Lecture 8

WKB Approximation, Variational Methods and the Harmonic Oscillator

Reading:

Notes and Brennan Chapter 2.5 & 2.6

Wentzel-Kramers-Brillouin (WKB) Approximation

•The WKB approximation is a "semiclassical calculation" in quantum mechanics in which the wave function is assumed an exponential function with amplitude and phase that slowly varies compared to the de Broglie wavelength, λ, and is then semiclassically expanded.

•While, Wentzel, Kramers, and Brillouin developed this approach in 1926, earlier in 1923, a mathematician, Harold Jeffreys, had already developed a more general method of approximating linear, second-order differential equations (the Schrödinger equation is a linear second order differential equation). Jeffreys is rarely given his proper credit.

•While technically this is an "Approximation method" not an "Exact solution" to the Schrödinger equation and thus should be covered when we discuss Approximation Methods in Chapter 4, it's very close relationship to the simple Plane Wave solutions warrants us discussing it now.

•The WKB method is most often applied to 1D problems but can be applied to 3D spherically symmetric problems as well (see Bohm 1951 for example).

•The WKB approximation will be especially useful in deriving the Tunnel Current in a tunnel diode (see Brennan section 11.6 for example). This topic will be covered in ECE 6453 in detail and only briefly introduced here.

Wentzel-Kramers-Brillouin (WKB) Approximation

The WKB approximation states that since in a constant potential, the wave function solutions of the Schrodinger Equation are of the form of simple plane waves,

$$\Psi(x) = Ae^{\pm ikx} \quad \text{where } k = 2\pi/\lambda = \sqrt{\frac{2m(E-U)}{\hbar^2}} = \text{constant}$$

if the potential , U→U(x), changes slowly with x, the solution of the Schrodinger equation is of the form,

(*)

$$\Psi(x) = Ae^{i\phi(x)}$$

Where $\phi(x)=xk(x)$. For the constant potential case, $\phi(x)=\pm kx$ so the phase changes linearly with x. In a slowly varying potential, $\phi(x)$ should vary slowly from the linear case, $\pm kx$.

For the two cases, E>U and E<U, let k(x) be defined as (so we only have to solve the problem once),

$$k(x) = \sqrt{\frac{2m(E-U(x))}{\hbar^2}} \quad \text{for } E > U(x)$$

$$k(x) = -i\sqrt{\frac{2m(U(x)-E)}{\hbar^2}} = -i\kappa(x) \quad \text{for } E < U(x)$$

Wentzel-Kramers-Brillouin (WKB) Approximation

Using the normalized version of (*) the Schrodinger Equation,

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x)+U(x)\Psi(x)=E\Psi(x)$$

Becomes,

$$i\frac{\partial^2\phi}{\partial x^2}-\left(\frac{\partial\phi}{\partial x}\right)^2+\left(k(x)\right)^2=0$$

The WKB approximation assumes that the potentials are slowly varying. If this is the case, k(x) is also slowly varying and so ϕ(x) slowly varying. **Thus, the 0th order WKB Approximation assumes**,

$$\frac{\partial^2\phi}{\partial x^2}\approx 0$$

and thus,

$$\left(\frac{\partial\phi_0}{\partial x}\right)^2=\left(k(x)\right)^2 \quad \text{or}$$

$$\boxed{\begin{array}{l}\phi_0(x)=\pm\int k(x)dx+C_0 \quad \text{and thus,}\\ \Psi(\mathrm{x})=e^{i\left(\pm\int k(x)dx+C_0\right)}\end{array}}$$

Note that the subscripts of zero, 0, emphasize that this solution comes from the 0th order approximation.

Wentzel-Kramers-Brillouin (WKB) Approximation

If a more accurate solution is required, we can rewrite our previous starting point as,

$$i\frac{\partial^2\phi}{\partial x^2}-\left(\frac{\partial\phi}{\partial x}\right)^2+\left(k(x)\right)^2=0 \quad\Rightarrow\quad \left(\frac{\partial\phi}{\partial x}\right)^2=\left(k(x)\right)^2+i\frac{\partial^2\phi}{\partial x^2} \quad \text{or}$$

$$\frac{\partial\phi}{\partial x}=\sqrt{\left(k(x)\right)^2+i\frac{\partial^2\phi}{\partial x^2}} \quad \text{so,}$$

$$\phi(x)=\pm\int\sqrt{\left(k(x)\right)^2+i\frac{\partial^2\phi}{\partial x^2}}dx+C_1$$

So far, no approximation has been made (i.e. this is an exact solution).

