The Uncertainty Principle: Fourier Analysis In Quantum Mechanics

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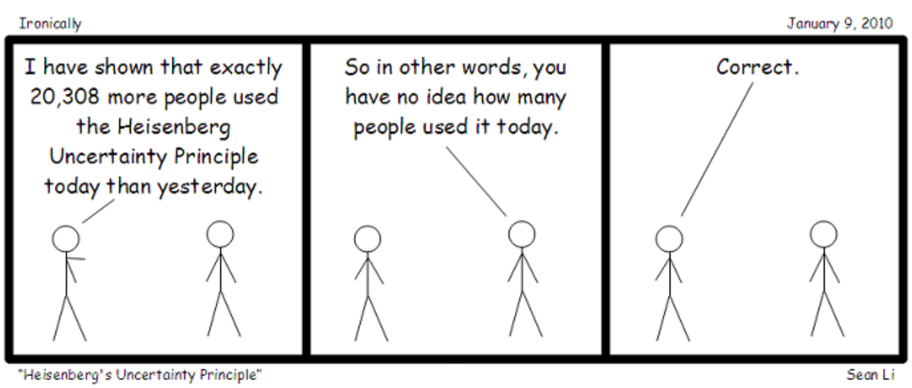
1 Introduction

Fourier Analysis is among the largest areas of applied mathematics and can be found in all areas of engineering and physics. Atomic physicists use the Fourier transform to characterize and understand molecular structures, optical physicist use Fourier series to decompose and resconstruct ultrafast photonic pulses and particle physicsts use the ideas of orthogonal basis and Fourier coefficients to describe the wave functions of particle states.

One of the most well known concepts in modern physics is the Heisenberg Uncertainty Principle which tells us that we cannot know both the position and momentum of a subatomic particle within a certain accuracy. To understand this principle in some detail, we look to the subject of Fourier analysis. We begin by motivating the idea that such a mathematical relationship exists and then proceed to derive and describe the uncertainty principle in the formal setting of Fourier analysis. After this, we discuss Fourier analysis as it is used and understoof by physicists in quantum mechanics for several simple examples. Finally, we will attempt to see the relationship between our formal discussion of the principle and some of the physical laws that govern the natural world.

This paper is written with the intent that the audiance is familiar with the material presented during the semester of math 472 and as such the statements and definitions regarding some topics taken to be well-understood are ommited. The proofs given are a combination of our own and those presented in various texts on the subject of Fourier analysis and wavelets.



2 The Balian-Low Theorem

2.1 Motivation: Gabor Functions and Orthornomal Basis of $L^2(\mathbb{R})$

Before we discuss formally the subject of uncertainty in Fourier analysis, we consider a few distinct but relavent ideas from which we can develope some intuition. Additionally, just as is the case in Fourier analysis, as we will see later the subject of quantum theory relies very heavily on the mathematics of orthonormal basis and the relationships between wave functions represented in these basis. As such a natural starting point for our discussion of uncertainty is to examine how we can create orthonormal basis using techniques we have already developed throughout the course such as translation and modulation. For example, consider a basis of $L^2(\mathbb{R})$ in which we choose $g = \chi_{[0,1]}$, the characteristic function over the closed interval $[0, 1]$ and let

$$g_{n,m} = e^{2\pi imx} g(x - n) \text{ for } n, m \in \mathbb{Z}.$$

We can see immediately that the basis is orthonormal because for any two elements in $\{g_{n,m}|n, m \in \mathbb{Z}\}$ are orthonormal since either the supports of the functions are disjoint or, when they have the same support, the orthonormality of the trigonometric functions take over. We conclude that

$$\langle g_{k,l}, g_{r,s}\rangle_{L^2(\mathbb{R})} = \int_{\mathbb{R}} g_{k,l}\overline{g_{r,s}}dx = \delta_{(k,r),(l,s)}$$

where the twice-indexed Kroncker delta is defined as

$$\delta_{(k,r),(l,s)} = \begin{cases} 0, & \text{for } k \neq r \text{ or } l \neq s \\ 1, & \text{for } k = r \text{ and } l = s \end{cases}$$

This is a Gabor basis where the functions $g_{n,m}$ are Gabor functions.

2.2 The Balian-Low Theorem

We now state a theorem that is used for specifying the conditions these functions must adhere to in order to form an orthonormal basis of the Hilbert space $L^2(\mathbb{R})$ and in doing so we will develope some notions about localizations of these fuctions.

