Quantum Physics I Notes

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Contents

1 Lec 1: Superposition Intuition

- Physical processes in the lab are unpredictable, nondeterminate, random
- Probability forced by observation

Uncertainty Principle: For incompatible properties, you cannot have an object w/ defined values for both properties at the same time

- ex. position and momentum
- If one property is determined, the object is in superposition of values for the other property
- Quantum effects negligible for large objects
- Quantum effects only significant for small objects w/ small energies
- ex. atoms, electrons, molecules

2 Lec 2: Physical Effects explained by Quantum Mechanics but not Classical Mechanics

1. Atoms exist
2. Randomness exists
3. Atomic Spectra are discrete and have structure
4. Photoelectric effect
5. Electron Diffraction
6. Bell's Poor Inequality

2.1 Atoms exist

- e^- orbiting nucleus in Bohr atom is an accelerating charged particle and so emits light (loses energy)
- Thus Bohr atom doesn't work classically because it collapses as the electron spirals around nucleus while releasing energy by radiation

2.2 Randomness exists

- Self explanatory

2.3 Atomic Spectra

$$\frac{1}{\lambda} = R \cdot \left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \text{ for } n_i \in \mathbb{Z}, n_2 > n_1 \tag{1}$$

- R is the Rydberg constant which depends on the element but is independent of the emission series
- This eqn shows that the atomic spectra are discrete and have structure, but classical mechanics doesn't have discrete energy levels (no energy quantization)

2.4 Photoelectric Effect

V_0**:** Stopping voltage req to stop e^- from being released by photoelectric effect
I**:** Current generated in circuit

Prediction	Result
• More intense beam $\implies$ e^- w/ higher KE • $V_0 \propto I$ • V_0 indep of frequnecy ν	• Same KE regardless of intensity • V_0 indep of intensity • $V_0 \propto \nu$

- Rate of e^- release depends on intensity
- But for $\nu < \frac{W}{h}$ (less than critical frequency), no e^- released regardless of intensity (not enough energy)
- Einstein's explanation: Light comes in chunks with defined energy $E = h\nu$

$$KE = h\nu - W \tag{2}$$

  where W is the work required to remove the e^-
- Recall $E = pc$ and $c = \lambda\nu$

$$\therefore \quad p = \frac{h}{\lambda} \tag{3}$$

- This implies that the discrete packets of light w/ wavelength λ have momentum p by above eqn (wave-particle duality)

2.4.1 Waves vs Particles

- Waves can interfere with themselves (Young's Double Slit)
- Waves are **not localized**; particles are
- An interference pattern (wave) implies that **amplitudes** but intensities do not

- Classical particles can pass through either top or bottom slit
- Passing classical particles through double slit leads to 2 peaks near the 2 openings

- e^- can interfere with themselves (wave behaviour) in double slit
- Each e^- takes superposition of the possible paths; We don't know if it took the top or bottom bath
- An e^- is neither strictly a particle nor strictly a wave

2.4.2 Light comes in chunks

- Light has an energy and momentum

$$E = h\nu \tag{4}$$
$$p = \frac{h}{\lambda} \tag{5}$$

2.5 Electron Diffraction

- Bragg's Law

$$\frac{1}{\lambda} = \frac{n}{2dsin\theta} \tag{6}$$
$$p = \frac{h}{\lambda} \tag{7}$$

2.6 Bell's Inequality

- For 3 binary properties A, B, C, **Bell's Inequality** states

$$N(A, \overline{B}) + N(B, \overline{C}) \geq N(A, \overline{C}) \tag{8}$$

  where $N(X, Y)$ is the number of objects with properties X and Y
- e^- have 3 binary properties (angular momentum about x-, y-, and z-axes)
- However, it violates Bell's Inequality

$$N(\uparrow_0, \downarrow_\theta) + N(\uparrow_\theta, \downarrow_{2\theta}) \leq N(\uparrow_0, \downarrow_{2\theta}) \tag{9}$$

- Can't add probabilities classically with basic addition

3 Lec 3: The Wave Function

3.1 de Broglie Relations

$$\begin{aligned} E &\sim \hbar \qquad & E &= h\nu \\ p &= \hbar k \qquad & p &= \frac{h}{\lambda} \end{aligned} \tag{10}$$

$$\hbar = \frac{h}{2\pi} \qquad \omega = 2\pi\nu \qquad k = \frac{2\pi}{\lambda} \tag{11}$$

ω **:** angular frequency [rad/s]
k **:** wavenumber [rad/m]

3.2 Systems in Classical Mechanics vs Quantum Mechanics

- In **Classical Mechanics**, an object's state is fully defined by its position and momentum vectors $\{\mathbf{x}, \mathbf{p}\}$
- All other properties can be found using $\mathbf{x}$ and $\mathbf{p}$
- ex. energy $E(\mathbf{x}, \mathbf{p})$ and angular momentum $\mathbf{L}(\mathbf{x}, \mathbf{p})$
- But in **Quantum Mechanics** (real life), there is uncertainty (Uncertainty Principle)

$$\Delta\mathbf{x}\Delta\mathbf{p} \gtrsim \hbar \tag{12}$$

3.3 Quantum Mechanics Postulates

1. The state of a quantum object is **completely** specified by a wavefunction $\Psi(x)$
2. $\mathbb{P} = |\Psi(x)|^2$ determines the probability density that the object in state $\Psi(x)$ will be found at x

- i.e. probability that upon measurement, the object is found at position x

3. Given two possible wavefunctions (or states) of a quantum system corresponding to distinct wavefunctions $\Psi_1(x)$ and $\Psi_2(x)$, the system can **also** be in a **superposition** of $\Psi_1(x)$ and $\Psi_2(x)$

$$\Psi(x) = \alpha\Psi_1(x) + \beta\Psi_2(x) \quad \alpha, \beta \in \mathbb{C} \tag{13}$$

such that $\Psi(x)$ is properly normalized

- Wavefunction can be expressed as a linear combination of 2 possible wavefunctions (superposition)
- i.e. superposition of 2 quantum states results in another valid quantum state

