

Some partial solutions and/or hints are given below. Watch out for misprints. If you catch an error, please let me know.

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1. Unitary matrices and operators.

- (a) Look up and report the definition of a unitary matrix.

**Solution/Hints/Discussion** →

A matrix is unitary if its hermitian conjugate (adjoint) is its inverse.  $U$  is unitary if  $U^\dagger = U^{-1}$ , i.e., if  $U^\dagger U = U U^\dagger = I$ .

*Comment (1):* The Hermitian conjugate is also known as the adjoint, or the conjugate transpose.

*Comment (2):* Sometimes, the conjugate transpose is also denoted with a star instead of with a dagger symbol, i.e.,  $U^*$  instead of  $U^\dagger$ . (E.g., as of Nov. 2020 the star notation is used in the wikipedia page for ‘Unitary Matrix’.) I strongly recommend using the dagger symbol, because in physics the star often represents the complex conjugate without transpose.

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- (b) Show that the matrix  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  is its own inverse.

**Solution/Hints/Discussion** →

A matrix  $A$  is its own inverse if  $AA = I$ . The matrix  $\sigma_x$  is its own inverse, because

$$\sigma_x \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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(c) Show that the three Pauli matrices are unitary.

**Solution/Hints/Discussion** →

We want to show

$$\sigma_x \sigma_x^\dagger = \sigma_x^\dagger \sigma_x = I \quad \sigma_y \sigma_y^\dagger = \sigma_y^\dagger \sigma_y = I \quad \sigma_z \sigma_z^\dagger = \sigma_z^\dagger \sigma_z = I$$

First for  $\sigma_x$ :

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_x^\dagger = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \sigma_x \quad \Longrightarrow \quad \begin{cases} \sigma_x \sigma_x^\dagger = \sigma_x \sigma_x = I \\ \sigma_x^\dagger \sigma_x = \sigma_x \sigma_x = I \end{cases}$$

using the fact that  $\sigma_x^2 = I$ , as shown previously.

Now for  $\sigma_y$ :

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_y^\dagger = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_y \quad \Longrightarrow \quad \begin{cases} \sigma_y \sigma_y^\dagger = \sigma_y \sigma_y = I \\ \sigma_y^\dagger \sigma_y = \sigma_y \sigma_y = I \end{cases}$$

where we have used the fact that

$$\sigma_y \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

And finally for  $\sigma_z$ :

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \sigma_z^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_z \quad \Longrightarrow \quad \begin{cases} \sigma_z \sigma_z^\dagger = \sigma_z \sigma_z = I \\ \sigma_z^\dagger \sigma_z = \sigma_z \sigma_z = I \end{cases}$$

where we have used the fact that

$$\sigma_z \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$$

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- (d) Show that the two-dimensional vector  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$  has the same norm as  $\sigma_y \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ , i.e., operating with  $\sigma_y$  keeps the norm unchanged.

**Solution/Hints/Discussion** →

$$\sigma_y \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} -i\beta \\ i\alpha \end{pmatrix}$$

whose norm is

$$|-i\beta|^2 + |i\alpha|^2 = |\beta|^2 + |\alpha|^2 = |\alpha|^2 + |\beta|^2$$

This is the same as the norm of  $\begin{pmatrix} \alpha \\ \beta \end{pmatrix}$ . Hence the norm is unchanged by operating with  $\sigma_y$ .

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- (e) If  $\hat{U}$  is a unitary operator, show that the state  $|\psi\rangle = \hat{U}|\phi\rangle$  has the same norm as the state  $|\phi\rangle$ .

**Solution/Hints/Discussion** →

$$|\psi\rangle = \hat{U}|\phi\rangle \quad \implies \quad \langle\psi| = \langle\phi|\hat{U}^\dagger$$

Thus the norm of  $|\psi\rangle$  is

$$\langle\psi|\psi\rangle = \langle\phi|\hat{U}^\dagger\hat{U}|\phi\rangle = \langle\phi|\phi\rangle$$

i.e., is equal to the norm of  $|\phi\rangle$ . Note we have used  $\hat{U}^\dagger\hat{U} = 1$ .

