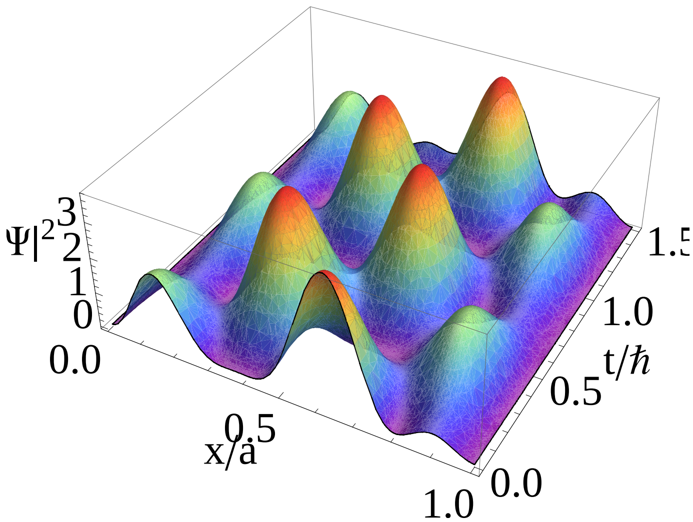
```
In[1]:= ClearAll["Global`*"]

In[2]:= (*These solutions cover the plotting portion of the
         homework. The math portion is self evident from the examples given*)
        (*Let's first set up some basic eigen states and energies that we will use throughout*)

In[3]:= (*Infinite Square Well*)

In[4]:= psiISW[n_, x_] := Sqrt[2 / a] Sin[π n x / a];
        EngISW[n_] := (n π ℏ / a) ^2 / (2 m);

In[6]:= (*Simple Harmonic Oscillator*)

In[7]:= A0 = (m ω / (π ℏ)) ^ .25;
        ξ[x_] := Sqrt[m ω / ℏ] x;
        psiSHO[n_, x_] := A0 / Sqrt[2^n n!] HermiteH[n, ξ[x]] Exp[-ξ[x] ^2 / 2];
        EngSHO[n_] := ℏ ω (n + .5);

In[11]:= (*Plane Wave*)

In[12]:= psiPW[k_, x_] := Exp[ⅈ k x];
         EngPW[k_] := (ℏ k) ^2 / 2 m;

In[14]:= (*Let us set c=ℏ=a=m=ω=1, so that x and t will be values of order unity. This
          is done because computers don't much like very small or very large numbers *)

In[15]:= c = 1; ℏ = 1; a = 1; m = 1; ω = 1;

In[16]:= (*Problem 1*)
         (*We are asked to use the following quantities*)

In[17]:= E1 = 10; E2 = 1; c1 = Sqrt[1 / 2]; c2 = c1;

In[18]:= (*For a linear combination of two states (non-complex),
         we can write it's Probability Density time evolution as PsiSq[x_,t_]:=
          c1^2 psi1[x]^2+c2^2 psi2[x]^2+2 c1 c2 psi1[x] psi2[x]
            Cos[(E2-E1) t/ℏ]. Let use immediately generalize this to complex states,
         since we will also use this for the plane wave state.*)

In[19]:= PsiSq[x_, t_] := Abs[c1 psi1[x]] ^2 + Abs[c2 psi2[x]] ^2 +
            2 Re[ Conjugate[c1 psi1[x]] c2 psi2[x] Exp[ⅈ (E2 - E1) t / ℏ]];

In[20]:= (*Let's use two orthogonal states of the infinite well. There
          is no way to pick eigenstates that match the the energies given since,
         n=m sqrt(E1/E2), must be an integer. Let's just use the 1st and 4th*)

In[21]:= psi1[x_] = psiISW[1, x]
         psi2[x_] = psiISW[4, x]

Out[21]= √2 Sin[π x]

Out[22]= √2 Sin[4 π x]
```