The **<u>1st order WKB approximation</u>** assumes that since,

$$\left(\frac{\partial\phi_0}{\partial x}\right)^2=\left(k(x)\right)^2 \quad \text{from the 0th order solution,}$$

$$\frac{\partial\phi_0}{\partial x}=\pm k(x) \quad \text{so,}$$

$$\frac{\partial^2\phi_0}{\partial x^2}=\pm\frac{\partial}{\partial x}k(x) \ \text{thus,}$$

$$\phi(x)=\pm\int\sqrt{\left(k(x)\right)^2\pm i\frac{\partial}{\partial x}k(x)}dx+C_1 \quad \text{and thus,}$$

$$\Psi(x)=e^{i\left(\pm\int\sqrt{\left(k(x)\right)^2\pm i\frac{\partial}{\partial x}k(x)}dx+C_1\right)}$$

Note that the subscripts of 1, emphasize that this solution comes from the 1st order approximation.

Wentzel-Kramers-Brillouin (WKB) Approximation

Some important points about the WKB Approximation:

1) We only need to know the shape of the potential to estimate the wave function since,

$$U(x) \Rightarrow k(x) \Rightarrow \phi(x) = \pm\int \sqrt{(k(x))^2 \pm i\frac{\partial}{\partial x}k(x)}\,dx + C_1 \;\Rightarrow\; \Psi(\mathrm{x}) = e^{i\left(\pm\int\sqrt{(k(x))^2 \pm i\frac{\partial}{\partial x}k(x)}\,dx + C_1\right)}$$

2) Since we are limited to slowly varying U(x) (compared to λ), then we can say,

$$\left|\frac{\partial}{\partial x}k(x)\right| << \left|(k(x))^2\right|$$

and thus, the 1st order approximation is only slightly different from the 0th order approximation

3) The WKB approximation breaks down at regions where E~U (points when classical particles will turn around and change directions – Classical Turning Points). In this case, the wavevector, k(x), approaches zero but its derivative does not.

$$k(x) = 0 \quad \text{but} \quad \frac{\partial k(x)}{\partial x} = -i\frac{\partial}{\partial x}\left(\sqrt{\frac{2m(E-U(x))}{\hbar^2}}\right) \neq 0$$

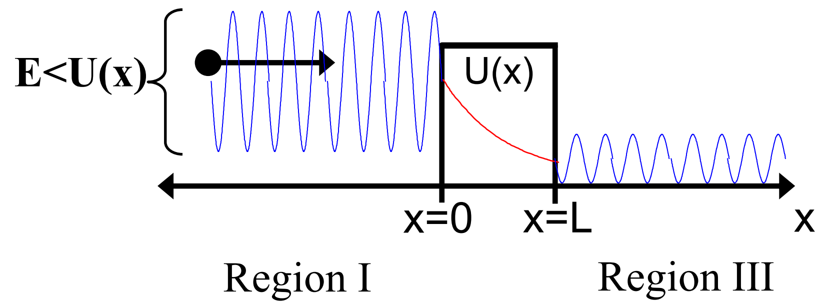
In this case, clearly $\left|\frac{\partial}{\partial x}k(x)\right| << \left|(k(x))^2\right|$ does not hold true!

In these special cases, connection formulas must be used to tie together regions on either side of the classical turning point. In all other regions WKB is valid (See Merzbacher 1970 for details).

Wentzel-Kramers-Brillouin (WKB) Approximation

Example:

Consider the tunneling probability at a finite width potential barrier.



$$T = \frac{\Psi^*(L)\Psi(L)}{\Psi^*(0)\Psi(0)} \quad \text{where} \quad \Psi(\mathrm{x}) = \Psi(0)e^{i\left(\pm\int k(x)dx + C_1\right)}$$

