## Problem 1 Path-connectedness of $SO(n)$

Show that $SO(n)$ is path connected using induction over $n$. *Hint:* It is enough to show that there is a path from each element to the identity.

*Solution to Problem 1*:

First, note that for all $M \in SO(2)$ we can find a $\theta \in [0, 2\pi)$, such that $M = M_\theta$, where

$$M_\theta = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}. \tag{1}$$

Any two $M_0, M_1 \in SO(2)$ can therefore be connected by the path

$$\gamma \;:\; [0,1] \to SO(2) \tag{2}$$
$$t \mapsto M_{\theta(t)}, \tag{3}$$

where $\theta(t) = \theta_0(1-t) + \theta_1$, $M_0 = M_{\theta_0}$, and $M_1 = M_{\theta_1}$. Hence, $SO(2)$ is path connected.

Let us now show that $SO(n)$ is path connected by induction. We thus assume that $SO(n-1)$ is path connected. It suffices to show that any $M \in SO(n)$ is path connected to the identity.

We consider a basis $\mathbf{e}_1, \ldots, \mathbf{e}_n$ of $\mathbb{R}^n$. We can characterize any $M \in SO(n)$ by the transformation of these basis elements to $M\mathbf{e}_1, \ldots, M\mathbf{e}_n$. In a first step, we focus on the transformation from $\mathbf{e}_1$ to $M\mathbf{e}_1$. Assuming they are not equal, these vectors $\mathbf{e}_1$ and $M\mathbf{e}_1$ span a plane. We can rotate $\mathbf{e}_1$ to $M\mathbf{e}_1$ by rotating this plane using $R \in SO(n)$. In a suitable basis $R$ can be written as $R = R_2 \oplus \mathbf{1}_{n-2}$, where $\mathbf{1}_{n-2}$ is the identity operator and $R_2 \in SO(2)$. Since $SO(2)$ is path connected, we can find a path $\gamma_1 : [0,1] \to SO(n)$ connecting $R$ to the identity.

In a second step, we try to find another rotation that maps all the remaining $\mathbf{e}_2, \ldots, \mathbf{e}_n$ to $M\mathbf{e}_2, \ldots, M\mathbf{e}_n$ at once. This is of course possible by a rotation in $SO(n-1)$ but we have to make sure that this rotation does not disturb the vector $M\mathbf{e}_1 = R\mathbf{e}_1$. The second rotation has to happen entirely in a subspace that is orthogonal to $M\mathbf{e}_1$. Let's check the initial points first: since $R$ is a rotation and the $\mathbf{e}_1, \ldots, \mathbf{e}_n$ are orthogonal, we have that all the $R\mathbf{e}_2, \ldots, R\mathbf{e}_n$ are orthogonal to $M\mathbf{e}_1 = R\mathbf{e}_1$. Moreover, also all the endpoints of the rotation, $M\mathbf{e}_2, \ldots, M\mathbf{e}_n$, are also orthogonal to $M\mathbf{e}_1$ since $M$ is a rotation. This means that such a rotation is indeed possible and since $SO(n-1)$ is path connected by assumption, we can describe this rotation continuously by a path $\gamma_2$. Composing both paths $\gamma_2 \circ \gamma_1$ connects $M$ to the identity in $SO(n)$.

## Problem 2 Time reversal in quantum mechanics

Operations $f(x)$ that conserve the modulus $|\langle f(x)|f(y)\rangle| = |\langle x|y\rangle|$, $\forall (x,y) \in \mathcal{H}^2$, where $\mathcal{H}$ is a Hilbert space with Hermitian product $\langle\cdot|\cdot\rangle$, can only be of a certain kind: Wigner's theorem states that $f$ can be recast as $f(x) = e^{i\theta(x)}U(x)$, where $\theta$ is real-valued and $U : \mathcal{H} \to \mathcal{H}$ obeys the following properties

$$\forall (x,y) \in \mathcal{H}^2 \qquad U(x+y) = U(x) + U(y) \tag{4}$$
$$\forall (\lambda, x) \in \mathbb{C} \times \mathcal{H} \qquad U(\lambda x) = \kappa(\lambda) U(x) \tag{5}$$
$$\forall (x,y) \in \mathcal{H}^2 \qquad \langle U(x)|U(y)\rangle = \kappa(\langle x|y\rangle) \tag{6}$$

where $\kappa(\lambda) = \lambda$ (unitary operators) or $\kappa(\lambda) = \bar{\lambda}$ (anti-unitary operators).

In this exercise, we focus on time reversal symmetry $T : \psi(\boldsymbol{r}) \mapsto \overline{\psi(\boldsymbol{r})}$.

1. Consider the Hamiltonian $\hat{H} = \hat{p}^2/2m + V(\hat{\boldsymbol{r}})$. Find an interpretation of $T$ by considering its action on solutions of Schrödinger's equation $i\hbar\partial_t\psi = \hat{H}\psi$.