3.4 The Wavefunction $\Psi(x)$

- Wavefunction $\Psi(x)$ is a complex function and **must** be single valued and continuous
- The probability $|\Psi(x)|^2$ is always real and nonnegative
- Probability density means

$$\mathbb{P}(x, x+dx) = \mathbb{P}(x)dx = |\Psi(x)|^2 dx \tag{14}$$

- Units of wavefunction are $[\Psi(x)] = \frac{1}{\sqrt{L}}$
- Recall that for complex numbers,

$$|\beta|^2 = \beta^* \beta \tag{15}$$
$$|e^{i\alpha}|^2 = e^{i\alpha} e^{-i\alpha} = 1 \tag{16}$$

3.5 Normalization of Wavefunctions

- Probability must be **normalized** such that the sum of probabilities is 1 over an interval

$$\int_{All} \mathbb{P}(x)dx = \int_{All} |\Psi(x)|^2 dx = 1 \tag{17}$$

- If wave function is not normalized, then use

$$\mathbb{P}(x) = \frac{|\Psi(x)|^2}{\int_{All} |\Psi(x)|^2 dx} \tag{18}$$

3.6 Plane Waves

- de Broglie says a particle with energy $E \sim \hbar\omega$ and momentum $p = \hbar k$ has a plane wave wavefunction
- General plane wave:

$$\Psi(x) = e^{i(kx-wt)} \tag{19}$$

- Note: plane wave is a complex function (need to remember that there is an imaginary component)
- But not all wavefunctions are plane waves; some are well localized

3.7 Superposition of 2 waves

- Using the rule $|\beta|^2 = \beta^*\beta$, the probability with superposition is:

$$\begin{aligned}
\mathbb{P} &= |\alpha\Psi_1 + \beta\Psi_2|^2 = (\alpha^*\Psi_1^* + \beta^*\Psi_2^*)(\alpha\Psi_1 + \beta\Psi_2) && (20)\\
&= |\alpha|^2|\Psi_1|^2 + |\beta|^2|\Psi_2|^2 + \alpha^*\Psi_1^*\beta\Psi_2 + \alpha\Psi_1\beta^*\Psi_2^* && (21)\\
&= \mathbb{P}_1 + \mathbb{P}_2 + \alpha^*\Psi_1^*\beta\Psi_2 + \alpha\Psi_1\beta^*\Psi_2^* && (22)
\end{aligned}$$

  where $\alpha^*\Psi_1^*\beta\Psi_2 + \alpha\Psi_1\beta^*\Psi_2^*$ are the **interference terms**
- The first term in the interference terms is the conjugate of the 2^{nd} term
- Therefore the interference term is real but not necessarily nonnegative, so the overall probability will still be real
- Note: Superposition principle and interpretation of probability as $|\Psi(x)|^2$ gives correction to classical probability (the interference terms)
- Shows that probabilities don't add as they do classically in Bell's Inequality (i.e. probability of both is **not** the sum of the individual probabilities)

Wavefunctions add; probabilities do not

3.8 Superposition of many waves

- As you add more plane waves to a superposition, the wavefunction and probability distribution become more localized (i.e. Δx decreases)
- For lots of plane waves, get a very narrow probability distribution and wavefunction
- There will be very few peaks, so particle is very likely to be found at those positions: $\Delta x \sim$ small
- But that requires a superposition of many momenta (each plane wave has a different λ and $p = \frac{h}{\lambda}$) so $\Delta p \sim$ large as required by the Uncertainty Principle

3.8.1 Fourier Transforms for wave functions

Theorem 1. *Any well behaved $f(x)$ can be built by superimposing enough plane waves e^{ikx}*

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{f}(k) e^{ikx} dk \tag{23}$$

where $\widetilde{f}(x)$ gives the amplitude of the plane wave with wavelength $\lambda = \frac{2\pi}{k}$

- Every mode has a definite wavelength $\lambda = \frac{2\pi}{k}$

- Note: Fourier Transform coefficients of x are all equivalent
- Can use Inverse Fourier Transform to get $\widetilde{f}(k)$ from $f(x)$

$$\widetilde{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx \tag{24}$$

- Physics Version: any $\Psi(x)$ can be expressed as the superposition of states with definite momentum $p = \hbar k$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\Psi}(x) e^{ikx} dk \tag{25}$$

- The Fourier Transform associates a magnitude and phase for each possible wave vector
- Note: if the wavefunction is well localized to a position, the Fourier Transform is not well localized ($\therefore$ not having definite momentum)
- Similarly, if there is definite momentum, position is not well defined, but the Fourier Transform will have a single peak (position very localized)

3.9 Probability density for Wavenumber/Momentum

- Similar to probability density for position x, the probability density for momentum p/wavenumber k is given by the norm squared of the wavefunction in the k-space

$$\mathbb{P}(k) = |\Psi(k)|^2 \tag{26}$$

3.10 Wavefunction Examples

3.10.1 Gaussian Wavefunctions

$$\Psi(x) = \frac{1}{0.5\sqrt{2\pi}} exp\Big(-\frac{(x+3)^2}{2 \cdot 0.5}\Big) \quad (27)$$

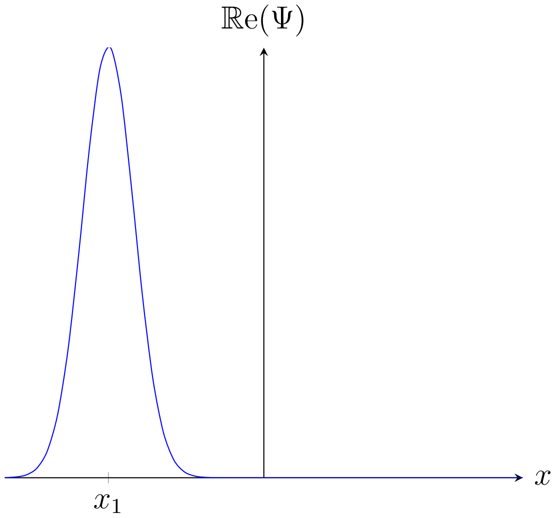

Figure 1: Ex. Gaussian Wavefunction

$$x \sim x_1 \quad (28)$$
$$\Delta x \sim \text{small} \quad (29)$$

$$\Psi(x) = \frac{1}{0.5\sqrt{2\pi}} exp\Big(-\frac{(x-2.5)^2}{2 \cdot 0.5}\Big) \quad (30)$$

