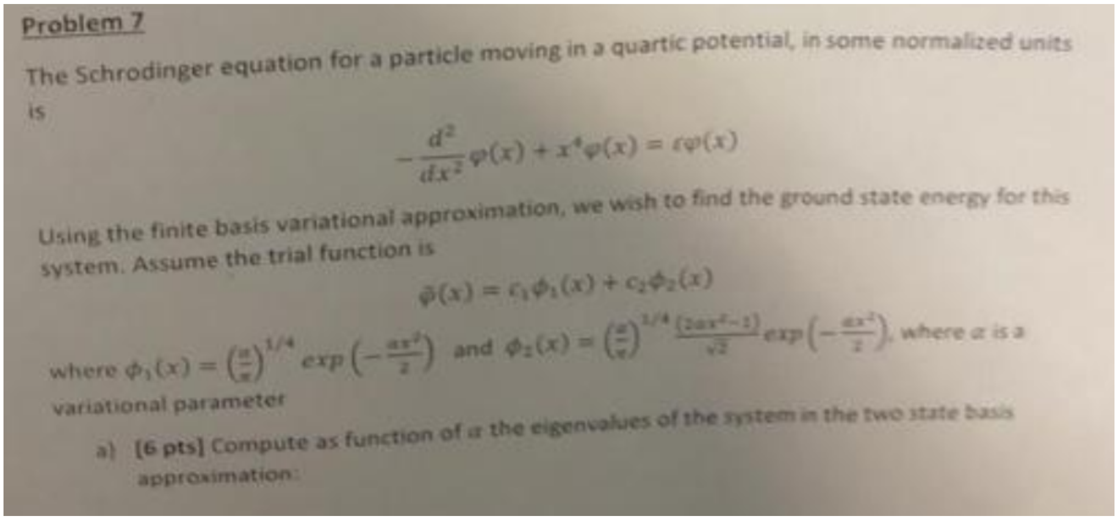
Problem 7



Problem 7

The Schrodinger equation for a particle moving in a quartic potential, in some normalized units is

$$-\frac{d^2}{dx^2}\varphi(x) + x^4\varphi(x) = \varepsilon\varphi(x)$$

Using the finite basis variational approximation, we wish to find the ground state energy for this system. Assume the trial function is

$$\tilde{\varphi}(x) = c_1\phi_1(x) + c_2\phi_2(x)$$

where $\phi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} exp\left(-\frac{\alpha x^2}{2}\right)$ and $\phi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4}\frac{(2\alpha x^2-1)}{\sqrt{2}} exp\left(-\frac{\alpha x^2}{2}\right)$, where α is a variational parameter

a) **[6 pts]** Compute as function of α the eigenvalues of the system in the two state basis approximation.

Alright so this one is the linear variational technique. In class, and in Professor Manassah's lectures, this method is also known as finite basis approximation (two-state, in this case).

Wait...this is literally Chapter 4 - Problem 6.
Hopefully you'll get this, but we'll just solve it and hopefully we all have the same answer!

Avocado and Mochi

Part A.

Compute as a function of α, the eigenvalues of the system in the two state basis approximation.

In[723]:=
```
Clear["Global`*"]
ϕ1[x_] = (α/Pi)^(1/4) * Exp[-(α * x^2)/2];
ϕ2[x_] = (α/Pi)^(1/4) * (2 * α * x^2 - 1)/Sqrt[2] * Exp[-(α * x^2)/2];
```

we know the Hamiltonian from the Schrodinger Equation

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Schrodinger's Equation (in some normalized units):

$$-\frac{d^2}{dx^2}\phi(x) + x^4\phi(x) = \epsilon\phi(x)$$

is:

Hamiltonian (in some normalized units):

$$H = -\frac{d^2}{dx^2} + x^4$$

Since we'll be using the finite basis approximation, we can build the matrix as such:

$$H = \begin{bmatrix} H_{11} - En & H_{12} \\ H_{21} & H_{22} - En \end{bmatrix}$$

Where we define

$$H_{nm} = \langle \phi_n | H | \phi_m \rangle \quad where\ H\ is\ the\ Hamiltonian$$

Performing this for n = 1, m = 1

In[726]:=
```
kineticEnergy11 = Integrate[ϕ1[x] * -1 * D[ϕ1[x], {x, 2}],
   {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];
potentialEnergy11 = Integrate[ϕ1[x] * x^4 * ϕ1[x],
   {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];

H11 = kineticEnergy11 + potentialEnergy11;
```

n = 1, m = 2

In[729]:=
```
kineticEnergy12 = Integrate[ϕ1[x] * -1 * D[ϕ2[x], {x, 2}],
   {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];
potentialEnergy12 = Integrate[ϕ1[x] * x^4 * ϕ2[x],
   {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];

H12 = kineticEnergy12 + potentialEnergy12;
```

n = 2, m = 1

In[732]:=
```
kineticEnergy21 = Integrate[ϕ2[x] * -1 * D[ϕ1[x], {x, 2}],
   {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];
potentialEnergy21 = Integrate[ϕ2[x] * x^4 * ϕ1[x],
   {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];

H21 = kineticEnergy21 + potentialEnergy21;
```

n = 2, m = 2

In[735]:=
```
kineticEnergy22 = Integrate[ϕ2[x] * -1 * D[ϕ2[x], {x, 2}],
    {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];
potentialEnergy22 = Integrate[ϕ2[x] * x^4 * ϕ2[x],
    {x, -Infinity, Infinity}, Assumptions → Re[α] > 0];

H22 = kineticEnergy22 + potentialEnergy22;
```

