P3317 HW from Lecture 2+3 and Recitation 2

Due Tuesday September 11

Q: What is polite and works for the phone company?
A: A deferential operator.

Problem 1. Gross-Pittaevskii Equation In class we modeled an atomic gas by saying that each particle was described by the same single particle wavefunction, $\psi(x)$, and that wavefunction obeyed the standard Schrodinger equation,

$$i\hbar\partial_t\psi(x) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x)\psi(x), \tag{1}$$

where $V(x)$ is the applied potential. This approach neglects the interactions between the particles. The simplest way to account for those interactions is to argue that each particle feels a potential created by the others. Since atomic interactions tend to be short ranged, one typically assumes

$$\begin{aligned} i\hbar\partial_t\psi(x) &= -\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V_{\text{eff}}(x)\psi(x), & (2)\\ V_{\text{eff}}(x) &= V(x) + gn(x), & (3) \end{aligned}$$

where g is a constant which depends on the atom. In class we argued that $n(x) \propto |\psi(x)|^2$. In particular $n(x) = N|\psi(x)|^2$, where N is the total number of particles. This then leads to the *non-linear Schrodinger equation*,

$$i\hbar\partial_t\psi(x) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x) + V(x)\psi(x) + gN|\psi(x)|^2\psi(x). \tag{4}$$

This is also known as the Gross-Pittaevskii equation. We will analyze this equation in the same way we analyzed the Schrodinger equation in the "continuity worksheet" from lecture 3. It may help to refer to that worksheet. As in that exercise, our goal is to interpret the equations of motion in terms of fluid dynamics.

1.1. Write the complex wavefunction as an amplitude and a phase

$$\psi(x,t) = f(x,t)e^{i\phi(x,t)}, \tag{5}$$

where both f and ϕ are real. Substitute this ansatz into the Gross-Pitaevskii equation, multiply by $e^{-i\phi}$ and take the real and imaginary parts to get two equations.

Solution 1.1. Making the substitution, we get:

$$i\hbar\partial_t\left(fe^{i\phi}\right) = -\frac{\hbar^2}{2m}\partial_x^2\left(fe^{i\phi}\right) + V(x)fe^{i\phi} + hNf^3e^{i\phi} \tag{6}$$

$$i\hbar\left(\dot{f} + if\dot{\phi}\right)e^{i\phi} = -\frac{\hbar^2}{2m}\partial_x\left[\left(f' + i\phi' f\right)e^{i\phi}\right] + Vfe^{i\phi} + gNf^3e^{i\phi} \tag{7}$$

$$\left(i\hbar\dot{f} - \hbar f\dot{\phi}\right)e^{i\phi} = -\frac{\hbar^2}{2m}\left(f'' + i\phi'' f + 2i\phi' f' - \phi'^2 f\right)e^{i\phi} + Vfe^{i\phi} + gNf^3e^{i\phi} \tag{8}$$

$$i\hbar\dot{f} - \hbar f\dot{\phi} = -\frac{\hbar^2}{2m}\left(f'' + i\phi'' f + 2i\phi' f' - \phi'^2 f\right) + Vf + gNf^3, \tag{9}$$

where a dot indicates a time derivative, and a prime indicates an x derivative. The real part gives:

$$\hbar f\dot{\phi} = \frac{\hbar^2}{2m}\left(f'' - \phi'^2 f\right) - Vf - gNf^3, \tag{10}$$

while the imaginary part gives:

$$\dot{f} = -\frac{\hbar}{2m}\left(\phi'' f + 2\phi' f'\right). \tag{11}$$

1.2. Show that one of these two equations can be interpreted as a continuity equation. Under this interpretation, what is the local velocity v?

Solution 1.2. Multiplying Eq. (11) by f gives:

$$\begin{aligned}\dot{f}f &= -\frac{\hbar}{2m}\left(\phi'' f^2 + 2\phi' f' f\right)\\ \frac{1}{2}\partial_t(f^2) &= -\partial_x\left(\frac{\hbar}{2m}f^2\phi'\right).\end{aligned} \tag{12}$$

This has the form of the continuity equation:

$$\partial_t\rho = -\nabla\cdot(\rho\vec{u}) \tag{13}$$

if we make the identifications:

$$\rho = f^2, \qquad v_x = \frac{\hbar}{m}\partial_x\phi. \tag{14}$$

In other words, the modulus squared behaves as a (probability) density, with the spatial variation of the phase measuring its 'fluid velocity'.