But for tunneling to occur, E<U so,

$$k(x) = -i\sqrt{\frac{2m(U(x)-E)}{\hbar^2}} \quad \text{for E < U(x) = U}$$

$$\Psi(\mathrm{x}) = \Psi(0)e^{i\left(\pm\int_0^x -i\sqrt{\frac{2m(U(x)-E)}{\hbar^2}}dx\right)}$$

$$\Psi(\mathrm{x}) = \Psi(0)e^{\left(-\int_0^x \sqrt{\frac{2m(U-E)}{\hbar^2}}dx\right)}$$

$$\Psi(\mathrm{x}) = \Psi(0)e^{\left(-\left(\sqrt{\frac{2m(U-E)}{\hbar^2}}\right)x\right)}$$

Thus,

$$T = \frac{\Psi^*(L)\Psi(L)}{\Psi^*(0)\Psi(0)} = \frac{\Psi(0)e^{\left(-\left(\sqrt{\frac{2m(U-E)}{\hbar^2}}\right)L\right)}\Psi(0)e^{\left(-\left(\sqrt{\frac{2m(U-E)}{\hbar^2}}\right)L\right)}}{\Psi(0)e^{\left(-\left(\sqrt{\frac{2m(U-E)}{\hbar^2}}\right)0\right)}\Psi(0)e^{\left(-\left(\sqrt{\frac{2m(U-E)}{\hbar^2}}\right)0\right)}} = \boxed{e^{\left(-2\left(\sqrt{\frac{2m(U-E)}{\hbar^2}}\right)L\right)}}$$

Variational Methods of Approximation

The concept behind the Variational method of approximating solutions to the Schrodinger Equation is based on:

a) An educated guess as to the functional form of the wave function. Often this is based on a similar problem that has an exact solution.

b) A "Variational parameter" that will be adjusted to obtain a minimum in the eigen energy.

c) Recognition that all natural systems seek the lowest energy state.

Using all of the above, one minimizes the expected energy by iterative methods.

Given,

$$\langle E \rangle = \langle \Psi(x,\alpha) | H | \Psi(x,\alpha) \rangle$$

Find the value of α for which $\langle \mathrm{E} \rangle$ is minimum. Thus,

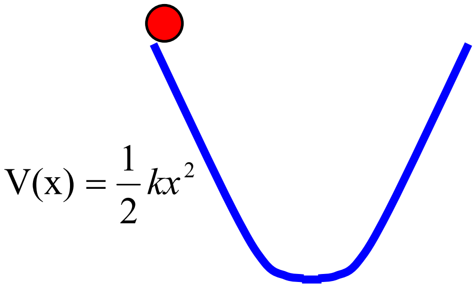
$$\frac{\mathrm{d}}{\mathrm{d}\alpha}\langle E \rangle = \frac{\mathrm{d}}{\mathrm{d}\alpha}\langle \Psi(x,\alpha) | H | \Psi(x,\alpha) \rangle = 0 \quad \text{and}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}\alpha^2}\langle E \rangle = \frac{\mathrm{d}^2}{\mathrm{d}\alpha^2}\langle \Psi(x,\alpha) | H | \Psi(x,\alpha) \rangle > 0$$

Harmonic Oscillator

In many physical systems, kinetic energy is continuously traded off with potential energy. Thus, as kinetic energy increases, potential energy is lost and vice versa in a cyclic fashion. When the equation of motion follows,

$$ma = m\frac{d^2x}{dt^2} = F = -kx$$



a Harmonic Oscillator results.

The term -kx is called the restoring force.

The radian frequency of such an oscillation is,

$\omega = \sqrt{\frac{k}{m}}$ while the potential can be found by integrating the force, F = -kx

$$V(x) = \frac{1}{2}kx^2$$

Thus, the Schrodinger equation for this potential is,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + \frac{1}{2}kx^2\Psi(x) = E\Psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + \frac{1}{2}m\omega^2x^2\Psi(x) = E\Psi(x)$$

Harmonic Oscillator Solution

The power series solution to this problem is derived in Brennan, section 2.6, p. 105-113 and is omitted for the sake of length. Instead we will only discuss the operator based solution. There is an infinite series of possible solutions described by:

$$\Psi_n(x) = \frac{C_n}{2^{\left(\frac{n}{2}\right)}} h_n(y) e^{-\left(\frac{y^2}{2}\right)} \quad \text{where } C_n \equiv \sqrt{\frac{\sqrt{\frac{m\omega}{\pi\hbar}}}{n!}} \quad \text{and} \quad \mathrm{y} \equiv \sqrt{\frac{m\omega}{\hbar}}x$$

