Report of Project 4

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Abstract

The Project 4 of PHY607 has only 1 exercises. The goal of this project is to solve a one dimensional simple harmonic potential.

1 Introduction

This exercise asks us to solve schrodinger equation for one dimensional simple harmonic potential. We set k, m, $\hbar$ equal one. The method we use is Numerov algorithm to solve this differential equation, and compare with analytical solutions.

2 Conclusion

2.1 Strategy and code

In this exercise, the equation we need to solve is

$$\left(-\frac{\hbar}{2m}\frac{d^2}{dx^2}+\frac{1}{2}kx^2\right)\psi = E\psi \tag{1}$$

If we set the parameters m, $\hbar$, k equal one, the equation becomes

$$\frac{d^2\psi}{dx^2}+(E-V)\,\psi = 0. \tag{2}$$

For a general differential equation, the form of equation is

$$\frac{d^2}{dx^2}y(x) = f(x, y(x)). \tag{3}$$

Then according to the hangout in class, the solution for $y_n(x)$ is

$$\left(1+\frac{h^2}{12}f_{n+1}\right)y_{n+1} = \left(2-\frac{5h^2}{12}f_n\right)y_n - \left(1+\frac{h^2}{12}f_{n-1}\right)y_{n-1}. \tag{4}$$

So the eigenstate of Eq.2 is

$$\left(1-\frac{h^2}{12}f_{i+1}\right)\psi_{i+1}=\left(2+\frac{5}{6}h^2f_i\right)\psi_i-\left(1-\frac{h^2}{12}f_{i-1}\right)\psi_{i-1}. \tag{5}$$

Because the hangout ask use even and odd function to solve the equation, they have different boundary condition, We define even and odd function as:

$$\psi(0)=1,\psi(h)=1+\frac{h^2}{2}f(0)+\frac{h^4}{24}(f''(0)+f^2(0));evensolutions \tag{6}$$

$$\psi(0)=0,\psi(h)=h+\frac{h^3}{6}f(0);oddsolutions \tag{7}$$

Then we can repeat Eq.5 to get more data, the code is shown below

```
#include <stdio.h>
#include <gsl/gsl_math.h>
#include <time.h>
#include <gsl/gsl_matrix.h>
#include <gsl/gsl_rng.h>
#include <gsl/gsl_permutation.h>
#include <gsl/gsl_linalg.h>

/* Dimension of Matrix and Vectors */

int main(void)
{

    /*int i, j;*/
    const gsl_rng_type * T;
    gsl_rng * r;

    gsl_rng_env_setup();
    T = gsl_rng_default;
    r = gsl_rng_alloc (T);
    int s;
    double det;

    double n = 500.0;

    FILE *fp;
    fp = fopen( "output.txt", "w" );
    for (int i = 0; i < 4; i ++) {
        clock_t start, finish;
        double  duration;
        /* duration of program */
        start = clock();
```

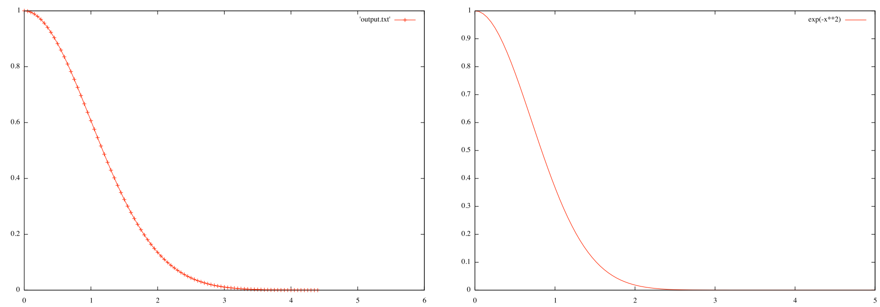

Figure 1: Ground state of harmonic oscillator. Left: numerical solution; Right: analytic solution

```
        gsl_matrix *m = gsl_matrix_alloc(n, n);

        for (int inter = 0; inter < n; inter++) {
            for (int inter2 = 0; inter2 < n; inter2++) {
                double u = gsl_rng_uniform (r);
                gsl_matrix_set(m, inter, inter2, u);
            }
        }

        gsl_permutation*p = gsl_permutation_calloc(n);
        gsl_linalg_LU_decomp (m, p, &s);
        det = gsl_linalg_LU_det(m, s);
        finish = clock();
        duration = (double)(finish - start) / CLOCKS_PER_SEC;
        printf( "%e %f seconds\n",log(n), log(duration) );
        fprintf(fp, "%e %e\n",log(n), log(duration));
        n = n + 500;
        gsl_permutation_free(p);
        gsl_matrix_free (m);
    }
    fclose( fp );
    gsl_rng_free (r);
    return 0;
}
```

2.2 Test for result

To test if our numerical solution is correct, we need to compare with analytic solution. we plot ground state and first exited state in Fig.1 and Fig.2. They are same curve, although they have different scalings.

