Cornell University

Department of Physics

Phys 480/680, Astro 690 February 8, 2000

Computational Physics, Spring 2000

Homework Assignment # 1

(Due Thursday, February 3 at 8:40 am in class.)

Agenda and readings for the week of February 1:

The readings are from *Numerical Recipes: The Art of Scientific Computing*, 2nd edition (in Fortran *or* C).

- Lec2, 01/27: Numerical integration in $d = 1$, Change of Variables; Potential energy in atoms.
  Reading: 4.0–4.1
- Lec3, 02/01: Runge-Kutta for Ord. Diff. Eq. including change of variables; Poisson's equation for atoms.
  Reading: 16.0–16.1
- Lab1, 02/03: Discuss code organization and explore changes of variables for atoms.

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1 Integration Routines

1.1 Trapezoidal Rule

In *either* Fortran or C, write a function subroutine of the form

```
C:        float trapint(float f[],float r[],float dr[],int N)

Fortran:  real function trapint(f,r,dr,N)
          integer N
          real f(N),r(N),dr(N)
```

which returns the result of using the trapezoidal rule to perform the integral

$$\int_{r(0)}^{r(1)} f(r)\,dr = \int_0^1 f(r(u))\,\frac{dr}{du}(u)\,du$$

from values at the $N+1$ points $u_i = 0, 1/N, 2/N, \ldots, (N-1)/N, 1$.

As input to this routine, the user supplies the values $r(u_i)$, $\frac{dr}{du}(u_i)$, and $f(r(u_i))$ in the arrays r, dr, and f, respectively.

1.2 Simpson's Rule

In *either* Fortran or C, write a function subroutine of the form

```
C:        float simpint(float f[],float r[],float dr[],int N)

Fortran:  real function simpint(f,r,dr,N)
          integer N
          real f(N),r(N),dr(N)
```

which returns the result of Simpson's rule for the same integral

$$\int_{r(0)}^{r(1)} f(r)\,dr = \int_0^1 f(r(u))\,\frac{dr}{du}(u)\,du$$

using the same inputs as your routine in (1.1).

2 Application to atoms

Note that, while for now you must rely on "outside sources" for $\psi_{1s}(r)$ and ϕ_{1s} below, soon your your own codes will compute them!

To use your integration routines for the problems below, you will need a change of variables function $r(u)$ for which $r(0) = 0$ and $r(1) = \infty$. One suitable choice is

$$r(u) = \frac{1}{1-u} - 1,$$

but you can get better results with other choices. You may wish to experiment...

2.1 Normalization

Write a main program which uses your subroutines (1.1,1.2) to check the normalization of the text-book ground state ("1s state") wave function for the hydrogen atom,

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi}} e^{-r}.$$

.

Specifically, use your routines to check that the total probability $\mathcal{P}(\vec{x}) = \psi^*(\vec{x})\,\psi(\vec{x})$ of finding the electron adds up to one,

$$\int \mathcal{P}_{1s}(\vec{x})\,dV = \int \psi^*_{1s}(\vec{x})\psi_{1s}(\vec{x})\,dV = \int_0^\infty \psi^2_{1s}(r)\,4\pi r^2\,dr = 1.$$

Your main program should allow you to easily select different values for N.

2.2 Electron-Nuclear potential energy

Write a main program which uses your subroutines to compute the electron-nuclear potential energy for a single electron in the 1s state,

$$V_{\mathrm{el-nuc}} = \int n(\vec{x}) V_{\mathrm{nuc}}(\vec{x})\,dV = \int_0^\infty \left(\psi^2_{1s}(r)\right)\left(-\frac{1}{r}\right) 4\pi r^2\,dr.$$

Note: because there is only one electron, $n_{1s}(\vec{x}) = \psi^2_{1s}(\vec{x})$.

2.3 Electron-electron potential energy

Write a main program which uses your subroutines to compute the "Hartree" electron-electron potential energy for the 1s state,

$$V_{\mathrm{el-el}} = \frac{1}{2}\int \phi(\vec{x})n(\vec{x})\,dV = \frac{1}{2}\int_0^\infty \left(\frac{1-e^{-2r}}{r} - e^{-2r}\right)\left(\psi_{1s}^2(r)\right) 4\pi r^2\,dr.$$

Note: For $n(\vec{x}) = \psi_{1s}^2(\vec{x})$, the potential from Poisson's equation $\nabla^2\phi_{1s}(\vec{x}) = -4\pi n_{1s}(\vec{x})$ is

$$\phi_{1s}(r) = \frac{1-e^{-2r}}{r} - e^{-2r}.$$