Which has Eigen Energy solutions of,

$$\mathrm{E_n} = \left(n + \frac{1}{2}\right)\hbar\varpi \quad \text{for} \quad \mathrm{n} = 0, 1, 2, 3 \ldots$$

The functions, $h_n(y)$ are Hermite polynomials defined by,

$$h_0(y) = 1$$

$$h_1(y) = 2y$$

$$h_2(y) = 4y^2 - 2$$

And the recursion relation,

$$h_{n+1}(y) = 2yh_n(y) - \frac{d}{dy}h_n(y) \quad \text{for } \mathrm{n} \geq 2$$

Harmonic Oscillator Operator Solution

Let us define two operators* as,

$$a^{-} = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)$$

which for reasons that will become obvious, we will call the annihilation or lowering operator and,

$$a^{+} = \frac{1}{\sqrt{2}}\left(y - \frac{d}{dy}\right)$$

which we will call the creation or raising operator.

Consider the product of these two operators:

$$a^{-}a^{+} = \frac{1}{2}\left(y + \frac{d}{dy}\right)\left(y - \frac{d}{dy}\right)$$

$$a^{-}a^{+} = \frac{1}{2}\left(y^{2} - \frac{d^{2}}{dy^{2}} - y\frac{d}{dy} + \frac{d}{dy}y\right)$$

$$a^{-}a^{+} = \frac{1}{2}y^{2} - \frac{1}{2}\frac{d^{2}}{dy^{2}} - \frac{1}{2}y\frac{d}{dy} + \left[\frac{1}{2}\frac{d}{dy}y\right]$$

Lets focus on this expression for a moment.

***Note: a^{+} and a^{-} are NOT Hermitian!**

Harmonic Oscillator Operator Solution

Cont'd:

$$a^-a^+ = \frac{1}{2}y^2 - \frac{1}{2}\frac{d^2}{dy^2} - \frac{1}{2}y\frac{d}{dy} + \left[\frac{1}{2}\frac{d}{dy}y\right]$$

Using the fact that $\frac{\mathrm{d}}{\mathrm{dy}}\left(ya(y)\right) = a(y)\frac{\mathrm{dy}}{\mathrm{dy}} + y\frac{\mathrm{d}}{\mathrm{dy}}\left(a(y)\right) = \left(1 + y\frac{\mathrm{d}}{\mathrm{dy}}\right)a(y)$

$$a^-a^+ = \frac{1}{2}y^2 - \frac{1}{2}\frac{d^2}{dy^2} - \frac{1}{2}y\frac{d}{dy} + \left[\frac{1}{2} + \frac{1}{2}y\frac{d}{dy}\right]$$

$$a^-a^+ = \frac{1}{2}y^2 - \frac{1}{2}\frac{d^2}{dy^2} + \frac{1}{2}$$

Let H' be defined as,

$\mathrm{H'} = \frac{1}{2}y^2 - \frac{1}{2}\frac{d^2}{dy^2}$ such that,

$\boxed{a^-a^+ = \mathrm{H'} + \frac{1}{2}}$ and since it can be shown that the commutation,

$a^-a^+ - a^+a^- = 1$ then,

$\boxed{a^+a^- = \mathrm{H'} - \frac{1}{2}}$ (alternatively the same approach could be taken to directly evaluate a^+a^-

Harmonic Oscillator Operator Solution

What we seek to do now is to eliminate the non-physical variable, y, and cast these results in terms of our physical variables x, ω, m, and momentum p.

$$y = \sqrt{\frac{m\varpi}{\hbar}}x \quad \text{and} \quad \frac{d}{dy} = \sqrt{\frac{\hbar}{m\varpi}}\frac{d}{dx}$$

Thus,

$$a^{-} = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)$$

$$a^{-} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\varpi}{\hbar}}x + \sqrt{\frac{\hbar}{m\varpi}}\frac{d}{dx}\right)$$

or using the fact that $p_x = \frac{\hbar}{i}\frac{d}{dx}$

$$a^{-} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\varpi}{\hbar}}x + \sqrt{\frac{\hbar}{m\varpi}}\frac{ip_x}{\hbar}\right)$$

$$a^{-} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\varpi}{\hbar}}x + i\sqrt{\frac{1}{m\hbar\varpi}}p_x\right)$$

