{2\pi}} \int dk k^2 \exp\left[-(k/\Delta k)^2/2\right] = \frac{2(\Delta k)^2}{\sqrt{\pi}} \int dt t^2 e^{-t^2} = (\Delta k)^2. \tag{11}$$

In order to show that the Gaussian wave function and the Fourier transformed wave function result in an optimal minimum product of uncertainties in position, Δx, and wavenumber, Δk, as shown in equation (3), it is useful to consider a general extremum analysis of the product of the position variance of the probability density in x space, as formulated in equation (7), times the wavenumber variance of the probability density in k space, as formulated in equation (11).

2. Simple Variational Analysis of Real Wave Function that is Centered about $x=0$

For the sake of convenience, it is simplest to limit this variational analysis by considering a real wave function, $\psi(x) = \psi^*(x)$, where the probability density in x space is $|\psi(x)|^2 = \psi^2(x)$, which is centered (or even) about the origin, $x=0$, where the position expectation value is zero, $\langle x\rangle = 0$. To generalize this analysis for a complex valued wave function, simply replace the pairings $\psi(x)$ and $\psi(x)$ with $\psi(x)$ and $\psi^*(x)$, as is shown in section 3. In addition, in this case, the probability density in k space, $|\varphi(k)|^2$, is also centered (or even) about the origin, $k=0$, where the wavenumber expectation value is also zero, $\langle k\rangle = 0$. Although this is the case for the Gaussian wave function, equation (1), the approach can easily be generalized for a complex valued wave function which has a non-zero expectation value, where $\langle x\rangle = x_0$, as is also shown in section 3.

The objective in the following is to look for optimal solutions of the wave function, $\psi(x) = \psi_{\text{opt}}(x)$, where the product of the variance (or second moment) of the probability density in x space, times the variance of the probability density in k space, is a minimum. This is variationally analyzed in the following, using the functional, J, where

$$J = \left(\int dx x^2 \left|\psi(x)\right|^2\right)\left(\int dk k^2 \left|\varphi(k)\right|^2\right). \tag{12}$$

However, this is also subject to the wave function normalization functional constraint, $I = 1$, where

$$I = \int dx \left|\psi(x)\right|^2. \tag{13}$$

Consequently, it is appropriate to consider the zero variation of the combined functional, where

$$\delta J + \lambda \delta I = 0, \tag{14}$$

using a Lagrange multiplier, λ, which is determined during the analysis.

Prior to proceeding with the variational analysis, it is helpful to first re-write the variance of the probability density in k space, instead as a spatial integral functional of the spatial derivative of the wavefunction, $d\psi / dx$. Using the Fourier transform of the wave function,

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \int dx \psi(x) e^{-ikx}, \tag{15}$$

in the variance of the probability density in k space calculation, then

$$\begin{aligned} \int dk k^2 \left|\varphi(k)\right|^2 &= \int dk k^2 \left| \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \psi(x) e^{-ikx} \right|^2 \\ &= \int dx \int dx' \psi(x) \psi(x') \left[\frac{1}{2\pi} \int dk k^2 e^{ik(x-x')} \right] \end{aligned}. \tag{16}$$

The last term in brackets can be analyzed (in the distribution sense of integration by parts, with respect to a family of infinitely differentiable test functions), using a second derivative of a Dirac delta function (see [6], for example). It is important to emphasize that any analyses using a Dirac delta function are done in the distribution sense. Using this convention, the transformation of the k space variance calculation, equation (16), begins by recalling that the Dirac delta function can be expressed as the following integral,

$$\delta(x - x') = \frac{1}{2\pi} \int dk e^{ik(x-x')}. \tag{17}$$

Consequently, using equation (17), the last term in brackets of equation (16), is given by

$$\frac{1}{2\pi} \int dk k^2 e^{ik(x-x')} = -\frac{\partial^2}{\partial x^2}\left[\delta(x - x')\right], \tag{18}$$

so that the variance calculation, equation (16), can alternatively be expressed as

$$\int dk k^2 \left|\varphi(k)\right|^2 = -\int dx \int dx' \psi(x) \psi(x') \frac{\partial^2}{\partial x^2}\left[\delta(x - x')\right]. \tag{19}$$