Theorem 2.1 (The Balian-Low Theorem). *Let $g \in L^2(\mathbb{R})$ and let*

$$g_{n,m} = e^{2\pi imx} g(x - n) \textit{ for } n, m, \in \mathbb{Z}$$

then, if $\{g_{n,m}|n, m \in \mathbb{Z}\}$ is an orthonormal basis of $L^2(\mathbb{R})$, either

$$\int_{\mathbb{R}} x^2|g(x)|^2dx = \infty$$

or

$$\int_{\mathbb{R}} \xi^2|\hat{g}(\xi)|^2d\xi = \infty.$$

Formally, this states that a window fuction (Gabor function) cannot be simultaniously well-localized in both time and frequency. Nor can it be compactly supported and smooth because if it were, both integrals would be finite contradicting the Balian-Low theorem.

Proof. *For this proof, we follow the elegant and approachable one given by Hernandez(1). First, let Q and P be operators defined outside of paradise on the space $\mathcal{S}'(\mathbb{R})$ of tempered distributions such that*

$$Qf(x) = xf(x) \quad \text{and} \quad Pf(x) = -if'(x)$$

Doing this allows us to rewrite the above integrals as

$$\int_{-\infty}^{\infty} x^2|g(x)|^2dx = \int_{-\infty}^{\infty} |Qg(x)|^2dx$$

and

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} \xi^2|\hat{g}(\xi)|^2d\xi = \int_{-\infty}^{\infty} |P\hat{g}(\xi)|^2d\xi.$$ [1]

At this point, it suffices to show that Qg and Pg cannot both be in $L^2(\mathbb{R})$ simultaneously. We have the following relations

$$\langle Qg, Pg\rangle = \sum_{n,m\in\mathbb{Z}} \langle Qg, g_{n,m}\rangle\langle g_{n,m}, Pg\rangle \tag{1}$$

$$\langle Qg, g_{n,m}\rangle = \langle g_{-m,-n}, Qg\rangle \ \forall m, n \in \mathbb{Z} \tag{2}$$

and also

$$\langle Pg, g_{n,m}\rangle = \langle g_{-m,-n}, Pg\rangle. \tag{3}$$

Together, these relations imply that

$$\langle Qg, Pg\rangle = \langle Pg, Qg\rangle. \tag{4}$$

If this is true however then it cannot be that Qg and Pg and both in $L^2(\mathbb{R})$ since we would have,

$$\langle Qg, Pg\rangle = \int_{-\infty}^{\infty} xg(x)\overline{(-ig'(x))}dx$$

[1] Note that the factor of $\frac{1}{2\pi}$ on the left side comes from the facts that $\langle f, g\rangle = \frac{1}{2\pi}\langle \hat{f}, \hat{g}\rangle$ and $\hat{f'}(\xi) = i\xi\hat{f}(\xi)$. The later of the two expressions is proved as an auxillary lemma in the next section. See 3.3

where integration by parts gives[2]

$$\int_{-\infty}^{\infty} xg(x)\overline{(-ig'(x))}dx = -i\int_{-\infty}^{\infty}(g(x)+xg'(x))\overline{g(x)}dx$$

$$= -i\langle g,g\rangle + \langle Pg, Qg\rangle.$$

However, since $g \in L^2(\mathbb{R})$ *is a Gabor function, and* $\langle g,g\rangle = ||g||_2^2 = 1$*, we have*

$$\langle Qg, Pg\rangle = -i + \langle Pg, Qg\rangle$$

which is a contradiction. We need also to verify that (1),(2), and (3) are true for $Qg, Pg \in L^2(\mathbb{R})$.

Lemma 2.2. *Let* Q *and* P *be operators and let* $g, Qg, Pg \in L^2(\mathbb{R})$*, and let* $\{g_{n,m}|n,m \in \mathbb{Z}\}$ *form and orthonormal basis of* $L^2(\mathbb{R})$ *then the equations*

$$\langle Qg, Pg\rangle = \sum_{n,m\in\mathbb{Z}} \langle Qg, g_{n,m}\rangle\langle g_{n,m}, Pg\rangle,$$

$$\langle Qg, g_{n,m}\rangle = \langle g_{-m,-n}, Qg\rangle \ \forall m,n \in \mathbb{Z},$$

and

$$\langle Pg, g_{n,m}\rangle = \langle g_{-m,-n}, Pg\rangle$$

hold.

