FYS4411 - Project 1

Scrap I/O and friends

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Abstract

This is where we put the abstract. It will be so good, like, the best. The greatest, probably.

1 Introduction

Lorem ipsum dolor amet

2   Theory

Sample text without lorem ipsum (or is it?)

3 Method

Keeping the stuff here for examples. Might even be relevant.

3.1 Randomization

Randomizing the transaction factor ϵ, and the picking of financial agents, `agent_one` and `agent_two`, was done by initializing the following random number generators (RNGs):

```cpp
std::random_device rd;
std::mt19937_64 gen(rd());
std::uniform_int_distribution<int> AgentPicker(0,NAgents-1);
std::uniform_real_distribution<double> TransactionFactorGenerator
    (0.0,1.0);
// Calling RNGs to initialize agents and transaction factor:
agent_one = AgentPicker(gen);
agent_two = AgentPicker(gen);
TransactionFactor = TransactionFactorGenerator(gen);
```

3.2 Conservation of money

A potential source of money "leaks" in the simulations is if `agent_one` = `agent_two`. In this case the system would "leak" an amount of money equal to $\epsilon(m_1 + m_2)$, propagating for each transaction where that agent is involved, and for each subsequent instance of the error. This was handled by a simple test

```cpp
if (agent_one == agent_two){
    continue;
}
```

which throws away the transactions where this would happen.

4 Results
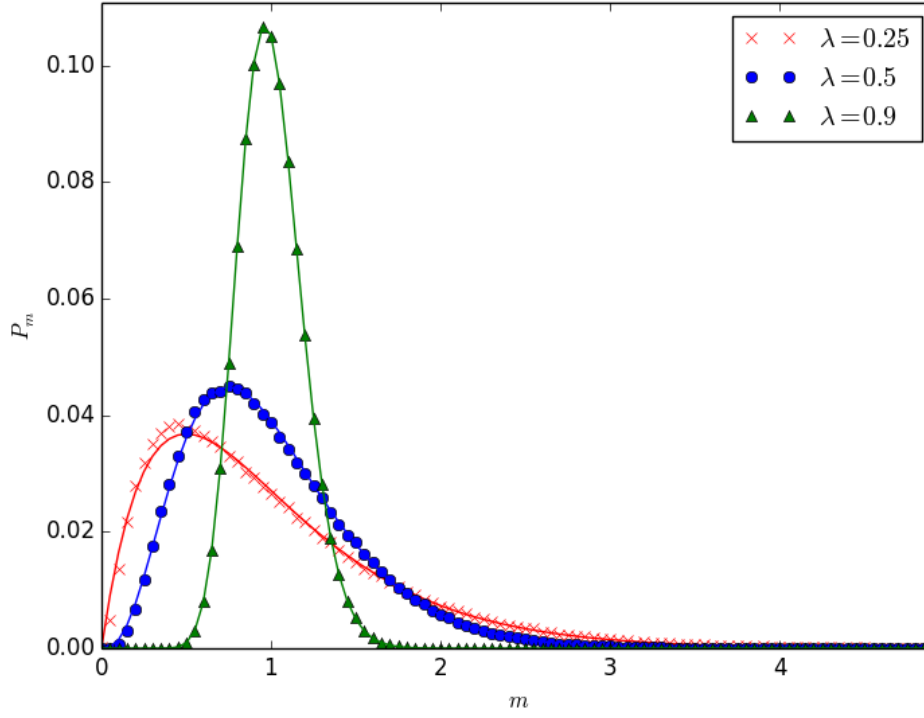
Keeping one figure as example

Figure 1: The wealth probability distribution of agents in the basic model where $\lambda = 0$ and $\eta = 0$

The data is normalized by dividing by the number of Monte Carlo cycles and the number of agents.

5   Discussion

Tekst

6   Conclusion

Herein lies the conclusions of yonder project, verily I say!