1.3. The other equation can be rewritten as

$$\partial_t\phi = -\frac{\hbar}{2m}\left(\partial_x\phi\right)^2 + \frac{\hbar}{2m}\frac{\partial_x^2 f}{f} - \frac{V}{\hbar} - \frac{gn}{\hbar} \tag{15}$$

By differentiating this equation with respect to x it takes on the form of the one-dimensional Euler equation from fluid dynamics

$$\partial_t v(x,t) + \frac{1}{2}\partial_x v^2(x,t) + \partial_x p(x,t) = 0, \tag{16}$$

where $p(x,t)$ is the local pressure. By identifying terms, what is the pressure of this interacting gas? [Note: this gas is essentially at $T = 0$, so the ideal gas law would predict $p = 0$. Unlike an ideal gas, interactions are very important here.]

Solution 1.3. The x derivative of Eq. (22) of the homework is given by:

$$\partial_t \phi' = -\frac{\hbar}{2m}\partial_t(\phi'^2) + \frac{\hbar}{2m}\frac{\partial_x^2 f}{f} - \frac{V}{\hbar} - \frac{gn}{\hbar}. \tag{17}$$

Replacing ϕ' by $vm/\hbar$ from Eq. (14), and multiplying by a factor of $\hbar/m$, gives:

$$\partial_t v(x,t) + \frac{1}{2}\partial_x(v^2) + \partial_x\left(\frac{V(x)}{m} + \frac{gn(x)}{m} - \frac{\hbar^2}{2m^2}\frac{f''}{f}\right). \tag{18}$$

Therefore, we have that the pressure is given by the final term:

$$p(x,t) = \frac{V(x)}{m} + \frac{gn(x)}{m} - \frac{\hbar^2}{2m^2}\frac{f''}{f}. \tag{19}$$

The first term represents the external forces. The last term is sometimes called a "quantum pressure" – it represents the momentum spread which comes from trying to localize particles. The second term is the contribution to pressure from interactions.

Problem 2. Consider the 1D time independent Schrodinger equation of a free particle:

$$-\frac{\hbar^2}{2m}\partial_x^2\psi(x) = E\psi(x). \tag{20}$$

This is a second order differential equation – thus it needs two boundary conditions to uniquely define the eigenstates.

As a mathematics problem, there are several different Canonical choices of boundary conditions. In your differential equations course, you may have seen the following boundary conditions in similar equations:

Dirichlet: $\psi(0) = 0$ and $\psi(L) = 0$.

Neuman: $\psi'(0) = 0$ and $\psi'(L) = 0$

Homogeneous: $\psi'(0) = \kappa\psi(0)$ and $\psi'(L) = \kappa\psi(L)$, where κ is a constant.

Note Dirichlet and Neuman are special cases of homogeneous boundary conditions with $\kappa = 0$ and $\kappa = \infty$.

Periodic: $\psi(L) = \psi(0)$ and $\psi'(0) = \psi'(L)$

Antiperiodic: $\psi(L) = -\psi(0)$ and $\psi'(0) = -\psi'(L)$

Twisted: $\psi(L) = e^{i\phi}\psi(0)$ and $\psi'(0) = e^{i\phi}\psi'(L)$ where ϕ is a constant.

Note, Periodic and Antiperiodic are special cases of twisted boundary conditions with $\phi = 0$ *and* $\phi = \pi$.

In PHYS 3316 you probably only used one of these: Dirichlet boundary conditions, more commonly known to physicists as "hard wall boundary conditions," as it represents confinement by a very steep potential. In recitation 2, you saw that in a finite difference approximation, you can incorporate different boundary conditions into the matrix which gives you derivatives.

2.1. With "hard wall" boundary conditions: $\psi(0) = 0, \psi(L) = 0$. What are the energies of the lowest 5 eigenstates of EQ. (20)? [Do this with pencil and paper – not the computer.]

Hint: The eigenstates are of the form $\psi(x) = \sin(kx)$. You just need to find k such that the boundary condition is satisfied.

