1 2-State Systems

(i)

Let’s work in the eigenbasis of $\sigma^3$, so that
\[
|b^{(\pm)}\rangle = |\pm\rangle \tag{1.1}
\]
\[
|a^{(\pm)}\rangle = (|+\rangle \pm |-\rangle)/\sqrt{2}. \tag{1.2}
\]

Then,
\[
U = \sum_{a=\pm} |b^{(a)}\rangle\langle a^{(a)}| = |b^{(+)}\rangle\langle a^{(+)}| + |b^{(-)}\rangle\langle a^{(-)}|
\]
\[
= |+\rangle \left( \frac{|+\rangle + |-\rangle}{\sqrt{2}} \right) + |-\rangle \left( \frac{|+\rangle - |-\rangle}{\sqrt{2}} \right) \tag{1.3}
\]
\[
= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.
\]

Thus, $U = (\sigma^1 - \sigma^3)/\sqrt{2}$, and since $\{\sigma^i, \sigma^j\} = 2\delta^{ij}$, we have
\[
U^\dagger U = \frac{1}{2}(\sigma^1 + \sigma^3)^2 = \frac{1}{2} ((\sigma^1)^2 + (\sigma^3)^2 + \{\sigma^1, \sigma^3\}) = 1. \tag{1.4}
\]

(ii)

Starting with $\hat{n} = \sin(\gamma)\hat{x} + \cos(\gamma)\hat{z}$, we find
\[
\left( \hat{n} \cdot \vec{S} \right) = \frac{\hbar}{2} \left( \sin(\gamma)\sigma^1 + \cos(\gamma)\sigma^3 \right) = \frac{\hbar}{2} \left( \begin{array}{cc} \cos(\gamma) & \sin(\gamma) \\ \sin(\gamma) & -\cos(\gamma) \end{array} \right). \tag{1.5}
\]

Now, we need to know the eigenvectors for this operator. They have eigenvalues $\pm \frac{\hbar}{2}$ and in terms of the $\sigma^3$ eigenbasis, they are
\[
|\pm\rangle_n = \cos(\gamma/2)|\pm\rangle \pm \sin(\gamma/2)|\mp\rangle. \tag{1.6}
\]

Since $S_x = \frac{\hbar}{2} |+\rangle\langle -| + \frac{\hbar}{2} |-\rangle\langle +|$, then in either of the states $|\pm\rangle_n$
\[
\langle S_x \rangle_{\pm n} = \frac{\hbar}{2} n(\pm) \left( |+\rangle\langle -| + |-\rangle\langle +| \right) |\pm\rangle_n
\]
\[
= \pm \hbar\cos(\gamma/2)\sin(\gamma/2) \tag{1.7}
\]
\[
= \pm \frac{\hbar}{2} \sin(\gamma).
\]
Now, $S_x^2 = \frac{\hbar^2}{4} \mathbf{1}$ and so

$$(\Delta S_x)^2 = \langle S_x^2 \rangle - \langle S_x \rangle^2 = \frac{\hbar^2}{4} \left(1 - (\pm \sin(\gamma))^2\right) = \frac{\hbar^2}{4} \cos^2(\gamma),$$

or simply $\Delta S_x = \frac{\hbar}{2} \cos(\gamma)$. For the special cases,

$$
\begin{array}{ccc}
\gamma & \langle S_x \rangle & \langle \Delta S_x \rangle \\
0 & 0 & \frac{\hbar}{2} \\
\frac{\pi}{4} & \pm \frac{\hbar}{2\sqrt{2}} & \frac{\hbar}{2\sqrt{2}} \\
\frac{\pi}{2} & \pm \frac{\hbar}{2} & 0
\end{array}
$$

which is exactly what we expect for a state that’s rotated for an even combination of two eigenvectors into a single one.

## 2 Evolution of a 2-State System

There’s a nice trick for solving this problem, which is to go to a rotating frame. By defining the coefficients

$$b_{\pm}(t) = e^{\pm i\omega t/2}c_{\pm}(t).$$

we obtain a new wavefunction

$$|\tilde{\psi}(t)\rangle = b_+(t)|+\rangle + b_-(t)|-\rangle$$

which obeys $i\hbar \partial_t |\tilde{\psi}(t)\rangle = \tilde{H}|\tilde{\psi}(t)\rangle$, where the new Hamiltonian

$$\tilde{H} = \frac{\hbar}{2} (-\Delta \omega \sigma^3 + \omega_1 \sigma^1)$$

is now time-independent! In the last step I introduced the quantities $\Delta \omega \equiv \omega - E_0/\hbar$ and $\omega_1 \equiv 2\epsilon/\hbar$.

