Software Packages in Physics
Mid-term Exam: Model Solutions and Marks
2nd semester 2004-2005
9-May-2005

■ ***Each problem below was marked out of 10.***

Name:

Problem 1: The Hydrogen Ion

■ Statement of the problem

Using the variational principle, find the ground-state energy for a hydrogen ion H_2^+ made up of two protons and a single electron, then comment on your result.

■ Physics of the problem

The use of the variational principle in quantum mechanics is based on a theorem that states that using a guessed (trial wavefunction) for a system whose actual wavefunction is unknown, we can say that:

$$E_g \leq \langle \psi \mid H \mid \psi \rangle \equiv \langle H \rangle$$

Based on the LCAO (Linear Combination of Atomic Orbitals) technique, a suitable trial wavefunction for the hydrogen ion is a linear combination of the ground states of the two protons:

$$\psi = A[\psi_g(r_1) + \psi_g(r_2)]$$

To solve the problem, we first normalize this wavefunction, by solving the following equation for A:

$$1 = \int |\psi|^2 \, d^3\mathbf{r}$$

where, $\mathbf{r}_1$ and $\mathbf{r}_2$ are the vectors separating the electron from the two protons, such that R is the distance between the two protons. We substitute the resulting value of A into our original function, and then calculate the expectation value of the Hamiltonian of the system:

$$\langle H \rangle = \left\langle \psi \left| -\frac{\hbar^2}{2\,m}\,\nabla^2 - \frac{e^2}{4\,\pi\,\epsilon_0}\left(\frac{1}{r_1} + \frac{1}{r_2}\right) \right| \psi \right\rangle$$

After calculating the relevant integrals, we end up with an expression for the total energy of the system as a function of R. In units of $-E_1$, and expressed as a function of $x \equiv R/a$ (where a is Bohr's radius), the total energy function $F(x)$ reads:

$$F(x) = -1 + \frac{2}{x}\left\{\frac{(1-(2/3)\,x^2)\,e^{-x} + (1+x)\,e^{-2\,x}}{1 + (1 + x + (1/3)\,x^2)\,e^{-x}}\right\}$$

E_1 mentioned above is the ground-state energy for the hydrogen atom:

$$E_1 = -\frac{e^2}{4\,\pi\,\epsilon_0}\,\frac{1}{2\,a}$$

■ Proposed steps for solution

1. Define the function $F(x)$ as a *Mathematica* function.
2. Plot that function in the range $x \in [0.5, 7]$.
3. Differentiate $F(x)$ with respect to x, and find the zero of the derivative using **`FindRoot[]`**.
4. Substitute the zero of $F'(x)$ back into $F(x)$ and transform the answer to become in units of electron-volt. (To do this last step, you might find the values of constants in the packages **`` Miscellaneous`PhysicalConstants` ``** to be useful.
5. Comment on the physical significance of the value of x that minimizes the energy function $F(x)$, and the value of energy (in eV) you get by minimization.

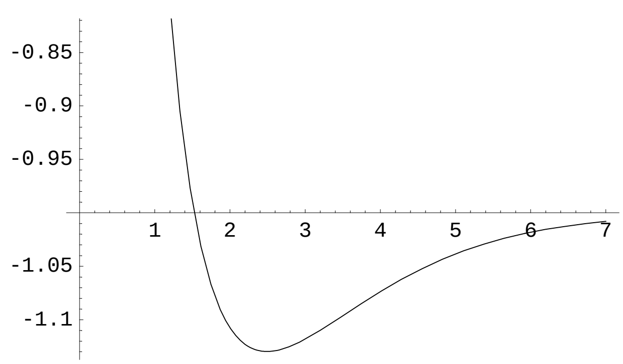
■ Your solution of problem 1:

```
(*Here' s a definition of F (x):*)
```

$$\texttt{F[x\_] := } -1 + \frac{2}{x}\,\frac{(1-(2/3)\,x^2)\,e^{-x} + (1+x)\,e^{-2\,x}}{1 + (1 + x + (1/3)\,x^2)\,e^{-x}}$$

```
(*Now its plot in the designated range:*)

Plot[F[x], {x, 0.5, 7}];
```



```
(*The derivative of F[x] with respect to x:*)

d = D[F[x], x]
```