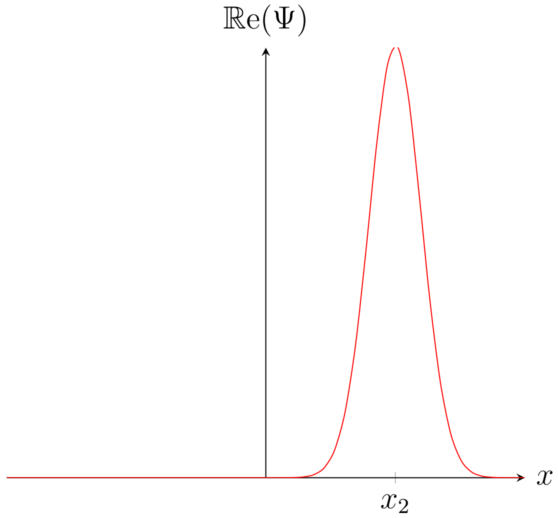

Figure 2: Ex. Gaussian Wavefunction

$$x \sim x_2 \quad (31)$$
$$\Delta x \sim \text{small} \quad (32)$$

- For both Gaussian wavefunctions above, there is no definite wavelength, so $\Delta p \sim large$

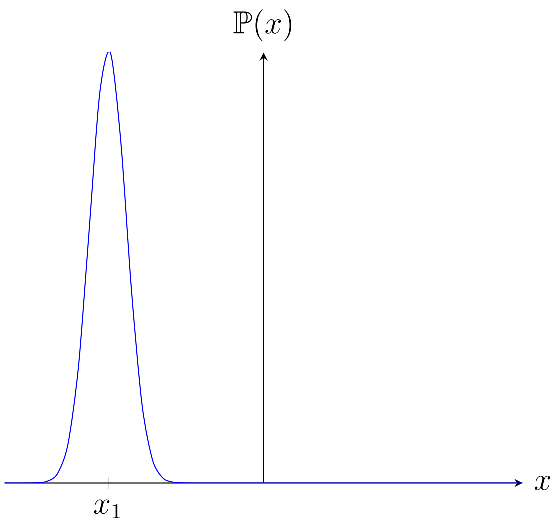

Figure 3: Probability density

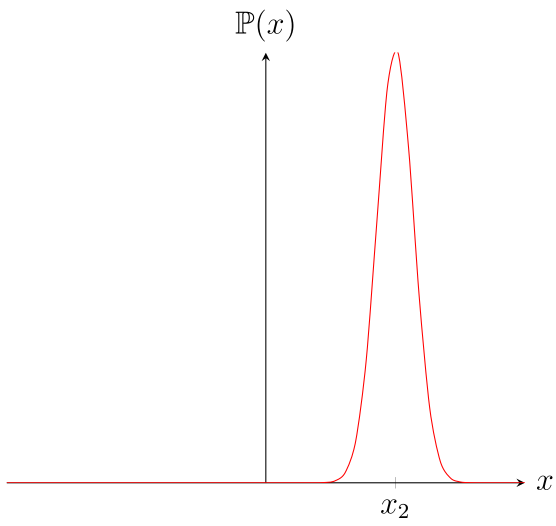

Figure 4: Probability density

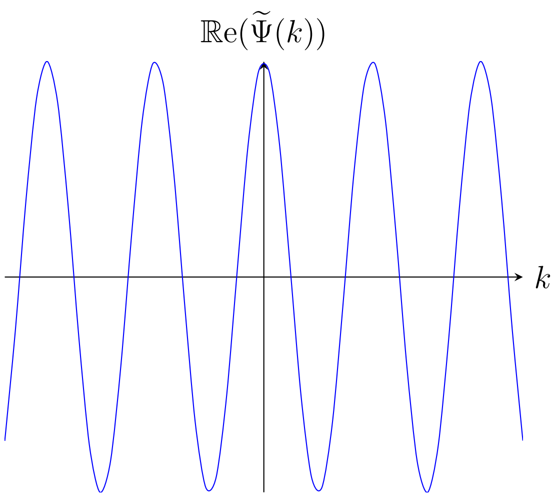

Figure 5: Wavefunction in k-space

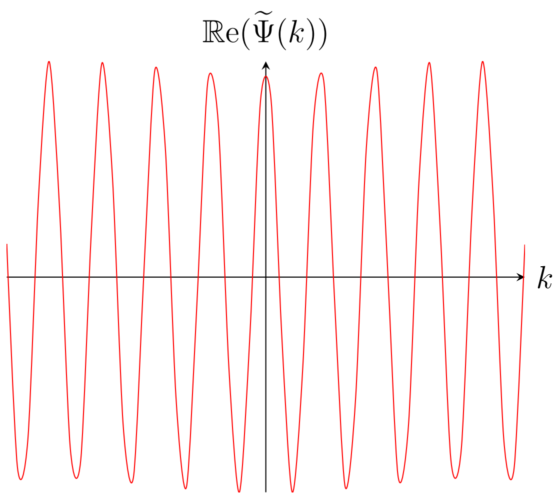

Figure 6: Wavefunction in k-space

$$p \sim ??? \tag{33}$$
$$\Delta p \sim large \tag{34}$$

$$p \sim ??? \tag{35}$$
$$\Delta p \sim large \tag{36}$$

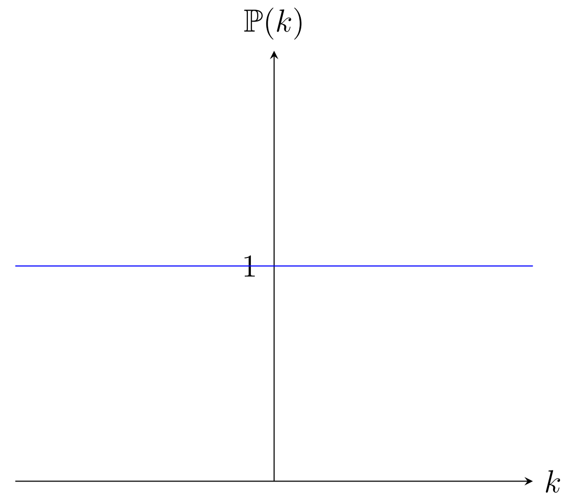

Figure 7: Probability density of wavefunction having specific wavenumbers k

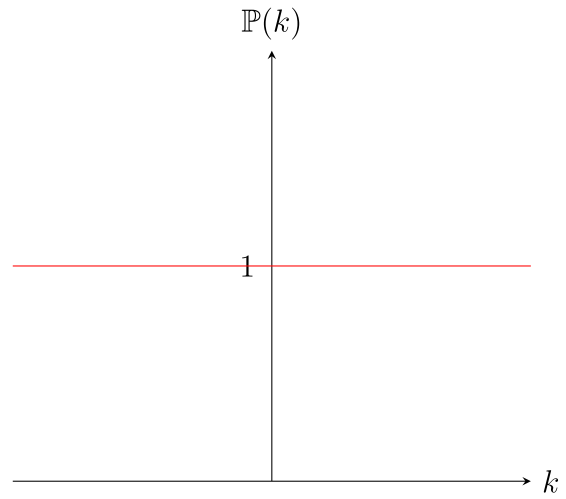

