



## Quantum Mechanics for Spin Systems & the Uncertainty Principle

### Homework Problems

#### 1. The Pauli matrices

Consider the three Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

- (i) Prove  $\sigma_j \sigma_k = \delta_{jk} \text{id}_{\mathbb{C}^2} + i \sum_{l=1}^3 \epsilon_{jkl} \sigma_l$  where  $\epsilon_{jkl}$  is the epsilon tensor.
- (ii) Prove that any  $2 \times 2$  matrix can be written as the linear combination of the identity and the three Pauli matrices with coefficients  $h_0$  and  $h = (h_1, h_2, h_3)$ ,

$$\text{Mat}_{\mathbb{C}}(2) \ni A = (a_{jk})_{1 \leq j, k \leq 2} = h_0 \text{id}_{\mathbb{C}^2} + \sum_{j=1}^3 h_j \sigma_j =: h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma. \quad (1)$$

**Hint:** Use that  $\text{Mat}_{\mathbb{C}}(2)$  is finite-dimensional.

- (iii) Now assume that the coefficients  $h_0, \dots, h_3$  in equation (1) are real. Show that then the resulting matrix  $H = h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma$  is hermitian. Compute the eigenvalues  $E_{\pm}(h_0, h)$  of  $H$  in terms of the coefficients  $h_0$  and  $h$ .
- (iv) Use (i) to prove that for real  $h_0, \dots, h_3$

$$P_{\pm}(h_0, h) = \frac{1}{2} \left( \text{id}_{\mathbb{C}^2} \pm \frac{h \cdot \sigma}{|h|} \right), \quad h \neq 0 \in \mathbb{R}^3, \quad |h| := \sqrt{h_1^2 + h_2^2 + h_3^2},$$

are the projections onto the eigenspaces for the two eigenvalues  $E_{\pm}(h_0, h)$  of  $H$ .

- (v) Compute the trace of  $H$ .

**Note:** In physics especially, one frequently writes  $h \cdot \sigma$  for  $\sum_{j=1}^3 h_j \sigma_j$  where  $h = (h_1, h_2, h_3)$ .

**Solution:**

(i) This follows from direct computation: for  $j = k$  we obtain

$$\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = \text{id}_{\mathbb{C}^2}$$

while for  $j < k$

$$\begin{aligned}\sigma_1 \sigma_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} = \begin{pmatrix} +i & 0 \\ 0 & -i \end{pmatrix} = i \sigma_3 \\ \sigma_1 \sigma_3 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = -i \sigma_2 \\ \sigma_2 \sigma_3 &= \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & +i \\ +i & 0 \end{pmatrix} = i \sigma_1\end{aligned}$$

In other words, we have shown (i) for  $j < k$ .

To show (i) in the remaining cases, we use that the  $\sigma_j = \sigma_j^*$  are hermitian matrices, and hence for  $j < k$  we obtain

$$\begin{aligned}\sigma_k \sigma_j &= (\sigma_j \sigma_k)^* = \left( \delta_{jk} \text{id}_{\mathbb{C}^2} + i \sum_{l=1}^3 \epsilon_{jkl} \sigma_l \right)^* \\ &= \delta_{jk} \text{id}_{\mathbb{C}^2} - i \sum_{l=1}^3 \epsilon_{jkl} \sigma_l = \delta_{jk} \text{id}_{\mathbb{C}^2} + i \sum_{l=1}^3 \epsilon_{kjl} \sigma_l.\end{aligned}$$

This proves (i).

- (ii) The vector space of  $2 \times 2$  matrices is four-dimensional,  $\dim \text{Mat}_{\mathbb{C}}(2) = 4$ , and seeing as the 4 vectors  $\{\text{id}_{\mathbb{C}^2}, \sigma_1, \sigma_2, \sigma_3\}$  are linearly independent, they form a basis of  $\text{Mat}_{\mathbb{C}}(2)$ .
- (iii) In case  $h_0, \dots, h_3$  are real,

$$\begin{aligned}H^* &= (h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma)^* = \overline{h_0} \text{id}_{\mathbb{C}^2} + \overline{h} \cdot \sigma \\ &= h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma = H\end{aligned}$$

is hermitian and we can compute both eigenvalues: the characteristic polynomial of  $H$  is

$$\begin{aligned}\chi(\lambda) &= \det(\lambda \text{id}_{\mathbb{C}^2} - H) = \det \begin{pmatrix} \lambda - h_0 - h_3 & h_1 - i h_2 \\ h_1 + i h_2 & \lambda - h_0 + h_3 \end{pmatrix} \\ &= ((\lambda - h_0) - h_3) ((\lambda - h_0) + h_3) - (h_1 - i h_2)(h_1 + i h_2) \\ &= (\lambda - h_0)^2 - (h_1^2 + h_2^2 + h_3^2) = (\lambda - h_0)^2 - |h|^2,\end{aligned}$$

and hence, the eigenvalues are  $E_{\pm}(h_0, h) = h_0 \pm |h|$ .