Proof. *This will again follow directly the proof given by Hernandez. Because* $\{g_{n,m}|n,m \in \mathbb{Z}\}$ *is an orthonormal basis, it must be that*

$$\langle Qg, Pg\rangle = \langle \sum_m \sum_n \langle Qg, g_{m,n}\rangle g_{m,n}, Pg\rangle$$

for which we can simply remove the sums from the inner product to give

$$\langle Qg, Pg\rangle = \sum_m \sum_n \langle Qg, g_{m,n}\rangle\langle g_{m,n}, Pg\rangle.$$

This proves the first expression. Now, for the second, we note that $n\langle g, g_{n,m}\rangle = 0 \ \forall n,m \in \mathbb{Z}$ *it must hold for both cases when* $n = 0$ *and when* $n \neq 0$*. For the later case, this imples that* $g = g_{0,0}$ *is orthogonal to* $g_{n,m}$ *so that*

$$\langle Qg, g_{n,m}\rangle = \langle Qg, g_{n,m}\rangle - n\langle g, g_{n,m}\rangle$$

$$= \int_{-\infty}^{\infty} e^{-2\pi imx} g(x)(x-n)\overline{g(x-n)}dx$$

if we let $x = y+n$*, and use the fact that* $e^{-2\pi inm} = 1$*, we have*

$$\int_{\mathbb{R}} e^{-2\pi i(y+n)m} g(y+n)y\overline{g(y)}dy = \int_{\mathbb{R}} e^{-2\pi iym} g(y+n)\overline{Qg(y)}dy$$

[2]If $g \in \mathcal{S}$ then it is clear that the boundary terms will cancel but here $xg, g' \in L^2(\mathbb{R})$, and that is sufficient to ensure this integration by parts formula holds in Sobolev space.

$$= \langle g_{-m,-n}, Qg \rangle$$

proving the second expression. Finally, we can integrate by parts and make the substitution $y = x - n$ *to see that*

$$\langle Pg, g_{n,m} \rangle = -i \int_{-\infty}^{\infty} e^{-2\pi imx} g'(x)\overline{g(x-n)}dx$$

$$= i \int_{-\infty}^{\infty} e^{-2\pi imx} g(x)(-2\pi im\overline{g(x-n)} + \overline{g'(x-n)})dx$$

$$= 2\pi m\delta_{-m,0}\delta_{0,n} + \int_{\mathbb{R}} e^{-2\pi imy} g(y+n)(\overline{-ig'(y)})dy = \langle g_{-m,-n}, Pg \rangle$$

which verifies the final expression. Thus, the lemma and the Balian-Low theorem hold.

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In discussing this theorem we are able to gain some motivation for expecting (at least analytically) a more general notion of localization of a function and its Fourier transform. The Balian-Low theorem tells us that we cannot have a function localized at once in both time and frequency but to actually characterize and quantify this, we now move into the idea of uncertainty.

3 The Uncertainty Principle

Indeed, as we expect, the term *uncertainty* comes from the fact that both a function and its Fourier transform cannot be localized at once. This means that if a function f is localized about a point, then its Fourier transform $\hat{f}$ will be non-localized. In terms of dispersion which we will see in a moment, this means that the cooresponding dispersion of $\hat{f}$ will be large. We will begin by restating several relavant theorems that are needed to understand the uncertainty principle.

Theorem 3.1 (Hölder's inequality). *Let $1 < p, q < \infty$ be such that $\frac{1}{p} + \frac{1}{q} = 1$. If $f \in L^p(\mathbb{R})$ and $g \in L^q(\mathbb{R})$, then $fg \in L^1(\mathbb{R})$ and $\int_{\mathbb{R}} |f(t)g(t)|dt \leq ||f||_p||g||_q$.*

Proof. *Let A=$||f||_p, B = ||g||_q$, if A or B then $f = 0$ in $L^p(\mathbb{R})$ or $g = 0$ in $L^q(\mathbb{R})$ then the result is trivial and we are done. Now let $a = \frac{|f(x)|}{A}$ and $b = \frac{|g(x)|}{B}$ and we will use Young's inequality[3] to obtain*

$$ab = \frac{|f(x)g(x)|}{AB} \leq \frac{|f(x)|^p}{pA^p} + \frac{|g(x)|^q}{qB^q}.$$

Using the middle inequality and taking the integral yields

$$\frac{1}{AB} \int_{\mathbb{R}} |f(x)g(x)|dx \leq \frac{1}{pA^p} \int_{\mathbb{R}} |f(x)|^p dx + \frac{1}{qB^q} \int_{\mathbb{R}} |g(x)|^q dx.$$