In[23]:=
```
Plot3D[PsiSq[x, t], {x, 0, 1}, {t, 0, 1.5}, AxesStyle → Directive[FontSize → 20], AxesLabel →
  {Style["x/a", FontSize → 20], Style["t/ℏ", FontSize → 20], Text[Style["|Ψ|^2", FontSize → 20]]},
 ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

Out[23]=



In[24]:=
```
(*you must use a t~ℏ/|E2-E1|
 to see the effect appropriately. Likewise the x axis should match the model used.*)
```

In[25]:=
```
(*Let's try two orthogonal states of the harmonic oscilator. Again,
there is no way to match the energies given to actual states*)
```

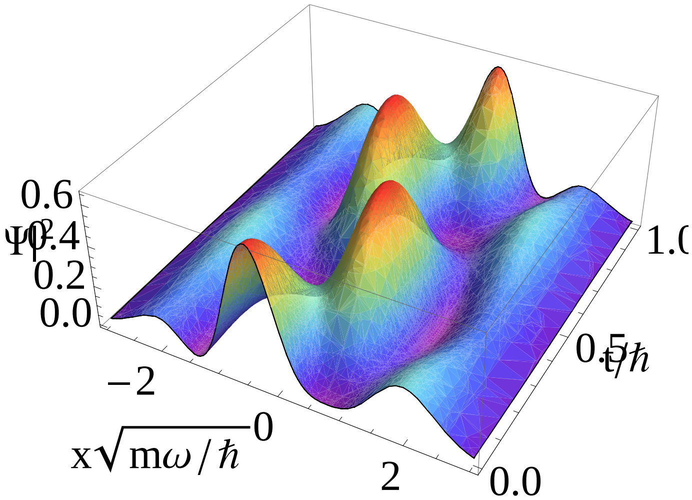
In[26]:=
```
psi1[x_] = psiSHO[0, x]
psi2[x_] = psiSHO[3, x]
```

Out[26]= $0.751126\, e^{-\frac{x^2}{2}}$

Out[27]= $0.108416\, e^{-\frac{x^2}{2}} \left(-12\, x + 8\, x^3\right)$

In[28]:=
```
Plot3D[PsiSq[x, t], {x, -3, 3}, {t, 0, 1}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x√mω / ℏ ", FontSize → 20], Style["t/ℏ", FontSize → 20],
   Text[Style["|Ψ|2", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

Out[28]=



In[29]:=
```
(*Finally, let's try two orthogonal states of the free particle (plane wave state).*)
```

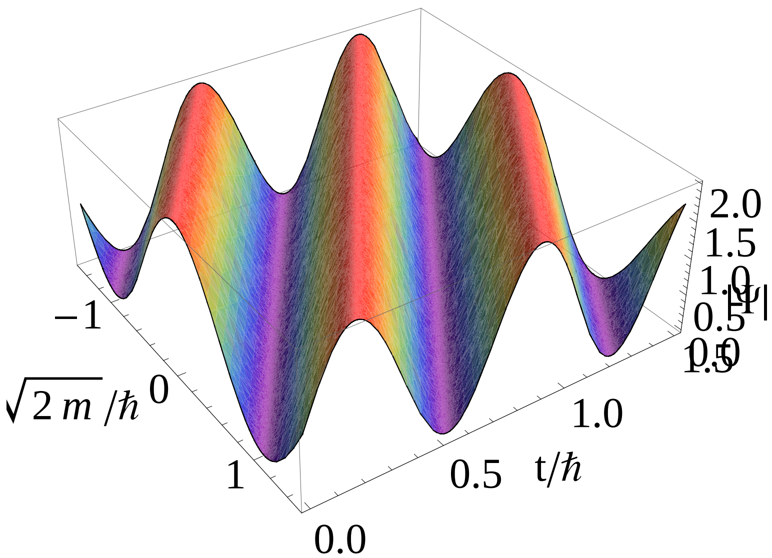
In[30]:=
```
k1 = Sqrt[2 m E1] / ℏ; k2 = Sqrt[2 m E2] / ℏ;
psi1[x_] = Exp[i k1 x]
psi2[x_] = Exp[i k2 x]
```