Finally, noting that the wave function and the derivative of the wave function have zero boundary conditions,

$$\left. \psi(x), \frac{d}{dx}\psi(x) \right|_{x=\pm\infty} = 0, \tag{20}$$

twice integration by parts of equation (19) gives the variance,

$$\int dk k^2 \left|\varphi(k)\right|^2 = -\int dx \int dx' \frac{\partial^2}{\partial x^2}\left[\psi(x)\right] \psi(x') \delta(x - x') = -\int dx \frac{\partial^2}{\partial x^2}\left[\psi(x)\right] \psi(x), \tag{21}$$

and after one final integration by parts, the variance is

$$\int dk k^2 \left|\varphi(k)\right|^2 = \int dx \left[\frac{\partial}{\partial x}\psi(x)\right]^2 . \tag{22}$$

The variance product functional, equation (12), which will be variationally analyzed, is

$$J = \left[\int dx x^2 \psi^2(x)\right]\left\{\int dx \left[\frac{\partial}{\partial x}\psi(x)\right]^2\right\} = \int dx \int dx' x^2 \psi^2(x)\left[\frac{\partial}{\partial x'}\psi(x')\right]^2 . \tag{23}$$

In order to analyze the variational problem, equation (14), it is useful to parameterize the variation of the wave function, $\delta\psi$, using trial wave functions,

$$\psi(x,\alpha) = \psi(x,0) + \alpha\eta(x), \tag{24}$$

which incorporate an α parameter, and an arbitrary variation function, $\eta(x)$, which has the usual zero boundary conditions at the end points,

$$\left.\eta(x)\right|_{x=\pm\infty} = 0 , \tag{25}$$

where the optimal (zero variation) solution is achieved at $\alpha = 0$, where

$$\left.\psi(x,\alpha)\right|_{\alpha=0} = \psi(x,0) = \psi_{\text{opt}}(x) . \tag{26}$$

Given the trial wave function parameterization, equation (24), it should be noted that the two functionals, Eqs. (13) and (23), are simply functions of the α parameter; consequently, the zero variation analysis, equation (14), can be achieved by setting to zero the ordinary derivative with respect to α , as

$$\left.\frac{d}{d\alpha}\left[J(\alpha) + \lambda I(\alpha)\right]\right|_{\alpha=0} = 0 . \tag{27}$$

With the aid of equation (24), applied to Eqs. (13) and (23), the extremum problem, equation (27), is

$$0 = \frac{d}{d\alpha}\left.\left\{\begin{aligned} &\iint dx dx' x^2 \left[\psi_{\text{opt}}(x) + \alpha\eta(x)\right]^2 \left\{\frac{\partial}{\partial x'}\left[\psi_{\text{opt}}(x') + \alpha\eta(x')\right]\right\}^2 \\ &\quad + \lambda \int dx \left[\psi_{\text{opt}}(x) + \alpha\eta(x)\right]^2 \end{aligned}\right\}\right|_{\alpha=0} . \tag{28}$$

After the derivative of the three separate terms is taken and α set to zero, the result is

$$\begin{aligned} 0 = {} & 2\int dx \left\{ x^2 \psi_{\text{opt}}(x)\left[\int dx' \left[\frac{d\psi_{\text{opt}}(x')}{dx'}\right]^2\right] + \lambda\psi_{\text{opt}}(x)\right\}\eta(x) \\ & + 2\int dx' \left[\frac{d\psi_{\text{opt}}(x')}{dx'}\frac{d\eta(x')}{dx'}\right]\left[\int dx x^2 \psi^2_{\text{opt}}(x)\right] \end{aligned} . \tag{29}$$

Integrating the last term by parts and utilizing the zero boundary condition from equation (25), and changing integration variables in the last term, the result is

$$0 = \int dx \left\{\begin{aligned} & x^2 \psi_{\text{opt}}(x)\left[\int dx' \left[\frac{d\psi_{\text{opt}}(x')}{dx'}\right]^2\right] + \lambda\psi_{\text{opt}}(x) \\ & \qquad - \frac{d^2\psi_{\text{opt}}(x)}{dx^2}\left[\int dx' x'^2 \psi^2_{\text{opt}}(x')\right] \end{aligned}\right\}\eta(x) . \tag{30}$$