(iv) The product

$$H P_{\pm} = (h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma) P_{\pm} = h_0 P_{\pm} + \frac{1}{2} \left( h \cdot \sigma \pm \frac{(h \cdot \sigma)^2}{|h|} \right)$$

involves the square of  $h \cdot \sigma$  which can be computed with the help of (i):

$$\begin{aligned}
(h \cdot \sigma)^2 &= \sum_{j,k=1}^3 h_j h_k \sigma_j \sigma_k \\
&= \sum_{j=1}^3 h_j^2 \text{id}_{\mathbb{C}^2} + \sum_{\substack{j,k,l=1,2,3 \\ j \neq k}} h_j h_k \mathbf{i} \epsilon_{jkl} \sigma_l \\
&= |h|^2 \text{id}_{\mathbb{C}^2} + \mathbf{i} \sum_{l=1}^3 \left( \sum_{\substack{j,k=1,2,3 \\ j \neq k}} h_j h_k \mathbf{i} \epsilon_{jkl} \right) \sigma_l = |h|^2 \text{id}_{\mathbb{C}^2}
\end{aligned}$$

Hence, we can factor out  $E_{\pm}$  and obtain (iv):

$$\begin{aligned}
H P_{\pm} &= h_0 P_{\pm} + \frac{1}{2} \left( h \cdot \sigma \pm \frac{|h|^2 \text{id}_{\mathbb{C}^2}}{|h|} \right) \\
&= h_0 P_{\pm} \pm |h| \frac{1}{2} \left( \text{id}_{\mathbb{C}^2} \pm \frac{h \cdot \sigma}{|h|} \right) \\
&= (h_0 \pm |h|) P_{\pm} = E_{\pm} P_{\pm}
\end{aligned}$$

(v) The trace is just the sum over the diagonal elements of the matrices, and clearly, the Pauli matrices are all traceless. Hence, we compute

$$\begin{aligned}
\text{tr} H &= \text{tr}(h_0 \text{id}_{\mathbb{C}^2} + h \cdot \sigma) \\
&= h_0 \text{tr} \text{id}_{\mathbb{C}^2} + \sum_{j=1}^3 h_j \text{tr} \sigma_j = 2h_0.
\end{aligned}$$

## 2. Functional calculus for $2 \times 2$ matrices

Let  $f$  be a piecewise continuous function and  $H = H^*$  a hermitian  $2 \times 2$  matrix. Then define

$$f(H) := \sum_{j=\pm} f(E_{\pm}) P_{\pm} \quad (2)$$

where  $E_{\pm}$  are the eigenvalues of  $H$  and  $P_{\pm}$  the two projections from problem 1.

(i) Compute  $f(H)$  defined as in equation (2) for  $H = h \cdot \sigma$ ,  $h \neq 0$ , and

$$f(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases}.$$

(ii) Show that  $f(H)$  for  $f(x) = e^{-itx}$  (defined via (2)) coincides with the matrix exponential, i. e.

$$f(H) = e^{-ith_0} \left( \cos(|h|t) - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right) = e^{-itH} = \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} H^n. \quad (3)$$

**Hint:** Use  $e^{-it(h_0+h\cdot\sigma)} = e^{-ith_0} e^{-ith\cdot\sigma}$ .

(iii) Assuming  $h_0, h_1, h_2, h_3$  are real, compute  $\psi(t)$  for the initial condition  $\psi(0) = \psi_0 \in \mathbb{C}^2$ :

(a)  $\frac{d}{dt}\psi(t) = (h_2 \sigma_2 + h_3 \sigma_3)\psi(t)$

(b)  $i \frac{d}{dt}\psi(t) = h_2 \sigma_2 \psi(t)$

(c)  $-i \frac{d}{dt}\psi(t) = (h_0 \text{id}_{\mathbb{C}^2} + h_3 \sigma_3)\psi(t)$