Now we can substitute $A^p = \int_{\mathbb{R}} |f(x)|^p dx$ and $B^q = \int_{\mathbb{R}} |g(x)|^q dx$ and get

$$\frac{1}{||f||_p||g||_q} ||fg||_1 \leq \frac{1}{p} + \frac{1}{q} = 1,$$

which gives our result

$$||fg||_1 \leq ||f||_p||g||_q.$$

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Theorem 3.2 (Plancherel's Theorem). *For $f \in L^2(\mathbb{R})$,*

$$\int_{\mathbb{R}} |f(t)|^2 dt = \frac{1}{2\pi} \int_{\mathbb{R}} |\hat{f}(w)|^2 dw$$

Proof. *Since $|f(t)|^2 = f(t)\overline{f(t)}$, we can take $\hat{g}(t) = \overline{f(t)}$ and $g(w) = \frac{1}{2\pi} \int_{\mathbb{R}} \overline{f(t)} e^{iwt} dt = \frac{1}{2\pi} \overline{\int_{\mathbb{R}} f(t) e^{-iwt} dt} = \frac{1}{2\pi} \overline{\widehat{f}(w)}$ and then we have*

$$\int_{\mathbb{R}} |f(t)|^2 dt = \int_{\mathbb{R}} f(t)\overline{f(t)} dt = \int_{\mathbb{R}} f(t)\widehat{g}(t) dt$$

$$= \int_{\mathbb{R}} \widehat{f}(t)g(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \widehat{f}(w)\overline{\widehat{f}(w)} dt = \frac{1}{2\pi} \int_{\mathbb{R}} |\hat{f}(w)|^2.$$

■

It is sufficient to discuss the Heisenberg uncertainty principle in one dimension using the $L^2(\mathbb{R})$ theory of the Fourier transform as is usually done. To do so we introduce the following definition of the dispersion of a function which tells us quantitatively how that function is distributed about a point x. We will focus on the simple case when $x = 0$.

[3] Young's inequality states that if $a, b > 0$ then $ab \leq \frac{a^p}{p} + \frac{b^q}{q}$ where $1 < p, q < \infty$ and $\frac{1}{p} + \frac{1}{q} = 1$.

Definition 3.1 (Dispersion Of A Function)**.** Let$f, xf \in L^2()\mathbb{R}$. The *dispersion* of a function f about $x = 0$ is given by

$$\Delta f = D_0(f) = \frac{\int_{\mathbb{R}} x^2|f(x)|^2dx}{\int_{\mathbb{R}} |f(x)|^2dx}. \tag{5}$$

Lemma 3.3 (Fourier Transform Of A Derivative)**.** *Let $f, xf \in L^2(\mathbb{R})$. We find $\widehat{f'}$ using the inversion formula then use integration by parts. First consider the case where $f \in \mathcal{S}$. Here we have*

$$\widehat{f'}(\xi) = \int_{\mathbb{R}} f'(x)e^{-i\xi x}dx = -\int_{\mathbb{R}} f(x)(-i\xi e^{-i\xi x})dx.$$

Since $f \in \mathcal{S}$ we know that $lim_{x\to\pm\infty}f(x) = 0$ so that

$$\widehat{f'}(\xi) = 0 + i\xi \int_{\mathbb{R}} f(x)e^{-i\xi x}dx = i\xi \hat{f}(\xi).$$

This all works sufficiently for functions in $\mathcal{S}$ however, since we are interested in functions f and f' in $L^2(\mathbb{R})$ where f' is now treated as a weak derivative (in the distribution sense) we can instead use the time-frequency dictionary to write $\widehat{f'}(\phi) = f'(\widehat{\phi'}) = f[(\widehat{\phi})]'$.

Theorem 3.4 (The Heisenberg Uncertainty Principle In One Dimension)**.** *Let $f, xf, \xi\hat{f}$ be in $L^2(\mathbb{R})$, then the product of the dispersion about zero of f with the dispersion about zero of $\hat{f}$ is such that*

$$\Delta f \Delta \hat{f} \geq \frac{1}{4} \tag{6}$$

Proof: We will start with $\int_{\mathbb{R}} x\overline{f(x)}f'(x)dx$ using integration by parts where, as before there are no boundary terms, and the fact that $f(x)\overline{f(x)} = |f(x)|^2$ we see

$$\int_{\mathbb{R}} x\overline{f(x)}f'(x)dx = -\int_{\mathbb{R}} f(x)(\overline{f(x)} + x\overline{f'(x)})dx = -\int_{\mathbb{R}} (|f(x)|^2 + xf(x)\overline{f'(x)})dx$$

and then rearranging the terms gives

$$\int_{\mathbb{R}} |f(x)|^2dx = -\int_{\mathbb{R}} x\overline{f(x)}f'(x)dx - \int_{\mathbb{R}} xf(x)\overline{f'(x)}dx$$
$$= -\int_{\mathbb{R}} [x\overline{f(x)}f'(x) + xf(x)\overline{f'(x)}]dx,$$

