Quantum Mechanics II: PHYS 314 (Spring 2021)
Problem Set 3–Solutions.

Overview

In this Problem Set you will practice manipulating operators and operator exponentials by studying the parity operator in three dimensions, and by investigating Galilean transformations in quantum mechanical systems Part (d) of Problem 2 is for **extra credit**. You do **not** need to complete this part of question to receive full marks for the Problem Set.

Question 1 [Griffiths 6.1] 20pts

Consider the parity operator in three dimensions.

(a) Show that $\psi'(\mathbf{r}) = \widehat{\Pi}\,\psi(\mathbf{r}) = \psi(-\mathbf{r})$ is equivalent to a mirror reflection followed by a rotation.

(b) Show that, for ψ expressed in polar coordinates, the action of the parity operator is

$$\widehat{\Pi}\,\psi(r,\theta,\phi) = \psi(r,\pi-\theta,\phi+\pi).$$

(c) Show that for the hydrogenic orbitals,

$$\widehat{\Pi}\,\psi_{n\ell m}(r,\theta,\phi) = (-1)^{\ell}\psi(r,\theta,\phi).$$

That is, $\psi_{n\ell m}$ is an eigenstate of the parity operator, with eigenvalue $(-1)^{\ell}$.

Solution 1

(a) A reflection across the (x, y)-plane gives

$$\psi'(x,y,z) = \widehat{M}\,\psi(x,y,z) = \psi(x,y,-z),$$

whereas a rotation by π in the (x, y)-plane leads to

$$\psi'(x,y,z) = \widehat{R}(\pi)\,\psi(x,y,z) = \psi(-x,-y,z).$$

Therefore, composing these two operations gives

$$\psi''(x,y,z) = \widehat{M}\cdot\widehat{R}(\pi)\,\psi(x,y,z) = \psi(-x,-y,-z) = \widehat{\Pi}\,\psi(x,y,z),$$

as required.

(b) The simplest way to solve this is to rewrite the Cartesian coordinates in polar coordinates,

$$x = r\sin\theta\cos\phi,$$
$$y = r\sin\theta\sin\phi,$$
$$z = r\cos\theta,$$

then, motivated by the form of the expression given, replace $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$ to obtain

$$x = r\sin(\pi-\theta)\cos(\pi+\phi) = r\sin\theta(\cos(-\phi)) = -x,$$
$$y = r\sin(\pi-\theta)\sin(\pi+\phi) = r\sin\theta(\sin(-\phi)) = -y,$$
$$z = r\cos(\pi-\theta) = r(-\cos\theta) = -z.$$

From this, we can see that this replacement is identical to changing the sign of the Cartesian coordinates. In other words,

$$\widehat{\Pi}\,\psi(r,\theta,\phi) = \psi(r,\pi-\theta,\phi+\pi),$$

as required.

(c) The hydrogenic orbitals can be written in the form

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)Y_\ell^m(\theta,\phi),$$

which is Equation 4.74 of Griffiths and Schroeter. Here R is the radial wavefunction and the Y_ℓ^m are the spherical harmonics, defined in Equation 4.32 of Griffiths and Schroeter,

$$Y_\ell^m(\theta,\phi) = K_\ell^m e^{im\phi} P_\ell^m(\cos\theta). \tag{1}$$

Here the K_ℓ^m are normalization constants that are independent of θ and ϕ, and $P_\ell^m(\cos\theta)$ are the associated Legendre functions. Substituting in $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$, we see that

$$Y_\ell^m(\pi-\theta,\phi+\pi) = K_\ell^m e^{im\phi} e^{im\pi} P_\ell^m(\cos(\pi-\theta)) = K_\ell^m e^{im\phi}(-1)^m P_\ell^m(-\cos\theta).$$

Now we use Equation 4.27 to show that

$$\begin{aligned} P_\ell^m(-x) &= (-1)^m(1-(-x)^2)^{m/2}\left(\frac{\mathrm{d}}{\mathrm{d}(-x)}\right)^m P_\ell(-x) \\ &= (-1)^m\left[(-1)^m(1-x^2)^{m/2}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^m P_\ell(-x)\right]. \end{aligned}$$

Finally, we apply Equation 4.28 to observe that

$$\begin{aligned} P_\ell(-x) &= \frac{1}{2^\ell \ell!}\left(\frac{\mathrm{d}}{\mathrm{d}(-x)}\right)^\ell ((-x)^2-1)^\ell \\ &= (-1)^\ell \left[\frac{1}{2^\ell \ell!}\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^\ell ((-x)^2-1)^\ell\right] \\ &= (-1)^\ell P_\ell(x). \end{aligned}$$