Appendix A - Problem 1

The local energy is given by

$$E_L(r) = \frac{1}{\Psi_T(r)} \hat{H} \Psi_T(r)$$

with trial wave equation

$$\Psi_T(r) = \prod_i g(\alpha, \beta, r_i) \prod_{i<j} f(a, |r_i - r_j|)$$

The Hamiltonian becomes

$$\hat{H} = \sum_i^N \left(\frac{-\hbar^2}{2m} \nabla_i^2 + V_{ext}(r_i) \right) + \sum_{i>j}^N V_{int}(r_i, r_j)$$

where

$$V_{ext}(r_i) = \begin{cases} \frac{1}{2} m\omega_{ho}^2 r^2 & (S) \\ \frac{1}{2} m[\omega_{ho}^2(x^2 + y^2) + \omega_z^2 z^2] & (E) \end{cases}$$

and

$$v_{int}(|r_i - r_j|) = \begin{cases} \infty & |r_i - r_j| \leq a \\ 0 & |r_i - r_j| > a \end{cases}$$

First only harmonic oscillator (a=0) and we use $\beta = 1$ for one particle in 1D. for one particle the trial wave equation and Hamiltonian becomes

$$\Psi_T(r) = g(\alpha, x) = e^{-\alpha x_i^2},$$

$$\hat{H} = \left(\frac{-\hbar^2}{2m} \nabla^2 + \frac{1}{2} m\omega_{ho}^2 x^2 \right)$$

$$E_L = \frac{1}{e^{-\alpha x^2}} \left(\frac{-\hbar^2}{2m} \nabla^2(e^{-\alpha x^2}) + \frac{1}{2} m\omega_{ho}^2 x^2 (e^{-\alpha x^2}) \right)$$

$$\nabla^2(e^{-\alpha x^2}) = \frac{d^2 e^{-\alpha x^2}}{dx^2}$$
$$= \frac{d}{dx} \left(\frac{d e^{-\alpha x^2}}{dx} \right)$$
$$= \frac{d}{dx} (-2\alpha x \cdot e^{-\alpha x^2})$$
$$= (4\alpha^2 x^2 - 2\alpha)e^{-\alpha x^2}$$

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$$E_L = \frac{e^{-\alpha x^2}}{e^{-\alpha x^2}} \left(\frac{-\hbar^2}{2m}(4\alpha^2 x^2 - 2\alpha) + \frac{1}{2}m\omega_{ho}^2 x^2 \right)$$

$$E_L = \frac{-\hbar^2}{2m}(4\alpha^2 x^2 - 2\alpha) + \frac{1}{2}m\omega_{ho}^2 x^2$$

Solving the same problem for one particle in 2D and 3D we get something similar,

$$E_L = (\frac{-\hbar^2}{2m})4\alpha^2(x^2 + y^2) - 4\alpha + \frac{1}{2}m\omega_{ho}^2(x^2 + y^2),$$

$$E_L = (\frac{-\hbar^2}{2m})4\alpha^2(x^2 + y^2 + z^2) - 6\alpha + \frac{1}{2}m\omega_{ho}^2(x^2 + y^2 + z^2).$$

ADD LOCAL ENERGY FOR N PARTICLES IN 3D!!!

Now we can try to solve the complete problem. The trial wave function is now

$$\Psi_T(r) = \prod_i g(\alpha, \beta, r_i) \prod_{i<j} f(a, |r_i - r_j|)$$

and first we rewrite it using

$$g(\alpha, \beta, r_i) = \exp -\alpha(x_i^2 + y_i^2 + \beta z_i^2) = \phi(r_i)$$

and

$$f(r_{ij}) \exp \left(\sum_{i<j} u(r_{ij}) \right)$$

getting

$$\Psi_T(r) = \prod_i \phi(r_i) \exp \left(\sum_{i<j} u(r_{ij}) \right).$$

The local energy for this problem becomes:

$$E_L = \frac{1}{\Psi_T(\boldsymbol{r})} \left(\sum_i^N \left(\frac{\hbar^2}{2m}\nabla_i^2 \Psi_T(r) + \frac{1}{2}m\omega_{ho}^2 r^2 \Psi_T(r) \right) + \sum_{i<j}^N V_{int}(r_i, r_j)\Psi_T(r) \right). \qquad (1)$$

