Problem Set 7

1. $$\tilde{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x)\, e^{i k x}\, dx$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a}} \int_{-\frac{a}{2}}^{\frac{a}{2}} \cos\left(\frac{\pi x}{a}\right) e^{-i k x}\, dx$$

$$= \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2}{a}} \int_{-\frac{a}{2}}^{\frac{a}{2}} \left(\frac{e^{i\pi x/a} + e^{-i\pi x/a}}{2}\right) e^{-i k x}\, dx$$

$$= \frac{1}{2\sqrt{a\pi}} \int_{-\frac{a}{2}}^{\frac{a}{2}} \left(e^{i\pi x/a} + e^{-i\pi x/a}\right) e^{-i k x}\, dx$$

$$= \frac{1}{2 i \left(\frac{\pi}{a} - k\right)\sqrt{a\pi}}\, e^{i\left(\frac{\pi}{a}-k\right)x}\Big|_{-\frac{a}{2}}^{\frac{a}{2}} - \frac{1}{2 i \left(\frac{\pi}{a} + k\right)\sqrt{a\pi}}\, e^{-i\left(\frac{\pi}{a}+k\right)x}\Big|_{-\frac{a}{2}}^{\frac{a}{2}}$$

$$= \frac{1}{\left(\frac{\pi}{a} - k\right)\sqrt{a\pi}} \sin\left(\left(\frac{\pi}{a} - k\right)\frac{a}{2}\right) + \frac{1}{\left(\frac{\pi}{a} + k\right)\sqrt{a\pi}} \sin\left(\left(\frac{\pi}{a} + k\right)\frac{a}{2}\right)$$

$$= \frac{2\sqrt{a\pi}}{(\pi^2 - a^2 k^2)} \cos\left(\frac{a k}{2}\right)$$

In[18]:= $\psi[x\_, a\_] := \text{Piecewise}\left[\left\{\left\{\sqrt{\frac{2}{a}}\ \text{Cos}\left[\frac{\pi}{a} x\right], x \le \frac{a}{2}\ \&\&\ x \ge -\frac{a}{2}\right\}, \left\{0, x < -\frac{a}{2}\ ||\ x > \frac{a}{2}\right\}\right\}\right];$

$$\frac{1}{\sqrt{2\pi}} \int_{-\frac{a}{2}}^{\frac{a}{2}} \sqrt{\frac{2}{a}}\ \text{Cos}\left[\frac{\pi}{a} x\right] E^{i k x}\, dx$$

(* Check that the $\tilde{\psi}(k)$ we calculated above is correct. *)

$$\tilde{\psi}[k\_] := \frac{2\sqrt{a\pi}\ \text{Cos}\left[\frac{a k}{2}\right]}{(-a^2 k^2 + \pi^2)};$$

$$\int_{-\infty}^{\infty} \text{Conjugate}[\tilde{\psi}[k]]\ \tilde{\psi}[k]\, dk$$

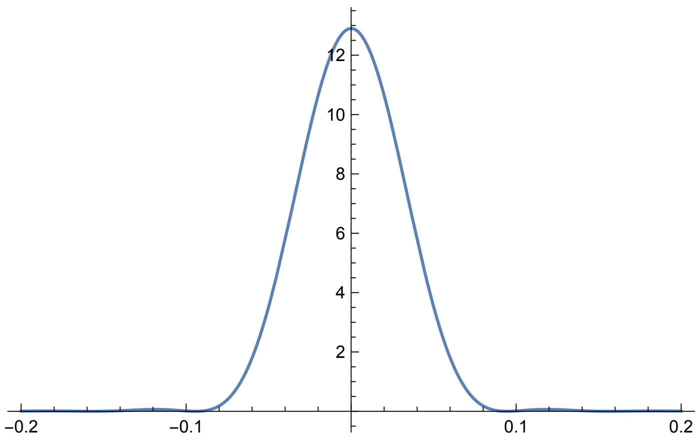
(* Check that $\tilde{\psi}(k)$ is normalized (for a>0). *)

Plot[Conjugate[$\tilde{\psi}$[k]] $\tilde{\psi}$[k] /. a → 100, {k, -0.2, 0.2}]