Plugging this into our expression for $P_\ell^m(-x)$, we see that

$$P_\ell^m(-x) = (-1)^{m+\ell} P_\ell^m(x).$$

This means that

$$\begin{aligned} Y_\ell^m(\pi-\theta, \phi+\pi) &= K_\ell^m e^{im\phi} e^{im\pi} P_\ell^m(\cos(\pi-\theta)) \\ &= K_\ell^m e^{im\phi}(-1)^m(-1)^{m+\ell} P_\ell^m(\cos\theta) \\ &= (-1)^\ell Y_\ell^m(\theta,\phi). \end{aligned}$$

The radial wavefunction is independent of these angles, so we have

$$\psi_{n\ell m}(r, \pi-\theta, \phi+\pi) = (-1)^\ell \psi(r,\theta,\phi),$$

We know that in three dimensions, applying the parity operator is equivalent to the angle replacements $\theta \to \pi - \theta$ and $\phi \to \phi + \pi$, so we can deduce that

$$\widehat{\Pi}\, \psi_{n\ell m}(r,\theta,\phi) = (-1)^\ell \psi(r,\theta,\phi),$$

as required.

Question 2 [Griffiths 6.35] 30pts

A **Galilean transformation** performs a boost from a reference frame $\mathcal{S}$ to a reference frame $\mathcal{S}'$ moving with velocity $-v$ with respect to $\mathcal{S}$ (the origins of the two frames coincide at $t = 0$). The unitary operator that carries out a Galilean transformation at time t is

$$\widehat{\Gamma}(v,t) = \exp\left[-\frac{i}{\hbar} v\,(t\widehat{p} - m\widehat{x})\right].$$

(a) Find $\widehat{x}' = \widehat{\Gamma}^\dagger \widehat{x} \widehat{\Gamma}$ and $\widehat{p}' = \widehat{\Gamma}^\dagger \widehat{p} \widehat{\Gamma}$ for an infinitesimal transformation with velocity δ. What is the physical meaning of your result?

(b) Show that

$$\widehat{\Gamma}(v,t) = \exp\left[\frac{i}{\hbar}\left(mv\widehat{x} - \frac{mv^2}{2}t\right)\right]\widehat{T}(vt)$$
$$= \widehat{T}(vt)\exp\left[\frac{i}{\hbar}\left(mv\widehat{x} + \frac{mv^2}{2}t\right)\right],$$

where $\widehat{T}$ is the spatial translation operator (Equation 6.3),

$$\widehat{T}(a) = \exp\left[-\frac{ia}{\hbar}\widehat{p}\right].$$

You will need to use the Baker-Campbell-Hausdorff formula (Problem 3.29)

$$\widehat{\Gamma} = e^{\widehat{A}+\widehat{B}} = e^{\widehat{A}}e^{\widehat{B}}e^{-\widehat{C}/2}.$$

(c) Show that if Ψ is a solution to the time-dependent Schrödinger equation with Hamiltonian

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + V(x)$$

then the boosted wavefunction $\Psi' = \widehat{\Gamma}(v,t)\Psi$ is a solution to the time-dependent Schrödinger equation with the potential $V(x)$ in motion:

$$\widehat{H} = \frac{\widehat{p}^2}{2m} + V(x - vt).$$

Note:

$$\frac{\mathrm{d}}{\mathrm{d}t}e^{\widehat{A}} = e^{\widehat{A}}\frac{\mathrm{d}\widehat{A}}{\mathrm{d}t}$$

only if

$$\left[\widehat{A}, \frac{\mathrm{d}\widehat{A}}{\mathrm{d}t}\right] = 0.$$

(d) [EXTRA CREDIT: 5 PTS]

Show that the result of Problem 2.50a,

$$\Psi(x,t) = \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x-vt|/\hbar^2}\exp\left\{-\frac{i}{\hbar}\left[\left(E + \frac{mv^2}{2}\right)t - mvx\right]\right\},$$

for a moving delta-function well $V(x,t) = -\alpha\delta(x - vt)$, is an example of this result [i.e. the result of part (c)].

Solution 2

(a) For an infinitesimal velocity, δ, we have

$$\begin{aligned}\widehat{x}' &= \widehat{\Gamma}^\dagger \widehat{x} \widehat{\Gamma} \\ &\simeq \left[1 + \frac{i}{\hbar}\delta\left(t\widehat{p} - m\widehat{x}\right)\right] \widehat{x} \left[1 - \frac{i}{\hbar}\delta\left(t\widehat{p} - m\widehat{x}\right)\right] \\ &\simeq \widehat{x} + \frac{i}{\hbar}\delta t[\widehat{p}, \widehat{x}] - \frac{i}{\hbar}\delta m[\widehat{x}, \widehat{x}] \\ &\simeq \widehat{x} + \delta t.\end{aligned}$$