Out[31]= $e^{2 i \sqrt{5} x}$

Out[32]= $e^{i \sqrt{2} x}$

In[33]:=
```
Plot3D[PsiSq[x, t], {x, -1.5, 1.5}, {t, 0, 1.5}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x√2 m /ℏ", FontSize → 20], Style["t/ℏ", FontSize → 20],
   Text[Style["|Ψ|²", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

Out[33]=



In[34]:=
```
(*Problem 2*)
```

In[35]:=
```
(*Let's define the wavefunction between 0 and a=1*)
```

In[36]:=
```
Psi0[x_] := Sqrt[30 / a^5] x (a - x);
```

In[37]:=
```
(*Let us approximate it using the eigen states of the infinite square
 well. The projection to eigen states gives their respective amplitudes*)
```

In[38]:=
```
cn[n_] = Integrate[psiISW[n, x] Psi0[x], {x, 0, a}]
```

Out[38]=

$$-\frac{2\sqrt{15}\,(-2+2\,\mathrm{Cos}[n\,\pi]+n\,\pi\,\mathrm{Sin}[n\,\pi])}{n^3\,\pi^3}$$

In[39]:=
```
(*Let's see the first 5 terms explicitly*)
```

In[40]:=
```
Table[cn[n], {n, 1, 5, 1}]
```

Out[40]=

$$\left\{\frac{8\sqrt{15}}{\pi^3},\ 0,\ \frac{8\sqrt{\frac{5}{3}}}{9\,\pi^3},\ 0,\ \frac{8\sqrt{\frac{3}{5}}}{25\,\pi^3}\right\}$$

In[41]:=
```
(*Only the n=odd terms survive*)
```

In[42]:=
```
(*We approximates the wavefunction as an expansion of the basis up to 5th order*)
```

In[43]:=
```
PsiApprox1 = Sum[cn[n] psiISW[n, x], {n, 1, 1}]
PsiApprox3 = Sum[cn[n] psiISW[n, x], {n, 1, 3}]
PsiApprox5 = Sum[cn[n] psiISW[n, x], {n, 1, 5}]
```

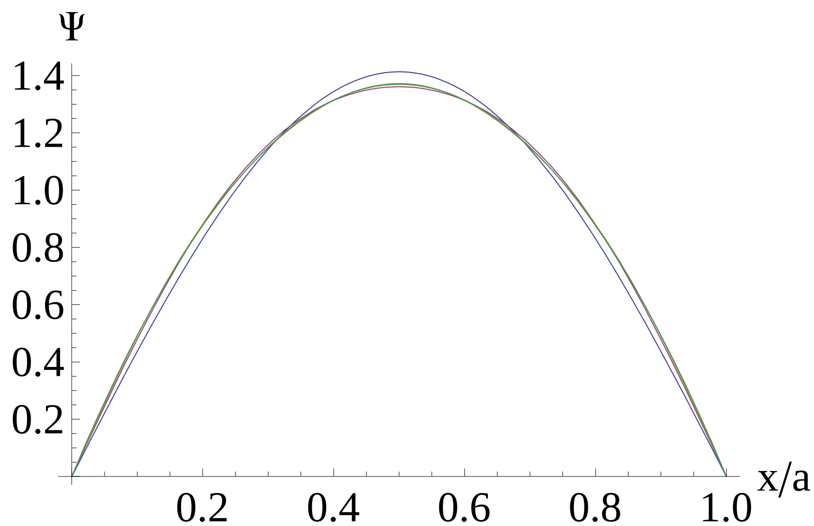
Out[43]= $\frac{8\sqrt{30}\,\text{Sin}[\pi x]}{\pi^3}$

Out[44]= $\frac{8\sqrt{30}\,\text{Sin}[\pi x]}{\pi^3} + \frac{8\sqrt{\frac{10}{3}}\,\text{Sin}[3\pi x]}{9\pi^3}$