Out[19]= $$\frac{2\sqrt{\pi}\ \text{Cos}\left[\frac{a k}{2}\right]}{\sqrt{\frac{1}{a}}\ (-a^2 k^2 + \pi^2)}$$

Out[21]= $\text{ConditionalExpression}\left[\frac{\text{Abs}[a]^2}{a^2}, a \in \text{Reals}\right]$

Out[22]=



2. $\tilde{\psi}(k) = \frac{2\sqrt{a\pi}}{(\pi^2 - a^2 k^2)} \cos\left(\frac{a k}{2}\right);$

$\tilde{\psi}^2(k) = \frac{4 a \pi}{(\pi^2 - a^2 k^2)^2} \cos^2\left(\frac{a k}{2}\right);$

Hence the first zero point $k_0 = \pm\frac{3\pi}{a}$; (* the k satisfying $\frac{a k}{2} = \frac{\pi}{2}$ is not a zero point since the denominator also approaches 0 at that k value. hence the first zero point of $\tilde{\psi}^2(k)$ is when $\frac{a k}{2} = \frac{3\pi}{2}$ *)

As the infinite well becomes wider, the k_0 becomes smaller;

Hence $\Delta x\, \Delta p = \hbar\, \Delta x\, \Delta k \sim \hbar\, a \frac{3\pi}{a} = 3\pi\hbar > \frac{\hbar}{2}$;

which is consistent with Heisenberg's uncertainty relation.

3.

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ψ$tilde[k_] := (20 Sqrt[π] Cos[50 k])/(-10 000 k^2 + π^2);
ψ$approx[x_, k_] := ψ$tilde[k] E^(i k x) / Sqrt[2 π];
Plot[ψ[x, 100], {x, -400, 400}, AxesLabel → {"x"},
 PlotLabel → "Wavefunction ψ(x)"]
(*  The wavefunction that we want.  *)
Plot[Re[ψ$approx[x, 0.03]], {x, -400, 400}, AxesLabel → {"x"},
 PlotLabel → "Approximated avefunction ψ(x) with k=0.03"]
(*  The approximation to the wavefunction with only k=0.03.   *)
(* The wavelength of the sin funciton wave is determined
 by the wavenumber k used to approximate the wavefunction. *)
plot$approx[start_, end_, incre_] :=
  Plot[Re[Sum[ψ$approx[x, i] * incre, {i, start, end, incre}]],
   {x, -400, 400}, PlotRange → All, AxesLabel → {"x"},
   PlotLabel → "Approximated wavefunciton ψ(x)"];
(*  The 'incre' here in the summation works as the 'dx' in an integration,
and is necessary if you want to reproduce
 the wavefunction with the same magnitude.  *)
plot$approx[0.03, 0.03, 0.01]
(* Check the previous result. *)
(*  Since 2π/a = 2π/100 ~0.5,
the contribution for k ∈ [-0.5,0.5] or so is most important. If we
  calculate the approximated wavefunction over this range of k's,
we should get a satisfying result.  *)
plot$approx[-0.01, 0.01, 0.001]
plot$approx[-0.07, 0.07, 0.01]
plot$approx[-0.1, 0.1, 0.01]
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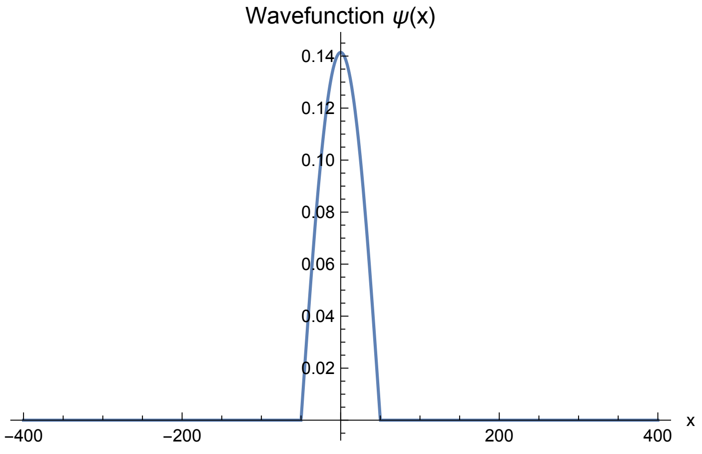
Out[25]=