We also have

$$\begin{aligned}\widehat{p}' &= \widehat{\Gamma}^\dagger \widehat{p} \widehat{\Gamma} \\ &\simeq \left[1 + \frac{i}{\hbar}\delta\left(t\widehat{p} - m\widehat{x}\right)\right] \widehat{x} \left[1 - \frac{i}{\hbar}\delta\left(t\widehat{p} - m\widehat{x}\right)\right] \\ &\simeq \widehat{p} + \frac{i}{\hbar}\delta t[\widehat{p}, \widehat{p}] - \frac{i}{\hbar}\delta m[\widehat{x}, \widehat{p}] \\ &\simeq \widehat{p} + \delta m.\end{aligned}$$

These equations tell us that: first, the origins of the two coordinate systems are displaced by an amount δt at time t; and second, that the velocity of the particle in the primed frame is just the unprimed velocity plus δ. [Note also there is typo in the equations for $\widehat{p}$ in the official textbook solutions and a mistake in the result for $\widehat{x}'$ in those solutions, too!]

(b) Define the operators

$$\widehat{A} = -\frac{ivt}{\hbar}\widehat{p}, \qquad \text{and} \qquad \widehat{B} = -\frac{ivt}{\hbar}\widehat{p},$$

which have commutator

$$\widehat{C} = [\widehat{A}, \widehat{B}] = \frac{mv^2 t}{\hbar}[\widehat{p}, \widehat{x}] = -imv^2 t.$$

We can then apply the Baker-Campbell-Hausdorff formula

$$\widehat{\Gamma} = e^{\widehat{A}+\widehat{B}} = e^{\widehat{A}} e^{\widehat{B}} e^{-\widehat{C}/2},$$

to obtain

$$\widehat{\Gamma} = \exp\left[-\frac{i}{\hbar}vt\widehat{p}\right] \exp\left[\frac{i}{\hbar}mv\widehat{x}\right] \exp\left[\frac{i}{\hbar}\frac{mv^2}{2}t\right].$$

The first exponential is the translation operator and so we have

$$\boxed{\widehat{\Gamma} = \widehat{T}\exp\left[\frac{i}{\hbar}\left(mv\widehat{x} + \frac{mv^2}{2}t\right)\right]}.$$

We can also switch the $\widehat{A}$ and $\widehat{B}$, which changes the sign of the commutator, so we have

$$\boxed{\widehat{\Gamma} = \exp\left[\frac{i}{\hbar}\left(mv\widehat{x} - \frac{mv^2}{2}t\right)\right]\widehat{T}}.$$

(c) We consider the "primed" wavefunction

$$\widehat{\Psi}' = \Gamma\Psi,$$

which satisfies

$$i\hbar\frac{\partial}{\partial t}\left(\widehat{\Gamma}\Psi\right) = i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Psi + i\hbar\Gamma\frac{\partial\Psi}{\partial t}.$$

Assuming Ψ satisfies the (time-independent) Schrödinger equation, with Hamiltonian H, we find

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left(\widehat{\Gamma}\Psi\right) &= i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Psi + \Gamma\widehat{H}\Psi \\ &= \left[i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Gamma^\dagger + \Gamma\widehat{H}\Gamma^\dagger\right]\Gamma\Psi, \end{aligned}$$

where in the second line we've inserted the identity in the form $\Gamma^\dagger\Gamma = \mathbb{I}$.

This equation can be cast into the form of the Schrödinger equation if the Hamiltonian is

$$\begin{aligned} H_\gamma &= \Gamma\widehat{H}\Gamma^\dagger + i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Gamma^\dagger \\ &= \exp\left[\frac{i}{\hbar}\left(mv\widehat{x} - \frac{mv^2}{2}t\right)\right]\widehat{T}(vt)\widehat{H}\widehat{T}^\dagger(vt)\exp\left[-\frac{i}{\hbar}\left(mv\widehat{x} - \frac{mv^2}{2}t\right)\right] + i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Gamma^\dagger \\ &= \exp\left[\frac{i}{\hbar}mv\widehat{x}\right]\left(\frac{\widehat{p}^2}{2m} + V(x-vt)\right)\exp\left[-\frac{i}{\hbar}mv\widehat{x}\right] + i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Gamma^\dagger. \end{aligned}$$