The difficulty in (1) is solving the derivatives of the wave equation given the complexity of the exponential. We begin with the first derivative.

$$\nabla_i^2 \prod_i \phi(r_i) \exp \left(\sum_{i<j} u(r_{ij}) \right) = \nabla_i \cdot \nabla_i \prod_i \phi(r_i) \exp \left(\sum_{i<j} u(r_{ij}) \right)$$

The first derivative of particle k:

$$\nabla_k \prod_i \phi(r_i) \exp\left(\sum_{i<j} u(r_{ij})\right) = \nabla_k \left(\prod_i \phi(r_i)\right) \exp\left(\sum_{i<j} u(r_{ij})\right) + \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij})\right)\right) \prod_i \phi(r_i)$$

$$\nabla_k \left(\prod_i \phi(r_i)\right) = \nabla_k(\phi(r_1)(\phi(r_2)...(\phi(r_k)..(\phi(r_N)))$$

$$= \nabla_k \left(e^{-\alpha(x_1^2+y_1^2+z_1^2)} e^{-\alpha(x_2^2+y_2^2+z_2^2)}...e^{-\alpha(x_k^2+y_k^2+z_k^2)}...e^{-\alpha(x_N^2+y_N^2+z_N^2)}\right)$$

$$= \nabla_k \phi(r_k) \left[\prod_{i \neq k} \phi(r_i)\right]$$

$$\nabla_k \exp\left(\sum_{i<j} u(r_{ij})\right) = \nabla_k \exp(u(r_{12}) + u(r_{13}) + ... + u(r_{23}) + ... + u(r_{kj}) + .. + u(r_{N-1,N}))$$

$$= \exp\left(\sum_{i<j} u(r_{ij})\right) \sum_{i \neq k} \nabla_k u(r_{kj})$$

And the first derivative of the trial wave equation is

$$\nabla_k \Psi_T(r) = \nabla_k \phi(r_k) \left[\prod_{i \neq k} \phi(r_i)\right] \exp\left(\sum_{i<j} u(r_{ij})\right) + \prod_i \phi(r_i) \exp\left(\sum_{i<j} u(r_{ij})\right) \sum_{j \neq k} \nabla_k u(r_{kj}).$$

FINAL EXPRESSION FOR TRIAL WAVE FUNCTION?
Now we find the second derivative of the wave function.

$$\frac{1}{\Psi_T(r)}\nabla_k^2\Psi_T(r) = \frac{1}{\nabla_k\prod_i\phi(r_i)\exp\left(\sum_{i<j}u(r_{ij})\right)}\left(\nabla_k\left(\nabla_k\phi(r_k)\left[\prod_{i\neq k}\phi(r_i)\right]\right)\cdot\exp\left(\sum_{i<j}u(r_{ij})\right)\right.$$

$$+\nabla_k\phi(r_k)\left[\prod_{i\neq k}\phi(r_i)\right]\cdot\nabla_k\left(\exp\left(\sum_{i<j}u(r_{ij})\right)\right)$$

$$+\nabla_k\left(\prod_i\phi(r_i)\right)\cdot\exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k u(r_{kj})$$

$$+\prod_i\phi(r_i)\cdot\nabla_k\left(\exp\left(\sum_{i<j}u(r_{ij})\right)\right)\sum_{j\neq k}\nabla_k u(r_{kj})$$

$$\left.+\prod_i\phi(r_i)\exp\left(\sum_{i<j}u(r_{ij})\right)\cdot\nabla_k\left(\sum_{j\neq k}\nabla_k u(r_{kj})\right)\right)$$

Solving these equations separately makes it easier.

