Diffusion equation approach to quantum systems

In this approach, the ground state of the system is found by modeling a diffusion process. There are several approaches to implementing this idea: we will develop programs for the Fokker-Planck and Diffusion Monte Carlo approaches.

Diffusion and random walks

Consider a random walk on a lattice with spacing a in one dimension. The rule for the walk is that if the walker is at position x at time t, then at time $t+h$, the walker moves to the neighbor sites $x \pm a$ with equal probabilities α and remains at x with probability $1-2\alpha$: the sum of the three probabilities add up to 1.

Let's consider an *ensemble* of a large number of such walkers. The number density of walkers is $\rho(x,t)$, which means that, at time t, the number of walkers between x and $x+\mathrm{d}x$ is $\rho(x,t)\mathrm{d}x$. Note: each walker moves on a lattice, but the lattices of different walkers are in general different.

The *master equation*

$$\rho(x,t+h) - \rho(x,t) = \alpha\rho(x+a,t) + \alpha\rho(x-a,t) - 2\alpha\rho(x,t) \ ,$$

says that the density of walkers at x increases in one time step h due to walkers from $x \pm a$ moving to x with probability α, and decreases due to walkers moving from x to $x \pm a$ with probability α.

If h and a are both small, the we can use Taylor expansions

$$\rho(x,t+h) = \rho(x,t) + h\frac{\partial\rho}{\partial t} + \ldots \qquad \rho(x \pm a,t) = \rho(x,t) \pm a\frac{\partial\rho}{\partial x} + \frac{1}{2}a^2\frac{\partial^2\rho}{\partial x^2} + \ldots$$

In the *continuum limit* $h \to 0$, $a \to 0$ with a^2/h held constant, we obtain the *diffusion equation*

$$\frac{\partial\rho}{\partial t} = \gamma\frac{\partial^2\rho}{\partial x^2} \ ,$$

where

$$\gamma \equiv \lim_{h,a\to 0} \frac{\alpha a^2}{h} \ ,$$

is called the *diffusion constant* for the system of walkers.

Green's function for the diffusion equation

The density of walkers at time t can be computed from the initial density using the formula

$$\rho(y,t) = \int \mathrm{d}x\, G(x,y;t)\rho(x,0)\ , \qquad G(x,y;t) = \frac{1}{\sqrt{4\pi\gamma t}} e^{-(x-y)^2/(4\gamma t)}\ ,$$

where $G(x,y;t)$ is a *Green's function* with the properties

$$G(x,y;0) = \delta(x-y)\ , \qquad \text{and} \qquad \int \mathrm{d}x\, G(x,y;t) = 1\ .$$

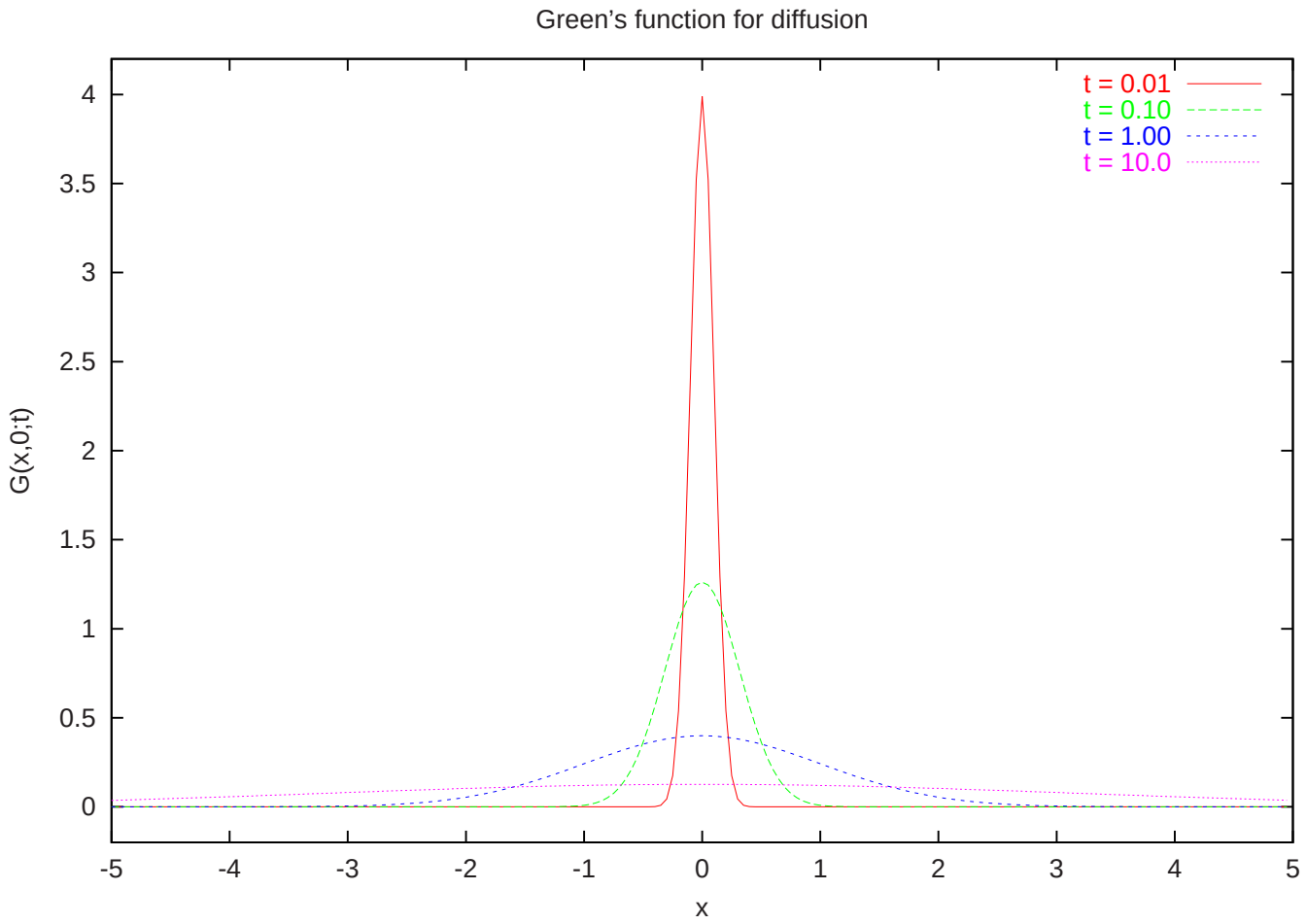
In fact, $G(x,y;t)$ is the probability that a walker at x (or y) at time $t=0$ moves to y (or x) at time t. This provides a way of implementing the random walk:

- Choose a step size Δt in time
- A walker at $x(t)$ at time t moves to $x(t+\Delta t) = x(t) + \eta\sqrt{\Delta t}$, where η is chosen randomly from a Gaussian distribution with variance $\sigma^2 = 2\gamma$.

Let's consider this step as a trial step in the Metropolis algorithm. Do we need to make a Metropolis type test before accepting the step? The answer is no, because the step is chosen according to a probability function which drives the distribution exactly to equilibrium as a function of time t.

Another way of seeing that every step can be accepted is from the physical meaning of diffusion. Typically, we have a dilute collection of non-interacting particles in a medium which can be considered to be a heat bath at constant temperature T. The particles undergo random thermal motion due to collisions with the molecules of the medium. The temperature of the medium determines the diffusion constant via Einstein's relation

$$\gamma = \frac{k_\mathrm{B}T}{\beta}\ ,$$



where β is the drag coefficient, e.g., $\beta = 6\pi\eta R$ for Brownian spheres of radius R moving in fluid with kinematic viscosity η (not to be confused with the Gaussian deviate in the step). Since the diffusing particles are non-interacting, there is no energy cost when they move.

The following program was used to generate data for this plot.

diffusion.cpp

```
#include <iostream>                                                    1
```

```
#include <fstream>                                                          2
#include <cmath>                                                            3
using namespace std;                                                        4
const double pi = 4*atan(1.0);                                              5

double f(double x, double t) {                                              7
    return exp(-x*x/2/t)/sqrt(2*pi*t);                                      8
}                                                                           9

int main() {                                                                11
    ofstream file;                                                          12
    char name[4][10] = {"0.01", "0.10", "1.00", "10.0"};                    13
    double t[4] = {0.01, 0.1, 1.0, 10.0};                                   14
    for (int i = 0; i < 4; i++) {                                           15
        file.open(name[i]);                                                 16
        for (int j = 0; j < 200; j++) {                                     17
            double x = -5 + j*0.005*10;                                     18
            file << x << '\t' << f(x,t[i]) << '\n';                         19
        }                                                                   20
        file.close();                                                       21
    }                                                                       22
    file.close();                                                           23
}                                                                           24
```

Fokker-Planck equation

Suppose we wish to find the average energy of a quantum system with a trial wave function $\Psi_{\rm T}(x)$. This can be done using a diffusion process with a density of walkers $\rho(x,\tau)$ such that

$$\lim_{t\to\infty}\rho(x,t)=\rho(x)=|\Psi_{\rm T}(x)|^2 \ .$$

Can we use the diffusion equation to generate $\rho(x)$? The problem with the diffusion equation is that the density of walkers $\rho(x,t)$ tends to a constant as $t\to\infty$.