Similarly,

$$a^{+} = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\varpi}{\hbar}}x - i\sqrt{\frac{1}{m\hbar\varpi}}p_x\right)$$

Harmonic Oscillator Operator Solution

Cont'd:

$$a^{-}=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\varpi}{\hbar}}x+i\sqrt{\frac{1}{m\hbar\varpi}}p_x\right)\quad \text{and,}\quad a^{+}=\frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\varpi}{\hbar}}x-i\sqrt{\frac{1}{m\hbar\varpi}}p_x\right)$$

$$a^{-}a^{+}=\frac{m\varpi}{2\hbar}x^2+\frac{1}{2m\hbar\varpi}p_x^2+i\sqrt{\frac{m\varpi}{\hbar}}\sqrt{\frac{1}{m\hbar\varpi}}p_x x - i\sqrt{\frac{m\varpi}{\hbar}}\sqrt{\frac{1}{m\hbar\varpi}}x p_x$$

$$a^{-}a^{+}=\frac{m\varpi}{2\hbar}x^2+\frac{1}{2m\hbar\varpi}p_x^2+\frac{i}{2\hbar}\left(p_x x - x p_x\right)$$

$$a^{-}a^{+}=\frac{1}{\hbar\varpi}\left(\frac{p_x^2}{2m}+\frac{1}{2}m\varpi^2x^2\right)+\frac{i}{2\hbar}\left[p_x, x\right]$$

$$\left[p_x, x\right]=\frac{\hbar}{i}$$

$$U(x)=\frac{1}{2}m\varpi^2x^2$$

$$H=\left(\frac{p_x^2}{2m}+U(x)\right)$$

Thus, $\quad a^{-}a^{+}=\dfrac{H}{\hbar\varpi}+\dfrac{1}{2}$

Harmonic Oscillator Operator Solution

Cont'd:

Comparing, $a^-a^+ = \frac{H}{\hbar\varpi} + \frac{1}{2}$ and $H' = a^-a^+ - \frac{1}{2}$ one sees,

$H' = \frac{H}{\hbar\varpi}$ which we called the normalized Hamiltonian (i.e. unitless)

Thus, solving for H and inserting in the Schrodinger equation,

$$\left(a^-a^+ - \frac{1}{2}\right)\hbar\varpi = H \quad \Rightarrow \quad \left(a^-a^+ - \frac{1}{2}\right)\hbar\varpi\Psi(x) = E\Psi(x)$$

or

$$\left(a^-a^+ - \frac{1}{2}\right)\Psi(x) = \frac{E}{\hbar\varpi}\Psi(x)$$

But since the commutator, $a^-a^+ - a^+a^- = 1$,

$$a^-a^+ = a^+a^- + 1$$

$$\left(a^-a^+ - \frac{1}{2}\right) = \left(a^+a^- + \frac{1}{2}\right)$$

We arrive at two new forms of the Schrodinger Equation :

$$\left(a^-a^+ - \frac{1}{2}\right)\Psi(x) = \frac{E}{\hbar\varpi}\Psi(x) \quad \text{and} \quad \left(a^+a^- + \frac{1}{2}\right)\Psi(x) = \frac{E}{\hbar\varpi}\Psi(x)$$

Using the new form of the Schrodinger Equation: Harmonic Oscillator Operator Solution

Cont'd:

The new forms of the Schrodinger Equation :

$$\left(a^{-}a^{+}-\frac{1}{2}\right)\Psi(x)=\frac{E}{\hbar\varpi}\Psi(x) \quad \text{and} \quad \left(a^{+}a^{-}+\frac{1}{2}\right)\Psi(x)=\frac{E}{\hbar\varpi}\Psi(x)$$

Acting on the Schrodinger Equation with the creation operator,

$$a^{+}\left(a^{-}a^{+}-\frac{1}{2}\right)\Psi(x)=a^{+}\frac{E}{\hbar\varpi}\Psi(x)$$

$$\left(a^{+}a^{-}-\frac{1}{2}\right)a^{+}\Psi(x)=\frac{E}{\hbar\varpi}a^{+}\Psi(x)$$

Adding $a^{+}\Psi(x)$ to both sides,

$$\left(a^{+}a^{-}+\frac{1}{2}\right)a^{+}\Psi(x)=\frac{(E+\hbar\varpi)}{\hbar\varpi}a^{+}\Psi(x)$$

Thus, if "Ψ" is an eigenfunction of $(a^{+}a^{-}+1/2)$ with energy eigenvalue, E/ħω, then so is "$a^{+}\Psi$" but with an energy eigenvalue of (E+ħω)/ħω. Thus, the raising/creation operator , a^{+}, raised the energy of the state by exactly one quantum, ħω.