As is usual for variational analysis, since $\eta(x)$ is arbitrary, the result is

$$x^2\psi_{\text{opt}}(x)\left[\int dx'\left[\frac{d\psi_{\text{opt}}(x')}{dx'}\right]^2\right]+\lambda\psi_{\text{opt}}(x)=\frac{d^2\psi_{\text{opt}}(x)}{dx^2}\left[\int dx'x'^2\psi^2{}_{\text{opt}}(x')\right]. \tag{31}$$

The integrals in equation (31) are precisely the variances of the probability density in x space,

$$\int dxx^2\psi^2{}_{\text{opt}}(x)=(\Delta x)^2, \tag{32}$$

and in k space,

$$\int dx\left[\frac{d\psi_{\text{opt}}(x)}{dx}\right]^2=\int dkk^2\left|\varphi_{\text{opt}}(k)\right|^2=(\Delta k)^2, \tag{33}$$

so it is convenient to parameterize them using the uncertainty in position, Δx, and wavenumber, Δk, notation, where $\varphi_{\text{opt}}(k)$ is the Fourier transform of the optimal wave function, $\psi_{\text{opt}}(x)$. Thus, the optimal extremum wave function satisfies the following differential equation, where

$$(\Delta k)^2\,x^2\psi_{\text{opt}}(x)+\lambda\psi_{\text{opt}}(x)=(\Delta x)^2\,\frac{d^2\psi_{\text{opt}}(x)}{dx^2}. \tag{34}$$

Finally, the extremum differential equation, equation (34), for the optimal wave function, is satisfied by the Gaussian wave function, equation (1), when the Lagrange multiplier is set to $\lambda=-1/2$. To see this result, consider the following: the optimal wave function is

$$\psi_{\text{opt}}(x)=\frac{1}{(2\pi)^{1/4}\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]; \tag{35}$$

the probability density in x space is

$$\left|\psi_{\text{opt}}(x)\right|^2=\frac{1}{\Delta x\sqrt{2\pi}}\exp\left[-(x/\Delta x)^2/2\right], \tag{36}$$

which is properly normalized, as

$$I=\int dx\left|\psi_{\text{opt}}(x)\right|^2=1, \tag{37}$$

and which has the correct parameterization for the variance in x space, as

$$\int dxx^2\psi^2{}_{\text{opt}}(x)=(\Delta x)^2; \tag{38}$$

the derivative of the optimal wave function is

$$\frac{d\psi_{\text{opt}}(x)}{dx}=\frac{-x}{2(2\pi)^{1/4}(\Delta x)^2\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]; \tag{39}$$

and the second derivative of the optimal wave function is

$$\begin{aligned}\frac{d^2\psi_{\text{opt}}(x)}{dx^2}&=\frac{-1}{2(2\pi)^{1/4}(\Delta x)^2\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]\\&+\frac{x^2}{4(2\pi)^{1/4}(\Delta x)^4\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]\end{aligned}. \tag{40}$$

Consequently, the extremum equation, equation (34), with $\lambda=-1/2$, is satisfied, where

$$\begin{aligned}&(\Delta k)^2 x^2 \frac{1}{(2\pi)^{1/4}\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]-\frac{1}{2(2\pi)^{1/4}\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]\\&=\frac{-1}{2(2\pi)^{1/4}\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]+\frac{x^2}{4(2\pi)^{1/4}(\Delta x)^2\sqrt{\Delta x}}\exp\left[-(x/\Delta x)^2/4\right]\end{aligned}, \quad (41)$$

which reduces to the correct optimal uncertainty relation, equation (3), where the variance product is

$$(\Delta x)^2(\Delta k)^2 = 1/4. \quad (42)$$

It should be noted that the optimal wave function Fourier transform,

$$\varphi_{\text{opt}}(k) = \frac{1}{(2\pi)^{1/4}\sqrt{\Delta k}}\exp\left[-(k/\Delta k)^2/4\right], \quad (43)$$

does indeed have the correct variance of the probability density in k space,

$$\int dk k^2 \left|\varphi_{\text{opt}}(k)\right|^2 = (\Delta k)^2, \quad (44)$$

so that ultimately the product of the variances is optimal, which can be expressed as

$$\left[\int dx x^2 \left|\psi_{\text{opt}}(x)\right|^2\right]\left[\int dk k^2 \left|\varphi_{\text{opt}}(k)\right|^2\right] = \frac{1}{4}. \quad (45)$$

