Problem 1: Operators that Commute with the Hamiltonian are Conserved
adapted from Griffiths 3.17

Here is a very important theorem for the time-dependence of an expectation value:

\[ \frac{d\langle \hat{Q} \rangle}{dt} = i\hbar \left( \frac{\langle \hat{H} \hat{Q} \rangle}{\hbar} + \langle \frac{\partial \hat{Q}}{\partial t} \rangle \right) \]

It’s a bit hard to see, but the take-away from this formula is a standard piece of QM knowledge:

An operator that commutes with the Hamiltonian is conserved.

That is what everyone remembers about this formula, but some “fine-print” is missing. To be exact,

\textit{The expectation value of} an operator that commutes with the Hamiltonian is conserved as long as the operator has no implicit time-dependence of its own.\(^1\)

(a) Derive the theorem in the box. Hint: see the formalism chapter of any QM textbook. Also, a question that you can only answer if you’ve worked through the derivation: does this theorem require the operator \(Q\) and/or the operator \(H\) (the Hamiltonian) to be Hermitian?

Next let’s try out our new formula. Calculate \(d\langle \hat{Q} \rangle / dt\) for the operators \(Q\) given below. In each case comment on the result with particular reference to one or more of these prior results or concepts:

- the time-independence of a particle’s total probability :
  \[ \frac{d}{dt} \int_{-\infty}^{\infty} \psi^* \psi \, dx = 0 \]

- Ehrenfest’s theorems #1 and #2 :
  \[ \langle p \rangle = m \frac{d\langle x \rangle}{dt} \quad \text{and} \quad \frac{d\langle p \rangle}{dt} = -\frac{d\langle V \rangle}{dx} \]

- conservation of energy

(b) \(Q = 1\)
(c) \(Q = H = \text{the Hamiltonian (assuming it has no explicit time-dependence)}\)
(d) \(Q = x = \text{the position operator}\)
(e) \(Q = p = \text{the momentum operator}\)

Problem 2: The Virial Theorem
adapted from Griffiths 3.31

The \textbf{Virial Theorem} is an extremely useful rule-of-thumb that every physicist should have in memory in some form. Here is the most common version of the theorem:

If a particle is held in a bound state by an inverse-square central force \(F(r) \sim 1/r^2\),
then its average kinetic energy is half its average \textit{potential energy}:

\[ \langle T \rangle = \frac{1}{2} \langle V \rangle. \]

This covers all bound states help together by \(1/r^2\) forces, which is a \textit{lot} as it includes anything held together by gravity (planets orbiting around stars) or electricity (electrons bound by nuclei). The absolute-value bars on potential energy \(\langle V \rangle\) are there because a particle in a bound state has negative potential energy (relative to its presumed zero at infinity, where the particle would be free). The average signs refer to the cycle average of \(T\)

\(^1\) This italicized piece of fine print refers to the right-hand term of the formula, \(<\partial \hat{Q}/\partial t>\). Can you think of a physical observable whose operator is explicitly time-dependent? It is tricky … Griffiths provides a nice example: \(Q = \text{the Hamiltonian for a simple-harmonic oscillator with a time-dependent spring constant } k(t) = -\hbar^2/2m \partial^2/\partial x^2 + \tfrac{1}{2} k(t) x^2.\)
and \( V \), i.e. the average over one period of their motion. This rule-of-thumb is really useful: you only have to calculate the kinetic energy or the potential energy, and you have the other one, nice! The total energy, by the way, is \( E = \langle T \rangle + \langle V \rangle = -\frac{1}{2} \langle V \rangle + \langle V \rangle = \frac{1}{2} \langle V \rangle = \) negative, as it must be for a bound state.

My personal visualization of the Virial Theorem is that a bound state is a particle in a well of negative potential energy \( V < 0 \), and its kinetic energy lets it climb half-way up the well, giving a total energy of \( \frac{1}{2} V \). My other take-away is how extraordinary it is that the potential and kinetic energies of all these bound states are always of the same order! They are only different by a factor of 2, when they could by different by 7 orders of magnitude or something. This is a BIG THING TO KNOW.

Attractive inverse-square central forces \( (F_r \sim -1/r^2) \) are described by potentials \( V \sim -1/r \). The General Virial Theorem in Classical Mechanics extends beyond \( 1/r \) potentials:

For a potential \( V(r) \sim r^n \), the Classical Virial Theorem is \( \langle T \rangle = n \langle V \rangle / 2 \).

For inverse-square forces, \( n = -1 \), so we recover the familiar \( \langle T \rangle = -\frac{1}{2} \langle V \rangle \). For a linear spring force \( \sim r \), the potential is \( \sim r^2 \) so \( n = 2 \), and we get \( \langle T \rangle = \langle V \rangle \). This is the second most common incidence of the virial theorem that folks have in their memories. The spring result is easy to understand because we know that the energy in an oscillating thing-on-a-spring system oscillates back and forth from all-potential at the endpoints (the turning-points where the “thing” stops before reversing direction) to all-kinetic at the midpoint (where the oscillating system is necessarily at equilibrium, so \( V = 0 \)).

That was the classical version. Now for the quantum version!

(a) Use our new boxed equation from problem 1 and the fact that the Hamiltonian \( H = T + V \) to derive this result:

\[
\frac{d\langle xp\rangle}{dt} = 2\langle T \rangle - \left\langle x \frac{dV}{dx} \right\rangle
\]

(b) Show that when the system is in an energy eigenstate, i.e. when the system’s wavefunction is

\[
\Psi(x, t) = \psi_E(x) e^{-iE t/\hbar} \quad \text{with} \quad \hat{H}\psi_E(x) = E\psi_E(x),
\]

then the left-hand side of the relation in part (a) is zero.

FYI: The word stationary state is often used to refer to energy eigenstates that are normalizable. Why? Because the space-time separation of such a state, \( \Psi(x, t) = \psi_E(x) e^{-iE t/\hbar} \), leads to these consequences:

- the probability density \( P(x, t) = \Psi^*\Psi \) is just \( \psi(x)^*\psi(x) \) and so is independent of time, and
- the expectation value \( \langle Q \rangle \) of any dynamical observable \( Q \) is independent of time.

Everything physical about this state is constant with time, hence “stationary”. This exercise allows you to remind yourself of the reason for that second property.

(c) Thus, when the system is in an energy eigenstate, we have

\[
2\langle T \rangle = \left\langle x \frac{dV}{dx} \right\rangle
\]

This is the quantum version of the Virial Theorem. Hmm, this looks quite different from the classical virial theorem, \( \langle T \rangle = n \langle V \rangle / 2 \) for a potential \( V(r) \sim r^n \) … but it’s not actually different. Show that the classical virial theorem can equivalently be written as \( 2\langle T \rangle = \langle r dV/dr \rangle \) (again under the assumption that \( V(r) \sim r^n \)).