Similarly, the lowering/annihilation operator, a^{-}, lowers the energy of a state by one quantum, ħω. (This is easily proved by the same procedures using a^{-} instead of a^{+} - see Brennan, page 117).

Using the new form of the Schrodinger Equation: Harmonic Oscillator Operator Solution

Cont'd:

Since the energy of the Harmonic Oscillator is never less than zero, some "ground state" Ψ_0 must exist for which lowering the energy with the lowering operator, a^-, must give zero energy.

$$\left(a^-a^+ - \frac{1}{2}\right)a^-\Psi_0(x) = \frac{(E_0 - \hbar\varpi)}{\hbar\varpi}a^-\Psi_0(x)$$

If $a^-\Psi_0(x) \neq$ Null State (0) then E_0 is not the lowest (ground state). Thus,

$a^-\Psi_0(x) = 0$ and,

$$\left(a^+a^- + \frac{1}{2}\right)\Psi_0(x) = \frac{E_0}{\hbar\varpi}\Psi_0(x)$$

$$\left(a^+\{a^-\Psi_0(x)\} + \frac{1}{2}\Psi_0(x)\right) = \frac{E_0}{\hbar\varpi}\Psi_0(x)$$

$$\left(a^+\{0\} + \frac{1}{2}\Psi_0(x)\right) = \frac{E_0}{\hbar\varpi}\Psi_0(x)$$

$$\frac{1}{2}\Psi_0(x) = \frac{E_0}{\hbar\varpi}\Psi_0(x)$$

$$E_0 = \frac{\hbar\varpi}{2}$$

Using the new form of the Schrodinger Equation: Harmonic Oscillator Operator Solution

Cont'd:

To arrive at all the other higher energy states, we simply apply the raising operator and require normalization. Thus,

$\Psi_n(x) = C_n\left(a^+\right)^n \Psi_0(x)$ Where C_n is the normalization coefficient (previously defined)

Similarly, the energy of the higher states is merely $n\hbar\varpi$ larger than the ground state energy

$$E_n = n\hbar\varpi + E_0 = \left(\frac{1}{2} + n\right)\hbar\varpi$$

But what is Ψ_0?

$$a^-\Psi_0(x) = 0$$

$$a^- = \frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)$$

$$\frac{1}{\sqrt{2}}\left(y + \frac{d}{dy}\right)\Psi_0(x) = 0$$

$$\frac{d\Psi_0(x)}{dy} = -y\Psi_0(x)$$

$$\Psi_0(x) = Ae^{-\left(\frac{y^2}{2}\right)}$$

Using the new form of the Schrodinger Equation: Harmonic Oscillator Operator Solution

Cont'd:

Finding the successive excited states is merely just applying the raising operator. For example the first excited state is:

$$\Psi_1(x) = a^+ \Psi_0(x)$$

$$\Psi_1(x) = a^+ \mathrm{A}_0 \mathrm{e}^{-\left(\frac{\mathrm{y}^2}{2}\right)}$$

$$\Psi_1(x) = \frac{1}{\sqrt{2}}\left(\mathrm{y} - \frac{\mathrm{d}}{\mathrm{dy}}\right)\mathrm{A}_0 \mathrm{e}^{-\left(\frac{\mathrm{y}^2}{2}\right)}$$

$$\Psi_1(x) = \frac{2}{\sqrt{2}} \mathrm{A}_0 \mathrm{y}\mathrm{e}^{-\left(\frac{\mathrm{y}^2}{2}\right)}$$

$$\Psi_1(x) = \mathrm{A}_1 \mathrm{y}\mathrm{e}^{-\left(\frac{\mathrm{y}^2}{2}\right)}$$

Other examples left as homework problems.