Solution 2.1. The solution is given by:

$$\psi(x) = \sin(kx), \qquad \text{with } k = \frac{s\pi}{L}, \quad s = 1, 2, 3, ... \tag{21}$$

for integer $s \geq 1$. The general solution has a cos piece as well as a sin piece, but the boundary conditions kill the cos. Plugging this into Schrodinger's equation gives:

$$E = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\left(\frac{s\pi}{L}\right)^2, \tag{22}$$

and so the first five Eigenvalues are

$$E = \frac{\hbar^2\pi^2}{2mL^2} \times \{1, 4, 9, 16, 25\}. \tag{23}$$

2.2. Physically it is also reasonable to consider the quantum mechanics of a particle on a ring (say manufactured in the Cornell Nanofabrication Facility). We will take L to be the circumference of the ring, and x is the distance along the ring. In such a setting, we should use periodic boundary conditions: $\psi(0) = \psi(L)$ and $\psi'(0) = \psi'(L)$. What are the energies $E_0, E_1, \cdots E_4$ of the lowest 5 eigenstates?

Hint: The eigenstates are of the form $\psi(x) = e^{ikx}$, you just need to find k such that the boundary condition are satisfied.

Solution 2.2. This time, the solutions are:

$$\psi(x) = e^{ikx}, \qquad \text{with } k = \pm\frac{2s\pi}{L}, s = 0, \pm1, \pm2, \pm3.... \tag{24}$$

Note that compared with the previous solution: (a) there is a zero mode with zero energy, and (b) the excited modes are twofold degenerate. This last fact corresponds to the presence of clockwise and anti-clockwise travelling modes. The first five modes have energies:

$$E = \frac{\hbar^2\pi^2}{2mL^2} \times \{0, 4, 4, 16, 16\}. \tag{25}$$

Aside: zero modes and degeneracy

In order to see why there is no $s = 0$ mode in the hard boundary case, consider what would be the corresponding eigenfunction:

$$\psi_{s=0}^{\text{hard}} \stackrel{?}{=} \sin(0x) = 0. \tag{26}$$

This is clearly not a normalizable state: it is not a state at all. Therefore, the energy levels of the hard box start at $n = 1$. In the periodic case, the zero mode is:

$$\psi_{s=0}^{\text{periodic}} = e^{i0x} = \text{const}. \tag{27}$$

This is normalizable, and satisfies Schrodinger's equation with $E = 0$. It is therefore the lowest lying energy state of the particle on a ring.

The reason that the hard box does not have degenerate states is that the states $\pm s$ differ only by a constant phase:

$$\sin\left(-\frac{s\pi x}{L}\right) = -\sin\left(\frac{s\pi x}{L}\right) = e^{i\pi}\sin\left(\frac{s\pi x}{L}\right). \tag{28}$$

They are therefore the same state. On the other hand, in the periodic case there are two distinct states for each non-zero energy that cannot be related simply by multiplication by a phase:

$$e^{ikx} \neq e^{i\phi}e^{-ikx}, \tag{29}$$

unless $k = 0$. Therefore, as long as $k \neq 0$ the energies come in pairs.

2.3. You should have found that the first excited state is two-fold degenerate when you have periodic boundary conditions. That is $E_1 = E_2$. Prove that $(\psi_1 - \psi_2)/(2i)$ is also an eigenstate, with this same energy. [Note, this is a generic result. If you ever have two eigenstates with the same eigenvalue, their sum is also an eigenstate.]

Solution 2.3. We have that:

$$\frac{\psi_1 - \psi_2}{2i} = \frac{e^{ikx} - e^{-ikx}}{2i} = \sin(kx). \tag{30}$$

This also satisfies the Schrodinger equation, with $E = \hbar^2 k^2/2m$:

$$-\frac{\hbar^2}{2m}\partial_x^2 \sin(kx) = \frac{\hbar^2 k^2}{2m}\sin(kx). \tag{31}$$

Although the question didn't ask, you could also take

$$\frac{\psi_1 + \psi_2}{2} = \frac{e^{ikx} + e^{-ikx}}{2} = \cos(kx). \tag{32}$$

2.4. Clearly the individual energies depend on the different boundary conditions. On the other hand, if you squint your eyes, the "coarse grained" spectra are very similar. More concretely, calculate the sum of the first 5 energies $E_s = E_0 + E_1 + E_2 + E_3 + E_4$ in each of these cases. What is the fractional difference $(E_s^{\text{periodic}} - E_s^{\text{hard}})/(E_s^{\text{periodic}} + E_s^{\text{hard}})$?