The most important conclusion of this analysis, which pertains to a general wave function, $\psi(x)$, and its Fourier transform, $\varphi(k)$, is that the product of variances in x space and in k space must always be greater than or equal to the limit given in equation (45), so that the variance inequality is

$$\left[\int dx x^2 \left|\psi(x)\right|^2\right]\left[\int dk k^2 \left|\varphi(k)\right|^2\right] \geq \frac{1}{4}. \quad (46)$$

Using Eqs. (32) and (33), but for a general wave function, $\psi(x)$, and its Fourier transform, $\varphi(k)$, the uncertainty inequality relation is given by

$$(\Delta x)^2(\Delta k)^2 \geq \frac{1}{4}. \quad (47)$$

3. General Variational Analysis of Complex Wave Function that is Centered about $x = x_0$

The variational uncertainty principle calculation of equation (46) is repeated here, with the generalization to a complex wave function, $\psi(x)$, which has a probability density in x space, $\left|\psi(x)\right|^2$, that is centered about $x = x_0$, where $\langle x\rangle = x_0$, as well as having a Fourier transformed wave function, $\phi(k)$, such that the probability density in k space, $\left|\varphi(k)\right|^2$, is centered about $k = k_0$, where $\langle k\rangle = k_0$. First, a complex wave function, $\psi(x)$, with a Fourier transform, $\varphi(k)$, is analyzed as having an uncertainty principle for the case that $\langle x\rangle = 0$ and $\langle k\rangle = 0$, where

$$\left[\int dx x^2 \left|\psi(x)\right|^2\right]\left[\int dk k^2 \left|\varphi(k)\right|^2\right] \geq \frac{1}{4}; \quad (48)$$

while the proper normalization of the wave function,

$$\int dx \left|\psi(x)\right|^2 = 1, \quad (49)$$

and the Fourier transformed wave function,

$$\int dk\left|\varphi(k)\right|^2=1, \tag{50}$$

are assumed. Next, an altered wave function, given by the transformation

$$\psi(x)\rightarrow e^{ik_0x}\psi(x-x_0), \tag{51}$$

with an altered Fourier transformed wave function, given by the transformation

$$\varphi(k)\rightarrow e^{-i(k-k_0)x_0}\varphi(k-k_0), \tag{52}$$

are shown to result in the general case, where the uncertainty principle is

$$\left[\int dx\left(x-x_0\right)^2\left|\psi(x)\right|^2\right]\left[\int dk\left(k-k_0\right)^2\left|\varphi(k)\right|^2\right]\geq\frac{1}{4}. \tag{53}$$

Prior to the general uncertainty principle case, equation (53), it is important to demonstrate that: i) the expectation value of position is $\langle x\rangle=x_0$, using the shifted wave function, equation (51), as

$$\langle x\rangle=\int dxx\left|e^{ik_0x}\psi(x-x_0)\right|^2=\int dx'\left(x'+x_0\right)\left|\psi(x')\right|^2=x_0\int dx\left|\psi(x)\right|^2=x_0, \tag{54}$$

where the substitution, $x'=x-x_0$, is made, as well as the prior assumption of $\int dxx\left|\psi(x)\right|^2=0$, is used; ii) the Fourier transform is given by the transformation in equation (52), using equation (51) and $x'=x-x_0$, where

$$\varphi(k)\rightarrow\int dxe^{ik_0x}\psi(x-x_0)e^{-ikx}=\int dx'\psi(x')e^{-i(k-k_0)(x_0+x')}=e^{-i(k-k_0)x_0}\varphi(k-k_0); \tag{55}$$

and iii) that the expectation value of wavenumber is $\langle k\rangle=k_0$, using the shifted Fourier transformed wave function, equation (52), and $k'=k-k_0$, where

$$\langle k\rangle=\int dkk\left|e^{-i(k-k_0)x_0}\varphi(k-k_0)\right|^2=\int dk'\left(k'+k_0\right)\left|\varphi(k')\right|^2=k_0\int dk\left|\varphi(k)\right|^2=k_0, \tag{56}$$

as the prior assumption of $\int dkk\left|\varphi(k)\right|^2=0$, is used.

