APPENDIX A

DERIVATION OF HEISENBERG UNCERTAINTY PRINCIPLE

Heisenberg uncertainty principles can be derived by different methods. This appendix uses the wave packet to derive the uncertainty principles. For the sake of simplicity, the case of the one-dimensional wave packet is presented here. Then the wave function only depends on x and t.

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int g(k) \mathrm{e}^{i(kx-\omega t)} \, \mathrm{d}k. \tag{A.1}$$

For t=0, we have

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int g(k) \mathrm{e}^{ikx} \, \mathrm{d}k \tag{A.2}$$

and

$$g(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x,0) \mathrm{e}^{-ikx} \, \mathrm{d}x \tag{A.3}$$

Thus, $g(\boldsymbol{k})$ is the Fourier transform of $\psi(\boldsymbol{r},0)$. The wave packet is given by x-dependent wave function expressed in Equation A.2. If $|g(\boldsymbol{k})|$ has the shape depicted in Fig. A1 and $\psi(x)$, instead of having the form shown in Equation A.2, is composed of three plane waves with wave vectors of $k_0, k_0 + \Delta k/2$, and $k_0 - \Delta k/2$ and amplitudes proportional to 1, $\frac{1}{2}$, and $\frac{1}{2}$, then one can write the new wave packet as

$$\psi(x) = \frac{g(k_0)}{\sqrt{2\pi}} \left[e^{ik_0 x} + \frac{1}{2} e^{i(k_0 - \Delta k/2)x} + \frac{1}{2} e^{i(k_0 + \Delta k/2)x} \right]$$

Introduction to Nanomaterials and Devices, First Edition. Omar Manasreh.

$$= \frac{g(k_0)}{\sqrt{2\pi}} e^{ik_0x} \left[1 + \cos\left(\frac{\Delta k}{2}x\right)\right]$$

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$$= \frac{g(k_0)}{\sqrt{2\pi}} \mathrm{e}^{ik_0x} \left[1 + \cos\left(\frac{\Delta k}{2}x\right)\right]. \tag{A.4}$$

From Fig. A1, $|\psi(x)|$ is maximum at $x = 0$. This result is due to the fact that when x is zero, the three waves are in phase and interfere constructively as shown in the figure. As one moves away from the value $x = 0$, the waves become more and more out of phase and $|\psi(x)|$ decreases. The interference becomes completely destructive when the phase shift between e^{ik_0x} and $\mathrm{e}^{i(k_0\pm\Delta k/2)x}$ is equal to $\pm\pi$ and $|\psi(x)| = 0$ when $x = \pm\Delta x/2$. In other words, $|\psi(x)| = 0$ when $\cos(\Delta k.\Delta x/4) = -1$. This leads to the following equation:

$$\Delta k \cdot \Delta x = 4\pi. \tag{A.5}$$

This equation shows that the larger the width of $|\psi(x)|$, the smaller the width of $g(\boldsymbol{k})$. Equation A.4, however, shows that $|\psi(x)|$ is periodic in x and therefore has a series of maxima and minima. This arises from the fact that $\psi(x)$ is the superposition of a finite number of waves. For a continuous superposition of an

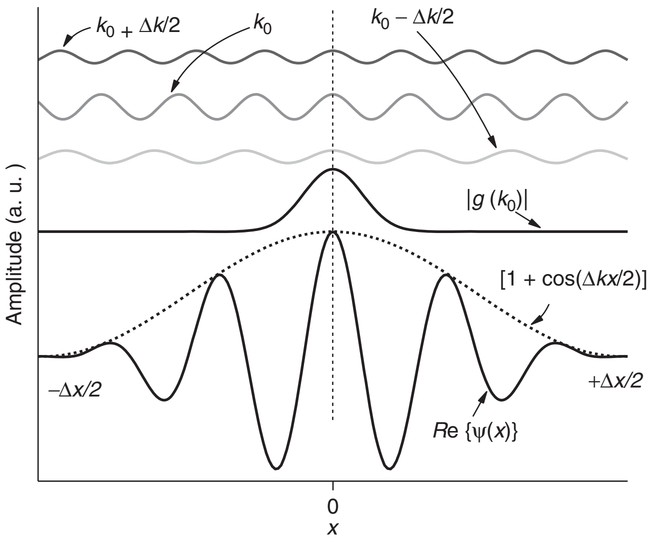

FIGURE A1 The shape of the function $|g(k)|$ is plotted along with the real parts of the three functions whose sum gives the function $\psi(x)$ of Equation A.3. The real part of $\psi(x)$ is also shown. The dashed-line curve corresponds to the function $[1 + \cos(\Delta kx/2)]$, which represents the form of the wave packet infinite number of waves as shown in Equation A.2, such a phenomenon does not exist and $|\psi(x,0)|$ can have only one maximum.