*Comment:*

Note that this is abstract and general, and makes no assumption about whether the Hilbert space is finite-dimensional or infinite-dimensional. We don't need a specific formula for the norm such as  $\int dx \psi^*(x)\psi(x)$  or  $\sum_j \psi_j^* \psi_j$ . The general bra-ket expression  $\langle\psi|\psi\rangle$  is good enough.

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2. The state  $|\mu_1\rangle$  is an eigenstate of  $\hat{M}$  with corresponding eigenvalue  $m_1$ .
- (a) Show that  $|\mu_1\rangle$  is also an eigenstate of  $\hat{M}^2$ , and find the corresponding eigenvalue. Show that  $|\mu_1\rangle$  is also an eigenstate of  $\hat{M}^n$ , where  $n$  is an integer, and find the corresponding eigenvalue.

**Solution/Hints/Discussion** →

Since  $\hat{M}|\mu_1\rangle = m_1|\mu_1\rangle$ , we have

$$\begin{aligned}\hat{M}^2|\mu_1\rangle &= \hat{M}(\hat{M}|\mu_1\rangle) = \hat{M}(m_1|\mu_1\rangle) = m_1(\hat{M}|\mu_1\rangle) \\ &= m_1(m_1|\mu_1\rangle) = m_1^2|\mu_1\rangle\end{aligned}$$

Thus  $|\mu_1\rangle$  is also an eigenstate of  $\hat{M}^2$ , with the eigenvalue  $m_1^2$ .

Similarly,  $|\mu_1\rangle$  is also an eigenstate of  $\hat{M}^n$ , for any positive integer  $n$ , with the eigenvalue  $m_1^n$ .

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- (b) How is the operator  $e^{\hat{M}}$  defined?  
How is  $e^{\alpha\hat{M}}$  defined, if  $\alpha$  is a complex number?  
Is  $|\mu_1\rangle$  an eigenstate of  $e^{\alpha\hat{M}}$ ? If so, find the corresponding eigenvalue.

**Solution/Hints/Discussion** →

$$\begin{aligned}e^{\hat{M}} &= \hat{1} + \hat{M} + \frac{1}{2!}\hat{M}^2 + \frac{1}{3!}\hat{M}^3 + \dots \\ e^{\alpha\hat{M}} &= \hat{1} + \alpha\hat{M} + \frac{\alpha^2}{2!}\hat{M}^2 + \frac{\alpha^3}{3!}\hat{M}^3 + \dots\end{aligned}$$

Is  $|\mu_1\rangle$  is an eigenstate of  $e^{\alpha\hat{M}}$ ? Let's try:

$$\begin{aligned}e^{\alpha\hat{M}}|\mu_1\rangle &= \left(\hat{1} + \alpha\hat{M} + \frac{\alpha^2}{2!}\hat{M}^2 + \frac{\alpha^3}{3!}\hat{M}^3 + \dots\right)|\mu_1\rangle \\ &= |\mu_1\rangle + \alpha m_1|\mu_1\rangle + \frac{\alpha^2}{2!}m_1^2|\mu_1\rangle + \frac{\alpha^3}{3!}m_1^3|\mu_1\rangle + \dots \\ &= \left(1 + \alpha m_1 + \frac{\alpha^2}{2!}m_1^2 + \frac{\alpha^3}{3!}m_1^3 + \dots\right)|\mu_1\rangle = e^{\alpha m_1}|\mu_1\rangle\end{aligned}$$

Yes, an eigenstate, with the eigenvalue  $e^{\alpha m_1}$ .

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3. We will consider a particle in one dimension subject to a negative (attractive) delta potential at  $x = 0$ :

$$V(x) = -\lambda\delta(x)$$

This system has a single bound state at some negative energy,  $E < 0$ . We will find the energy and wavefunction of this bound state.

**Comment** →

The wikipedia page titled “Delta potential” is recommended reading. Also described there is the motivation for studying this artificial-looking potential.

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- (a) Consider the left half-line ( $x < 0$ ). Write down the general solution of the Schroedinger equation in this region. Remember: we are considering  $E < 0$ .