$$-\left(2\left(e^{-2x}(1+x)+e^{-x}\left(1-\frac{2x^2}{3}\right)\right)\left(e^{-x}\left(1+\frac{2x}{3}\right)-e^{-x}\left(1+x+\frac{x^2}{3}\right)\right)\right)\Big/\left(x\left(1+e^{-x}\left(1+x+\frac{x^2}{3}\right)\right)^2\right)+$$
$$\frac{2\left(e^{-2x}-\frac{4e^{-x}x}{3}-2e^{-2x}(1+x)-e^{-x}\left(1-\frac{2x^2}{3}\right)\right)}{x\left(1+e^{-x}\left(1+x+\frac{x^2}{3}\right)\right)}-\frac{2\left(e^{-2x}(1+x)+e^{-x}\left(1-\frac{2x^2}{3}\right)\right)}{x^2\left(1+e^{-x}\left(1+x+\frac{x^2}{3}\right)\right)}$$

```
(*From the plot,
 one can see that the root resulting in minimum energy is somewhere near x=2.5,
 therefore:*)

e = FindRoot[d == 0, {x, 2.5}]

{x → 2.49283}

(*The value of the function F[x] at this root is:*)

f = F[x] /. e

-1.12966

(*We now call the package PhysicalConstants to calculate the value of the ground-
  state energy of a hydrogen atom E1 in electron volts:*)

<< Miscellaneous`PhysicalConstants`
```

$$E1 = -\frac{\text{ElectronCharge}^2}{4\pi\,\text{VacuumPermittivity}}\;\frac{1}{2\,\text{BohrRadius}}\;\text{//.}\;\left\{\text{Ampere}\to\frac{\text{Coulomb}}{\text{Second}},\ \text{Coulomb}\to\text{Joule}/\text{Volt},\ \text{Joule}\to\frac{\text{Coulomb}}{\text{ElectronCharge}}\,\text{eV}\right\}$$

```
-13.6057 eV

(*And finally, we transform our answer into electron volts:*)

f * (-E1)

-15.3698 eV
```

Problem 2: The Function `Divisors[]`

■ Statement of the problem

Build a *Mathematica* function in the style of procedural programming, that calculates the divisors of an integer, and outputs them as a list in ascending order (from lowest to highest).
Then use that function to calculate the divisors of 3628800. Use an appropriate *Mathematica* built-in function to count how many numbers your resulting list has.

Mathematica already has a built-in function that calculates divisors, it is called **`Divisors[]`**. Here's how it is used to find the divisors of 120:

```
Divisors[120]
```

```
{1, 2, 3, 4, 5, 6, 8, 10, 12, 15, 20, 24, 30, 40, 60, 120}
```

Your function should be able to do the same.

■ Proposed steps for solution

Let *m* be the integer whose divisors we are looking for. The basic idea then is to form a loop that will check every number $n \in [1, m]$; if *n* divides *m* then it is included in our list, if not, then it is discarded.

A useful function that checks if a number *n* divides another *m* is **`Mod[]`**, which calculates the remainder of dividing *m* by *n*. If *n* divides *m*, then clearly the answer of **`M[m,n]`** is zero. If *n* does not divide *m* then the answer is the remainder of the division:

```
Mod[4, 2]
```

```
0
```

```
Mod[4, 3]
```

```
1
```

If in a given loop, *n* divides *m*, then *n* needs to be appended to an accumulator (the list which will eventually be given as output). You can use **`Append[]`** or **`AppendTo[]`** for that purpose.

Your accumulator needs to be initialized in order to be usable, here's how to do it:

```
y = {}
```

Notice the following snippet:

```
y = {1, 2}; AppendTo[y, 3]; y
```

```
{1, 2, 3}
```

It is a good idea to do all this within a **`Module[]`**.