Solution 2.4. We have that:

$$E_s^{\text{periodic}} = \frac{\hbar^2\pi^2}{2L^2m}(0+4+4+16+16) = 20\frac{\hbar^2\pi^2}{L^2m} \tag{33}$$

$$E_s^{\text{hard}} = \frac{\hbar^2\pi^2}{2L^2m}(1+4+9+16+25) = \frac{55}{2}\frac{\hbar^2\pi^2}{L^2m}, \tag{34}$$

and therefore:

$$\frac{E_s^{\text{periodic}} - E_s^{\text{hard}}}{E_s^{\text{periodic}} + E_s^{\text{hard}}} = \frac{40-55}{40+55} = -\frac{3}{19} \simeq -\frac{1}{6}. \tag{35}$$

This ratio gets smaller and smaller as you include more and more states. In the thermodynamic limit the choice of boundary condition is irrelevant.

Problem 3. Finite Differences in Time – Part 2 Recall that last homework you were approximating solutions to the differential equation

$$\begin{pmatrix} i\hbar\partial_t\psi_0(t) \\ i\hbar\partial_t\psi_1(t) \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}. \tag{36}$$

With initial conditions $\psi_0(0) = 1, \psi_1(0) = 0$. Physically $|\psi_0|^2$ and $|\psi_1|^2$ are the probabilities of finding the particle at positions r_0 and r_1.

3.1. Deriving Backward Euler Similar to what we did last week, we will turn this differential equation into a difference equation via Taylor's theorem. We will use a slightly different approximation though, this time we will use the following form of Taylor's Theorem

$$f(t - \delta t) = f(t) - \delta t f'(t) + \frac{(\delta t)^2}{2!} f''(t) + \cdots. \tag{37}$$

If δt is small, we can truncate this at the second term, approximating

$$f(t-\delta t) \approx f(t) - \delta t f'(t), \tag{38}$$

or equivalently

$$f'(t) \approx \frac{f(t)-f(t-\delta t)}{\delta t}. \tag{39}$$

Taking $f=\psi_0$ and $f=\psi_1$, we can substitute this expression into EQ. (36) to get an equation of the form

$$\mathbb{W}\begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t-\delta t) \\ \psi_1(t-\delta t) \end{pmatrix}, \tag{40}$$

where $\mathbb{W}$ is a 2×2 matrix. Find $\mathbb{W}$.

Solution 3.1. As was pointed out in an email, the $\hbar$ in Eq. (36) was erroneous. Keeping it doesn't change anything except the limit of the graph.
Starting from:

$$i\partial_t \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}, \tag{41}$$

we use Eq. (39) to get:

$$\frac{i}{\delta t} \begin{pmatrix} \psi_0(t)-\psi_0(t-\delta t) \\ \psi_1(t)-\psi_1(t-\delta t) \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}. \tag{42}$$

Multiply through be $-i\delta t$ and rearrange terms to get:

$$\begin{pmatrix} 0 & -i\delta t \\ -i\delta t & 0 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t-\delta t) \\ \psi_1(t-\delta t) \end{pmatrix} \tag{43}$$

$$\begin{pmatrix} 1 & -i\delta t \\ -i\delta t & 1 \end{pmatrix} \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix} = \begin{pmatrix} \psi_0(t-\delta t) \\ \psi_1(t-\delta t) \end{pmatrix}. \tag{44}$$

Therefore:

$$\mathbb{W} = \begin{pmatrix} 1 & -i\delta t \\ -i\delta t & 1 \end{pmatrix}. \tag{45}$$

3.2. Solving the Backward Euler Equations – the eigenvalue problem: From EQ. (40), one has

$$\begin{pmatrix} \psi_0(t=N\delta t) \\ \psi_1(t=N\delta t) \end{pmatrix} = \mathbb{W}^{-N} \begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} \tag{46}$$

This means you find the inverse matrix $\mathbb{W}^{-1}$, which satisfies $\mathbb{W}^{-1}\mathbb{W} = \mathbb{1}$, then raise it to the N'th power. We would like to have a closed form expression for $\psi_0(N\delta t)$ and $\psi_1(N\delta t)$ when $\psi_0(0)=1$ and $\psi_1(0)=0$. [If we were doing this on a computer it would be trivial – we just do a bunch of matrix multiplications by the inverse matrix $\mathbb{W}^{-1}$. Here, however, we want to do it by hand.]