The final resultant general uncertainty principle, equation (53), can be shown as being correct, given equation (48), since the analysis of equation (53), with the substitution of Eqs. (51) and (52) into equation (53), provides

$$\left[\int dx\left(x-x_0\right)^2\left|e^{ik_0x}\psi(x-x_0)\right|^2\right]\left[\int dk\left(k-k_0\right)^2\left|e^{-i(k-k_0)x_0}\varphi(k-k_0)\right|^2\right]\geq\frac{1}{4}, \tag{57}$$

and with the changes of variables, $x'=x-x_0$ and $k'=k-k_0$, the result is

$$\left[\int dx'x'^2\left|\psi(x')\right|^2\right]\left[\int dk'k'^2\left|\varphi(k')\right|^2\right]\geq\frac{1}{4}. \tag{58}$$

Consequently, given equation (48), or the equivalent equation (58), the general uncertainty principle result, equation (53), is correct.

The generalization of the variational analysis of the complex wave function, $\psi(x)$, where $\langle x\rangle=0$ and $\langle k\rangle=0$, proceeds by considering the uncertainty product functional, J from equation (12), combined with the normalization functional constraint, I from equation (13). The generalization of the variance of the probability density in k space, equation (22), is found by starting with equation (16), which is replaced by

$$\int dkk^2 \left|\varphi(k)\right|^2 = \int dkk^2 \left| \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\psi(x) e^{-ikx} \right|^2 \\ = \int dx \int dx' \psi^*(x)\psi(x') \left[\frac{1}{2\pi} \int dkk^2 e^{ik(x-x')} \right]. \tag{59}$$

With the aid of equation (18), then the replacement of the variance in equation (59) is

$$\int dkk^2 \left|\varphi(k)\right|^2 = -\int dx \int dx' \psi^*(x)\psi(x') \frac{\partial^2}{\partial x^2}\left[\delta(x-x')\right]. \tag{60}$$

Utilizing boundary conditions, equation (20), and the integration by parts in equations (21) and (22), then equation (22) is replaced by

$$\int dkk^2 \left|\varphi(k)\right|^2 = \int dx \left| \frac{\partial}{\partial x}\psi(x) \right|^2 . \tag{61}$$

Consequently, the variance product, equation (12), is replaced by

$$J = \left[\int dxx^2 \left|\psi(x)\right|^2 \right] \left[\int dx \left| \frac{\partial}{\partial x}\psi(x)\right|^2 \right] = \int dx \int dx' x^2 \left|\psi(x)\right|^2 \left| \frac{\partial}{\partial x'}\psi(x')\right|^2 . \tag{62}$$

Utilizing the parameterization of the variation of the wave function, equation (24), with equations (25) and (26), the extremum problem, using the zero variation analysis, equation (27), with equations (13) and (62), is

$$0 = \frac{d}{d\alpha} \left\{ \begin{aligned} & \iint dxdx' x^2 \left|\psi_{\text{opt}}(x) + \alpha\eta(x)\right|^2 \left| \frac{\partial}{\partial x'}\left[\psi_{\text{opt}}(x') + \alpha\eta(x')\right] \right|^2 \\ & + \lambda \int dx \left|\psi_{\text{opt}}(x) + \alpha\eta(x)\right|^2 \end{aligned} \right\} \Bigg|_{\alpha=0} . \tag{63}$$