We can use the fact that $2Re(z+\overline{z}) = z+\overline{z}$ and $Re\big(\int_{\mathbb{R}} F(x)dx\big) = \int_{\mathbb{R}} Re(F(x))dx$ and that the integral on the left is real to combine the two integrals on the left to get

$$\int_{\mathbb{R}} |f(x)|^2dx = -2Re\left(\int_a^b x\overline{f(x)}f'(x)dx\right).$$

Note that the integral on the left is real as required since the right side is a real number. Now, using the fact that $|Re(z)| \leq |z|$ and the Cauchy-Schwarz inequality we obtain, after squaring both sides and employing the triangle inequality for integrals,

$$\left(\int_{\mathbb{R}} |f(x)|^2 dx\right)^2 \leq 4\left(\int_{\mathbb{R}} |x\overline{f(x)}f'(x)|dx\right)^2 \leq 4\bigg(\int_{\mathbb{R}} x^2|f(x)|^2 dx\bigg)\bigg(\int_{\mathbb{R}} |f'(x)|^2 dx\bigg).$$

Now we can use Plancherel's theorem on the right integral term and get

$$\int_{\mathbb{R}} |f'(x)|^2 dx = \frac{1}{2\pi}\int_{\mathbb{R}} |\widehat{f'}(\xi)|^2 d\xi$$

and applying 3.3,

$$\int_{\mathbb{R}} |f'(x)|^2 dx = \frac{1}{2\pi}\int_{\mathbb{R}} \xi^2|\widehat{f}(\xi)|^2 d\xi.$$

Substituting back into the inequality yields

$$\left(\int_{\mathbb{R}} |f(x)|^2 dx\right)^2 \leq \frac{4}{2\pi}\bigg(\int_{\mathbb{R}} x^2|f(x)|^2 dx\bigg)\bigg(\int_{\mathbb{R}} \xi^2|\widehat{f}(\xi)|^2 d\xi\bigg).$$

Now we can apply Plancherel's theorem to the left hand side, giving

$$\left(\frac{1}{2\pi}\int_{\mathbb{R}} |f(x)|^2 dx\right)\left(\int_{\mathbb{R}} |\widehat{f}(\xi)|^2 d\xi\right) \leq \frac{4}{2\pi}\left(\int_{\mathbb{R}} x^2|f(x)|^2 dx\right)\left(\int_{\mathbb{R}} \xi^2|\widehat{f}(\xi)|^2 d\xi\right)$$

$$\Rightarrow \frac{1}{4} \leq \frac{\int_{\mathbb{R}} x^2|f(x)|^2 dx}{\int_{\mathbb{R}} |f(x)|^2 dx}\frac{\int_{\mathbb{R}} \xi^2|\widehat{f}(\xi)|^2 d\xi}{\int_{\mathbb{R}} |\widehat{f}(\xi)|^2 d\xi}.$$

Finally, using the definition of dispersion we get the result that

$$\frac{1}{4} \leq \Delta f(x)\Delta\hat{f}(\xi).$$

■

This concludes our development and description of the uncertainty principle as a purely mathematical idea. In the next section, we are going to look at this principle from the perspective of quantum mechanics to see how such an abstract mathematical result arising from the properties of the Fourier transform manifests itself in such a far-reaching natural way.

4 The Heisenberg Uncertainty Principle And Quantum Mechanics

Attempting to say what defines quantum mechanics and how one should think about it is a difficult task that many scientists still do not agree on. The quantum world, even though its properties are the most fundemental found in nature (at least at this point in the history of our understanding), is very much different from the macroscopic world that we live in. The physical objects that obey these laws are of atomic scales so small that attempting to vizualize these properties is often analogous to trying to draw a four-dimesnional figure on a chalk board - impossible. Because of this, the comic given in the introduction is a good example of an incorrect use of the uncertainty principle as it is being applied in a macroscopic situation.