Out[45]= $\frac{8\sqrt{30}\,\text{Sin}[\pi x]}{\pi^3} + \frac{8\sqrt{\frac{10}{3}}\,\text{Sin}[3\pi x]}{9\pi^3} + \frac{8\sqrt{\frac{6}{5}}\,\text{Sin}[5\pi x]}{25\pi^3}$

In[46]:=
```
Plot[{PsiApprox1, PsiApprox3, PsiApprox5, Psi0[x]},
 {x, 0, a}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x/a", FontSize → 20], Text[Style["Ψ", FontSize → 20]]}]
```

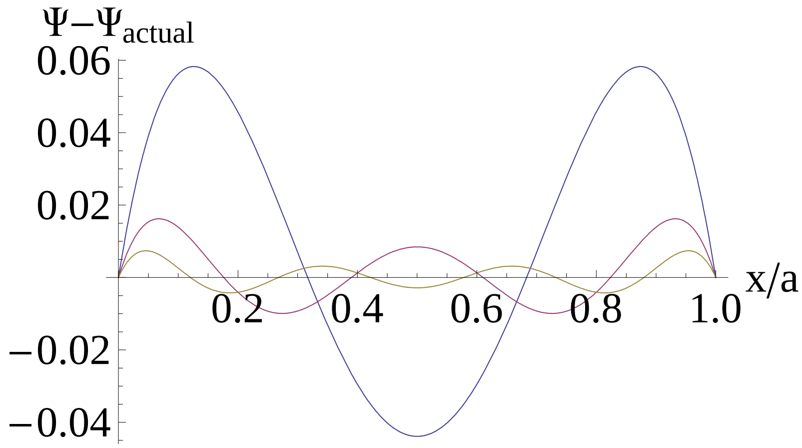
Out[46]=



In[47]:=
```
(*To get a better idea of how well it approximates,
we plot also the difference from the actual*)
```

In[48]:=
```
Plot[{Psi0[x] - PsiApprox1, Psi0[x] - PsiApprox3, Psi0[x] - PsiApprox5},
 {x, 0, 1}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x/a", FontSize → 20], Text[Style["Ψ-Ψactual", FontSize → 20]]}]
```

Out[48]=



In[49]:=
```
(*Now let them evolve in time*)
```

In[50]:=
```
(*We have chosen, m=1, which is not really a reasonable value for atoms,
but gives the correct qualitative solution regardless*)
```

In[51]:=
```
PsiApprox[x_, t_] = Sum[cn[n] psiISW[n, x] Exp[i EngISW[n] t], {n, 1, 5}]
```

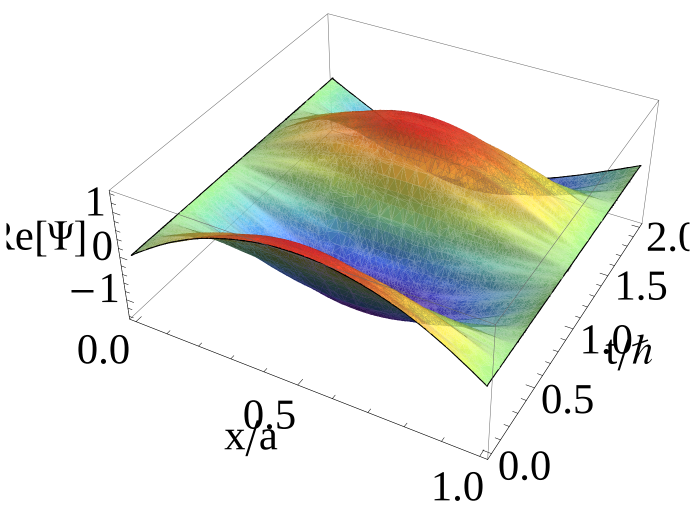
Out[51]=

$$\frac{8\sqrt{30}\,e^{\frac{1}{2} i \pi^2 t}\,\mathrm{Sin}[\pi x]}{\pi^3} + \frac{8\sqrt{\frac{10}{3}}\,e^{\frac{9}{2} i \pi^2 t}\,\mathrm{Sin}[3 \pi x]}{9 \pi^3} + \frac{8\sqrt{\frac{6}{5}}\,e^{\frac{25}{2} i \pi^2 t}\,\mathrm{Sin}[5 \pi x]}{25 \pi^3}$$

In[52]:=
```
(*The real part of Psi(x,t) *)
```

In[53]:=
```
Plot3D[Re[PsiApprox[x, t]], {x, 0, 1},
 {t, 0, 2}, AxesStyle → Directive[FontSize → 20], AxesLabel →
  {Style["x/a", FontSize → 20], Style["t/ℏ", FontSize → 20], Text[Style["Re[Ψ]", FontSize → 20]]},
 ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