After the derivative of the three terms is achieved, with α set to zero, the equation (29) is replaced by

$$0 = \int dx \left\{ \begin{aligned} & x^2 \left[\eta^*(x)\psi_{\text{opt}}(x) + \psi^*_{\text{opt}}(x)\eta(x) \right] \left[\int dx' \left| \frac{d\psi_{\text{opt}}(x')}{dx'} \right|^2 \right] \\ & + \lambda \left[\eta^*(x)\psi_{\text{opt}}(x) + \psi^*_{\text{opt}}(x)\eta(x) \right] \end{aligned} \right\} \\ + \int dx' \left[\frac{d\eta^*(x')}{dx'} \frac{d\psi_{\text{opt}}(x')}{dx'} + \frac{d\psi^*_{\text{opt}}(x')}{dx'} \frac{d\eta(x')}{dx'} \right] \left[\int dxx^2 \left|\psi_{\text{opt}}(x)\right|^2 \right] . \tag{64}$$

Using the same parameterization of the integrals in equation (64), as in Eqs. (32) and (33),

$$\int dxx^2 \left|\psi_{\text{opt}}(x)\right|^2 = (\Delta x)^2 , \tag{65}$$

and

$$\int dx \left| \frac{d\psi_{\text{opt}}(x)}{dx} \right|^2 = \int dkk^2 \left|\varphi_{\text{opt}}(k)\right|^2 = (\Delta k)^2 , \tag{66}$$

then, after the appropriate integration by parts, the equivalent of equation (30) is

$$0 = 2\,\text{Re} \left\{ \int dx \left[(\Delta k)^2 x^2 \psi_{\text{opt}}(x) + \lambda\psi_{\text{opt}}(x) - (\Delta x)^2 \frac{d^2\psi_{\text{opt}}(x)}{dx^2} \right] \eta^*(x) \right\} . \tag{67}$$

Consequently, for arbitrary $\eta^*(x)$, the variational differential equation, equivalent to equation (34), is

$$(\Delta k)^2 x^2 \psi_{\text{opt}}(x) + \lambda \psi_{\text{opt}}(x) = (\Delta x)^2 \frac{d^2 \psi_{\text{opt}}(x)}{dx^2}. \tag{68}$$

As previously shown using the Gaussian wave function, equation (35), with $\lambda = -1/2$, the extremum solution of equation (68), as shown in equation (41), is equivalent to the result of equation (3), which provides that general result

$$\left[\int dx x^2 \left|\psi_{\text{opt}}(x)\right|^2\right]\left[\int dk k^2 \left|\varphi_{\text{opt}}(k)\right|^2\right] = \frac{1}{4}. \tag{69}$$

However, for the case that the expectation value of position is non-zero, where $\langle x \rangle = x_0$, as pointed out in equations (51) and (52), the more general optimal Gaussian wave function is given by

$$\psi_{\text{opt}}(x) = \frac{1}{(2\pi)^{1/4}\sqrt{\Delta x}} e^{ik_0 x} \exp\left[-\left(\frac{x - x_0}{\Delta x}\right)^2 / 4\right], \tag{70}$$

where the Fourier transform is

$$\varphi_{\text{opt}}(k) = \frac{1}{(2\pi)^{1/4}\sqrt{\Delta k}} e^{-i(k-k_0)x_0} \exp\left[-\left(\frac{k - k_0}{\Delta k}\right)^2 / 4\right], \tag{71}$$

which achieves the optimal uncertainty product relation, equation (3), as

$$\Delta x \Delta k = 1/2. \tag{72}$$

Most generally, the equivalent of equation (72), is the optimal variance product relation, where

$$\left[\int dx (x - x_0)^2 \left|\psi_{\text{opt}}(x)\right|^2\right]\left[\int dk (k - k_0)^2 \left|\varphi_{\text{opt}}(k)\right|^2\right] = \frac{1}{4}. \tag{73}$$

Consequently, as this is the optimal product of variances, equation (73), which occurs for the optimal Gaussian wave function, equation (70), for the case of a general wave function, $\psi(x)$, and its Fourier transform, $\varphi(k)$, the general uncertainty inequality relation, equation (53), is achieved as

$$\left[\int dx (x - x_0)^2 \left|\psi(x)\right|^2\right]\left[\int dk (k - k_0)^2 \left|\varphi(k)\right|^2\right] \geq \frac{1}{4}. \tag{74}$$