■ Your solution of problem 2:

```
OurDivisors[x_] := Module[{y = {}, i}, Do[If[Mod[x, i] == 0, AppendTo[y, i]], {i, x}]; y]
```

```
OurDivisors[3628800]
Length[%]
```

```
{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 12, 14, 15, 16, 18, 20, 21, 24, 25, 27, 28, 30, 32, 35,
 36, 40, 42, 45, 48, 50, 54, 56, 60, 63, 64, 70, 72, 75, 80, 81, 84, 90, 96, 100, 105,
 108, 112, 120, 126, 128, 135, 140, 144, 150, 160, 162, 168, 175, 180, 189, 192, 200,
 210, 216, 224, 225, 240, 252, 256, 270, 280, 288, 300, 315, 320, 324, 336, 350, 360,
 378, 384, 400, 405, 420, 432, 448, 450, 480, 504, 525, 540, 560, 567, 576, 600,
 630, 640, 648, 672, 675, 700, 720, 756, 768, 800, 810, 840, 864, 896, 900, 945,
 960, 1008, 1050, 1080, 1120, 1134, 1152, 1200, 1260, 1280, 1296, 1344, 1350, 1400,
 1440, 1512, 1575, 1600, 1620, 1680, 1728, 1792, 1800, 1890, 1920, 2016, 2025, 2100,
 2160, 2240, 2268, 2304, 2400, 2520, 2592, 2688, 2700, 2800, 2835, 2880, 3024, 3150,
 3200, 3240, 3360, 3456, 3600, 3780, 3840, 4032, 4050, 4200, 4320, 4480, 4536, 4725,
 4800, 5040, 5184, 5376, 5400, 5600, 5670, 5760, 6048, 6300, 6400, 6480, 6720, 6912,
 7200, 7560, 8064, 8100, 8400, 8640, 8960, 9072, 9450, 9600, 10080, 10368, 10800,
 11200, 11340, 11520, 12096, 12600, 12960, 13440, 14175, 14400, 15120, 16128, 16200,
 16800, 17280, 18144, 18900, 19200, 20160, 20736, 21600, 22400, 22680, 24192,
 25200, 25920, 26880, 28350, 28800, 30240, 32400, 33600, 34560, 36288, 37800,
 40320, 43200, 44800, 45360, 48384, 50400, 51840, 56700, 57600, 60480, 64800,
 67200, 72576, 75600, 80640, 86400, 90720, 100800, 103680, 113400, 120960, 129600,
 134400, 145152, 151200, 172800, 181440, 201600, 226800, 241920, 259200, 302400,
 362880, 403200, 453600, 518400, 604800, 725760, 907200, 1209600, 1814400, 3628800}
```

```
270
```

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Problem 1: Calculating The Ground-State Energy For The Harmonic Oscillator Using The Variational Principle

■ Statement of the problem

Using the variational principle, find the ground-state energy for the one-dimensional harmonic oscillator using the trial wavefunction $\psi(x; b) = A\, e^{-b\, x^4}$, where A is the normalization constant, and b is an adjustable parameter. Then comment on your result.

■ Physics of the problem

The use of the variational principle in quantum mechanics is based on a theorem that states that using a guessed (trial wavefunction) for a system whose actual wavefunction is unknown, we can say that:

$$E_g \leq \langle \psi \mid H \mid \psi \rangle \equiv \langle H \rangle$$

We are given a trial wavefunction to use:

$$\psi = A\, e^{-b\, x^4}$$

To solve the problem, we first normalize this wavefunction, by solving the following equation for A:

$$1 = \int |\, \psi\, |^2\, d^3\, \mathbf{r}$$

Then, we find the expectation value of the Hamiltonian. For the problem at hand, the Hamiltonian operator is:

$$\hat{H} = -\frac{\hbar^2}{2\, m} \frac{d^2}{dx^2} + \frac{1}{2}\, m\, \omega^2\, \hat{x}^2$$

and its expectation value is then:

$$\langle \hat{H} \rangle = \left\langle \psi \left| -\frac{\hbar^2}{2\,m} \frac{d^2}{dx^2} + \frac{1}{2}\, m\, \omega^2\, \hat{x}^2 \right| \psi \right\rangle$$

The result of calculating this expectation value is a function of *b*. According to the theorem we mentioned at the start, to get an estimate of the ground-state energy, we should minimize the resulting function with respect to *b*.