There is a modified diffusion equation, however, for which the density of walkers tends to a non-constant funtion as $t\to\infty$. This is the *Fokker-Planck* equation

$$\frac{\partial\rho(x,t)}{\partial t}=\frac{1}{2}\frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}-F(x)\right]\rho(x,t) \ ,$$

where the "Force" is determined by the desired density at $t=\infty$:

$$F(x)=\frac{1}{\rho(x)}\frac{{\rm d}\rho(x)}{{\rm d}x} \ .$$

Note that the Fokker-Planck equation can be written

$$\frac{\partial\rho(x,t)}{\partial t}=\frac{1}{2}\left[\frac{\partial^2\rho(x,t)}{\partial x^2}-\frac{\rho(x,t)}{\rho(x)}\frac{{\rm d}^2\rho(x)}{{\rm d}x^2}+\frac{\rho(x,t)}{\rho^2(x)}\left(\frac{{\rm d}\rho(x)}{{\rm d}x}\right)^2-\frac{1}{\rho(x)}\frac{{\rm d}\rho(x)}{{\rm d}x}\frac{\partial\rho(x,t)}{\partial x}\right] \ .$$

The right hand side vanishes if $\rho(x,t)=\rho(x)$, and hence $\partial\rho/\partial t$ tends to zero, and the density becomes independent of time in this limit.

Approximate Green's function for the Fokker-Planck equation

Unfortunately, a closed form for the Green's function cannot be obtained for arbitrary $F(x)$. However, we can use the following *approximate* form

$$G(x,y;\Delta t) = \frac{1}{\sqrt{2\pi\Delta t}} e^{-[y-x-F(x)\Delta t/2]^2/(2\Delta t)} ,$$

which has the necessary properties

$$\lim_{\Delta t\to 0} G(x,y;\Delta t) = \delta(x-y) , \qquad \int \mathrm{d}y\, G(x,y;\Delta t) = 1 ,$$

for a probability interpretation. This function does not however obey the Fokker-Planck equation: but if Δt is small, then the error is of order Δt^2.

To implement a random walk with this Green's function, suppose the walker is at position x at time t, then he moves to y which is Gaussian-distributed around $x + F(x)\Delta t/2$ with variance Δt:

$$x(t+\Delta t) = x(t) + F(x)\Delta t/2 + \eta\sqrt{\Delta t} ,$$

where η is chosen from a Gaussian distribution with unit variance.

Metropolis correction to Fokker-Planck walk

If the Green's function for the Fokker-Planck equation were exact, then the random walk algorithm given above would inevitably drive any initial distribution to the desired equilibrium distribution $\rho(x)$, just as in the case of the diffusion equation. However, the Green's function is *not* exact, and there will be errors in the evolution of the distribution of $\mathcal{O}(\Delta t^2)$. If Δt is chosen small, the errors will be small, but it will take a long time to generate $\rho(x)$.

These errors can be corrected using the Metropolis algorithm. The Fokker-Planck step from $x(t)$ to $x(t+\Delta t)$ is considered as a *trial step* for the Metropolis algorithm. If the Green's function were exact, then we would have for the ratio of step probabilities

$$\frac{T(x\to y)}{T(y\to x)} = \frac{G(x,y;\Delta t)}{G(y,x;\Delta t)} = \frac{\rho(y)}{\rho(x)} .$$

Since the Green's function is not exact, we need to push the ratio

$$w = \frac{T(y \to x)\rho(y)}{T(x \to y)\rho(x)} = \frac{G(y, x; \Delta t)\rho(y)}{G(x, y; \Delta t)\rho(x)}$$

toward unity. If $T(x \to y)$ is too small compared with $T(y \to x)$, this will tend to make $w > 1$: in this case the step from x to y should always be accepted. Conversely, if $T(x \to y)$ is too large compared with $T(y \to x)$, then accepting the step conditionally by checking whether w is larger than a uniform deviate will tend to correct the problem.

Fokker-Planck equation approach to VMC

The algorithms described above are coded in the following program `vmc-fp.cpp`. The system chosen is the Harmonic Oscillator moving in one dimension. For trial wave function, we choose a Gaussian:

$$\Psi_{\mathrm{T}}(x) \sim e^{-\alpha x^2} , \qquad \rho(x) \sim |\Psi_{\mathrm{T}}(x)|^2 \sim e^{-2\alpha x^2} ,$$

where α is a variational parameter. The "Force" in the Fokker-Planck equation is then

$$F(x) = \frac{1}{\rho(x)} \frac{\mathrm{d}\rho(x)}{\mathrm{d}x} = -4\alpha x .$$

Note that this "Force" acts towards the equilibrium position $x = 0$ of the oscillator, which is reasonable!