4. EXAMPLE OF A NON-OPTIMAL WAVE FUNCTION UNCERTAINTY RELATION

As an informative example of a wave function, $\psi(x)$, that does not produce the optimal variance product relation, consider the two sided (symmetric) exponential wave function, where

$$\psi(x) = \frac{1}{\sqrt{2\Delta x}} \exp(-|x| / 2\Delta x), \tag{75}$$

and the x space probability density is

$$\left|\psi(x)\right|^2 = \frac{1}{2\Delta x} \exp(-|x| / \Delta x). \tag{76}$$

First note that this wave function is properly normalized, where

$$\int_{-\infty}^{\infty} dx \left|\psi(x)\right|^2 = \frac{1}{2\Delta x} \int_{-\infty}^{\infty} dx \exp(-|x| / \Delta x) = \int_{0}^{\infty} dt \exp(-t) = 1, \tag{77}$$

and due to the symmetry, the x space expectation value is zero, where $\langle x \rangle = 0$. As a result of the symmetry, it should also be noted that the variance of the x space probability density is

$$\int_{-\infty}^{\infty} dx x^2 \left|\psi(x)\right|^2 = \frac{1}{2\Delta x}\int_{-\infty}^{\infty} dx x^2 \exp\left(-|x|/\Delta x\right)$$
$$= \left(\Delta x\right)^2 \int_0^{\infty} dt t^2 \exp(-t) = 2!\left(\Delta x\right)^2 = 2\left(\Delta x\right)^2 . \quad (78)$$

The Fourier transform of the wave function is calculated as

$$\varphi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx \psi(x) e^{-ikx} = \frac{1}{\sqrt{2\pi}\sqrt{2\Delta x}}\int_{-\infty}^{\infty} dx \exp\left(-\frac{|x|}{2\Delta x} - ikx\right)$$
$$= \frac{1}{\sqrt{2\pi}\sqrt{2\Delta x}}\left[\int_0^{\infty} dx \exp\left(-\frac{x}{2\Delta x} - ikx\right) + \int_{-\infty}^{0} dx \exp\left(\frac{x}{2\Delta x} - ikx\right)\right]$$
$$= \frac{2}{\sqrt{2\pi}\sqrt{2\Delta x}} \operatorname{Re}\left\{\int_0^{\infty} dx \exp\left[-\left(\frac{1}{2\Delta x} + ik\right)x\right]\right\} = \frac{2}{\sqrt{2\pi}\sqrt{2\Delta x}}\left[\frac{2\Delta x}{1+\left(2\Delta x k\right)^2}\right] . \quad (79)$$
$$= \frac{1}{\sqrt{2\pi}} \frac{2^{3/2}\sqrt{\Delta x}}{1+\left(2\Delta x k\right)^2}$$

Furthermore, as the k space probability density,

$$\left|\varphi(k)\right|^2 = \frac{1}{2\pi}\frac{2^3 \Delta x}{\left[1+\left(2\Delta x k\right)^2\right]^2} , \quad (80)$$

is symmetric, where the k space expectation value is zero, as $\langle k \rangle = 0$, the variance of the k space probability density is

$$\int_{-\infty}^{\infty} dk k^2 \left|\varphi(k)\right|^2 = \frac{8\Delta x}{2\pi}\int_{-\infty}^{\infty} dk \frac{k^2}{\left[1+\left(2\Delta x k\right)^2\right]^2} = \frac{1}{2\pi\left(\Delta x\right)^2}\int_{-\infty}^{\infty} dz \frac{z^2}{\left(1+z^2\right)^2} = \frac{1}{4\left(\Delta x\right)^2} . \quad (81)$$

Here, it should be noted that the integral in equation (81) can be obtained using a closed loop contour integration, with the second order pole at $z = i$, and the derivative of the residue theorem, where

$$\int_{-\infty}^{\infty} dz \frac{z^2}{\left(1+z^2\right)^2} = \frac{\pi}{2} . \quad (82)$$

Consequently, the product of the variances for the exponential wave function is not optimal, where

$$\left(\int_{-\infty}^{\infty} dx x^2 \left|\psi(x)\right|^2\right)\left(\int_{-\infty}^{\infty} dk k^2 \left|\varphi(k)\right|^2\right) = \left[2\left(\Delta x\right)^2\right]\left[\frac{1}{4\left(\Delta x\right)^2}\right] = \frac{1}{2} > \frac{1}{4} , \quad (83)$$