There are several approaches to this sort of problem, but one classic approach starts with finding the eigenvalues s, s' and eigenvectors of $\mathbb{W}$:

$$\mathbb{W}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = s\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \tag{47}$$

and

$$\mathbb{W}\begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = s'\begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \tag{48}$$

Equivalently, these equations can be written

$$\frac{1}{s}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \mathbb{W}^{-1}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} \tag{49}$$

and

$$\frac{1}{s'}\begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \mathbb{W}^{-1}\begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \tag{50}$$

One then finds coefficients A and B such that

$$\begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = A\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} + B\begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \tag{51}$$

Matrices are *linear* operators, so

$$\mathbb{W}^{-n}\begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = A\mathbb{W}^{-n}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} + B\mathbb{W}^{-n}\begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \tag{52}$$

We can now use EQ. (49) and (50) to get

$$\mathbb{W}^{-n}\begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = A \times (s)^{-n}\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} + B \times (s')^{-n}\begin{pmatrix} b_0 \\ b_1 \end{pmatrix}. \tag{53}$$

Find $s, s', a_0, a_1, b_0, b_1$.

Solution 3.2. Finding the eigenvalues s amounts to solving the determinant equation:

$$\begin{vmatrix} 1-s & -\frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 1-s \end{vmatrix} = 0 \tag{54}$$

$$(1-s)^2 + \frac{\delta t^2}{\hbar} = 0 \tag{55}$$

$$s^2 - 2s + 1 + \frac{\delta t^2}{\hbar} = 0 \tag{56}$$

and so:

$$s = 1 + i\frac{\delta t}{\hbar}, \quad s' = 1 - i\frac{\delta t}{\hbar}, \tag{57}$$

to first order in δt. Now we wish to solve:

$$\begin{pmatrix} 1 & -\frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \left(1 + i\frac{\delta t}{\hbar}\right) \begin{pmatrix} a_0 \\ a_1 \end{pmatrix}. \tag{58}$$

This has solution:

$$\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{59}$$

Similarly, the Eigenvector equation:

$$\begin{pmatrix} 1 & -\frac{i\delta t}{\hbar} \\ -\frac{i\delta t}{\hbar} & 1 \end{pmatrix} \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \left(1 - i\frac{\delta t}{\hbar}\right) \begin{pmatrix} b_0 \\ b_1 \end{pmatrix} \tag{60}$$

has solution:

$$\begin{pmatrix} b_0 \\ b_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{61}$$

3.3. Find A and B.

Solution 3.3. We are given:

$$\begin{pmatrix} \psi_0(0) \\ \psi_1(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{62}$$

We therefore have $A = B = 1/2$.