$$\frac{\nabla_k^2\phi(r_k)\left[\prod_{i\neq k}\phi(r_i)\right]\cdot\exp\left(\sum_{i<j}u(r_{ij})\right)}{\nabla_k\prod_i\phi(r_i)\exp\left(\sum_{i<j}u(r_{ij})\right)} = \frac{\nabla_k^2\phi(r_k)}{\phi(r_k)}$$

$$\frac{\nabla_k\phi(r_k)\left[\prod_{i\neq k}\phi(r_i)\right]\cdot\nabla_k\left(\exp\left(\sum_{i<j}u(r_{ij})\right)\right)}{\nabla_k\prod_i\phi(r_i)\exp\left(\sum_{i<j}u(r_{ij})\right)} = \frac{\nabla_k\phi(r_k)}{\phi(r_k)}\sum_{j\neq k}\nabla_k u(r_{kj})$$

$$\frac{\nabla_k\left(\prod_i\phi(r_i)\right)\cdot\exp\left(\sum_{i<j}u(r_{ij})\right)\sum_{j\neq k}\nabla_k u(r_{kj})}{\nabla_k\prod_i\phi(r_i)\exp\left(\sum_{i<j}u(r_{ij})\right)} = \frac{\nabla_k\phi(r_k)}{\phi(r_k)}\sum_{j\neq k}\nabla_k u(r_{kj})$$

$$\frac{\prod_i \phi(r_i) \cdot \nabla_k \left(\exp\left(\sum_{i<j} u(r_{ij})\right)\right) \sum_{j\neq k} \nabla_k u(r_{kj})}{\nabla_k \prod_i \phi(r_i) \exp\left(\sum_{i<j} u(r_{ij})\right)} = \sum_{i\neq k} \nabla_k u(r_{ki}) \sum_{j\neq k} \nabla_k u(r_{kj})$$

$$\frac{\prod_i \phi(r_i) \exp\left(\sum_{i<j} u(r_{ij})\right) \cdot \nabla_k \left(\sum_{j\neq k} \nabla_k u(r_{kj})\right)}{\nabla_k \prod_i \phi(r_i) \exp\left(\sum_{i<j} u(r_{ij})\right)} = \sum_{j\neq k} \nabla_k^2 u(r_{kj})$$

Putting them together again we get the following

$$\frac{1}{\Psi_T(r)} \nabla_k^2 \Psi_T(r) = \frac{\nabla_k^2 \phi(r_k)}{\phi(r_k)} + 2\frac{\nabla_k \phi(r_k)}{\phi(r_k)} \sum_{j\neq k} \nabla_k u(r_{kj}) + \sum_{i\neq k} \nabla_k u(r_{ki}) \sum_{j\neq k} \nabla_k u(r_{kj}) + \sum_{j\neq k} \nabla_k^2 u(r_{kj})$$

$$(2)$$

We solve the first and second derivatives of $u(r_{kj})$.

$$\nabla_k u(r_{kj}) = \left(\vec{i}\frac{\partial}{\partial x_k} + \vec{j}\frac{\partial}{\partial y_k} + \vec{k}\frac{\partial}{\partial z_k}\right) u(r_{kj}) \tag{3}$$

From Rottmann p. 128 we have that

$$\frac{\partial u(r_{kj})}{\partial x_k} \vec{i} = \frac{\partial u(r_{kj})}{\partial r_{kj}} \frac{\partial r_{kj}}{\partial x_k} \vec{i}$$

$$= u'(r_{kj}) \frac{\partial \sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}}{\partial x_k} \vec{i}$$

$$= u'(r_{kj}) \frac{1}{2} 2|x_k - x_j| \frac{1}{r_{kj}} \vec{i}$$

$$= \frac{u'(r_{kj})|x_k - x_j|}{r_{kj}} \vec{i}$$

$$\frac{\partial u(r_{kj})}{\partial y_k} \vec{j} = \frac{u'(r_{kj})|y_k - y_j|}{r_{kj}} \vec{j}$$

$$\frac{\partial u(r_{kj})}{\partial z_k} \vec{k} = \frac{u'(r_{kj})|z_k - z_j|}{r_{kj}} \vec{k}$$

where we have used the fact that $r_{kj} = \sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}$. Now equation (3) becomes

$$\nabla_k u(r_{kj}) = u(r_{kj}) \frac{(|x_k - x_j|\vec{i} + |y_k - y_j|\vec{j} + |z_k - z_j|\vec{k})}{r_{kj}}$$