Which clearly satisfies the uncertainty relation, equation (46) or more generally equation (74), as it must, since it is not the optimal Gaussian wave function.,

5. Results and Discussion: As an Application to the Quantum Mechanical Heisenberg Uncertainty Principle

As a related topic associated with this uncertainty principle inequality conclusion, it is important to make the connection of this Fourier transform inequality identity, equation (46) or equation (74), to quantum mechanics. This can be achieved with a short review of the de Broglie wave concept of quantum particles, and the resultant Schrödinger wave equation. Specifically, de Broglie proposed that a free quantum particle, which has a precise momentum, p, could be modeled as an infinite extent quantum wave function, where

$$\psi(x) = \psi_0 e^{ikx}, \tag{84}$$

which has a precise wavenumber, k, that is associated with the momentum, as

$$p = \hbar k, \tag{85}$$

where $\hbar$ is the normalized Planck's constant, h, as $\hbar = h/2\pi = 1.05\times10^{-34}$ Js. With the additional Einstein concept of the frequency, ω, of the free particle wave function being associated with the precise energy, E, as

$$E = \hbar\omega, \tag{86}$$

the time dependent wave function,

$$\psi(x,t) = \psi_0 e^{i(kx-\omega t)}, \tag{87}$$

also satisfies the Schrödinger wave function equation for a free particle,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t), \tag{88}$$

as it is essentially an energy balance equation, where the energy of a free particle is

$$E = \hbar\omega = p^2/2m = (\hbar k)^2/2m. \tag{89}$$

In order to extend the concept of the infinite extent wave function, equation (84), to the situation that the quantum particle might have a finite spatial extent, Δx, it was necessary to consider an infinite linear superposition of precise momentum, or wavenumber eigenstate, wave functions, with $p = \hbar k$, using a Fourier integral representation approach, where

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\varphi(k)e^{ikx}. \tag{90}$$

However, the unfortunate consequence of this construct is that the Fourier components,

$$\varphi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\psi(x)e^{-ikx}, \tag{91}$$

imply that there must be an infinite spectrum of momentum components of such a wave function, since each wavenumber component has the property that $p = \hbar k$, and thus, if the particle has a finite spatial extent, Δx, then it will also have a finite wavenumber extent, Δk, which indicates that it also has a finite momentum extent, $\Delta p = \hbar\Delta k$. Consequently, due to the inverse variance, or uncertainty width relation, between Δx and Δk, found from the Fourier transform and the variational analysis given above, the quantum uncertainty principle is given by

$$\Delta x\Delta p \geq \hbar/2. \tag{92}$$

This is, of course, the famous Heisenberg uncertainty principle, which puts a limit on the joint uncertainty that one can obtain, associated with the precision that one can know a particle's location, Δx, and the particle's momentum, Δp. It should be interesting to the reader that the quantum uncertainty relation, equation (92), is a direct consequence of the optimization analysis associated with a general wave function, $\psi(x)$, and its Fourier transform, $\varphi(k)$, where the optimal solution is a Gaussian wave function, $\psi_{\text{opt}}(x)$, given by equation (70).

As proposed at the outset, the Heisenberg uncertainty principle is a direct consequence of the more general Fourier transforms pair optimization principle, that the Gaussian wave function provides the minimum product of the uncertainty in position and the uncertainty in wavenumber, for any general wave function that can be used to represent a quantum particle. Furthermore, with respect to achieving insightful instruction of quantum physics students, this is a profound result, which should help to advance quantum physics pedagogy applied to future students. Clearly, as Fourier transform analyses are used in most quantum mechanics discussions of quantum particles, being the key mathematical tool used to represent the solution of the Schrödinger equation, it is far superior to emphasize to the students the inherent mathematical constraint associated with the product of the uncertainty in position times the uncertainty in wavenumber, applicable to general wave functions, in contrast to focusing the student's attention towards the derivation of the uncertainty principle using the Schwartz inequality.

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