Let us return to the general wave packet formula shown in Equation A.2. Its form results from an interference phenomenon. Let $\alpha(\mathbf{k})$ be the argument of the function $g(\boldsymbol{k})$, that is,

$$g(k) = |g(k)|\ \mathrm{e}^{i\alpha(k)} \tag{A.6}$$

Assume that $\alpha(\boldsymbol{k})$ varies sufficiently smoothly within the interval $[k_0 - \Delta k/2, k_0 + \Delta k/2]$, where $|g(k)|$ is appreciable. Hence, when $\Delta\boldsymbol{k}$ is small enough, one can expand $\alpha(k)$ around $k \approx k_0$ such that $\alpha(k) \approx \alpha(k_0) + (k - k_0)\mathrm{d}\alpha/\mathrm{d}k|_{k=k0}$, which enables us to rewrite Equation A.2 in the following form:

$$\psi(x,0) \approx \frac{\mathrm{e}^{i[k_0 x + \alpha(k_0)]}}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} |g(k)|\mathrm{e}^{i(k-k_0)(x-x_0)}\mathrm{d}k, \tag{A.7}$$

where $x_0 = -[\mathrm{d}\alpha/\mathrm{d}k]_{k=k0}$. Equation A.7 is very useful for studying the variation of $|\psi(x)|$ in terms of x. When $|x - x_0|$ is large as compared to $1/(\Delta\boldsymbol{k})$, the wave function oscillates rapidly within the interval $\Delta\boldsymbol{k}$ as shown in Fig. A2. On the other hand, when $|x - x_0|$ is small as compared to $1/(\Delta\boldsymbol{k})$, the wave function oscillates only once as shown in the figure. Thus, when x moves away from x_0, $|\psi(x)|$ decreases. The decrease becomes appreciable if $\mathrm{e}^{i(k-k_0)(x-x_0)}$ oscillates approximately once. That is, when

$$\Delta k \cdot (x - x_0) \approx 1. \tag{A.8}$$

If Δx is the approximate width of the wave packet, one can write

$$\Delta \mathrm{k} \cdot \Delta x \geq 1 \tag{A.9}$$

This classic relation relates the widths of two functions that are Fourier transforms of each other. The important fact is that the product $\Delta k \cdot \Delta x$ has a lower bound, which depends on the precise definition of the each width.

With the help of the relation $\Delta\mathbf{p} = \hbar\Delta\mathbf{k}$, Equation A.9 can be rewritten as

$$\Delta \mathrm{p} \cdot \Delta x \geq \hbar \tag{A.10}$$

The relationship is called the *Heisenberg uncertainty principle*. The same procedure can be repeated by assuming

$$\psi(r,t) = A\mathrm{e}^{i\omega t} \tag{A.11}$$

to obtain a wave packet that is localized in time and frequency with their widths being related by

$$\Delta\omega \cdot \Delta t \approx 1. \tag{A.12}$$

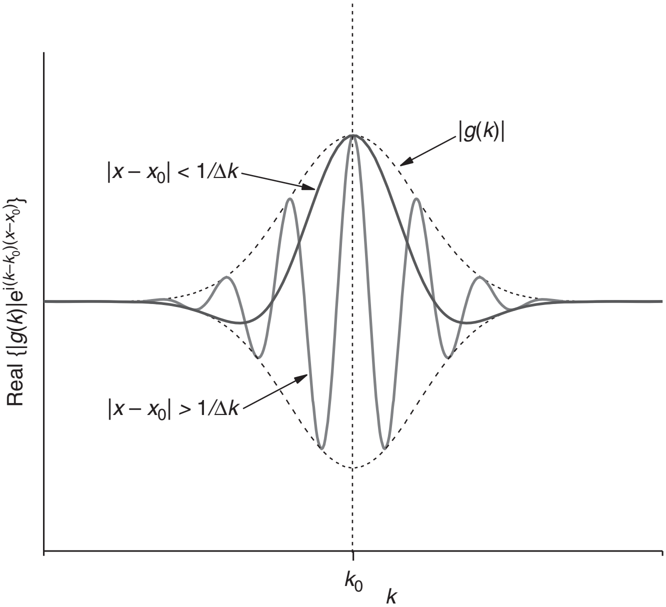

FIGURE A2 Variation of the wave function versus k. When $|x - x_0| > 1/\Delta \boldsymbol{k}$, we see several oscillations, but when $|x - x_0| < 1/\Delta \boldsymbol{k}$, we see only one oscillation

With the aid of the relation $\Delta E = \hbar \Delta\omega$, the uncertainty principle becomes

$$\Delta E \cdot \Delta t \geq \hbar. \tag{A.13}$$

These inequalities shown in Equations 1.34 and 1.37 are introduced to show that $\hbar$ is the lower limit. It is possible that one can construct wave packets for which the products of the quantities in these equations are larger than $\hbar$.