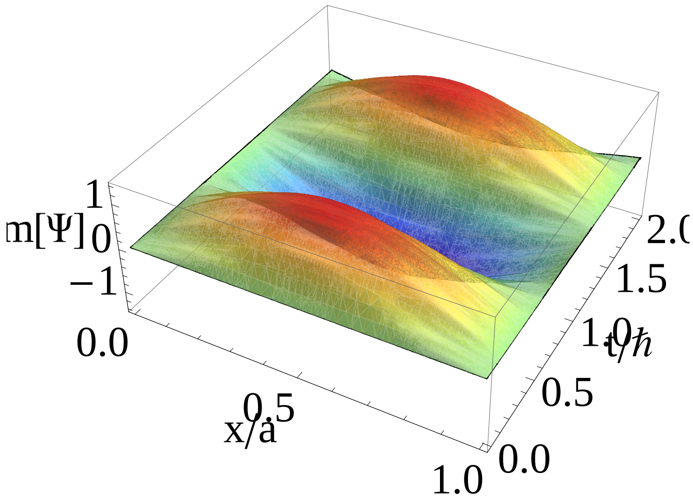
Out[53]=



In[54]:=
```
(*The imaginary part of Psi(x,t) *)
```

In[55]:=
```
Plot3D[Im[PsiApprox[x, t]], {x, 0, 1},
 {t, 0, 2}, AxesStyle → Directive[FontSize → 20], AxesLabel →
  {Style["x/a", FontSize → 20], Style["t/ℏ", FontSize → 20], Text[Style["Im[Ψ]", FontSize → 20]]},
 ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

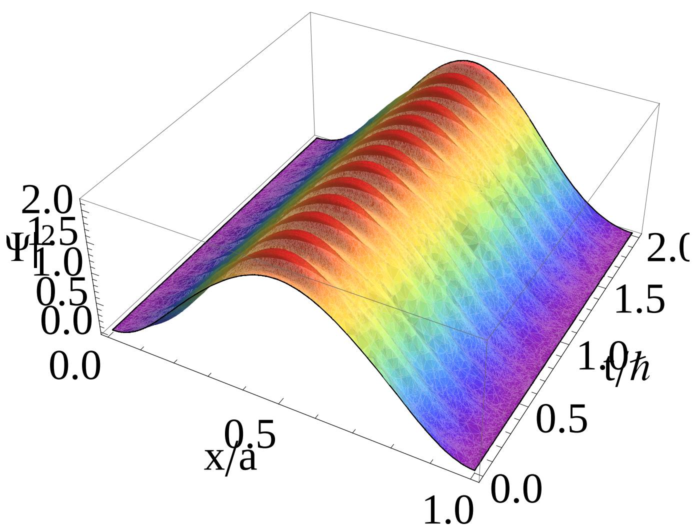
Out[55]=



In[56]:=
```
(*The probability |Psi(x,t)|^2 *)
```

In[57]:=
```
Plot3D[Abs[PsiApprox[x, t]]^2, {x, 0, 1},
 {t, 0, 2}, AxesStyle → Directive[FontSize → 20], AxesLabel →
  {Style["x/a", FontSize → 20], Style["t/ℏ", FontSize → 20], Text[Style["|Ψ|^2", FontSize → 20]]},
 ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

Out[57]=



In[58]:=
```
(*As expected the solution evolves in time very near the first energy eigenstate*)
```

In[59]:=
```
(*Problem 3*)
```

In[60]:=
```
(*<H≥ = <Ψ|H|Ψ> = ∑n<Ψ|H|ψn><ψn|Ψ> = ∑n En|cn|^2 *)
```

In[61]:=
```
(*With En=n^2/(2m)*(πℏ/a)^2,  |cn|^2=960/(πn)^6 for n odd and zero for n even*)
```

