

## Problem 2.

**Problem 2**

A voltage is applied externally across an infinite quantum well. We wish to apply the variational technique to compute the approximate ground state energy of a particle in this well.

The one-dimensional time-independent Schrodinger equation inside the well is given in normalized units by:

$$\epsilon \varphi(x) = -\frac{d^2}{dx^2} \varphi(x) + x v_0 \varphi(x)$$

subject to the boundary conditions  $\varphi(x=0) = \varphi(x=1) = 0$ . Using the variational function

$$\varphi_t(x) = C \sin(\pi x) \exp(-\alpha x)$$

Compute for  $v_0 = 100$  :

- a) [2 pts]  $C =$
- b) [2 pts]  $\left\langle \varphi_t \left| -\frac{d^2}{dx^2} \right| \varphi_t \right\rangle =$
- c) [2 pts]  $\langle \varphi_t | x | \varphi_t \rangle =$
- d) [3 pts]  $\frac{\partial E_t}{\partial \alpha} = 0$  for  $\alpha =$
- e) [3 pts]  $E_{\text{grd}} \approx$

So this problem is just the variational technique. The way he's writing this problem makes you believe that you need the linear variational technique (finite basis) but you can't use that method with a single finite basis state.

Anyway, this problem should be the same (just a lot uglier) than chapter 4 - Problem 2-4

- Avocado and Mochi♥

### Part A.

Part A is the normalization constant of the wave equation.

```
In[288]:= Clear["Global`*"]
vo = 100;
Element[α, Reals]; (* Assume that alpha is real for this part...
the normalization constant is just less ugly this way*)
φ[x_] = Sin[Pi * x] * Exp[-α * x];
c = 
$$\frac{1}{\sqrt{\text{Integrate}[\phi[x] * \phi[x], \{x, 0, 1\}]}}$$

```

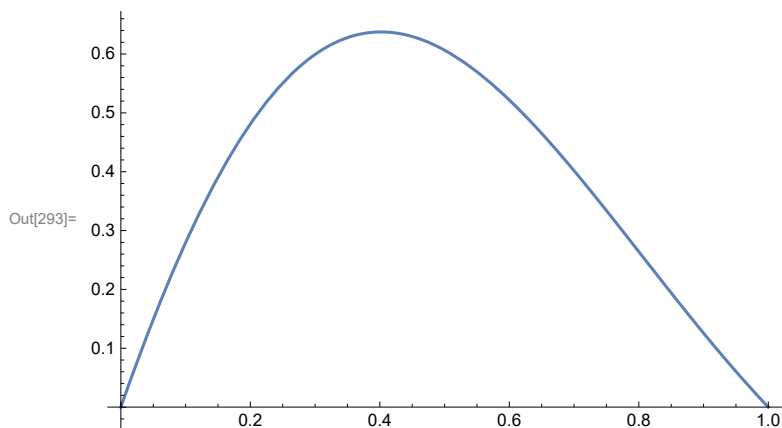
```
Out[292]= 
$$\frac{1}{\pi \sqrt{\frac{e^{-\alpha} \text{Sinh}[\alpha]}{2 \pi^2 \alpha + 2 \alpha^3}}}$$

```

I don't really trust my solution for this because it's so ugly, but the math is working out. Maybe it's just like that ... I don't judge :)

This next part is just to see the trial wave equation in the range. You can go ahead and disregard it if you're not interested.

```
In[293]:= Plot[Sin[Pi * x] * Exp[-x], {x, 0, 1}]
```



This is a good trial wave equation to estimate the ground state energy within the given range. The trial wave equation has no nodes (i.e. no zeros) within the range [0,1]. Then by the Strum's Theorem, this wave equation will be okay for estimating ground state energy. Strum's theorem is also known as Node Theorem (MIT open course ware) or Interlacing Theorem (Professor Mannasah).

## Part B.

Now we can begin using the Variational technique. The next four parts is the variational technique broken into steps. I guess this is his way of providing partial credit.

```
In[294]:= nφ[x_] = c * Sin[Pi * x] * Exp[-α * x];
(* normalized wave equation *)
```

Part B is basically the kinetic energy given by the Hamiltonian.

Anyway to solve this part, you have to know that:

$$\left\langle \psi \left| \frac{-d}{dx^2} \right| \psi \right\rangle = \int \psi^* \frac{-d}{dx^2} \psi dx$$

Make sure to integrate in the given range. If no range is given, it's from  $-\infty$  to  $\infty$ .

```
In[295]:= kineticEnergy = Integrate[nφ[x] * (-1 * D[nφ[x], {x, 2}]), {x, 0, 1}]
```

```
Out[295]= π² + α²
```

## Part C.

Alright so this part, is part of the potential energy given from the Hamiltonian. I guess we're going to kind of ignore  $V_0$  for now. I think the professor is trying to check that you're paying attention (at the end). If you're not paying attention, you'll end up forgetting  $V_0$  in your final answer. So be careful of that later.