**Solution:**

(i)  $f(H) = f(|h|) P_+ + f(-|h|) P_- = P_+$

(ii) For  $h = 0$ ,  $H$  is a scalar multiple of the identity matrix and equation (3) holds. So let us assume  $h \neq 0$ . Then we first compute the left-hand side:

$$\begin{aligned} e^{-itx}(H) &= e^{-it(h_0+|h|)} P_+ + e^{-it(h_0-|h|)} P_- \\ &= \frac{1}{2} \left( e^{-it(h_0+|h|)} + e^{-it(h_0-|h|)} \right) \text{id}_{\mathbb{C}^2} + \frac{1}{2} \left( e^{-it(h_0+|h|)} - e^{-it(h_0-|h|)} \right) \frac{h \cdot \sigma}{|h|} \\ &= e^{-ith_0} \left( \cos(|h|t) - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right) \end{aligned}$$

To obtain the right-hand side, we note

$$\begin{aligned} (h \cdot \sigma)^2 &= \sum_{j,k=1,2,3} h_j h_k \sigma_j \sigma_k = \sum_{j=1,2,3} h_j^2 \sigma_j^2 + \sum_{\substack{j,k=1,2,3 \\ j \neq k}} h_j h_k \sigma_j \sigma_k \\ &= \sum_{j=1,2,3} h_j^2 \text{id}_{\mathbb{C}^2} + \sum_{l=1,2,3} \sum_{\substack{j,k=1,2,3 \\ j \neq k}} h_j h_k \epsilon_{jkl} \sigma_l = h^2, \end{aligned}$$

and thus we identify a pattern in  $(h \cdot \sigma)^n$ :

$$\begin{aligned} (h \cdot \sigma)^{2n} &= |h|^{2n} \text{id}_{\mathbb{C}^2} \\ (h \cdot \sigma)^{2n+1} &= (h \cdot \sigma)^{2n} h \cdot \sigma = |h|^{2n} h \cdot \sigma \end{aligned}$$

This means that we can compute the matrix exponential after splitting the sum into even and odd terms:

$$\begin{aligned}
e^{-itH} &= e^{-ith_0} e^{-ith \cdot \sigma} = e^{-ith_0} \sum_{n=0}^{\infty} \frac{(-it)^n}{n!} (h \cdot \sigma)^n \\
&= e^{-ith_0} \sum_{n=0}^{\infty} \frac{(-it)^{2n}}{(2n)!} (h \cdot \sigma)^{2n} + e^{-ith_0} \sum_{n=0}^{\infty} \frac{(-it)^{2n+1}}{(2n+1)!} (h \cdot \sigma)^{2n+1} \\
&= e^{-ith_0} \sum_{n=0}^{\infty} (-1)^n \frac{(|h|t)^{2n}}{(2n)!} \text{id}_{\mathbb{C}^2} - \frac{i}{|h|} e^{-ith_0} \sum_{n=0}^{\infty} (-1)^n \frac{(|h|t)^{2n+1}}{(2n+1)!} h \cdot \sigma \\
&= e^{-ith_0} \left( \cos(|h|t) \text{id}_{\mathbb{C}^2} - \frac{i}{|h|} \sin(|h|t) h \cdot \sigma \right)
\end{aligned}$$

Thus, left- and right-hand side agree.

(iii) (a)

$$\begin{aligned}
\psi(t) &= e^{tH} \psi_0 = e^{t|h|} P_+(0, 0, h_2, h_3) + e^{-t|h|} P_-(0, 0, h_2, h_3) \\
&= \frac{1}{2} (e^{+t|h|} + e^{-t|h|}) \psi_0 + \frac{1}{2} \frac{e^{+t|h|} - e^{-t|h|}}{|h|} (h_2 \sigma_2 + h_3 \sigma_3) \psi_0 \\
&= \cosh(t|h|) \psi_0 + \sinh(t|h|) (h_2 \sigma_2 + h_3 \sigma_3) \psi_0
\end{aligned}$$

$$(b) \quad \psi(t) = e^{-itH} \psi_0 = \cos(t|h_2|) \psi_0 - i \frac{h_2}{|h_2|} \sin(t|h_2|) \sigma_2 \psi_0$$

$$(c) \quad \psi(t) = e^{+itH} \psi_0 = e^{+ith_0} \cos(t|h_2|) \psi_0 + i e^{+ith_0} \frac{h_3}{|h_3|} \sin(t|h_3|) \sigma_3 \psi_0$$