$$= u(r_{kj}) \frac{(\boldsymbol{r_k} - \boldsymbol{r_j})}{r_{kj}}.$$

And for the second derivative have that

$$\nabla_k^2 u(r_{kj}) = \left(\frac{\partial^2}{\partial x_k^2} + \frac{\partial^2}{\partial y_k^2} + \frac{\partial^2}{\partial z_k^2} \right) u(r_{kj}) \tag{4}$$

and use Rottmann p. 128 again and see that

$$\frac{\partial^2 u(r_{kj})}{\partial x_{kj}^2} = \frac{\partial^2 u(r_{kj})}{\partial r_{kj}^2} \left(\frac{\partial r_{kj}}{\partial x_{kj}} \right)^2 + \frac{\partial u(r_{kj})}{\partial r_{kj}} \frac{\partial^2 r_{kj}}{\partial x_{kj}^2}$$

$$= u''(r_{kj}) \frac{(x_k - x_j)^2}{r_{kj}^2} + u'(r_{kj}) \frac{\partial^2 r_{kj}}{\partial x_{kj}^2}$$

$$\frac{\partial^2 r_{kj}}{\partial x_{kj}^2} = \frac{\partial^2 \sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}}{\partial x_{kj}^2}$$

$$= \frac{\partial \frac{x_k - x_j}{\sqrt{|x_k - x_j|^2 + |y_k - y_j|^2 + |z_k - z_j|^2}}}{\partial x_{kj}}$$

$$= \frac{r_{kj} - \frac{1}{2}(x_k - x_j) \cdot \frac{2(x_k - x_j)}{r_{kj}}}{r_{kj}^2}$$

$$= \frac{1}{r_{kj}} - \frac{(x_k - x_j)^2}{r_{kj}^3}.$$

These equations put together and solving with respect to y and z we get

$$\frac{\partial^2 u(r_{kj})}{\partial x_{kj}^2} = u''(r_{kj}) \frac{(x_k - x_j)^2}{r_{kj}^2} + u'(r_{kj}) \left(\frac{1}{r_{kj}} - \frac{(x_k - x_j)^2}{r_{kj}^3} \right),$$

$$\frac{\partial^2 u(r_{kj})}{\partial y_{kj}^2} = u''(r_{kj}) \frac{(y_k - y_j)^2}{r_{kj}^2} + u'(r_{kj}) \left(\frac{1}{r_{kj}} - \frac{(y_k - y_j)^2}{r_{kj}^3} \right),$$

$$\frac{\partial^2 u(r_{kj})}{\partial z_{kj}^2} = u''(r_{kj}) \frac{(z_k - z_j)^2}{r_{kj}^2} + u'(r_{kj}) \left(\frac{1}{r_{kj}} - \frac{(z_k - z_j)^2}{r_{kj}^3} \right).$$

Now we can add them all together and equation (4) becomes

$$\nabla_k^2 u(r_{kj}) = \frac{u''(r_{kj})}{r_{kj}^2}((x_k - x_j)^2 + (y_k - y_j)^2 + (z_k - z_j)^2)$$

$$+ u'(r_{kj})\left(\frac{3}{r_{kj}} - \frac{(x_k - x_j)^2 + (y_k - y_j)^2 + (z_k - z_j)^2}{r_{kj}^3}\right)$$

$$= \frac{u''(r_{kj})r_{kj}^2}{r_{kj}^2} + u'(r_{kj})\left(\frac{3}{r_{kj}} - \frac{r_{kj}^2}{r_{kj}^3}\right)$$

$$= u''(r_{kj}) + u'(r_{kj})\frac{2}{r_{kj}}$$

Now we can write out the complete second derivative, equation (2)

$$\frac{1}{\Psi_T(r)}\nabla_k^2\Psi_T(r) = \frac{\nabla_k^2\phi(r_k)}{\phi(r_k)} + 2\frac{\nabla_k\phi(r_k)}{\phi(r_k)}\sum_{j\neq k}\frac{(\boldsymbol{r_k} - \boldsymbol{r_j})}{r_{kj}}u'(r_{kj})$$

$$+ \sum_{ij\neq k}\frac{(\boldsymbol{r_k} - \boldsymbol{r_i})}{r_{ki}}\frac{(\boldsymbol{r_k} - \boldsymbol{r_j})}{r_{kj}}u'(r_{ki})u'(r_{kj}) + \sum_{j\neq k}\left(u''(r_{kj}) + \frac{2}{r_{kj}}u'(r_{kj})\right).$$