In[740]:=
```
det = (H11 - en) * (H22 - en) - (H12) * (H21)
```

Out[740]=
$$\left(-en+\frac{3}{4\,\alpha^2}+\frac{\alpha}{2}\right)\left(-en+\frac{39}{4\,\alpha^2}+\frac{5\,\alpha}{2}\right)-\left(\frac{3}{\sqrt{2}\,\alpha^2}-\frac{\alpha}{\sqrt{2}}\right)^2$$

In[741]:=
```
Solve[det == 0, en]
```

Out[741]=
$$\left\{\left\{en\to\frac{1}{4}\left(\frac{21}{\alpha^2}+6\,\alpha-\frac{2\sqrt{3}\,\sqrt{33+8\,\alpha^3+2\,\alpha^6}}{\alpha^2}\right)\right\},\left\{en\to\frac{1}{4}\left(\frac{21}{\alpha^2}+6\,\alpha+\frac{2\sqrt{3}\,\sqrt{33+8\,\alpha^3+2\,\alpha^6}}{\alpha^2}\right)\right\}\right\}$$

These are the two “lambdas” that the Professor is looking for.

Part B.

We just have to find the lowest one out of these two equations, after solving and plugging in α.

In[746]:=
$$en1 = \frac{1}{4}\left(\frac{21}{\alpha^2}+6*\alpha-\frac{2*\sqrt{3}*\sqrt{33+8*\alpha^3+2*\alpha^6}}{\alpha^2}\right);$$

$$en2 = \frac{1}{4}\left(\frac{21}{\alpha^2}+6*\alpha+\frac{2*\sqrt{3}*\sqrt{33+8*\alpha^3+2*\alpha^6}}{\alpha^2}\right);$$

In[748]:=
```
denergy1 = D[en1, {α, 1}];
denergy2 = D[en2, {α, 1}];
```

In[751]:=
```
Solve[denergy1 == 0, {α}]
```

Out[751]=
$$\left\{\left\{\alpha\to-(-11)^{1/3}\right\},\left\{\alpha\to-(-3)^{1/3}\right\},\left\{\alpha\to3^{1/3}\right\},\left\{\alpha\to(-1)^{2/3}\,3^{1/3}\right\},\right.$$
$$\left\{\alpha\to11^{1/3}\right\},\left\{\alpha\to(-1)^{2/3}\,11^{1/3}\right\},\left\{\alpha\to\left(\frac{1}{2}\left(8-\sqrt{34}\right)\right)^{1/3}\right\},$$
$$\left.\left\{\alpha\to(-1)^{2/3}\left(\frac{1}{2}\left(8-\sqrt{34}\right)\right)^{1/3}\right\},\left\{\alpha\to-\left(\frac{1}{2}\left(-8+\sqrt{34}\right)\right)^{1/3}\right\}\right\}$$

These are the roots corresponding to the first energy equation. Now we just have to use the real parts, and see what the energy is at that point.

In[764]:=
```
α = 3^(1/3);
N[en1]
α = 11^(1/3);
N[en1]
α = (1/2 (8 - √34))^(1/3);
N[en1]
```

Out[765]= 1.08169

Out[767]= 1.06145

Out[769]= 1.07084

so far, our winner is $\alpha = 11^{1/3}$ but before we decide, we have to repeat the process for the second energy equation.

In[771]:=
```
Clear[α]
Solve[denergy2 == 0, {α}]
```

Out[772]= $\left\{\left\{\alpha \to -\left(\frac{1}{2}\left(-8-\sqrt{34}\right)\right)^{1/3}\right\}, \left\{\alpha \to \left(\frac{1}{2}\left(8+\sqrt{34}\right)\right)^{1/3}\right\}, \left\{\alpha \to (-1)^{2/3}\left(\frac{1}{2}\left(8+\sqrt{34}\right)\right)^{1/3}\right\}\right\}$

In[775]:=
```
α = (1/2 (8 + √34))^(1/3);
N[en2]
```

Out[776]= 7.54028

our winner is definitely $\alpha = 11^{1/3}$, so our corresponding lowest energy value is :

$$en_{min} = \lambda_{min} = 1.06145$$

In some normalized units.