Figure 8: Probability density of wavefunction having specific wavenumbers k

3.10.2 Plane Waves (Complex Exponential Form)

$$\Psi(x) = -e^{ik_1 x} \tag{37}$$

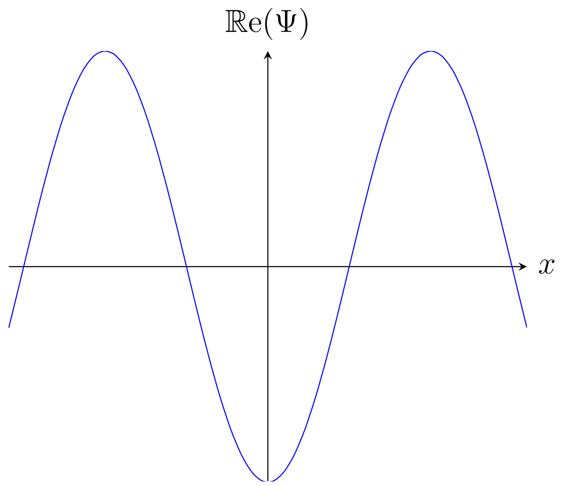

Figure 9: Ex. Plane Wavefunction

$$x \sim ??? \tag{38}$$
$$\Delta x \sim \text{large} \tag{39}$$
$$\tag{40}$$

$$\Psi(x) = e^{ik_2 x} \tag{41}$$

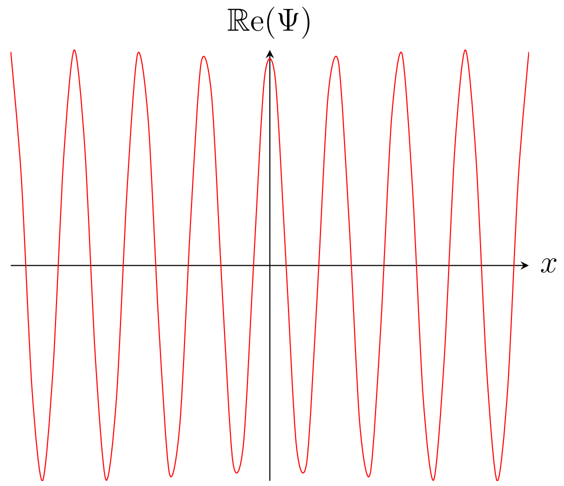

Figure 10: Ex. Plane Wavefunction

$$x \sim ??? \tag{42}$$
$$\Delta x \sim \text{large} \tag{43}$$

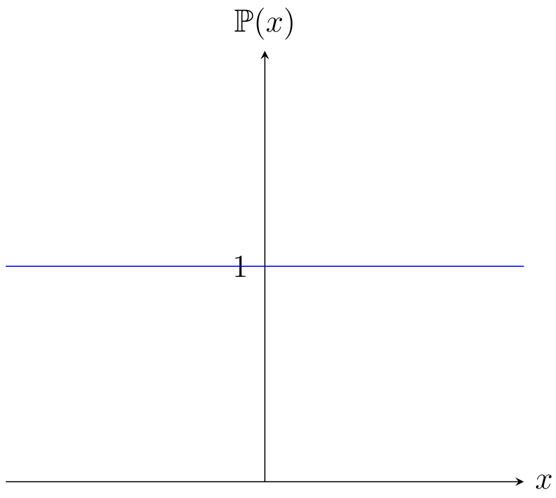

Figure 11: Probability density

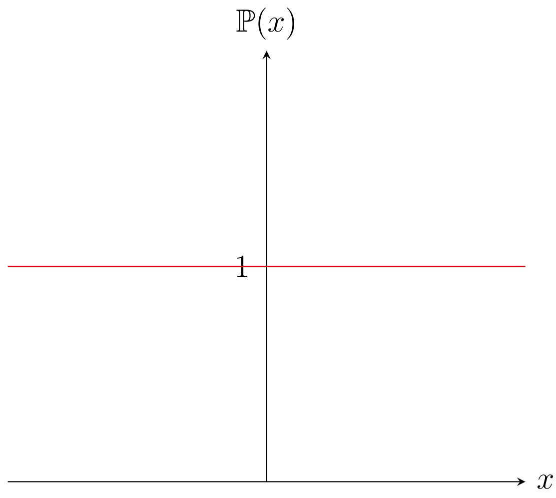

Figure 12: Probability density

- Note: wavefunction is not properly normalized
- Particle can be anywhere ($\Delta x \sim$ large)
- But $\Psi(x)$ has a very defined wavelength and wavenumber, so the particle has a defined momentum $p = \hbar k$