For the full analytical solution of the interacting problem we solve each term by it self.

$$\frac{1}{\phi(r_k)}\nabla_k^2\phi(r_k) = \frac{\nabla_k^2\, exp(-\alpha(x_k^2 + y_k^2 + \beta z_k^2))}{exp(-\alpha(x_k^2 + y_k^2 + \beta z_k^2))}$$

$$= ((2\alpha(2\alpha x_k^2 - 1)) + (2\alpha(2\alpha y_k^2 - 1)) + (2\alpha\beta(2\alpha\beta z_k^2 - 1))) \cdot \frac{\phi(r_k)}{\phi(r_k)}$$

$$= -4\alpha^2 - 2\alpha\beta + 4\alpha^2(x_k^2 + y_k^2 + \beta z_k^2)$$

$$\frac{1}{\phi(r_k)}\nabla_k\phi(r_k) = \frac{\nabla_k\, exp(-\alpha(x_k^2 + y_k^2 + \beta z_k^2))}{exp(-\alpha(x_k^2 + y_k^2 + \beta z_k^2))}$$

$$= (2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k}) \cdot \frac{\phi(r_k)}{\phi(r_k)}$$

$$= (2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k})$$

Wolfram alpha gives to solution the first and second derivatives of function $u(r_{kj})$.

$$u'(r_{kj}) = \frac{d(\ln f(r_{kj}))}{dr_{kj}}$$

$$= \frac{d \ \ln\left(1 - \frac{a}{(r_k - r_j)}\right)}{dr_{kj}}$$

$$= -\frac{a}{ar_{kj} - r_{kj}^2}$$

$$u''(r_{kj}) = \frac{d^2(\ln f(r_{kj}))}{dr_{kj}^2}$$

$$= \frac{a(a - 2r_{kj})}{r_{kj}^2(a - r_{kj})^2}$$

Putting all of this together we end up with the following expression for the second derivative of the wave equation divided by it self:

$$\frac{1}{\Psi_T(r)}\nabla_k^2\Psi_T(r) = -4\alpha^2 - 2\alpha\beta + 4\alpha^2(x_k^2 + y_k^2 + \beta z_k^2)$$

$$+ 2((2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k}))\sum_{j\neq k}\left(\frac{(x_k - x_j)\vec{i} + (y_k - y_j)\vec{j} + (z_k - z_j)\vec{k}}{r_{kj}}\left(\frac{-a}{ar_{kj} - r_{kj}^2}\right)\right)$$

$$+ \sum_{j\neq k}\left(\frac{(x_k - x_i)\vec{i} + (y_k - y_i)\vec{j} + (z_k - z_i)\vec{k}}{r_{ki}}\right)\left(\frac{(x_k - x_j)\vec{i} + (y_k - y_j)\vec{j} + (z_k - z_j)\vec{k}}{r_{kj}}\right)$$

$$* \left(\frac{-a}{ar_{ki} - r_{ki}^2}\right)\left(\frac{-a}{ar_{kj} - r_{kj}^2}\right)$$

$$+ \sum_{j\neq k}\left(\frac{a(a - 2r_{kj})}{r_{kj}^2(a - r_{kj})^2} + \frac{2}{r_{kj}} - \frac{a}{ar_{kj} - r_{kj}^2}\right)$$

Drift force:
Add calculations later.... OBS OBS

$$\nabla u(r_{kj}) = -\frac{a(\vec{r_k} - \vec{r_j})}{ar_{kj}^2 - r_{kj})^3}$$

$$F = (2\alpha x_k\vec{i} + 2\alpha y_k\vec{j} + 2\alpha\beta z_k\vec{k}) + \sum_{j\neq k}\left(-\frac{a(\vec{r_k} - \vec{r_j})}{ar_{kj}^2 - r_{kj})^3}\right)$$