Argue why one of the terms of the general solution can be dropped.

**Solution/Hints/Discussion** →

Away from  $x = 0$ , the potential is zero, so the Schroedinger equation is

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi$$

$$\implies \psi''(x) - \alpha^2 \psi(x) = 0 \quad \text{with} \quad \alpha = \sqrt{-\frac{2mE}{\hbar^2}}$$

The general solution is

$$\psi_L(x) = A_L e^{\alpha x} + B_L e^{-\alpha x}$$

I'm using the indices L and R for the left half-line and right half-line respectively.

The second term diverges for  $x \rightarrow -\infty$ , and so is unphysical, and so needs to be dropped:

$$\psi_L(x) = A_L e^{\alpha x}$$

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- (b) Similarly find the general solution on the right half-line ( $x > 0$ ), and identify the term that should be dropped.

**Solution/Hints/Discussion** →

On the right side, same general solution:

$$\psi_R(x) = A_R e^{\alpha x} + B_R e^{-\alpha x}$$

The first term diverges for  $x \rightarrow +\infty$ , and so is unphysical, and so needs to be dropped:

$$\psi_R(x) = B_R e^{-\alpha x}$$

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- (c) Explain why the derivative of the wavefunction,  $\psi'(x)$ , need not be continuous at  $x = 0$ .

**Solution/Hints/Discussion** →

The derivative needs to be continuous if the potential is everywhere finite. The potential here is  $-\infty$  at  $x = 0$ , i.e., not finite everywhere. Hence the derivative  $\psi'(x)$  does not need to be continuous.

We can also think about this by looking directly at the Schrodinger equation:

$$\begin{aligned} -\frac{\hbar^2}{2m}\psi''(x) - \lambda\delta(x)\psi(x) &= E\psi(x) \\ \implies -\frac{\hbar^2}{2m}\psi''(x) &= \lambda\delta(x)\psi(x) + E\psi(x) \end{aligned}$$

Since the right hand side is not finite at  $x = 0$ , this means that  $\psi''(x)$  is not finite at  $x = 0$ . This is consistent with  $\psi'(x)$  having a jump (discontinuity) at  $x = 0$ . (If a function has a jump, its derivative is infinite at that point.) Hence it is expected that  $\psi'(x)$  will have a jump at  $x = 0$ .

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- (d) Let  $\epsilon$  be an infinitesimally small positive number. By integrating both sides of the Schroedinger equation from  $-\epsilon$  to  $\epsilon$ , show that the derivative of the wavefunction has the following discontinuity around the  $x = 0$  point:

$$\psi'(\epsilon) - \psi'(-\epsilon) = -\frac{2m\lambda}{\hbar^2}\psi(0) + \text{infinitesimal term}$$

**Solution/Hints/Discussion**  $\rightarrow$

The Schroedinger equation is

$$\begin{aligned} -\frac{\hbar^2}{2m}\psi''(x) - \lambda\delta(x)\psi(x) &= E\psi(x) \\ \implies \psi''(x) &= -\frac{2m\lambda}{\hbar^2}\delta(x)\psi(x) - \frac{2mE}{\hbar^2}\psi(x) \end{aligned}$$

Integrating both sides from  $x = -\epsilon$  to  $x = +\epsilon$ , one obtains

$$\int_{-\epsilon}^{\epsilon} \psi''(x)dx = -\frac{2m\lambda}{\hbar^2} \int_{-\epsilon}^{\epsilon} \delta(x)\psi(x)dx - \frac{2mE}{\hbar^2} \int_{-\epsilon}^{\epsilon} \psi(x)dx$$

The first integral is equal to  $\psi'(\epsilon) - \psi'(-\epsilon)$  because  $\frac{d}{dx}\psi'(x) = \psi''(x)$ . (Fundamental Theorem of Calculus.)

The second integral is  $\psi(0)$  due to the property of the Dirac delta function.

Since  $\psi(x)$  is continuous, the last integral can be approximated for very small  $\epsilon$  as  $\psi(0)2\epsilon$ , which is an infinitesimal quantity.