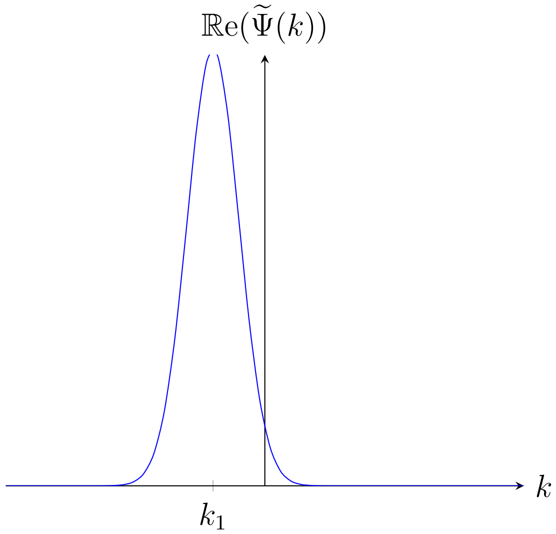

Figure 13: Wavefunction in k-space

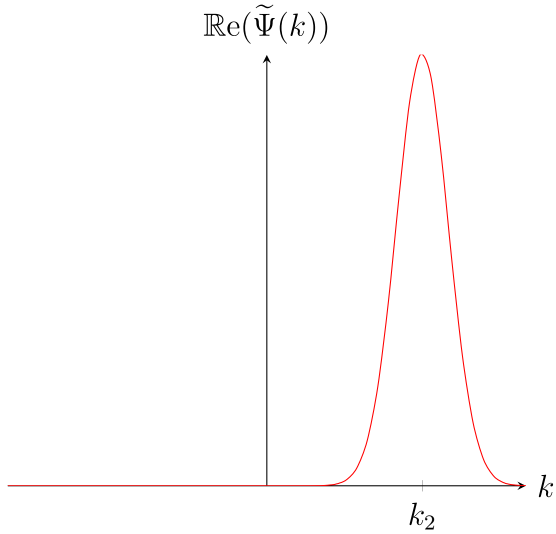

Figure 14: Wavefunction in k-space

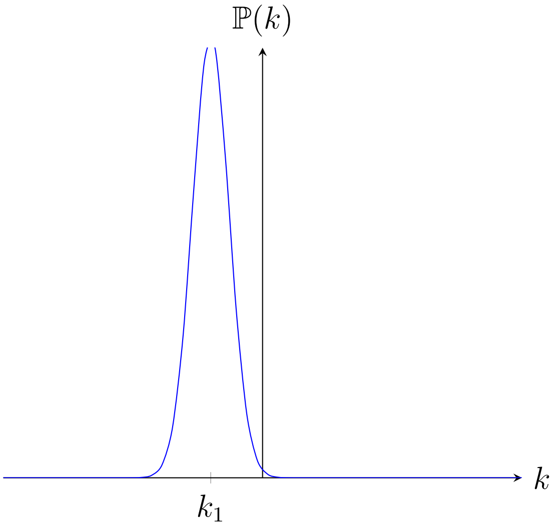

Figure 15: Probability density of wavefunction having specific wavenumbers k

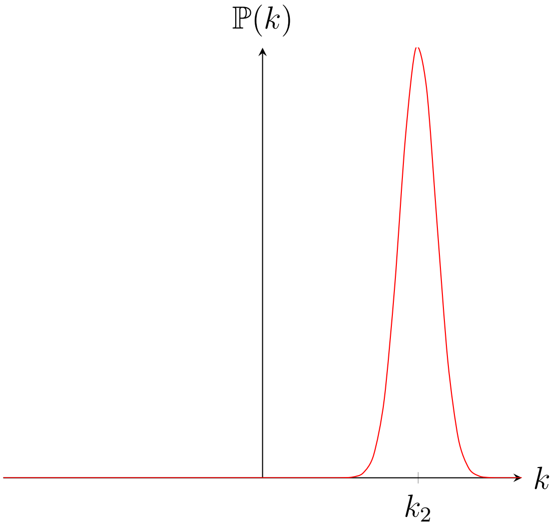

Figure 16: Probability density of wavefunction having specific wavenumbers k

$$p \sim \hbar k_1 \tag{44}$$
$$\Delta p \sim small \tag{45}$$

$$p \sim \hbar k_2 \tag{46}$$
$$\Delta p \sim small \tag{47}$$

3.10.3 Superposition of 2 Wavefunctions

$$\Psi(x) = \frac{1}{4}\frac{1}{0.5\sqrt{2\pi}}exp\Big(-\frac{(x+3)^2}{2\cdot 0.5}\Big) \tag{48}$$
$$+\frac{3}{4}\frac{1}{0.5\sqrt{2\pi}}exp\Big(-\frac{(x-2.5)^2}{2\cdot 0.5}\Big) \tag{49}$$

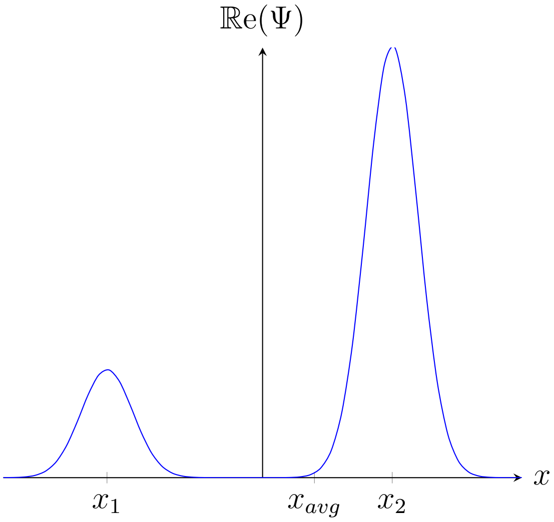

Figure 17: Ex. Superposition of 2 Gaussian Wavefunctions

$$x \sim \text{in betw } x_1 \text{ and } x_2 \text{ on avg} \tag{50}$$
$$\Delta x \sim (x_1 - x_2) \tag{51}$$

$$\Psi(x) = e^{ik_1x} + e^{ik_2x} \tag{52}$$
$$= -e^{ix} + 0.25e^{5ix} \tag{53}$$