### 3. Uncertainty of Gauß functions

Compute the right-hand side of Heisenberg's uncertainty principle

$$\sigma_\psi(\hat{x}) \sigma_\psi(-i\hbar\partial_x)$$

in one dimension for

(i)  $\psi_\lambda(x) = \sqrt[4]{\frac{\lambda}{\pi}} e^{-\frac{\lambda}{2}x^2}$ ,  $\lambda > 0$ , and

(ii)  $\varphi_\lambda(x) = \sqrt[4]{\frac{\lambda}{\pi}} e^{+ix\xi_0} e^{-\frac{\lambda}{2}(x-x_0)^2}$ ,  $\lambda > 0$ ,  $x_0, \xi_0 \in \mathbb{R}$ .

Here, the standard deviation

$$\sigma_\psi(H) := \sqrt{\mathbb{E}_\psi\left(\left(H - \mathbb{E}_\psi(H)\right)^2\right)}$$

for a selfadjoint operator  $H = H^*$  with respect to  $\psi$ ,  $\|\psi\| = 1$ , is defined as in the lecture notes via the expectation value

$$\mathbb{E}_\psi(H) := \langle \psi, H\psi \rangle.$$

**Solution:**

(i) First of all, since  $\psi(-x) = \psi(x)$  the expectation value

$$\mathbb{E}_{\psi_\lambda}(\hat{x}) = \int_{\mathbb{R}} dx \sqrt{\frac{\lambda}{\pi}} x e^{-\lambda x^2} = 0$$

necessarily vanishes. Similarly,

$$\begin{aligned} \mathbb{E}_{\psi_\lambda}(-i\hbar\partial_x) &= -i\hbar \langle \psi_\lambda, \partial_x \psi_\lambda \rangle = -i\hbar \langle \mathcal{F}\psi_\lambda, \mathcal{F}\partial_x \psi_\lambda \rangle \\ &= \hbar \langle \psi_{1/\lambda}, \hat{\xi} \psi_{1/\lambda} \rangle = 0 \end{aligned}$$

is also 0, because the Fourier transform of a Gaußian is also a Gaußian.

That means we can compute the first standard deviation by partial integration:

$$\begin{aligned} \sigma_{\psi_\lambda}(\hat{x})^2 &= \mathbb{E}_{\psi_\lambda}\left(\left(\hat{x} - \mathbb{E}_{\psi_\lambda}(\hat{x})\right)^2\right) = \mathbb{E}_{\psi_\lambda}(\hat{x}^2) = \sqrt{\frac{\lambda}{\pi}} \int_{\mathbb{R}} dx x^2 e^{-\lambda x^2} \\ &= \frac{1}{\lambda \sqrt{\pi}} \int_{\mathbb{R}} dx x^2 e^{-x^2} = \left[ -\frac{1}{2\lambda \sqrt{\pi}} x e^{-x^2} \right]_{-\infty}^{+\infty} + \frac{1}{2\lambda \sqrt{\pi}} \int_{\mathbb{R}} dx e^{-x^2} = \frac{1}{2\lambda} \end{aligned}$$

To compute the other standard deviation, we note that since the Fourier transform of a Gaußian is a Gaußian with inverse width,

$$(\mathcal{F}\psi_\lambda)(\xi) = \sqrt[4]{\frac{\lambda}{\pi}} (\mathcal{F}e^{-\frac{\lambda}{2}x^2})(\xi) = \frac{1}{\sqrt[4]{\lambda\pi}} e^{-\frac{1}{2\lambda}\xi^2} = \psi_{1/\lambda},$$

we can relate  $\sigma_{\psi_\lambda}(-i\hbar\partial_x)$  to  $\sigma_{\psi_\lambda}(\hat{x})$ ,

$$\begin{aligned} \sigma_{\psi_\lambda}(-i\hbar\partial_x)^2 &= -\hbar^2 \langle \psi_\lambda, \partial_x^2 \psi_\lambda \rangle = -\hbar^2 \langle \mathcal{F}\psi_\lambda, \mathcal{F}\partial_x^2 \psi_\lambda \rangle \\ &= +\hbar^2 \langle \mathcal{F}\psi_{1/\lambda}, \hat{\xi}^2 \psi_{1/\lambda} \rangle = \frac{\hbar^2}{2\lambda^{-1}}. \end{aligned}$$