2. Show that $T$ is an anti-unitary operator.

3. Consider a 1D problem and assume $V$ has compact support.

   (a) Prove the existence of the two families of solutions:

$$\psi_+(x) = \begin{cases} e^{ikx} + r_+ e^{-ikx} & x \to -\infty \\ t_+ e^{ikx} & x \to +\infty \end{cases}, \quad \psi_-(x) = \begin{cases} t_- e^{-ikx} & x \to -\infty \\ e^{-ikx} + r_- e^{ikx} & x \to +\infty \end{cases}. \tag{7}$$

   (b) Assuming the solution has time reversal symmetry, find the relations between $r_\pm$ and $t_\pm$.

4. Is the interpretation of $T$ as a solution of the Schrödinger equation after time reversal still valid if we add an external magnetic field, $\hat{H} = \frac{1}{2m}\left(-i\hbar\nabla + \frac{q}{c}\mathbf{A}\right)^2 + V(\hat{\boldsymbol{r}})$?

*Solution to Problem 2*:

1. Let $\psi(\mathbf{r}, t)$ be a solution of the Schrödinger equation:

$$i\hbar\partial_t\psi(\mathbf{r}, t) = [\hat{p}^2/2m + V(\hat{\boldsymbol{r}})]\psi(\mathbf{r}, t). \tag{8}$$

   Complex conjugation on both sides yields

$$-i\hbar\partial_t\overline{\psi(\mathbf{r}, t)} = [\hat{p}^2/2m + V(\hat{\boldsymbol{r}})]\overline{\psi(\mathbf{r}, t)}, \tag{9}$$

   or

$$i\hbar\partial_{-t}\overline{\psi(\mathbf{r}, t)} = [\hat{p}^2/2m + V(\hat{\boldsymbol{r}})]\overline{\psi(\mathbf{r}, t)}. \tag{10}$$

   In other words $T[\psi(\mathbf{r}, t)]$ is a solution to a modified Schrödinger equation where we replace $t$ by $-t$.

2. We consider

$$\begin{aligned} T[\psi_1(\mathbf{r}) + \psi_1(\mathbf{r})] &= \overline{\psi_1(\mathbf{r}) + \psi_1(\mathbf{r})} \\ &= \overline{\psi_1(\mathbf{r})} + \overline{\psi_1(\mathbf{r})} \\ &= T[\psi_1(\mathbf{r})] + T[\psi_2(\mathbf{r})], \end{aligned} \tag{11}$$

   and

$$T[c\psi(\mathbf{r})] = \overline{c\psi(\mathbf{r})} = \bar{c}T[\psi(\mathbf{r})]. \tag{12}$$

   Moreover,

$$\begin{aligned} \langle T[\psi_1] | T[\psi_2] \rangle &= \langle \overline{\psi_1} | \overline{\psi_2} \rangle \\ &= \int d\mathbf{r} \psi_1(\mathbf{r}) \overline{\psi_2(\mathbf{r})} \\ &= \overline{\int d\mathbf{r} \overline{\psi_1(\mathbf{r})} \psi_2(\mathbf{r})} \\ &= \overline{\langle \psi_1 | \psi_2 \rangle}. \end{aligned} \tag{13}$$

3. a) Since the support of $V$ is bounded, the potential vanishes at $\pm\infty$ and plane waves are a solution to the Schrödinger equation without potential, where $\hbar k$ is the momentum. This means these solutions exist. They can be interpreted as an incoming plane wave that is in part reflected and in part transmitted.

   b) Time reversal symmetry tells us that $T[\psi_+(x)]$ is a solution of the Schrödinger equation

$$T[\psi_+(x)] = \begin{cases} e^{-ikx} + \bar{r}_+ e^{ikx} & x \to -\infty \\ \bar{t}_+ e^{-ikx} & x \to +\infty \end{cases}. \tag{14}$$

Let us expand it in terms of $\psi_+(x)$ and $\psi_-(x)$ as

$$T[\psi_+(x)] = a\psi_+(x) + b\psi_-(x). \tag{15}$$

We find at $x \to -\infty$ that

$$e^{-ikx} + \bar{r}_+ e^{ikx} = ae^{ikx} + ar_+ e^{-ikx} + bt_- e^{-ikx}, \tag{16}$$

whereas at $x \to \infty$:

$$\bar{t}_+ e^{-ikx} = at_+ e^{ikx} + be^{-ikx} + br_- e^{ikx}. \tag{17}$$

Comparing coefficients, we obtain from (16) that

$$ar_+ + bt_- = 1 \tag{18}$$
$$\bar{r}_+ = a. \tag{19}$$

From the condition (17) we obtain

$$at_+ + br_- = 0 \tag{20}$$
$$\bar{t}_+ = b. \tag{21}$$

Inserting Eqs. (19) and (21) into Eq. (18) yields

$$|r_+|^2 + \bar{t}_+ t_- = 1 \tag{22}$$

and from the conservation of probability we have that $|r_+|^2 + |t_+|^2 = 1$, leading to

$$\bar{t}_+ t_- = |t_+|^2, \tag{23}$$

implying that $t_+ = t_-$. Inserting Eqs. (19) and (21) into Eq. (20) yields

$$\bar{r}_+ t_+ + \bar{t}_+ r_- = 0. \tag{24}$$

This tells us that $|r_-| = |r_+|$.