Thus

$$\psi'(\epsilon) - \psi'(-\epsilon) = -\frac{2m\lambda}{\hbar^2}\psi(0) + \text{infinitesimal term}$$

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- (e) Determine the energy of the bound state and the constants in the wavefunction.

You can use continuity of  $\psi(x)$  and the normalization of the full wavefunction. In addition, the relation above for the discontinuity of  $\psi'(x)$  can be used as a boundary condition:

$$\psi'_R(0) - \psi'_L(0) = -\frac{2m\lambda}{\hbar^2}\psi_L(0)$$

where  $\psi_L(x)$  and  $\psi_R(x)$  are the wavefunctions on the left half-line and right half-line respectively.

**Solution/Hints/Discussion** →

The wavefunction is  $\psi_L(x) = A_L e^{\alpha x}$  on the left and  $\psi_R(x) = B_R e^{-\alpha x}$  on the right.

Continuity of the wavefunction:

$$\psi_L(0) = \psi_R(0) \quad \implies \quad A_L = B_R$$

Normalization:

$$\begin{aligned} & \int_{-\infty}^0 |\psi_L(x)|^2 dx + \int_0^{\infty} |\psi_R(x)|^2 dx = 1 \\ \implies & |A_L|^2 \int_{-\infty}^0 e^{2\alpha x} dx + |A_L|^2 \int_0^{\infty} e^{-2\alpha x} dx = 1 \\ \implies & |A_L|^2 \frac{1}{2\alpha} + |A_L|^2 \frac{1}{2\alpha} = 1 \\ \implies & |A_L|^2 = \alpha = \sqrt{-\frac{2mE}{\hbar^2}} \end{aligned}$$

Discontinuity of  $\psi'$ :

$$\begin{aligned} -\alpha A_L - \alpha A_L &= -\frac{2m\lambda}{\hbar^2} A_L & \begin{cases} \text{using } \psi'_L(0) = A_L(\alpha)e^0 = \alpha A_L \\ \text{and } \psi'_R(0) = B_R(-\alpha)e^0 = -\alpha A_L \end{cases} \\ \implies \alpha &= \frac{m\lambda}{\hbar^2} & \implies E = -\frac{\hbar^2 \alpha^2}{2m} = -\frac{m\lambda^2}{2\hbar^2} \end{aligned}$$

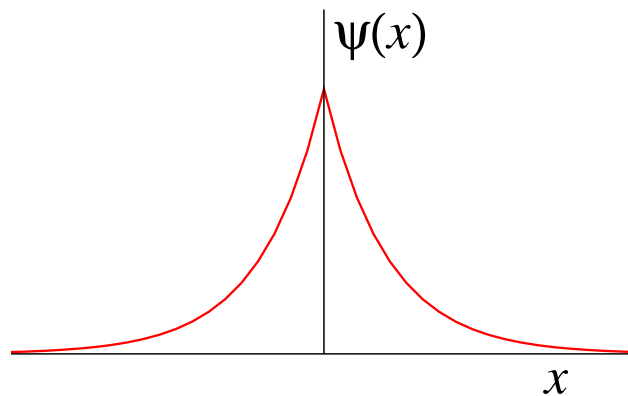
Thus we have found the energy and the overall constant to be

$$E = -\frac{m\lambda^2}{2\hbar^2} \quad A_L = \sqrt{\alpha} = \sqrt{\frac{m\lambda}{\hbar^2}}$$

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- (f) Plot the wavefunction as a function of position. Make sure the (dis)continuity at  $x = 0$  is clearly visible.

**Solution/Hints/Discussion** →



Note that the wavefunction from either side DOES NOT diverge at  $x = 0$ , because both functions  $e^{\alpha x}$  and  $e^{-\alpha x}$  go to unity at  $x = 0$ . i.e., the wavefunction is very finite.

The wavefunction  $\psi(x)$  itself is continuous – there is no jump.

The derivative of the wavefunction is discontinuous – this appears as a ‘kink’ in the curve at  $x = 0$ .

**Exercise:** Plot the derivative,  $\psi'(x)$ , as a function of position.