Hence,  $\psi_\lambda$  minimizes the uncertainty relation,

$$\sigma_{\psi_\lambda}(\hat{x}) \sigma_{\psi_\lambda}(-i\hbar\partial_x) = \frac{1}{\sqrt{2\lambda}} \sqrt{\frac{\hbar^2 \lambda}{2}} = \frac{\hbar}{2} \geq \frac{\hbar}{2}.$$

(ii) We will reuse the results from (i) as much as possible: the mean of  $\varphi_\lambda$  is  $x_0$ :

$$\begin{aligned}\mathbb{E}_{\varphi_\lambda}(\hat{x}) &= \int_{\mathbb{R}} \mathbf{d}x \, x \left| e^{+ix\xi_0} \psi_\lambda(x - x_0) \right|^2 = \int_{\mathbb{R}} \mathbf{d}x \, (x + x_0) |\psi_\lambda(x)|^2 \\ &= x_0 \|\psi_\lambda(x)\|^2 = x_0\end{aligned}$$

Hence, the standard deviation of  $\varphi_\lambda$  coincides with that of  $\psi_\lambda$ :

$$\begin{aligned}\sigma_{\varphi_\lambda}(\hat{x})^2 &= \mathbb{E}_{\varphi_\lambda}((\hat{x} - x_0)^2) = \int_{\mathbb{R}} \mathbf{d}x \, (x - x_0)^2 \left| e^{+ix\xi_0} \psi_\lambda(x - x_0) \right|^2 \\ &= \int_{\mathbb{R}} \mathbf{d}x \, x^2 |\psi_\lambda(x)|^2 = \frac{1}{2\lambda}\end{aligned}$$

Since the Fourier transform intertwines taking derivatives with multiplying by monomials and maps Gaussians on Gaussians of inverse width,

$$(\mathcal{F}\varphi_\lambda)(\xi) = (\mathcal{F}e^{+ix\xi_0} \psi_\lambda(\cdot - x_0))(\xi) = (\mathcal{F}\psi_\lambda(\cdot - x_0))(\xi - \xi_0) = e^{-i\xi x_0} \psi_{1/\lambda}(\xi - \xi_0),$$

we obtain the same integral (up to  $\hbar^2$ ) where  $\lambda$  is replaced by  $\lambda^{-1}$ ,

$$\sigma_{\varphi_\lambda}(-i\hbar\partial_x)^2 = \frac{\hbar^2\lambda}{2}.$$

Hence, also shifted Gaussians have minimal uncertainty,

$$\sigma_{\varphi_\lambda}(\hat{x}) \sigma_{\varphi_\lambda}(-i\hbar\partial_x) = \frac{\hbar}{2} \geq \frac{\hbar}{2}.$$

#### 4. The framework of physical theories (optional)

Identify (1) states, (2) observables and (3) dynamical equations for the following physical theories:

- (i) Classical mechanics on  $\mathbb{R}^d$
- (ii) Classical electromagnetism

##### Solution:

- (i) (1) *States*: Probability measures on phase space  $\mathbb{R}^{2d}$
- (2) *Observables*: Smooth functions on phase space  $\mathbb{R}^{2d}$
- (3) *Dynamical equations*: Given a hamiltonian (energy function)  $h$ , we can either propose Hamilton's equations of motion,

$$\begin{pmatrix} \dot{q} \\ \dot{p} \end{pmatrix} = \begin{pmatrix} +\nabla_p h \\ -\nabla_q h \end{pmatrix},$$

or equivalently

$$\frac{d}{dt}f(t) = \{h, f(t)\}, \quad f(0) = f,$$

where  $\{f, g\} = \nabla_p f \cdot \nabla_q g - \nabla_q f \cdot \nabla_p g$  is the Poisson bracket

- (ii) (1) *States*: Electromagnetic fields  $(\mathbf{E}, \mathbf{B})$ , i. e. vector fields on  $\mathbb{R}^3$  which satisfy the two source Maxwell equation:

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \rho \\ \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

where  $\rho$  is a charge density

- (2) *Observables*: Functionals  $\mathcal{F}(\mathbf{E}, \mathbf{B}) \in \mathbb{R}$  on the fields
- (3) *Dynamical equations*: the dynamical Maxwell equations

$$\begin{aligned} \partial_t \mathbf{E} &= +\nabla \wedge \mathbf{B} - \mathbf{j} \\ \partial_t \mathbf{B} &= -\nabla \wedge \mathbf{E} \end{aligned}$$

where  $\mathbf{j}$  is the current density