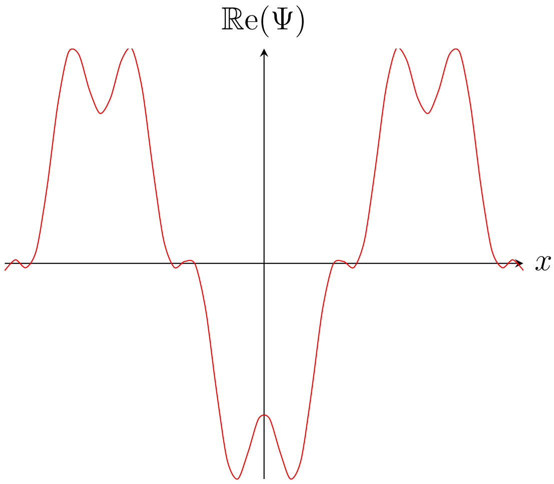

Figure 18: Ex. Superpositions of 2 Plane Wavefunctions

$$x \sim \text{some info} \tag{54}$$
$$\Delta x \sim \text{huge} \tag{55}$$

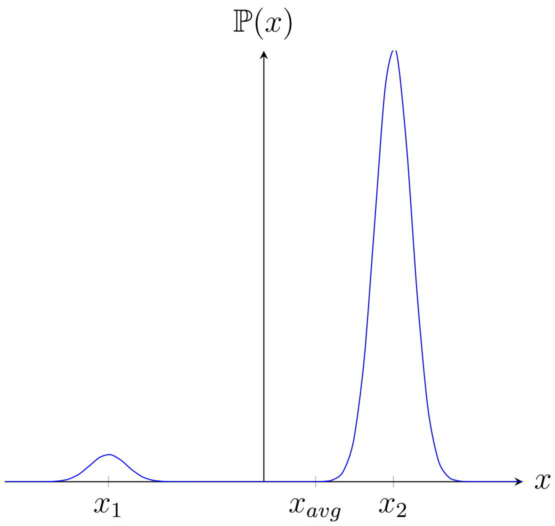

Figure 19: Probability density

$$\Psi(x) = e^{ikx_1} + e^{ikx_2} \quad (56)$$
$$= e^{ix} + 0.3e^{5ix} \quad (57)$$

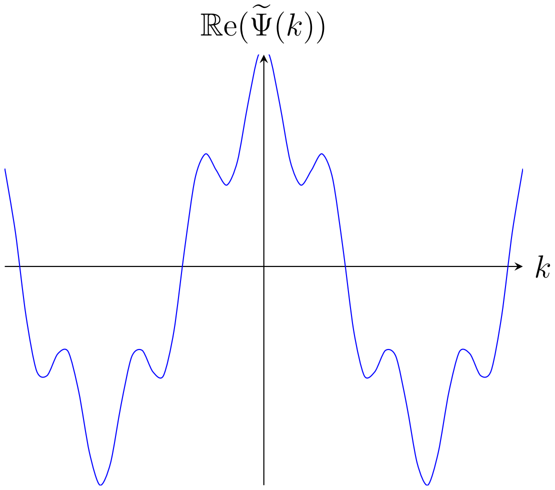

Figure 21: Wavefunction in k-space

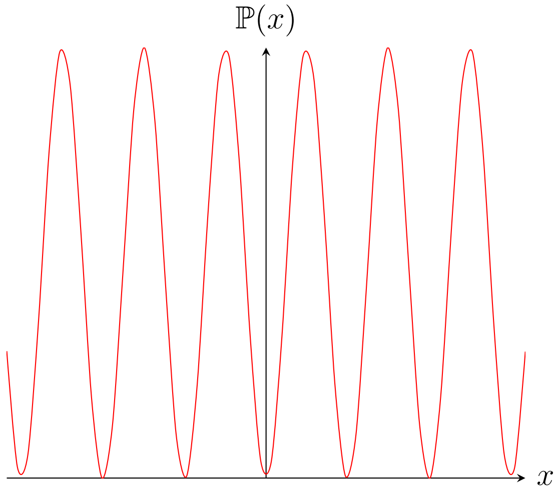

Figure 20: Probability density

$$\Psi(x) = \frac{1}{4}\frac{1}{0.5\sqrt{2\pi}} exp\Big(-\frac{(x+3)^2}{2\cdot 0.5}\Big) \quad (58)$$
$$+\frac{1}{0.5\sqrt{2\pi}} exp\Big(-\frac{(x-2.5)^2}{2\cdot 0.5}\Big) \quad (59)$$

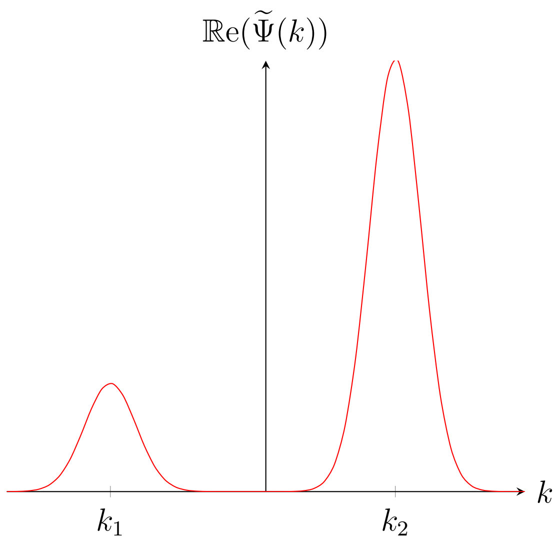

Figure 22: Wavefunction in k-space

4 Aside: More about Fourier Transforms

4.1 Fourier Series

- Can represent any periodic function $f(x)$ with a Fourier series

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n cos(nx) + \sum_{n=1}^{\infty} b_n sin(nx) \tag{60}$$