In[62]:=
```
Sum[n^2 / (2) * (π ) ^2 * 960 / (π n) ^6, {n, 1, ∞, 2}]
```
Out[62]= 5

In[63]:=
```
(*Thus, E=<H>=5(ℏ/a)^2/m. Notice that E1=π^2/2*(ℏ/a)^2/m, which is just smaller than E*)
```

In[64]:=
```
(*Problem 4*)
(*Let's return to the harmonic oscillator and create an arbitrary linear combination*)
```

In[65]:=
```
Psi[x_, t_] := Sqrt[.3] psiSHO[1, x] Exp[ⅈ EngSHO[1] t / ℏ] +
   Sqrt[.4] psiSHO[3, x] Exp[ⅈ EngSHO[3] t / ℏ] + Sqrt[.3] psiSHO[4, x] Exp[ⅈ EngSHO[4] t / ℏ];
```

In[66]:=
```
(*We can see that this is normalized and
 remains normalized (up to some error in calculation)*)
```

In[67]:=
```
Table[Integrate[Conjugate[Psi[x, t]] Psi[x, t], {x, -∞, ∞}], {t, 0, 1, .1}]
```

Out[67]= $\{1. + 0.\, i,\ 1. - 5.15746\times10^{-17}\, i,\ 1. + 2.34383\times10^{-16}\, i,\ 1. + 2.01704\times10^{-16}\, i,\ 1. - 2.01812\times10^{-16}\, i,\ 1. - 2.49127\times10^{-16}\, i,\ 1. + 1.03466\times10^{-16}\, i,\ 1. - 8.70323\times10^{-17}\, i,\ 1. - 1.04707\times10^{-16}\, i,\ 1. - 1.58526\times10^{-16}\, i,\ 1. - 7.64107\times10^{-17}\, i\}$

In[68]:=
```
(*The Energy of this state is*)
```

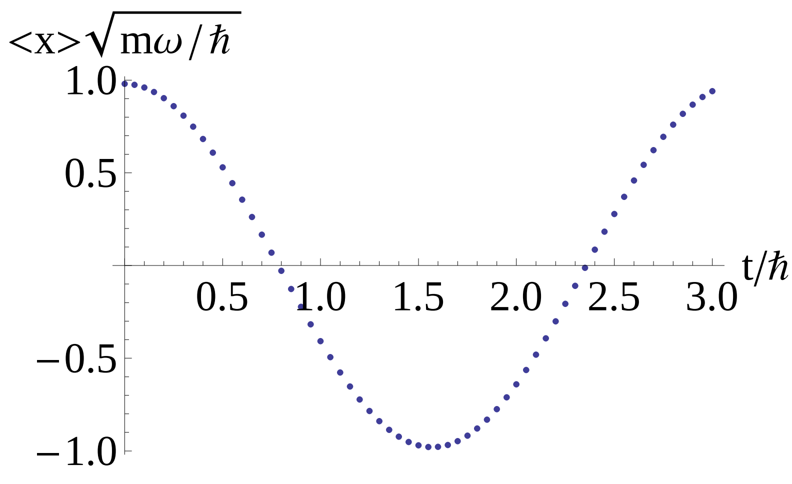
In[69]:=
```
.3 EngSHO[1] + .4 EngSHO[3] + .3 EngSHO[4]
```
Out[69]= 3.2

In[70]:=
```
(*Given ω=2π/sec, this would be ~10^-13 eV*)
```

In[71]:=
```
(*The average position oscillates*)
```

In[72]:=
```
pos = Table[Re[Integrate[x Conjugate[Psi[x, t]] Psi[x, t], {x, -∞, ∞}]], {t, 0, 6, .1}];
```

In[73]:=
```
ListPlot[pos, DataRange → {0, 3}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["t/ℏ", FontSize → 20], Text[Style["<x>√(mω / ℏ) ", FontSize → 20]]}]
```