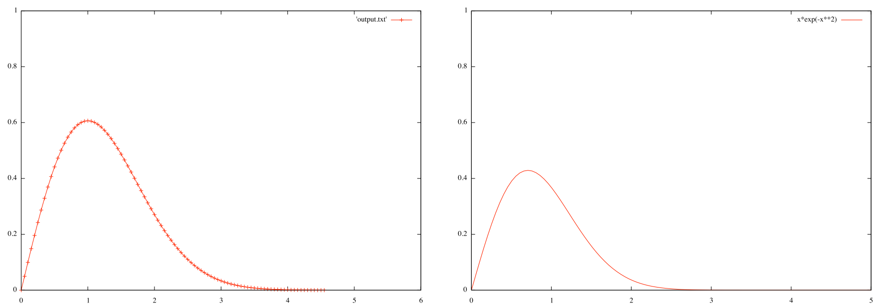

Figure 2: Exited state of harmonic oscillator. Left: numerical solution; Right: analytic solution

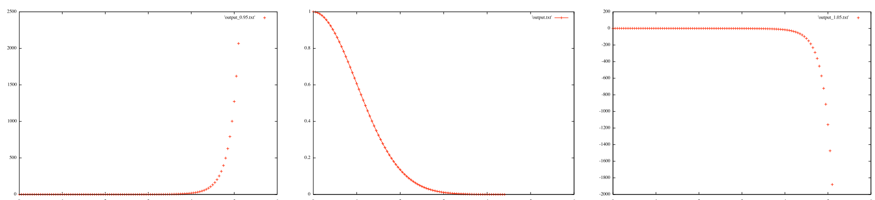

Figure 3: Ground state of harmonic oscillator. Left: E = 0.95; Center: E = 1; Right: E = 1.05

2.3 Change parameter

If we change our parameter, $h = 0.05$, $x = 5$, set $E = 0.95$, $E = 1.0$ and $E = 1.05$, and plot them in Fig.3. We find that the curve sensitive to energy, energy change a little bit, but eigenstate change a lot.

I guess the reason comes from Eq.2, the coefficient of ψ_{i+1} is depends on E and x. If E change or x increase the curve can change strikingly. So we increase x to a large number, we find that eigenfunction is very different from analytic solution and plot them in Fig.4.

2.4 Solutions of E = 3, 5 and 7

Finally, we plot the solution of E = 3, 5 and 7. We know that the eigenstate of E = 3, 5, 7 should be odd function, even function and odd function. The graph is shown in Fig.5, it is self consist with our exception.

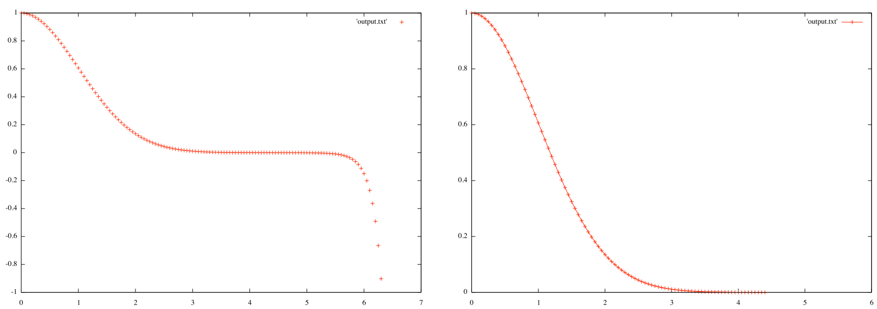

Figure 4: Ground state of harmonic oscillator. Left: up band of x is 5; Right: up band of x is 6.5. Left graph diverse at large x, but Right graph goes to zero, which is correct for ground state

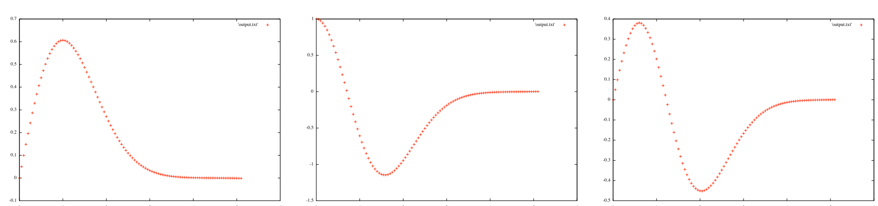

Figure 5: Eigenstate of E = 3, 5, 7