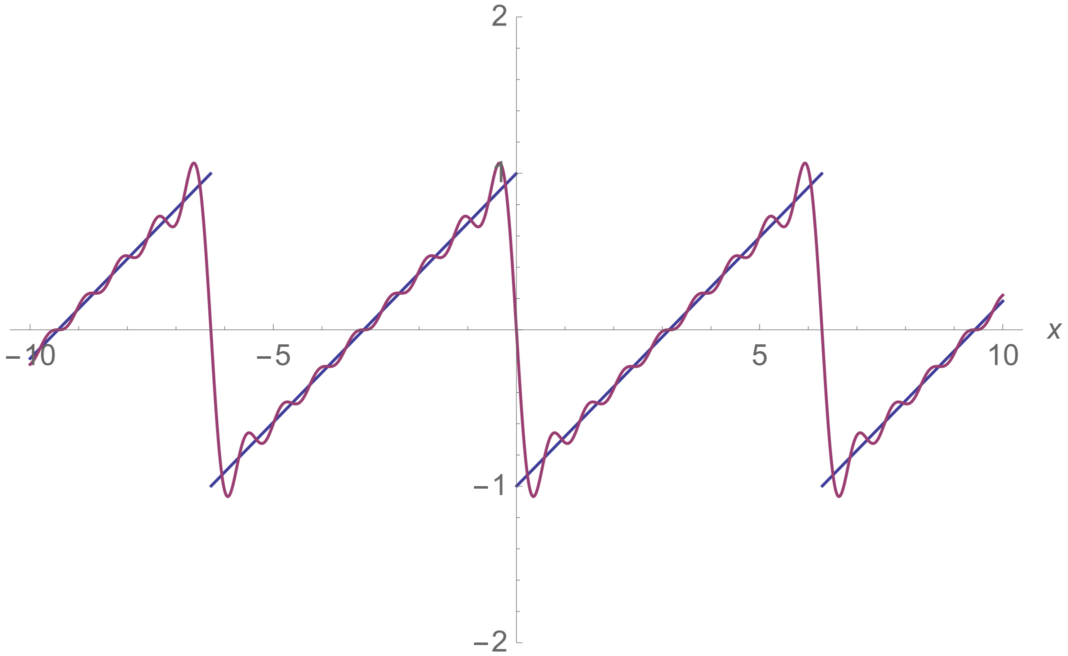

Figure 23: Graph of a periodic sawtooth function in the real x-space

4.2 Fourier k-space (Frequency domain)

- Can also describe the Fourier representation by plotting the strength of each sine/cosine term as a function of frequency/wavenumber (k), $\widetilde{f}(k)$
- Frequency representation is obtained by applying the Fourier Transform to the original function in the time domain

– Wavenumber used as dependent variable on x-axis

– Fourier coefficients a_n or b_n are then used as the amplitude of each wavenumber

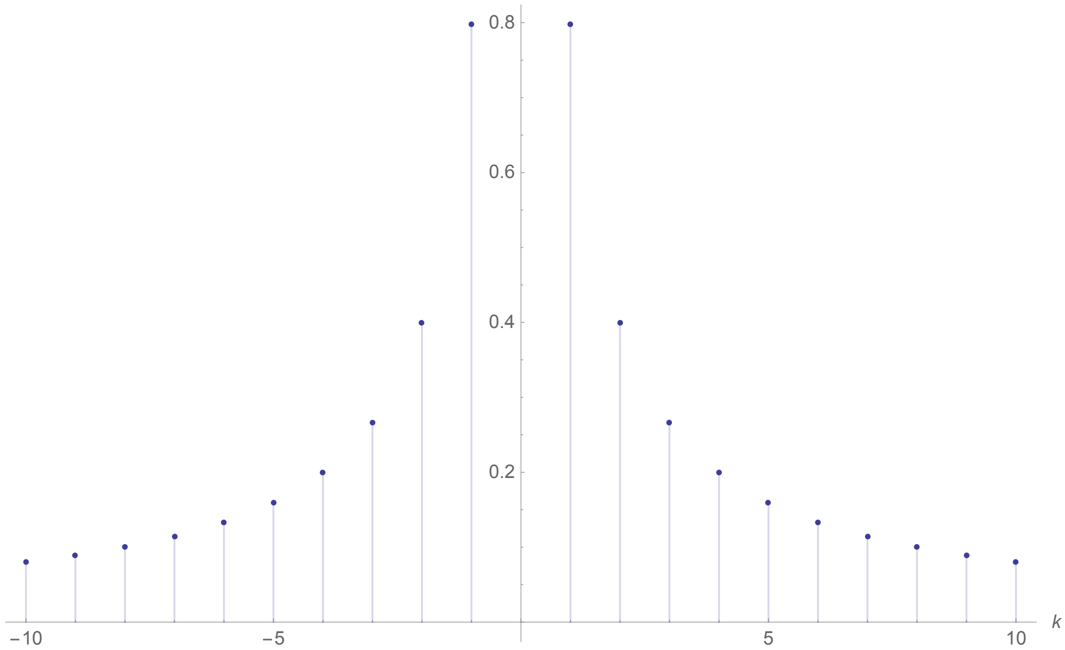

Figure 24: Graph of a periodic sawtooth function in Fourier k-space

- For the Fourier Transform of the sawtooth function, the k-space graph has discrete nonzero values for only specific wavenumbers, which means that ”in-between” frequencies/wavenumbers are not needed
- Note: amplitude of the function is large for small wavenumbers k and decreases for larger k
- Therefore, high frequency terms can be considered negligible (can approximate Fourier series with the first few terms)

4.3 How Period Length affects the Fourier Transform

- Can represent any function in the ”real x-space” (wiggly function) or in the ”Fourier k-space” (spiky function)
- The shorter the period of the original function, the sparser the Fourier representation; i.e. less wavenumbers required (Red sawtooth function)
- The longer the period, the denser the Fourier representation (Blue sawtooth function)
- The main contributing wavenumbers are condensed centrally closer to the small k-values
- Since $k = \frac{2\pi}{\lambda} = \frac{2\pi}{cT}$, $k \sim \frac{1}{T}$
- So if the original function has a longer period T, its Fourier series needs sinusoids with longer periods (smaller k)
- i.e. the more ”stretched out” a function is in the real space (longer period), the more centralized/”squished” it is in the Fourier space
- Note: ”periodic” functions with infinite period are aperiodic functions (never repeats itself)
- As the period approaches infinity, spikes in the k-space get infinitely squished together and

form a continuous function

- Therefore, while a periodic function can be represented by a discrete set of sines and cosines (only some wavenumbers), an aperiodic function (most functions) can only be formed from a **continuous** sum of sines and cosines (include all intermediate wavenumbers)