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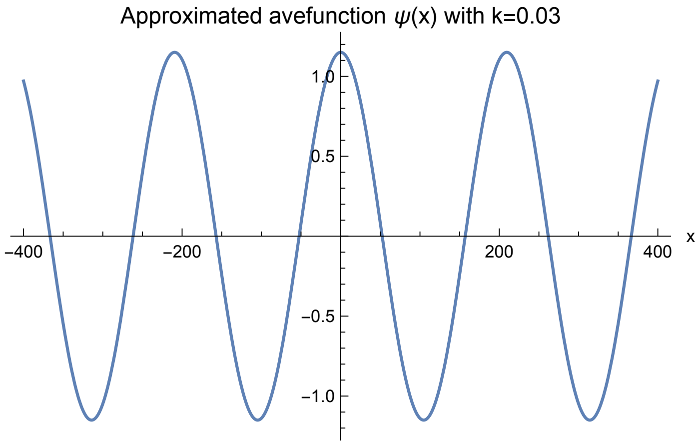

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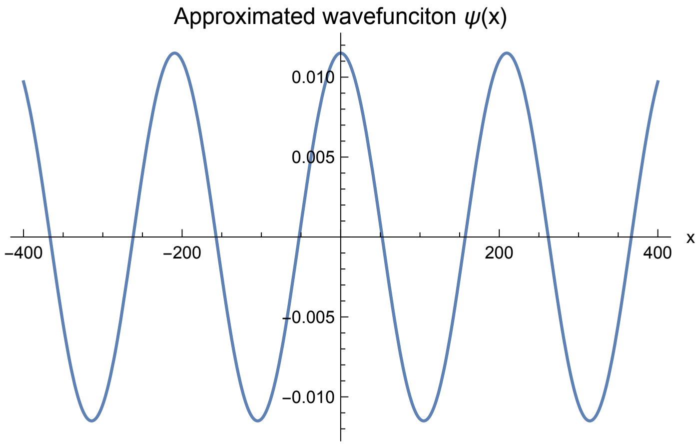

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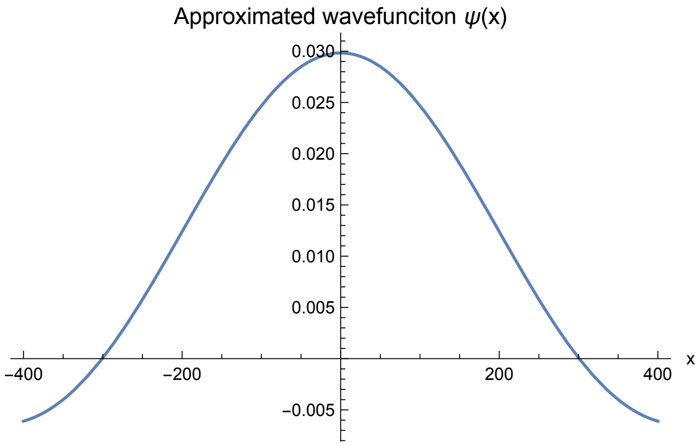

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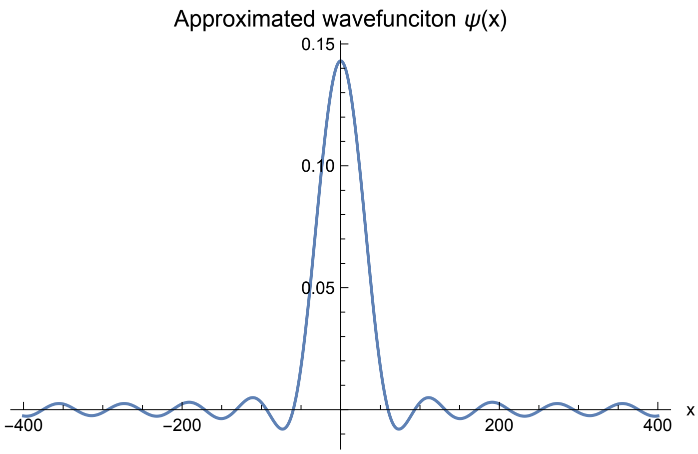

Out[31]=