▪ Proposed steps for solution

1. Calculate the normalization integral using **`Integrate[]`** (along with appropriate **`Assumptions`**), and set it to 1, then use **`Solve[]`** on the resulting equation to find *A*.
2. Construct the normalized wavefunction as function of *b*.
3. Find the expectation value of the Hamiltonian $E(b) = \int \psi^*(x;\, b)\, \hat{H}\, \psi(x;\, b)\, dx$. The result should be a function of *b*.
4. Minimize $E(b)$ with respect to *b*. You can do that by differentiating $E(b)$, then setting the result to zero, and solving the resulting equation with the help of **`Solve[]`**, then substituting that value back in the expression for $E(b)$.
5. The resulting expression may appear complicated; to simplify it you can apply one (or all) of the following functions on it:

    `Simplify[]`, **`FullSimplify[]`**, **`PowerExpand[]`**, and **`N[]`**.

▪ Your solution of problem 1:

```
(*We start with the normalization integral:*)

normalization = Integrate[(A ⅇ^(-b x^4))^2, {x, -∞, ∞}]

A^2 If[Re[b] > 0, (2^(3/4) Gamma[5/4])/b^(1/4), Integrate[ⅇ^(-2 b x^4), {x, -∞, ∞}, Assumptions → Re[b] ≤ 0]]

(*The assumption Re[b]>0 needs to be added:*)

normalization = Integrate[(A ⅇ^(-b x^4))^2, {x, -∞, ∞}, Assumptions → Re[b] > 0]

(2^(3/4) A^2 Gamma[5/4])/b^(1/4)

(*Therefore, the normalization constant is:*)

norm = Solve[normalization == 1, A]

{{A → -b^(1/8)/(2^(3/8) Sqrt[Gamma[5/4]])}, {A → b^(1/8)/(2^(3/8) Sqrt[Gamma[5/4]])}}

(*And the normalized wavefunction reads:*)

ψ[x_, b_] := A ⅇ^(-b x^4) /. norm[[2]]
```

```
(*Our choice of positive solution was conventional,
 since a wavefunction' s phase will have no effect on our calculations. Moving now
  to the expectation value of the Hamiltonian using our trial wavefunction:*)

Energy[b_] := (-ℏ^2)/(2 m) Integrate[ψ[x, b] D[ψ[x, b], {x, 2}], {x, -∞, ∞}, Assumptions → Re[b] > 0]
  1/2 ω^2 m Integrate[x^2 ψ[x, b]^2, {x, -∞, ∞}, Assumptions → Re[b] > 0]

(*Differentiating, setting to zero, then solving for b,
 we get the value of b that minimizes the expectation value of the Hamiltonian:*)

a = Solve[D[Evaluate[Energy[b]], b] == 0, b]
```

$$\left\{\left\{b \to \frac{m^2\,\omega^2\,\text{Gamma}\left[\frac{3}{4}\right]\,\text{Gamma}\left[\frac{5}{4}\right]}{\hbar^2\,\text{Gamma}\left[\frac{1}{4}\right]\,\left(3\,\text{Gamma}\left[\frac{3}{4}\right]-2\,\text{Gamma}\left[\frac{7}{4}\right]\right)}\right\}\right\}$$

```
PowerExpand[Energy[b] /. a] // N
```

$\{0.585414\,\omega\,\hbar\}$

```
(*As expected, this value is above the true value obtained analytically,
 which is 0.5 ω ℏ. Our value is slightly above the true value,
 because e^(-b x^4) behaves very similar to the true solution e^(-b x^2),
 and therefore, upon minimization, we get a really close answer.*)
```

Problem 2: Taylor Expansions

Statement of the problem

Build a *Mathematica* function that calculates the Taylor expansion of a function $f(x)$ up to order n, *i.e.* returning a polynomial of degree n in the variable x.
Mathematica already offers the function **`Series[]`** to perform this task.
Use your function to find the first 10 terms in the expansion of the function $h(x) = \sin\sqrt{x^2+1}$ around $x = 1$, and check your answer with that of **`Series[]`**.

