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hw7_sol_alex.txt      Mon Apr 27 16:12:32 2009      1

/*
Problem number 1

*/
/*
numerov.cc: mumerov method to find eigenvalues and eigenfunctions of
a particle in a potential well.

*/
#include <iostream>
#include <cmath>
#include <fstream>

using namespace std;

const double V0 = -83.0;                      // depth of potential well in MeV
const double E_min = -83.0;                     // energy band to find
const double E_max = 0.0;                       // energy eigenvalue
const double eps = 1E-6;                        // matching tolerance
double h = 0.004;                             // step size
                                                // well is assumed 4 fm wide
                                                // universe is 8 fm wide
                                                // 2000 total steps

double k2(int i, double E);                    /* returns potential at x */
double diff(double E);                        /* difference of derivatives */
void write_data(double E);                    /* saved data for final plot */

int main()
{
    double E_mid, E_lo, E_hi;                  // counter for iterations
    int i=0;

    E_lo = E_min;
    E_hi = E_max;

    do
    {
        ++i;
        E_mid =(E_lo + E_hi)/2.0;           // first guess for energy eigenvalue
        if (diff(E_mid)*diff(E_hi) < 0.0) E_lo = E_mid; // the bisection algorithm
        else E_hi = E_mid;
    }while(fabs(diff(E_mid))>eps);

    cout << "Eigenvalue E = " << E_mid << endl;
    cout << "after " << i << " iterations." << endl;
    write_data(E_mid);
    return 0;
}

/*----- end of main program -----*/
/* function returns difference between left and right wavefunction */
double diff(double E)
{
    double psi_now, psi_last, psi_next, psi_left, psi_right;
    int i;

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psi_last = 0.0;
psi_now = 0.00001;
for (i=1; i<=1500; ++i)           /* left side first */
{
    psi_next = (2*psi_now*(1 - ((5./12.)*h*h*k2(i,E))-
                           (1. + ((1./12.)*h*h)*k2(i-1,E))*psi_last)/(1. + ((h*h)/12.)*k2(i+1,E))
;
    psi_last = psi_now;
    psi_now = psi_next;
}
psi_left = psi_now;                /* value at matching point */

psi_last = 0.0;                   /* reset starting conditions */
psi_now = 0.00001;
for (i=1; i<500; ++i)           /* now the right side */
{
    psi_next = (2*psi_now*(1 - ((5./12.)*h*h*k2(i,E))-
                           (1. + ((1./12.)*h*h)*k2(i-1,E))*psi_last)/(1. + ((h*h)/12.)*k2(i+1,E))
;

    psi_last = psi_now;
    psi_now = psi_next;
}
psi_right = psi_now;              /* value at matching point */
return((psi_left - psi_right));
}

/*-----*/
// function returns k^2 depending on position i
double k2(int i, double E)
{
    const double units_convert = 0.4829;          // MeV^1 fm^-2
    if (i<500) return(units_convert*E);           // outside the well
    if (500<=i && i < 1000) return (units_convert*(E-(V0/2)*0.004*(i-500)));      // inside the well ( change here for different shapes of wells.)
    if (i >= 1000) return (units_convert*(E-(V0*(1-(0.5*0.004*(i-1000))))));
}
/*-----*/
/* write data for eigenfunction into files left.dat, right.dat */
void write_data(double E)
{
    double psi_last, psi_now, psi_next;
    int i;

    ofstream out_file_left;
    ofstream out_file_right;

    out_file_left.open("left.dat");    // save data in files
    out_file_right.open("right.dat");

    psi_last = 0.0;
    psi_now = 0.00001;
    for (i=1; i<=1500; i++)         // left side first
    {
        psi_next = (2*psi_now*(1- ((5./12.)*h*h*k2(i,E))-
                               (1 + ((1./12.)*h*h)*k2(i-1,E))*psi_last)/(1 + ((h*h)/12.)*k2(i+1,E));
        out_file_left << (i-1000)*h << "\t" << psi_next/3.0 << endl;
        psi_last = psi_now;
    }
}
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    psi_now = psi_next;
}

psi_last = 0.0;                                /* reset starting conditions */
psi_now = 0.00001;
for (i=1; i<500; i++)           /* now the right side */
{
    psi_next=(2*psi_now*(1- ((5./12.)*h*h*k2(i,E))-
        (1 + ((1./12.)*h*h)*k2(i-1,E))*psi_last)/(1 + ((h*h)/12.)*k2(i+1,E));

    out_file_right << (1000 -i)*h << "\t" << psi_next/3.0 << endl;

    psi_last = psi_now;
    psi_now = psi_next;
}
out_file_left.close();
out_file_right.close();
cout << "data saved in left.dat and right.dat" << endl;
}

/*
use gnuplot to plot left.dat and right.dat. modify the energy scale to find different b
ound states.

*/
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