4.1 Preliminaries: Operators, Observables, & Eigenstates

The mathematics governing quantum theory is group theory or more specifically, that of Lie groups and representation theory. Though we do not need much of this explicitly for the purpose of this discussion, it will be helpful to understand the way that quantum mechanics is treated to give context to how the uncertainty principle is used.

Quantum mechanics takes place in a complex vector space (usually a Hilbert space), $\mathcal{H}$ called a state space endowed with a Hermitian inner product. In general, for our purposes here, the objects in this space are *wavefunctions*. We say that the state ψ of a quantum mechanical object, is specified by the complex vector

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix}$$

called a *ket* vector. Every such vector has a dual[4] vector called a *bra* vector that is given by

$$\langle\psi| = \begin{pmatrix} \overline{\psi_1} & \dots & \overline{\psi_n}. \end{pmatrix}.$$

To obtain a more precise idea of what these abstract vectors are, consider two *spin-states* of a particle such as an electron. We call them $|\psi\rangle$ and $|\phi\rangle$. The probability amplitude of a particle in state $|\psi\rangle$ to be found (measured) in state $|\phi\rangle$ is given by the *bra-ket*

$$\langle\phi|\psi\rangle$$

where, we take the normalization requirement[5]

$$\langle\psi|\psi\rangle = 1$$

To see this further, we introduce the idea of an observable. We are talking about the discrete set of states available for the spin of a particle (we will see

[4] The linear vector space spanned by the bra vectors $\langle\psi|$ forms a dual space of $\mathcal{H}$

[5] This is axiomatic to the probabilistic interpretation of quantum mechanics. Formally, we postulate the existance of a positive-definite metric $\langle\psi|\psi\rangle \geq 0$

the continuous case in position and momentum later). By *observable* we mean a quantity A, such that a measurement of A will take discrete values $a_1, a_2, \ldots$. Then the general state of a quantum mechanical object can be written as the superposition,

$$|\psi\rangle = c_1|a_1\rangle + c_2|a_2\rangle + \ldots = \sum_{n\in\mathbb{Z}} c_n|a_n\ \rangle \tag{7}$$

and

$$\langle\psi| = c_1^*\langle a_1| + c_2^*\langle a_2| + \ldots = \sum_{n\in\mathbb{Z}} c_n^*\langle a_n|, \tag{8}$$

where

$$c_n = \langle a_n|\psi\rangle$$

and the complex conjugate is

$$c_n^* = \langle a_n|\psi\rangle^* = \langle\psi|a_n\rangle,$$

where any two vectors are orthonormal so that,

$$\langle a_i|a_j\rangle = \delta_{i,j}.$$

The set of possible measured states of A form a set of orthonormal basis vectors. It is not hard to see that we can write the probabilities under this requirement as

$$1 = \langle\psi|\psi\rangle = \left(\sum_i c_i^*\langle a_i|\right)\left(\sum_j c_j|a_j\rangle\right) = \sum_i\sum_j c_i^* c_j\langle a_i|a_j\rangle = \sum_i\sum_j c_i^* c_j\delta_{i,j} = \sum_i c_i^* c_i.$$

Thus, the probability of measuring a_i from a measurement of A is given by

$$|c_i|^2 = |\langle a_i|\psi\rangle|^2$$

and will sum to one. That is, There is a one hundred percent chance that $|\psi\rangle$ is in one of those states. We will now introduce the *expectation value* of A which is given as the average

$$\langle A\rangle = \sum_n |c_n|^2 a_n, \tag{9}$$

and the uncertainty of this measurement is then given by

$$\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}, \tag{10}$$

where

$$\langle A^2\rangle = \sum_n |c_n|^2 a_n^2.$$

We are almost ready to define and develope an uncertainty relation from these ideas. Before this however we will define one more idea that is central to the mathematics of quantum mechanics called an operator. An observable A such as spin or energy of a quantum system is represented as an operator . Informally, the observables of a quantum system are the eigenvalues of a self-adjoint (Hermitian) linear operator on $\mathcal{H}$. We will define an operator as

$$\Delta A := A - \langle A \rangle.$$

Note that all operators considered here are self-adjoint so that $A = A^{\dagger}$.