4. If we add an external magnetic field, the Schrödinger equation reads

$$i\hbar\partial_t \psi(\mathbf{r}, t) = \left[\frac{1}{2m}\left(-i\hbar\nabla + \frac{q}{c}\mathbf{A}\right)^2 + V(\hat{\boldsymbol{r}})\right]\psi(\mathbf{r}, t), \tag{25}$$

If we attempt to do the same procedure as before, we obtain after complex conjugation

$$-i\hbar\partial_t\overline{\psi(\mathbf{r},t)} = \left[\frac{1}{2m}\left(i\hbar\nabla + \frac{q}{c}\mathbf{A}\right)^2 + V(\hat{\boldsymbol{r}})\right]\overline{\psi(\mathbf{r},t)}. \quad (26)$$

Changing $t \to -t$ yields

$$i\hbar\partial_{-t}\overline{\psi(\mathbf{r},t)} = \left[\frac{1}{2m}\left(i\hbar\nabla + \frac{q}{c}\mathbf{A}\right)^2 + V(\hat{\boldsymbol{r}})\right]\overline{\psi(\mathbf{r},t)}. \quad (27)$$

Hence, unless we also replace $\frac{q}{c}\mathbf{A} \to -\frac{q}{c}\mathbf{A}$, the function $T[\psi(\mathbf{r},t)]$ will not be a solution after time reversal.

## Problem 3 (Bonus) Crystal symmetries and Pockels effect

In dielectric media, the displacement field $\mathbf{D} \in \mathbb{R}^3$ is related to the electric field $\mathbf{E} \in \mathbb{R}^3$ by the relation $D^i = \epsilon^i_j E^j$, where the $\epsilon^i_j$ are the components of the permittivity tensor (we make use of the sum convention). The Pockels effect describes a change of the permittivity tensor due to an electric field as $\epsilon^i_j = L^i_{jk}E^k$, where $L^i_{jk}$ are the components of a rank-3 tensor.

1. Identify the most general form of the permittivity tensor in a crystal with $C_4$ symmetry.
2. Show that the Pockels effect cannot be observed in crystals with inversion symmetry.

*Solution to Problem 3*:

1. The permittivity tensor must have the same symmetry as the crystal, so it must be invariant under the symmetry operations of $C_4$. We can construct a representation of $C_4$ on $\mathbb{R}^3$ by considering the $z$-axis as the rotation axis (of course if we pick a different axis, the result will be modified accordingly). This yields

$$r[g] = \begin{pmatrix} 0 & 1 & \\ -1 & 0 & \\ & & 1 \end{pmatrix}. \quad (28)$$

All other elements of the group can be generated from $r[g]$. Let us check explicitly the invariance of $\boldsymbol{\epsilon} = r[g]^{-1}\boldsymbol{\epsilon}r[g]$:

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -\epsilon_{12} & \epsilon_{11} & \epsilon_{13} \\ -\epsilon_{22} & \epsilon_{21} & \epsilon_{23} \\ -\epsilon_{32} & \epsilon_{31} & \epsilon_{33} \end{pmatrix} \quad (29)$$

$$= \begin{pmatrix} \epsilon_{22} & -\epsilon_{21} & -\epsilon_{23} \\ -\epsilon_{12} & \epsilon_{11} & \epsilon_{13} \\ -\epsilon_{32} & \epsilon_{31} & \epsilon_{33} \end{pmatrix}. \quad (30)$$

In order to be invariant, we have the conditions

$$\begin{aligned} \epsilon_{12} &= -\epsilon_{21} \\ \epsilon_{23} &= \epsilon_{13} = 0 \\ \epsilon_{31} &= \epsilon_{32} = 0 \\ \epsilon_{22} &= \epsilon_{11}. \end{aligned} \quad (31)$$

Invariance under $r[g]$ implies invariance under all powers of $r[g]$ and therefore invariance under the entire group. Hence, the most general form of the dielectric permittivity tensor for a crystal with $C_4$ symmetry is

$$\boldsymbol{\epsilon} = \begin{pmatrix} \epsilon_{11} & \epsilon_{12} & 0 \\ -\epsilon_{12} & \epsilon_{11} & 0 \\ 0 & 0 & \epsilon_{33} \end{pmatrix}. \tag{32}$$

2. Inversion symmetry is described in $\mathbb{R}^3$ by

$$r[\text{inv}] = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{33}$$

The rank-3 tensor $\mathbf{L}$ transforms under inversion as

$$\begin{aligned} L^i_{jk} &= (-\delta^i_a)(-\delta^b_j)(-\delta^c_k)L^a_{bc} \\ &= -L^i_{jk}. \end{aligned} \tag{34}$$

We see that all elements of this tensor must be zero in inversion-symmetric materials and therefore there can be no Pockels effect.