Review

Recall that the Taylor expansion of a function $f(x)$ about a point $x = x_0$ has the form:

$$f(x) = \sum_{p=0}^{\infty} \frac{f^{(p)}(x_0)}{p!}\,(x - x_0)^p$$

If only terms of degrees not exceeding n are kept, this series is truncated, and the result is:

$$f(x) \simeq \sum_{p=0}^{n} \frac{f^{(p)}(x_0)}{p!}(x - x_0)^p$$

Proposed steps for solution

1. Build a function **`TaylorExpansion[f_,{x_,x0_,n_}]`**, where **`f`** is the **name** of the function.
2. Make the function first test whether $f(x)$ is already a polynomial; if it is, let your function display a message notifying the user that the input funcion is already in polynomial form. You may find the function **`PolynomialQ[]`** useful in doing this.
3. Perform a Taylor expansion on the function. You may find **`Sum[]`** to be useful here.
4. To write the jth derivative of f at $x = x_0$, you can use the function **`Derivative[]`**.

Here is an example of how your function should operate:

```
g[x_] := LegendreP[2, x]
TaylorExpansion[g, {x, x0, 5}]
```

```
g is already a polynomial in x.
```

$$-\frac{1}{2} + \frac{3}{2}(x - x0)^2 + 3(x - x0)\, x0 + \frac{3\, x0^2}{2}$$

And here is another example:

```
g[x_] := Sin[x]
TaylorExpansion[g, {x, 0, 7}]
```

$$x - \frac{x^3}{6} + \frac{x^5}{120} - \frac{x^7}{5040}$$

Your solution of problem 2:

```
TaylorExpansion[f_, {x_, x0_, n_}] :=
 (If[PolynomialQ[f[x], x], Print[f, " is already a polynomial in ", x, "."]];
  Sum[Derivative[i][f][x0]/i! (x - x0)^i, {i, 0, n}])
```

```
h[x_] := Sin[Sqrt[x^2 + 1]]
```

TaylorExpansion[h, {x, 1, 10}]

$$\frac{(-1+x)\,\text{Cos}[\sqrt{2}]}{\sqrt{2}}+\frac{(-1+x)^8\left(-\frac{3059\,\text{Cos}[\sqrt{2}]}{128\sqrt{2}}-\frac{13285\,\text{Sin}[\sqrt{2}]}{128}\right)}{40320}+$$
$$\frac{1}{720}(-1+x)^6\left(-\frac{15\,\text{Cos}[\sqrt{2}]}{32\sqrt{2}}-\frac{169\,\text{Sin}[\sqrt{2}]}{32}\right)+\frac{1}{6}(-1+x)^3\left(-\frac{5\,\text{Cos}[\sqrt{2}]}{4\sqrt{2}}-\frac{3\,\text{Sin}[\sqrt{2}]}{4}\right)+$$
$$\frac{1}{2}(-1+x)^2\left(\frac{\text{Cos}[\sqrt{2}]}{2\sqrt{2}}-\frac{\text{Sin}[\sqrt{2}]}{2}\right)+\frac{1}{120}(-1+x)^5\left(\frac{19\,\text{Cos}[\sqrt{2}]}{16\sqrt{2}}+\frac{5\,\text{Sin}[\sqrt{2}]}{16}\right)+$$
$$\text{Sin}[\sqrt{2}]+\frac{1}{24}(-1+x)^4\left(-\frac{3\,\text{Cos}[\sqrt{2}]}{8\sqrt{2}}+\frac{11\,\text{Sin}[\sqrt{2}]}{8}\right)+\frac{(-1+x)^7\left(\frac{307\,\text{Cos}[\sqrt{2}]}{64\sqrt{2}}+\frac{1701\,\text{Sin}[\sqrt{2}]}{64}\right)}{5040}+$$
$$\frac{(-1+x)^9\left(\frac{9403\,\text{Cos}[\sqrt{2}]}{256\sqrt{2}}+\frac{40797\,\text{Sin}[\sqrt{2}]}{256}\right)}{362880}+\frac{(-1+x)^{10}\left(\frac{218385\,\text{Cos}[\sqrt{2}]}{512\sqrt{2}}+\frac{976439\,\text{Sin}[\sqrt{2}]}{512}\right)}{3628800}$$

Series[h[x], {x, 1, 10}] - TaylorExpansion[h, {x, 1, 10}]

$O[x-1]^{11}$