Now we proceed as usual, finding the eigenvalues and eigenvectors of this $2 \times 2$ Hamiltonian matrix. The results of this are: the eigenvalues

$$E_{\pm} = \pm \frac{\hbar}{2} \tilde{\omega} \quad \text{with} \quad \tilde{\omega} = \sqrt{(\Delta \omega)^2 + \omega_1^2}$$

and the associated eigenvectors

$$|\psi_{\pm}\rangle = \frac{\pm \omega_1 |+\rangle + \omega_2 |\mp\rangle}{\sqrt{\omega_1^2 + \omega_2^2}} \quad \text{with} \quad \omega_2 = \tilde{\omega} + \Delta \omega.$$
In terms of the original basis, we have $|\pm\rangle = (\pm \omega_1 |\psi_+\rangle + \omega_2 |\psi_-\rangle)/\sqrt{\omega_1^2 + \omega_2^2}$. Now we are in a position to find the time-evolved wavefunction:

$$|\tilde{\psi}(t)\rangle = e^{-i\hat{H}t/\hbar} |\tilde{\psi}(0)\rangle = e^{-i\hat{H}t/\hbar} |\psi_+\rangle = \frac{1}{\sqrt{\omega_1^2 + \omega_2^2}} \left[ e^{-i\tilde{\omega}t/2\omega_2} |\psi_+\rangle - e^{i\tilde{\omega}t/2\omega_1} |\psi_-\rangle \right]$$

$$= \frac{1}{\omega_1^2 + \omega_2^2} \left[ e^{-i\tilde{\omega}t/2\omega_2} (\omega_1 |+\rangle + \omega_2 |-) - e^{i\tilde{\omega}t/2\omega_1} (\omega_2 |+\rangle - \omega_1 |-) \right]$$  \hspace{1cm} (2.6)

Now, making use of the identity $\omega_1^2 + \omega_2^2 = 2\tilde{\omega}\omega_2$ and rotating back to our original $c_{\pm}(t)$ variables, we find

$$c_+(t) = e^{-i\tilde{\omega}t/2\omega_1} \sin \left( \frac{\tilde{\omega}t}{2} \right)$$  \hspace{1cm} (2.7)

$$c_-(t) = \frac{e^{i(\omega+\tilde{\omega})t/2\omega_2}}{2\tilde{\omega}\omega_2} \left[ \omega_1^2 + \omega_2^2 e^{-i\tilde{\omega}t} \right].$$  \hspace{1cm} (2.8)

For completeness, we recall the various frequencies which have been defined throughout:

$$\Delta \omega = E_0/\hbar - \omega$$

$$\omega_1 = 2\epsilon/\hbar$$

$$\tilde{\omega} = \sqrt{(\Delta \omega)^2 + \omega_1^2}$$

$$\omega_2 = \Delta \omega + \tilde{\omega}$$

As a check on this result, it’s good to verify that $|c_+(t)|^2 + |c_-(t)|^2 = 1$.

**Note:** Be careful not to try to diagonalize $H(t)$ directly, because this will not work for a rather subtle reason. While it’s true that we can find a basis in which $H$ is diagonal, with entries $\pm E \equiv \pm \sqrt{E_0^2/4 + \epsilon^2}$, the resulting eigenvectors are time-dependant and so $i\partial_t$ is no longer diagonal.