Now we need to calculate the derivative

$$\begin{aligned}
\frac{\mathrm{d}\Gamma}{\mathrm{d}t} &= \left(\frac{\mathrm{d}}{\mathrm{d}t}\widehat{T}(vt)\right)\exp\left[\frac{i}{\hbar}\left(mv\widehat{x}+\frac{mv^2}{2}t\right)\right]+\widehat{T}(vt)\frac{\mathrm{d}}{\mathrm{d}t}\exp\left[\frac{i}{\hbar}\left(mv\widehat{x}+\frac{mv^2}{2}t\right)\right] \\
&= -\frac{i}{\hbar}v\widehat{p}\widehat{T}(vt)\exp\left[\frac{i}{\hbar}\left(mv\widehat{x}+\frac{mv^2}{2}t\right)\right] \\
&\qquad +\widehat{T}(vt)\frac{i}{\hbar}\left(\frac{mv^2}{2}\right)\exp\left[\frac{i}{\hbar}\left(mv\widehat{x}+\frac{mv^2}{2}t\right)\right] \\
&= -\frac{i}{\hbar}\left(v\widehat{p}-\frac{mv^2}{2}\right)\widehat{\Gamma}.
\end{aligned}$$

This means that

$$i\hbar\frac{\mathrm{d}\Gamma}{\mathrm{d}t}\Gamma^\dagger = i\hbar\left[-\frac{i}{\hbar}\left(v\widehat{p}-\frac{mv^2}{2}\right)\widehat{\Gamma}\right]\Gamma^\dagger = v\widehat{p}-\frac{mv^2}{2}.$$

Next we need

$$\begin{aligned}
&\exp\left[\frac{i}{\hbar}mv\widehat{x}\right]\left(\frac{\widehat{p}^2}{2m}+V(x-vt)\right)\exp\left[-\frac{i}{\hbar}mv\widehat{x}\right] \\
&= \frac{1}{2m}\exp\left[\frac{i}{\hbar}mv\widehat{x}\right]\widehat{p}^2\exp\left[-\frac{i}{\hbar}mv\widehat{x}\right]+V(x-vt) \\
&= \frac{1}{2m}\exp\left[\frac{i}{\hbar}mv\widehat{x}\right]\widehat{p}\exp\left[-\frac{i}{\hbar}mv\widehat{x}\right]\exp\left[\frac{i}{\hbar}mv\widehat{x}\right]\widehat{p}\exp\left[-\frac{i}{\hbar}mv\widehat{x}\right]+V(x-vt).
\end{aligned}$$

To calculate this, we use

$$\begin{aligned}
\left[\exp\left[\frac{i}{\hbar}mv\widehat{x}\right],\widehat{p}\right] &= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{imv}{\hbar}\right)^n[\widehat{x}^n,\widehat{p}] \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{imv}{\hbar}\right)^n i\hbar n\widehat{x}^{n-1} \\
&= -mv\sum_{n=1}^{\infty}\frac{1}{(n-1)!}\left(\frac{imv}{\hbar}\widehat{x}\right)^{n-1} \\
&= -mv\exp\left[\frac{imv}{\hbar}\widehat{x}\right].
\end{aligned}$$

Using this, we can calculate

$$\exp\left[\frac{i}{\hbar}mv\widehat{x}\right]\widehat{p}\exp\left[-\frac{i}{\hbar}mv\widehat{x}\right] = \widehat{p}-mv.$$

Now we have to put all these pieces together, which leads to

$$\begin{aligned}\widehat{H}_\gamma &= \frac{1}{2m}(\widehat{p} - mv)^2 + V(x - vt) + v\widehat{p} - \frac{mv^2}{2} \\ &= \frac{\widehat{p}^2}{2m} + V(x - vt).\end{aligned}$$

(d) [THIS PART OF THE SOLUTION IS WORTH 5 PTS EXTRA CREDIT. IT IS NOT NECESSARY TO COMPLETE THIS QUESTION TO OBTAIN FULL MARKS OF 50/50.]

The solution in the frame with the stationary potential is

$$\Psi(x, t) = \psi_0(x)e^{-iEt/\hbar},$$

where E is the bound-state energy. In the moving frame, the result of part (c) tells us the solution is

$$\begin{aligned}\Psi'(x, t) &= \widehat{\Gamma}\Psi \\ &= \exp\left[\frac{i}{\hbar}\left(mv\widehat{x} - \frac{mv^2}{2}t\right)\right]\widehat{T}(vt)\frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x|^2/\hbar^2}e^{-iEt/\hbar} \\ &= \exp\left[\frac{i}{\hbar}\left(mv\widehat{x} - \frac{mv^2}{2}t\right)\right]\frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x-vt|^2/\hbar^2}e^{-iEt/\hbar} \\ &= \frac{\sqrt{m\alpha}}{\hbar}e^{-m\alpha|x-vt|/\hbar^2}\exp\left\{-\frac{i}{\hbar}\left[\left(E + \frac{mv^2}{2}\right)t - mv\widehat{x}\right]\right\}.\end{aligned}$$

This is exactly the solution in Problem 2.50.