The equation to solve this part is:

$$\left\langle \psi \left| x \right| \psi \right\rangle = \int \psi^* x \psi dx$$

Integrated within the given range ([0,1] in our case). If no range is given, it will be integrated from  $-\infty$  to  $\infty$ .

```
In[296]:=
```

```
partC = Integrate[nφ[x] * x * nφ[x], {x, 0, 1}]
potentialEnergy = Integrate[nφ[x] * v0 * x * nφ[x], {x, 0, 1}];
```

```
Out[296]= 1/2 (1 + 1/α + 2α/(π² + α²) - Coth[α])
```

## Part D.

Alright, so now that we have the kinetic energy and potential energy. We know that the energy as a function of  $\alpha$  is the linear combination of those two. From General Physics 1 we know that Energy = Kinetic Energy + Potential Energy

Basically we're going to follow the law of conservation of energy. Except all these energies are a function of  $\alpha$ .

```
In[298]:= energy = kineticEnergy + potentialEnergy
```

```
Out[298]= π² + α² + 50 (1 + 1/α + 2α/(π² + α²) - Coth[α])
```

Now we know from Calculus I, to find the maxima or minima (extrema) of a function, we have to take the derivative of the function. Then find when this derivative is equal to 0.

Basically this is a turning point of a given function - this turning point is a local extrema.

In[299]:= **denenergy** = **D**[**energy**, { $\alpha$ , 1}]

Out[299]= 
$$2\alpha + 50 \left( -\frac{1}{\alpha^2} - \frac{4\alpha^2}{(\pi^2 + \alpha^2)^2} + \frac{2}{\pi^2 + \alpha^2} + \text{Csch}[\alpha]^2 \right)$$

In[300]:= **Solve**[**denenergy** == 0,  $\alpha$ ]

 **Solve:** This system cannot be solved with the methods available to Solve.

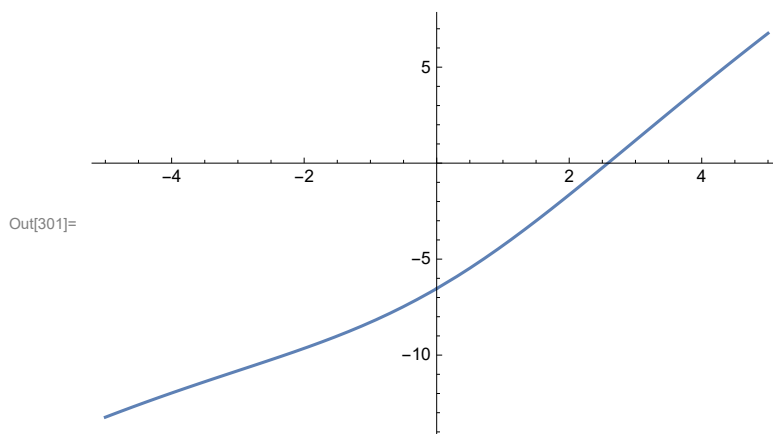
Out[300]= **Solve**  $\left[ 2\alpha + 50 \left( -\frac{1}{\alpha^2} - \frac{4\alpha^2}{(\pi^2 + \alpha^2)^2} + \frac{2}{\pi^2 + \alpha^2} + \text{Csch}[\alpha]^2 \right) = 0, \alpha \right]$

**Alright it looks like Mathematica can solve this problem!**

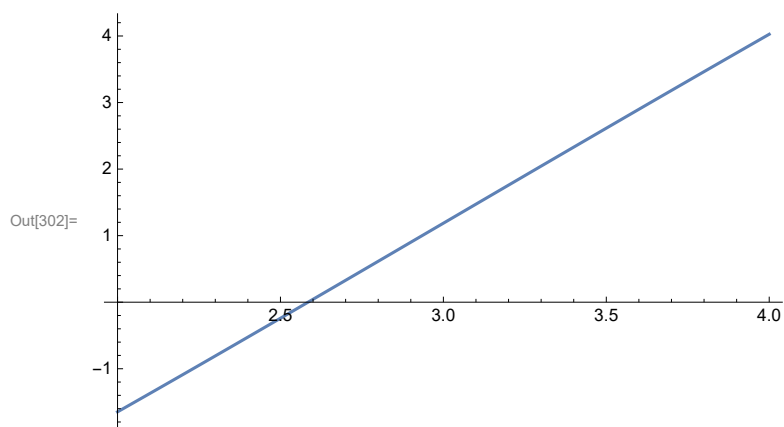
**Oh no! I guess it's time to give up!**

Nah, it's not. We just have to think outside the box a little. We're engineers right ? :)

In[301]:= **Plot**[**denenergy** == 0, { $\alpha$ , -5, 5}]



In[302]:= **Plot**[denenergy == 0, { $\alpha$ , 2, 4}]



Would you look at that!

Now we can use FindRoot to find our zero instead :)

In[303]:= **FindRoot**[denenergy == 0, { $\alpha$ , 2.6}]

Out[303]= { $\alpha \rightarrow 2.5847$ }

There we go, an  $\alpha$  value!

In[306]:=  $\alpha = 2.5847027304579955$ ;  
groundStateEnergy = energy

Out[307]= 50.9401