Theorem 4.1 (Uncertainty Relation From Operators)**.** *Let A and B be observables as defined above on the Hilbert space $\mathcal{H}$ such that*

$$|a\rangle = \Delta A|\psi\rangle$$

and

$$|b\rangle = \Delta B|\psi\rangle$$

then

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq \frac{1}{4}|\langle[A, B]\rangle|^2$$

where $[A, B]$ is the commutator of the operators A and B given as,

$$[A, B] = AB - BA \tag{11}$$

and the anti-commutator is

$$\{A, B\} = AB + BA \tag{12}$$

Note that these commutators are elements of subspaces of the state space $\mathcal{H}$. We will not discuss this here as the algebra becomes very cumbersome quickly. Proof. First, we consider the Schwarz inequality,

$$\langle a|a\rangle\langle b|b\rangle \geq |\langle a|b\rangle|^2$$

Substituting the definition of the operators into this expression, we get

$$\langle a|a\rangle = \langle\psi|(A - \langle A\rangle)^2|\psi\rangle = \langle(\Delta A)^2\rangle$$

and

$$\langle b|b\rangle = \langle\psi|(B - \langle B\rangle)^2|\psi\rangle = \langle(\Delta B)^2\rangle$$

The Schwarz inequality then becomes,

$$\langle(\Delta A)^2\rangle\langle(\Delta B)^2\rangle \geq |\langle(\Delta A\Delta B)\rangle|^2$$

To get to the next step, we will write $\Delta A\Delta B$ in terms of the commutator and the anti-commutator as

$$\langle\Delta A\Delta B\rangle = \frac{1}{2}\langle[\Delta A, \Delta B]\rangle + \frac{1}{2}\langle\{\Delta A, \Delta B\}\rangle$$

Where $[\Delta A, \Delta B]^\dagger = -[\Delta A, \Delta B]$ *(not Hermitian) and* $\{\Delta A, \Delta B\}^\dagger = \{\Delta A, \Delta B\}$ *(Hermitian). Since the expectation value of a Hermitian operator is real and the expectation value of a non-Hermitian operator is purely imaginary, this enables us to write the right side of the inequality as*

$$|\langle(\Delta A \Delta B)\rangle|^2 = \frac{1}{4}|\langle[\Delta A, \Delta B]\rangle|^2 + \frac{1}{4}|\langle\{\Delta A, \Delta B\}\rangle|^2.$$

We conclude by the Schwarz inequality, that the theorem holds. Note that the uncertainty principle as a physical law in quantum mechanics comes directly from the fact that $[x, p] = i\hbar$ *where* x *and* p *are the position and momentum operators that we will see in the next section.*

Now, let us move on to the Heisenberg's uncertainty principle in quantum mechanics.

4.2 Variance And Uncertainty Of A Particle

We will now move in to the continuous case of position and momentum. In this case we will follow the standard treatment given in all quantum mechanics books. Specifically, See Cahill(2) for a further description. To do this let us first define the position and momentum operators. For simplicity, we will consider a particle confined to move in one dimension.

Unlike the previous case, we now consider an observable over a continuous set of states. The position operator $\hat{x}$ [6] acting on a position state $|x\rangle$ is given by the following relation

$$\hat{x}|x\rangle = x|x\rangle$$

where the state of a particle in *position space* is now written as

$$|\psi\rangle = \int_{-\infty}^{\infty} dx|x\rangle\langle x|\psi\rangle.$$

We define the one-dimensional wave function in position space as

$$\langle x|\psi\rangle := \psi(x) \tag{13}$$

where the average (expectation) value for a measurement of the position of a particle is now given as

$$\langle x\rangle = \langle\psi|\hat{x}|\psi\rangle = \int_{\mathbb{R}} dx\langle\psi|\hat{x}|x\rangle\langle x|\psi\rangle$$

$$= \int_{\mathbb{R}} x|\psi(x)|^2 dx.$$

[6] Often in physics, the *hat* notation is used for operators and matracies and a tilde such as $\tilde{f}(x)$ is used to denote the Fourier transform.