Specifically, if we denote the diagonalized Hamiltonian as $\hat{H}$, let $S(t)$ be the similarity transform between $H(t)$ and $\hat{H}$, and also write $|\tilde{\psi}(t)\rangle = S(t) |\psi(t)\rangle$ for the wavefunction in this basis, then the time-dependant Schrödinger equation becomes

$$\hat{H} |\tilde{\psi}\rangle = \hat{H} |\tilde{\psi}\rangle = (\hat{H} - i\hbar \partial_t S^{-1}) |\tilde{\psi}\rangle.$$

And so, we’re left with a new Schrödinger equation to solve,

$$i\hbar \partial_t |\tilde{\psi}\rangle = (\hat{H} - i\hbar S \partial_t S^{-1}) |\tilde{\psi}\rangle.$$

(2.9)
It’s straightforward enough to work out $S(t)$, since its columns are just the eigenvectors, and it is

$$S(t) = \frac{1}{\sqrt{1 + \gamma^2}} \begin{pmatrix} 1 & -\gamma e^{-i\omega t} \\ \gamma e^{i\omega t} & 1 \end{pmatrix}$$

(2.11)

where $\gamma = (E - E_0/2)/\epsilon$. Then,

$$iS\partial_t S^{-1} = \frac{\omega \gamma}{1 + \gamma^2} \begin{pmatrix} -\gamma & e^{-i\omega t} \\ e^{i\omega t} & \gamma \end{pmatrix}$$

(2.12)

and in particular $(\hat{H} - i\hbar S\partial_t S^{-1})$ is no longer diagonal, nor is it time-independent. Thus, we arrive back essentially where we started. The “extra term” (2.12) is the reason that we cannot simply exponentiate $\hat{H}$ to obtain the evolution operator, and these cannot be overlooked.

### 3 Particle in a Suddenly Expanding Box (5.2.1)

With the particle constrained to lie in $|x| \leq L/2$, the groundstate wavefunction is

$$\psi_1 = \begin{cases} \sqrt{\frac{2}{L}} \cos \left( \frac{\pi x}{L} \right), & |x| \leq \frac{L}{2} \\ 0, & |x| \geq \frac{L}{2} \end{cases}.$$  

(3.1)

When the box expands, the new groundstate of the system is

$$\psi'_1 = \begin{cases} \sqrt{\frac{1}{L}} \cos \left( \frac{\pi x}{2L} \right), & |x| \leq L \\ 0, & |x| \geq L \end{cases}.$$  

(3.2)

The probability of finding our state (3.1) in the new groundstate depends on the overlap amplitude

$$\langle \psi_1 | \psi'_1 \rangle = \frac{\sqrt{2}}{L} \int_{-\pi/4}^{\pi/4} (\cos(3\theta) + \cos(\theta)) d\theta = \frac{\sqrt{2}}{\pi} \left( \frac{2}{3} \sin \left( \frac{3\pi}{4} \right) + 2 \sin \left( \frac{\pi}{4} \right) \right) = \frac{8}{3\pi}.$$  

(3.3)

having used the relation

$$\cos(2\theta) \cos(\theta) = \frac{e^{2i\theta} + e^{-2i\theta}}{4} \frac{(e^{i\theta} + e^{-i\theta})}{4} = \frac{e^{3i\theta} + e^{-3i\theta} + e^{i\theta} + e^{-i\theta}}{4} = \frac{\cos(3\theta) + \cos(\theta)}{2}.$$  

(3.4)

Then, the probability of finding the particle in the new groundstate is

$$\mathcal{P}(n' = 1) = |\langle \psi_1 | \psi'_1 \rangle|^2 = \left( \frac{8}{3\pi} \right)^2.$$  

(3.5)
4 Existence of Bound States in One-Dimension (5.2.2)

a) Suppose we have a complete set of energy eigenfunctions $|\psi_n\rangle$, with

$$H|\psi_n\rangle = E_n|\psi_n\rangle.$$  \hfill (4.1)

By definition, the ground state has the lowest energy, so $E_n \geq E_0, \forall n$. We can expand any state in terms of the energy eigenbasis,

$$|\psi\rangle = \sum_n c_n|\psi_n\rangle,$$  \hfill (4.2)

for some (complex) coefficients $c_n$, normalized such that $\sum_n |c_n|^2 = 1$. Then, it follows directly that

$$\langle \psi | H | \psi \rangle = \sum_{m,n} c_m^* c_n \langle \psi_m | H | \psi_n \rangle = \sum_{m,n} c_m^* c_n E_n \langle \psi_m | \psi_n \rangle$$

$$= \sum_{m,n} c_m^* c_n E_n \delta_{m,n} = \sum_n |c_n|^2 E_n$$

$$\geq E_0 \sum_n |c_n|^2 = E_0.$$  \hfill (4.3)

b) We need to show that negative energy states exist in all attractive potentials. Following the hint, let’s choose our zero-level such that $V(x) \rightarrow 0$ as $x \rightarrow \pm \infty$. Then $V(x) \leq 0, \forall x$, and we can write $V(x) = -|V(x)|$. Now, we consider the wavefunction

$$\psi_\alpha(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}.$$  \hfill (4.4)