vmc-fp.cpp

```
// Fokker-Planck equation approach to VMC                    1

#include <cmath>                                             3
#include <cstdlib>                                           4
#include <fstream>                                           5
#include <iostream>                                          6
#include "rng.h"                                             7
```

```
using namespace std;

int N;                          // number of walkers
double *x;                      // positions of walkers
double alpha;                   // variational parameter
double tStep;                   // time step
int seed = -987654321;          // for random ran2 and gasdev

double eSum;                    // accumulator to find energy
double eSqdSum;                 // accumulator to find fluctuations in E

void initialize() {

    x = new double [N];
    for (int i = 0; i < N; i++)
        x[i] = qadran() - 0.5;
    tStep = 0.1;
}

void zeroAccumulators() {
    eSum = eSqdSum = 0;
}

double eLocal(double x) {

    // compute the local energy
    return alpha + x * x * (0.5 - 2 * alpha * alpha);
}
```

```
int nAccept;                    // accumulator for number of accepted steps
```

The changes from the simple VMC program `vmc.cpp` are in the following function. The chosen walker is provisionally moved to to a new position

$$y = x + \eta\sqrt{\Delta t} + \frac{1}{2}F(x)\Delta t \ ,$$

where

$$F(x) = -4\alpha x \ .$$

vmc-fp.cpp

```
void MetropolisStep(int n) {

    // make a trial move
    double x = ::x[n];              // ::  chooses the global x
    double Fx = - 4 * alpha * x;
    double y = x + gasdev(seed) * sqrt(tStep) + Fx * tStep / 2;
```

The Metropolis test involves the ratio

$$w = \frac{G(y,x;\Delta t)\rho(y)}{G(x,y;\Delta t)\rho(x)} = \frac{e^{-(x-y-F(y)\Delta t/2)^2/(2\Delta t)}}{e^{-(y-x-F(x)\Delta t/2)^2/(2\Delta t)}}\frac{e^{-2\alpha y^2}}{e^{-2\alpha x^2}} \ ,$$

vmc-fp.cpp

```
    // compute ratio for Metropolis test
    double rhoRatio = exp( - 2 * alpha * (y * y - x * x));
    double oldExp = y - x - Fx * tStep / 2;
    double Fy = - 4 * alpha * y;
    double newExp = x - y - Fy * tStep / 2;
```

```
        double GRatio = exp( -(newExp * newExp - oldExp * oldExp) / (2 * tStep));
        double w = rhoRatio * GRatio;

        // Metropolis test
        if (w > ran2(seed)) {
            ::x[n] = x = y;
            ++nAccept;
        }

        // accumulate energy and wave function
        double e = eLocal(x);
        eSum += e;
        eSqdSum += e * e;
    }

    void oneMonteCarloStep() {

        // perform N Metropolis steps
        for (int n = 0; n < N; n++) {
            MetropolisStep(n);
        }
    }
```

The `main` function is almost identical to that in `vmc.cpp`. Following Thijssen's Fortran program, time step size Δt is adjusted in the thermalization phase of the Monte Carlo so that the acceptance ratio for the Metropolis tests is 90%. This is reasonable because the Metropolis test would not be needed were it not for the fact that the Green's function is not exact.

vmc-fp.cpp

```
    int main() {
```

```
cout << " Fokker-Planck approach to VMC: Harmonic Oscillator\n"
     << " ------------------------------------------------\n"
     << " Enter number of walkers:  ";
cin >> N;
cout << " Enter variational parameter alpha:  ";
cin >> alpha;
cout << " Enter number of Monte Carlo steps:  ";
int MCSteps;
cin >> MCSteps;

initialize();

// perform 20% of MCSteps as thermalization steps
// and adjust time step size so acceptance ratio ~90%
int thermSteps = int(0.2 * MCSteps);
int adjustInterval = int(0.1 * thermSteps) + 1;
nAccept = 0;
cout << " Performing " << thermSteps << " thermalization steps ..."
     << flush;
for (int i = 0; i < thermSteps; i++) {
    oneMonteCarloStep();
    if ((i+1) % adjustInterval == 0) {
        tStep *= nAccept / (0.9 * N * adjustInterval);
        nAccept = 0;
    }
}
cout << "\n Adjusted time step size = " << tStep << endl;
```

```
    // production steps                                                    104
    zeroAccumulators();                                                    105
    nAccept = 0;                                                           106
    cout << " Performing " << MCSteps << " production steps ..." << flush; 107
    for (int i = 0; i < MCSteps; i++)                                      108
        oneMonteCarloStep();                                               109

    // compute and print energy                                            111
    double eAve = eSum / double(N) / MCSteps;                              112
    double eVar = eSqdSum / double(N) / MCSteps - eAve * eAve;             113
    double error = sqrt(eVar) / sqrt(double(N) * MCSteps);                 114
    cout << "\n <Energy> = " << eAve << " +/- " << error                   115
         << "\n Variance = " << eVar << endl;                              116
}                                                                          117
```