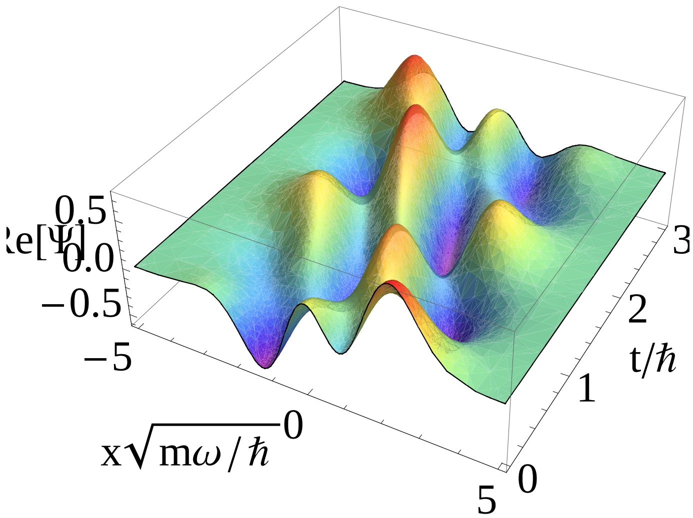
Out[73]=


In[74]:=
```
(*Notice that if we had a 1kg particle in this state, the maximal average
 displacement would be on the order of 10^-8 Angstroms (rediculously small)*)
```

In[75]:=
```
(*The Real part*)
```

In[76]:=
```
Plot3D[Re[Psi[x, t]], {x, -5, 5}, {t, 0, 3}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x√mω / ℏ", FontSize → 20], Style["t/ℏ", FontSize → 20],
   Text[Style["Re[Ψ]", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

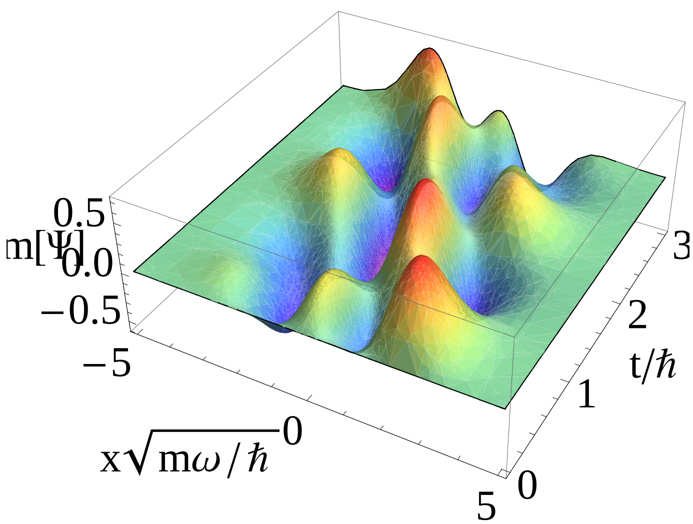
Out[76]=



In[77]:=
```
(*The Imaginary part*)
```

In[78]:=
```
Plot3D[Im[Psi[x, t]], {x, -5, 5}, {t, 0, 3}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x√mω / ℏ", FontSize → 20], Style["t/ℏ", FontSize → 20],
   Text[Style["Im[Ψ]", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