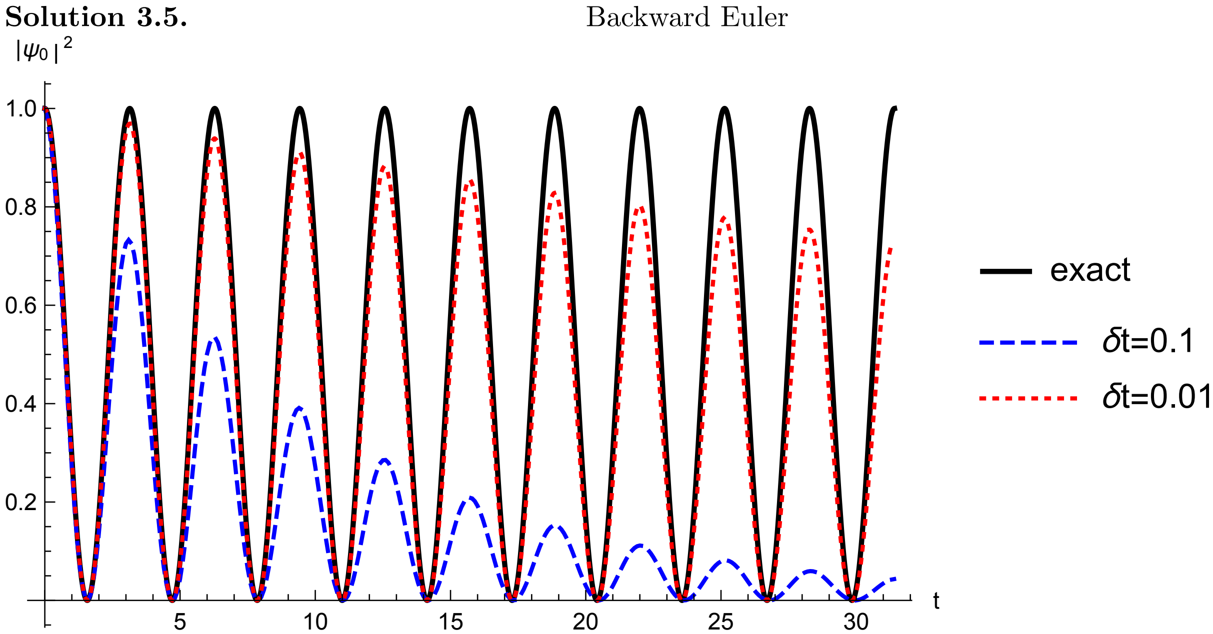
3.4. Find $\psi_0(N\delta t)$ and $\psi_1(N\delta t)$.

Solution 3.4. Putting everything together, we arrive at:

$$\begin{pmatrix} \psi_0(N\delta t) \\ \psi_1(N\delta t) \end{pmatrix} = \begin{pmatrix} \frac{1}{2}\left(1 - i\frac{\delta t}{\hbar}\right)^{-N} + \frac{1}{2}\left(1 + i\frac{\delta t}{\hbar}\right)^{-N} \\ \frac{1}{2}\left(1 - i\frac{\delta t}{\hbar}\right)^{-N} - \frac{1}{2}\left(1 + i\frac{\delta t}{\hbar}\right)^{-N} \end{pmatrix} \tag{63}$$

3.5. Comparison We want to understand how good our approximation is. Use a computer to make a plot which has time on the horizontal axis, and $|\psi_0|^2$ on the vertical axis. Plot the exact result for $0 < t < 10\pi$. Also plot the result of the Backward Euler Approximation, using timesteps $\delta t = 0.1$ and $\delta t = 0.01$. Properly label the axes, and include a legend.

Solution 3.5.



3.6. Comparison with Forward Euler Look at your homework from last week (or the solutions). What is the qualitative difference between the forward and backward Euler approximations? In Recitation 3, you will see an approximation for which the probabilities neither grow nor shrink.

Solution 3.6. With forward Euler the overall probability gradually increased increased with time, violating unitarity (conservation of probability). We can see that backward Euler has a steadily decreasing overall probability, again violating unitarity. The approximation used in recitation: the Unitary Euler approximation, conserves probability – thus it ends up being much more accurate at long times.

Problem 4. Heisenberg Equations of Motion

This is not a long problem. I just repeat in the statement of the question a summary of the technique which you should have seen in P3316. This technique will also be used in lecture 4 – so if this is a bit mysterious, wait until after lecture 4 to start this problem.

In this problem we will try to study the time dependence of $\langle x \rangle$ for a 1D simple harmonic oscillator. We will introduce a trick which lets us calculate such quantities *without* calculating the wavefunction or its time dependence. Recall from our first lecture that for any operator

$$\langle \hat{O} \rangle(t) = \int dx\, \psi^*(x,t)\hat{O}\psi(x,t). \tag{64}$$

If we take the time derivative of this expression we get

$$\partial_t \langle \hat{O} \rangle(t) = \int dx\, (\partial_t \psi^*(x,t))\hat{O}\psi(x,t) + \psi^*(x,t)\hat{O}\partial_t \psi(x,t). \tag{65}$$

But

$$\partial_t \psi(x,t) = \frac{1}{i\hbar}\hat{H}\psi(x,t), \tag{66}$$

and

$$\partial_t \psi^*(x,t) = \frac{i}{\hbar}[\hat{H}\psi(x,t)]^*, \tag{67}$$

Thus

$$\partial_t \langle \hat{O} \rangle(t) \;\; = \;\; \frac{i}{\hbar}\int dx\, [\hat{H}\psi(x,t)]^* \hat{O}\psi(x,t) - \psi^*(x,t)\hat{O}\hat{H}\psi(x,t). \tag{68}$$

The Hamiltonian has the property that it is Hermitian, meaning that for any wavefunctions ψ and ϕ,

$$\int dx\, [\hat{H}\psi(x,t)]^*\phi(x,t) = \int dx\, \psi(x,t)^* \hat{H}\phi(x,t). \tag{69}$$

[To prove this result, you just integrate by parts twice.]