For the *momentum* operator given such that $\hat{p}|p\rangle = p|p\rangle$ in momentum space, The above definitions follow exactly the same so that the wave function in position space is

$$\langle p|\psi\rangle = \psi(p).$$

Now, let us write the invese Fourier transform of $\psi(x)$ as

$$\psi(x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \tilde{\psi}(k) e^{ikx} dk = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\hbar}} \frac{\tilde{\psi}(p/\hbar)}{\sqrt{\hbar}} e^{i(p/\hbar)x} dp$$

where we have made the substitution for the wavenumber $k = \frac{p}{\hbar}$. Now, for the normalized wave function $\psi(x)$, we use Parseval's theorem to write

$$1 = \int_{\mathbb{R}} |\psi(x)|^2 dx = \int_{\mathbb{R}} |\tilde{\psi}(k)|^2 dk = \int_{\mathbb{R}} \Big| \frac{\tilde{\psi}(p/\hbar)}{\sqrt{\hbar}} \Big|^2 dp$$

or equivalently, in Dirac notation, where $\psi(x) = \langle x|\psi\rangle$ and $\phi(p) = \langle p|\psi\rangle = \frac{\widehat{\psi}(p/\hbar)}{\sqrt{\hbar}}$

$$1 = \langle\psi|\psi\rangle = \int_{\mathbb{R}} \langle\psi|x\rangle\langle\psi|x\rangle dx = \int_{\mathbb{R}} |\psi(x)|^2 dx = \int_{\mathbb{R}} |\psi(p)|^2 dp = \int_{\mathbb{R}} \langle\psi|p\rangle\langle\psi|p\rangle dp.$$

The Fourier transform that connects momentum and position space wave functions is then

$$\psi(x) = \int_{\mathbb{R}} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \phi(p) dp \tag{14}$$

and the inverse is given as

$$\phi(p) = \int_{\mathbb{R}} \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \psi(x) dx. \tag{15}$$

Differentiating equation (14), we get

$$\frac{\hbar}{i} \frac{d}{dx} \psi(x) = \int_{\mathbb{R}} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} p\phi(p) dp \tag{16}$$

however, recognizing that

$$\langle x|p|\psi\rangle = \int_{\mathbb{R}} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} p\phi(p) dp,$$

we see that we have the equation

$$\frac{\hbar}{i} \frac{d}{dx} \psi(x) = \langle x|p|\psi\rangle$$

where $\hat{p} = \frac{\hbar}{i} \frac{d}{dx}$ is the momentum operator in the *position basis.*

Now, we want to normalize the Gaussian wave $\psi(x) = Ne^{-(x/a)^2}$ to 1 in $\mathbb{R}$ as

$$1 = N^2 \int_{\mathbb{R}} e^{-2(x/a)^2} dx = N^2 a \sqrt{\frac{\pi}{2}}$$

so that $N^2 = \sqrt{2}\pi a^2$ and the *normalized Gaussian wave function* is

$$\psi(x) = \langle x|\psi\rangle = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \frac{1}{\sqrt{a}} e^{-(x/a)^2}$$

Notice that since the Gaussian is an even function, the expectation value of the position operator is zero.

$$\langle \hat{x}\rangle = \langle \psi|\hat{x}|\psi\rangle = \int_{\mathbb{R}} x|\psi(x)|^2 dx = 0$$

and the variance of $\hat{x}$, given as $(\Delta\hat{x})^2 = \langle\psi|(\hat{x} - \langle\hat{x}\rangle)^2|\psi\rangle$ is

$$\langle\psi|(\hat{x} - \langle\hat{x}\rangle)^2|\psi\rangle = \langle\psi|(\hat{x} - 0)^2|\psi\rangle = \langle\psi|\hat{x}^2|\psi\rangle = \int_{\mathbb{R}} x^2|\psi(x)|^2 = \frac{a^2}{4}.$$

Using the Fourier transform, we can also compute the variance of the momentum operator to get the gaussian wave function in momentum space as

$$\phi(p) = \sqrt{\frac{a}{2\hbar}} \left(\frac{2}{\pi}\right)^{\frac{1}{4}} e^{-(ap)^2/(2\hbar)^2}$$

and so, computing the variance of the momentum operator $\hat{p}$, we get that

$$(\Delta p)^2 = \int_{\mathbb{R}} p^2|\phi(p)|^2 dp = \sqrt{(}\frac{2}{\pi}) \int_{\mathbb{R}} p^2 \frac{a}{2\hbar} e^{-(ap)^2/2\hbar^2} dp = \frac{\hbar^2}{2}.$$

Multiplying the two variances together, we get

$$(\Delta x)^2(\Delta p)^2 = \frac{\hbar^2 a^2}{4a^2} = \frac{\hbar^2}{4}.$$

This is an example of uncertainty in quantum mechanics showing that the product of the variances cannot be made smaller than $\frac{\hbar^2}{4}$. As a physical law, Heisenberg's uncertainty principle states that,

$$(\Delta x)^2(\Delta p)^2 \geq \frac{\hbar^2}{4}.$$

5 Bibliography

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