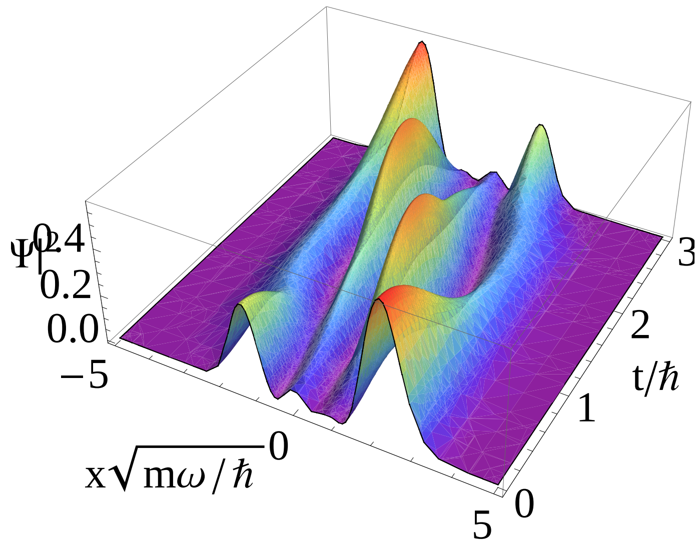
Out[78]=



In[79]:=
```
(*The probabilty density*)
```

In[80]:=
```
Plot3D[Abs[Psi[x, t]]^2, {x, -5, 5}, {t, 0, 3}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["x√mω/ℏ", FontSize → 20], Style["t/ℏ", FontSize → 20],
   Text[Style["|Ψ|²", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None, MaxRecursion → 5]
```

Out[80]=



In[81]:=
```
(*Problem 5*)
```

In[82]:=
```
(*In addition to the solution in the book,
I will state that the virial theorem for a single particel is simply 2<T>=-<rF>. Since,
for the Harmonic Oscillator F=-kr, <T>=<1/2*kr^2=<V>. And since <E>=<T>+<V>,
it follows that <V>=<E>/2*)
```

In[83]:=
```
(*Problem 6*)
```

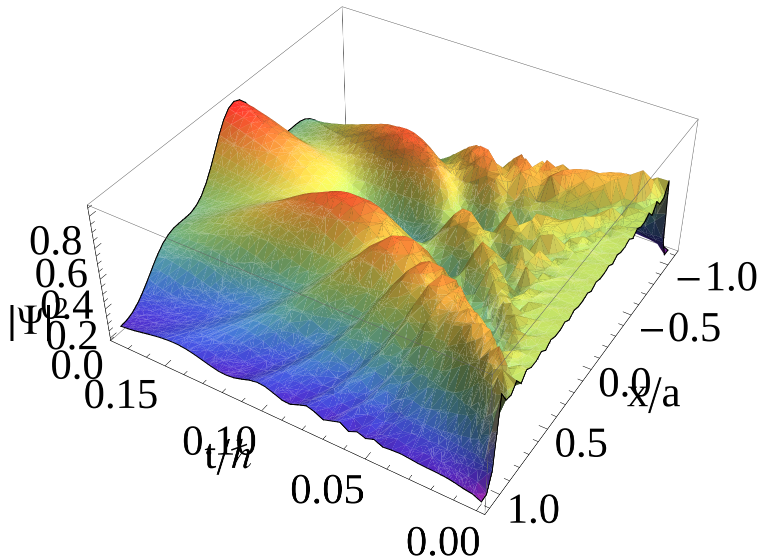
In[84]:=
```
Phi[k_, x_, t_] := 1 / (π Sqrt[2 a]) Sin[k a] / k Exp[i (k x - ℏ k^2 / (2 m) t)];
```

In[85]:=
```
Timing[Psi = Table[Abs[NIntegrate[Phi[k, x, t], {k, -50 / a, 50 / a}]]^2,
    {x, -1.1, 1.1, .05}, {t, 0, .176, .004}];]
```

Out[85]=
```
{99.86, Null}
```

In[86]:=
```
ListPlot3D[Psi, DataRange → {{0, .176}, {-1.1, 1.1}}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["t/ℏ", FontSize → 20], Style["x/a", FontSize → 20],
   Text[Style["|Ψ|^2", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None]
```

Out[86]=



In[90]:=
```
Timing[Psi =
   Table[Abs[NIntegrate[Phi[k, x, t], {k, -20 / a, 20 / a}]]^2, {x, -2, 2, .025}, {t, 0, 1, .05}];]
```

Out[90]= {139.687, Null}

In[91]:=
```
ListPlot3D[Psi, DataRange → {{0, 1}, {-2, 2}}, AxesStyle → Directive[FontSize → 20],
 AxesLabel → {Style["t/ℏ", FontSize → 20], Style["x/a", FontSize → 20],
   Text[Style["|Ψ|^2", FontSize → 20]]}, ColorFunction → "Rainbow", Mesh → None]
```

Out[91]=