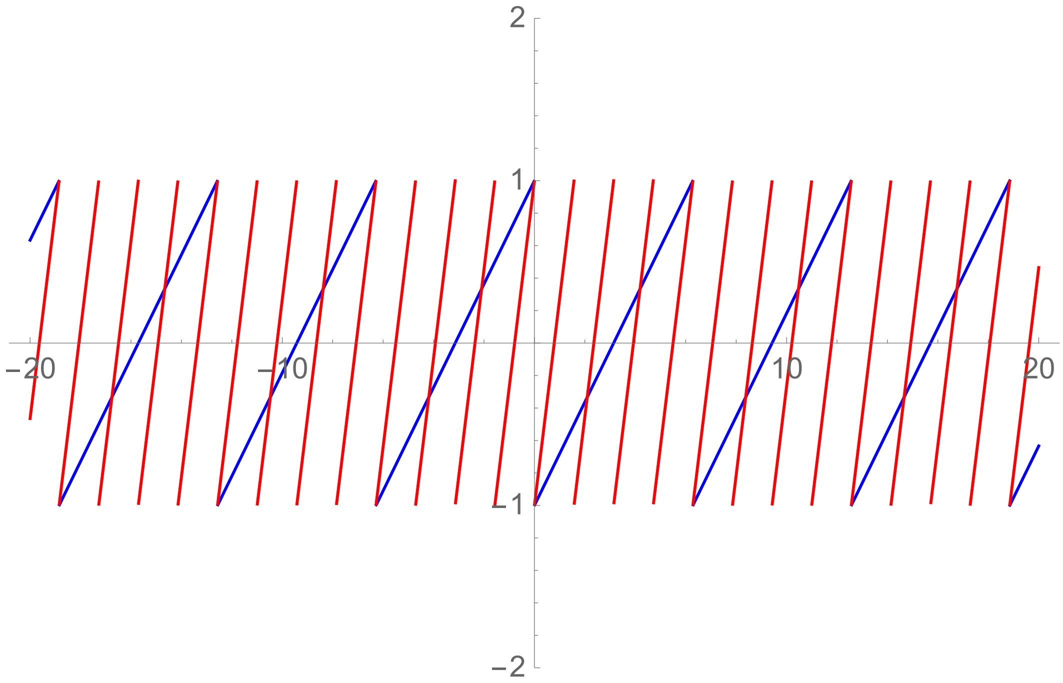

Figure 25: Graph of 2 sawtooth functions with different periods. The blue function has a longer period, while the red function has a shorter period.

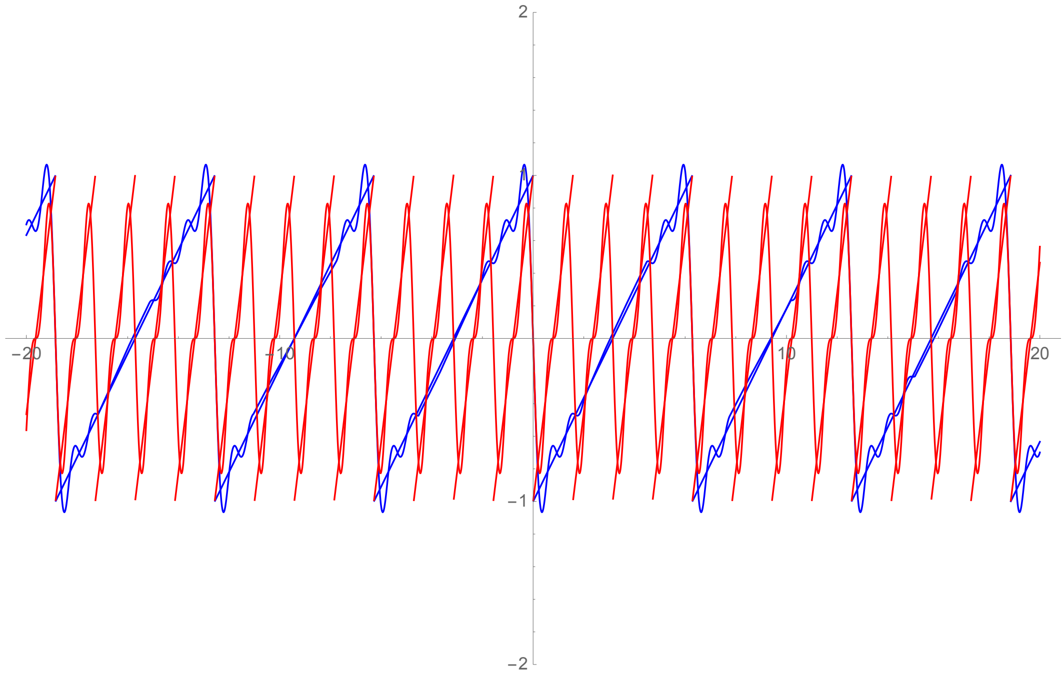

Figure 26: Graph of 2 sawtooth functions approximated with the first few terms of their Fourier series (real space)

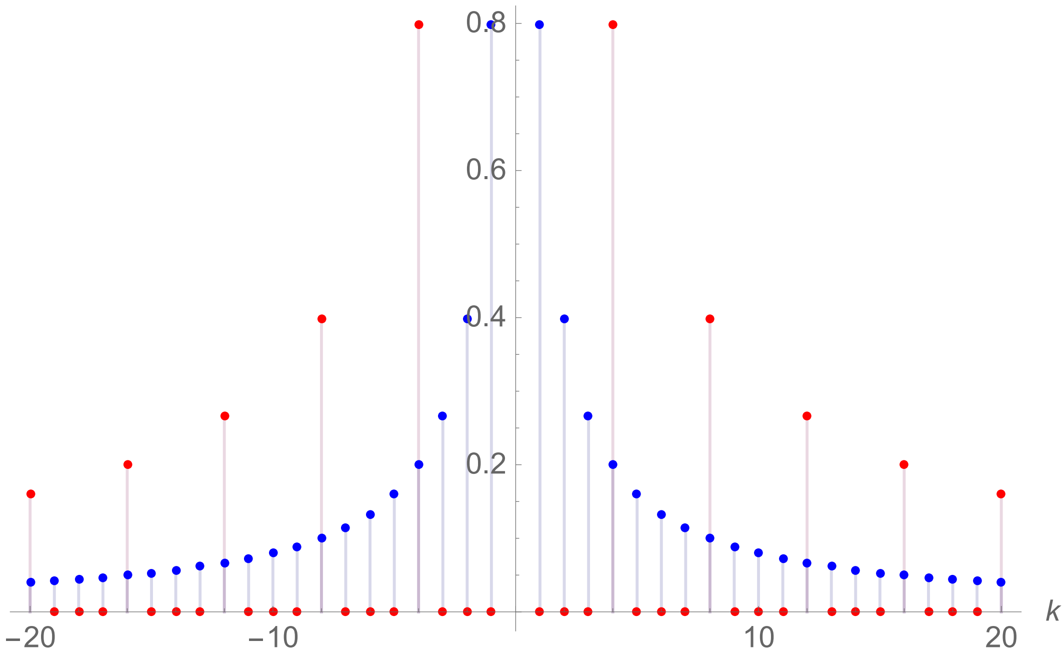

Figure 27: Graph of 2 sawtooth functions in Fourier k-space