We note that this wavefunction is properly normalized. We can compute the average energy of this state:

$$\langle \psi_\alpha | H | \psi_\alpha \rangle = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2/2} \left(-\frac{\hbar^2}{2m} \partial_{xx} - |V(x)|\right) e^{-\alpha x^2/2} dx$$

$$= \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2} \left(-\frac{\hbar^2}{2m} \left(-\alpha + \alpha^2 x^2\right) - |V(x)|\right) dx$$

$$= \frac{\hbar^2 \alpha}{4m} - \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha x^2} |V(x)| dx.$$  \hfill (4.5)

In the limit $\alpha \rightarrow 0$, the wavefunction becomes very short and flat, which means its gradients (and kinetic energy) go to zero. At the same time, the wavefunction spreads out and “sees” more of the negative potential. So the average total energy should become potential dominated, and indeed

$$\lim_{\alpha \rightarrow 0} \langle \psi_\alpha | H | \psi_\alpha \rangle \approx -\sqrt{\frac{\alpha}{2}} \int_{-\infty}^{\infty} 1 \cdot |V(x)| dx + \frac{\hbar^2 \alpha}{4m} + O(\alpha^{3/2}).$$  \hfill (4.6)
For \( \alpha \) “sufficiently small” the leading term will dominate, and drive the average energy negative. Then, using the results of the previous part, we have

\[
E_0 \leq \langle \psi_\alpha | H | \psi_\alpha \rangle \leq 0 \tag{4.7}
\]

and so there exist bound states.

**Note:** We should be a little careful what we say here, because \( \alpha \) is dimensionful, and so we must specify what length scale \( \alpha \) is small compared to. More precisely, we need some length \( L \) such that the combination \( \sqrt{\alpha} L \) is a small parameter. But what \( L \) should we chose? The answer depends on \( V \), and so is model dependent. Generally speaking, a potential will have a characteristic energy \( \mathcal{E} \) and length scale \( L \) associated to it.\(^1\) Roughly, these should satisfy

\[
\mathcal{E} L \approx \int_{-\infty}^{\infty} |V(x)| \, dx. \tag{4.8}
\]

Taking \( \sqrt{\alpha} L \) small then means that the wavelength of the particle is long compared to the size \( L \) of the potential, so indeed it makes sense to approximate the probability density by a constant in that region. (Outside that region the potential should be roughly zero, so the wavefunction doesn’t matter.)

So what we really mean is in (4.6) is

\[
\lim_{\alpha \to 0} \langle \psi_\alpha | H | \psi_\alpha \rangle \approx -\mathcal{E} \sqrt{\frac{2}{\alpha L}} + \left( \frac{\hbar^2}{4mL^2} \right) (\alpha L^2) + O \left( (\sqrt{\alpha L})^3 \right). \tag{4.9}
\]

Notice that in many examples that you know and are used to (such as hydrogen and the harmonic oscillator), the typical energy and length scales are related to the mass by

\[
\mathcal{E} \approx \frac{\hbar^2}{2mL^2}, \tag{4.10}
\]

in which case we have

\[
\lim_{\alpha \to 0} \langle \psi_\alpha | H | \psi_\alpha \rangle \approx \mathcal{E} \left( -\frac{1}{\sqrt{2}} (\sqrt{\alpha} L) + \frac{1}{2} (\alpha L^2) + \ldots \right). \tag{4.11}
\]

For \( \sqrt{\alpha} L \ll 1 \) we are guaranteed this will be negative.

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\(^1\)Think of hydrogen, with \( \mathcal{E} \sim eV \) and \( L \sim \text{Å} \). For the harmonic oscillator \( \mathcal{E} \sim \hbar \omega \) and \( L \sim \hbar/m\omega \). Even for the delta function, we have \( \mathcal{E} = \infty \) and \( L = 0 \), but still \( \mathcal{E} L \approx g \int \delta(x) = g \).