Using the Hermitian property,

$$\begin{aligned} \partial_t \langle \hat{O} \rangle(t) &= \frac{1}{i\hbar}\int dx\, \psi^*(x,t)(\hat{O}\hat{H} - \hat{H}\hat{O})\psi(x,t) && (70) \\ &= \frac{1}{i\hbar}\langle [\hat{O},\hat{H}] \rangle. && (71) \end{aligned}$$

Lets specialize to the simple harmonic oscillator Hamiltonian:

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega_0^2\hat{x}^2, \tag{72}$$

and recall that

$$\begin{aligned} [\hat{x},\hat{p}] &= i\hbar && (73) \\ [\hat{x},\hat{p}^2] &= 2i\hbar\hat{p} && (74) \\ [\hat{x},\hat{x}] &= 0 && (75) \\ [\hat{x},\hat{x}^2] &= 0 && (76) \\ [\hat{p},\hat{x}] &= -i\hbar && (77) \\ [\hat{p},\hat{x}^2] &= -2i\hbar\hat{x} && (78) \\ [\hat{p},\hat{p}] &= 0 && (79) \\ [\hat{p},\hat{p}^2] &= 0. && (80) \end{aligned}$$

4.1. Use Eq. (71) to write $\partial_t \langle \hat{x} \rangle$ in terms of $\langle \hat{p} \rangle$.

Solution 4.1.

$$\begin{aligned}
\partial_t \langle \hat{x} \rangle &= \frac{1}{i} \left\langle \left[\hat{x}, \hat{H}\right] \right\rangle \\
&= \frac{1}{i} \left\langle \left[\hat{x}, \frac{\hat{p}^2}{2m}\right] + \left[\hat{x}, \frac{1}{2} m\omega_0^2 \hat{x}^2\right] \right\rangle \\
&= \frac{1}{2mi} \left\langle \left[\hat{x}, \hat{p}^2\right] \right\rangle \\
&= \frac{1}{m} \hat{p}
\end{aligned} \tag{81}$$

4.2. Use Eq. (71) to write $\partial_t \langle \hat{p} \rangle$ in terms of $\langle \hat{x} \rangle$.

Solution 4.2.

$$\begin{aligned}
\partial_t \langle \hat{p} \rangle &= \frac{1}{i} \left\langle \left[\hat{p}, \hat{H}\right] \right\rangle \\
&= \frac{1}{i} \left\langle \left[\hat{p}, \frac{\hat{p}^2}{2m}\right] + \left[\hat{p}, \frac{1}{2} m\omega_0^2 \hat{x}^2\right] \right\rangle \\
&= \frac{1}{2i} m\omega_0^2 \left\langle \left[\hat{x}, \hat{p}^2\right] \right\rangle \\
&= -m\omega_0^2 \langle \hat{x} \rangle
\end{aligned} \tag{82}$$

4.3. Solve these coupled differential equations. For notational simplicity, it is best to write $X = \langle \hat{x} \rangle$, and $P = \langle \hat{p} \rangle$.

Solution 4.3. We have the coupled equations:

$$\dot{X} = \frac{1}{m} P, \tag{83}$$

$$\dot{P} = -m\omega_0^2 X. \tag{84}$$

Taking a time derivative of the first equation, and then substituting in the second equation, we obtain a second order differential equation for X:

$$\ddot{X} = \frac{1}{m} \dot{P} \tag{85}$$

$$= -\omega_0^2 X. \tag{86}$$

This equation has solution:

$$X = X_0 \cos(\omega_0 t + \phi), \tag{87}$$

and for P:

$$P = -\omega_0 m X_0 \sin(\omega_0 t + \phi). \tag{88}$$

Problem 5. Feedback

5.1. How long did this homework take?

5.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair