Sheet 06: Fields II. Matrices I

(b)[2](E/M/A) means: problem (b) counts 2 points and is easy/medium hard/advanced
Suggestions for central tutorial: example problems 4, 5(bii), 1.
Videos exist for example problems 1 (V3.4.1), 5 (V3.7.3).

Optional Problem 1: Wave functions of two-dimensional harmonic oscillator (polar coordinates) [4]

Points: (a)[0,5](E); (b)[0,5](E); (c)[3](M)

The quantum mechanical treatment of a two-dimensional harmonic oscillator leads to so-called 'wave functions',

$$\Psi_{nm} : \mathbb{R}^2 \to \mathbb{C}, \mathbf{r} \mapsto \Psi_{nm}(\mathbf{r}), \quad \text{with} \quad n \in \mathbb{N}_0, \quad m \in \mathbb{Z}, \quad m = -n, -n+2, \ldots, n-2, n,$$

which have a factorized form when written in terms of polar coordinates, $\Psi_{nm}(\mathbf{r}) = R_{n|m|}(\rho) Z_m(\phi)$, with $Z_m(\phi) = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\mathrm{i}m\phi}$. The wave functions satisfy the following 'orthogonality relation':

$$O_{nn'}^{mm'} \equiv \int_{\mathbb{R}^2} \mathrm{d}S \, \overline{\Psi}_{nm}(\mathbf{r}) \Psi_{n'm'}(\mathbf{r}) = \delta_{nn'} \delta_{mm'} \, .$$

Verify these for $n = 0$, 1 and 2, where the radial wave functions have the form:

$$R_{00}(\rho) = \sqrt{2} \mathrm{e}^{-\rho^2/2}, \quad R_{11}(\rho) = \sqrt{2} \rho \mathrm{e}^{-\rho^2/2}, \quad R_{22}(\rho) = \rho^2 \, \mathrm{e}^{-\rho^2/2}, \quad R_{20}(\rho) = \sqrt{2} [\rho^2 - 1] \mathrm{e}^{-\rho^2/2}.$$

Proceed as follows. Due to the product form of the wave function Ψ, each area integral separates into two factors that can be calculated separately, $O_{nn'}^{mm'} = P_{nn'}^{|m||m'|} \widetilde{P}^{mm'}$, where P is a radial integral and $\widetilde{P}$ an angular integral.

(a) Find general expressions for P and $\widetilde{P}$ as integrals over R- or Z-functions, respectively.

(b) Compute the angular integral $\widetilde{P}^{mm'}$ for arbitrary values of m and m'.

(c) Now compute those radial integrals that arise in combination with $\widetilde{P} \neq 0$, namely P_{00}^{00}, P_{11}^{11}, P_{22}^{22}, P_{22}^{00} and P_{20}^{00}.

Hint: The Euler identity, $\mathrm{e}^{\mathrm{i}2\pi k} = 1$ if $k \in \mathbb{Z}$, is useful for evaluating the angular integral, and $\int_0^\infty \mathrm{d}x \, x^n \mathrm{e}^{-x} = n!$ for the radial integrals.

Background information: The functions $\Psi_{nm}(\mathbf{r})$ are the 'eigenfunctions' of a quantum mechanical particle in a two-dimensional harmonic potential, $V(\mathbf{r}) \propto \mathbf{r}^2$, where n and m are 'quantum numbers' that specify a particular 'eigenstate'. A particle in this state is found with probability $|\Psi_{nm}(\mathbf{r})|^2 \mathrm{d}S$ within the area element $\mathrm{d}S$ at position $\mathbf{r}$. The total probability of being found anywhere in $\mathbb{R}^2$ equals 1, hence the normalization integral yields $O_{nn}^{mm} = 1$ for *every* eigenfunction $\Psi_{nm}(\mathbf{r})$. The fact that the area integral of two eigenfunctions vanishes if their quantum numbers are not equal, reflects the fact that the eigenfunctions form an orthonormal basis in the space of square-integrable complex functions on $\mathbb{R}^2$.

Optional Problem 2: Wave functions of the hydrogen atom (spherical coordinates) [4]
Points: [2](M); (b)[2](M); (c)[2](M,Bonus)

Show that the volume integral, $P_{nlm} = \int_{\mathbb{R}^3} \mathrm{d}V |\Psi_{nlm}(\mathbf{r})|^2$, for the following functions $\Psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_l^m(\theta,\phi)$, with spherical coordinates $\mathbf{r} = \mathbf{r}(r,\theta,\phi)$, yields $P_{nlm} = 1$:

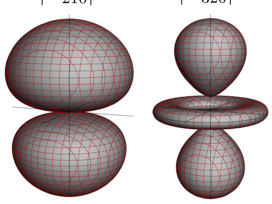
(a) $\Psi_{210}(\mathbf{r}) = R_{21}(r) Y_1^0(\theta,\phi), \quad R_{21}(r) = \dfrac{r\mathrm{e}^{-r/2}}{\sqrt{24}}, \quad Y_1^0(\theta,\phi) = \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta$

(b) $\Psi_{320}(\mathbf{r}) = R_{32}(r) Y_2^0(\theta,\phi), \quad R_{32}(r) = \dfrac{4\, r^2 \mathrm{e}^{-r/3}}{81\sqrt{30}}, \quad Y_2^0(\theta,\phi) = \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1)$

(c) Show that the 'overlap integral' $O = \int_{\mathbb{R}^3} \mathrm{d}V\, \overline{\Psi}_{320}(\mathbf{r}) \Psi_{210}(\mathbf{r})$ yields zero.

Hint: $I_n = \int_0^\infty \mathrm{d}x\, x^n\, \mathrm{e}^{-x} = n!$

Background information: The $\Psi_{nlm}(\mathbf{r})$ are quantum mechanical 'eigenfunctions' of the hydrogen atom, where n, l and m are 'quantum numbers' which specify the quantum state of the system. A particle in this state is found with probability $|\Psi_{nm}(\mathbf{r})|^2 \mathrm{d}V$ within the volume element $\mathrm{d}V$ at position $\mathbf{r}$. The total probability for being found anywhere in $\mathbb{R}^3$ equals 1, hence $P_{nlm} = 1$ holds for *every* eigenfunction $\Psi_{nm}(\mathbf{r})$.



The figures each show a surface on which $|\Psi_{nlm}|^2$ has a constant value. The eigenfunctions form an orthonormal basis in the space of square-integrable complex functions on $\mathbb{R}^3$, hence the volume integral of two eigenfunctions vanishes if their quantum numbers are not equal.

Optional Problem 3: Spin-$\frac{1}{2}$ matrices: commutation relations [2]
Points: (a)[0,5](E); (b)[1,5](E).

The 'spin' of a quantum mechanical particle is a type of internal angular momentum. The description of quantum mechanical spin requires three matrices, S_x, S_y and S_z, whose commutators satisfy the SU(2) algebra. The commutator of two matrices is defined as $[A, B] \equiv AB - BA$. The $\mathrm{SU}(2)$ algebra is defined by the relations $[S_i, S_j] = \mathrm{i}\epsilon_{ijk} S_k$, where ϵ_{ijk} is the antisymmetric Levi-Civita symbol (with $\epsilon_{xyz} = 1$, $\epsilon_{yxz} = -1$, etc.). The description of quantum mechanical particles with spin s, where $s \in \frac{1}{2}\mathbb{Z}$, utilizes a representation of the $\mathrm{SU}(2)$ algebra in terms of matrices of dimension $(2s+1) \times (2s+1)$. They have the property that the matrix $\mathbf{S}^2 \equiv S_x^2 + S_y^2 + S_z^2$ equals $s(s+1)\mathbb{1}$.

The following matrices are used to describe quantum mechanical particles with spin $s = \frac{1}{2}$:

$$S_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_y = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(a) Compute $\mathbf{S}^2$. Is the result consistent with the expected form $s(s+1)\mathbb{1}$?

(b) Verify that S_x, S_y and S_z satisfy the $\mathrm{SU}(2)$ algebra $[S_i, S_j] = \mathrm{i}\epsilon_{ijk} S_k$.

Optional Problem 4: Spin-1 matrices: commutation relations [2]
Points: (a)[0,5](E); (b)[1,5](E)

The following matrices are used to describe quantum mechanical particles with spin $s = 1$:

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

(a) Compute $\mathbf{S}^2 \equiv S_x^2 + S_y^2 + S_z^2$. Is the result consistent with the expected form $s(s+1)\mathbb{1}$?

(b) Verify that S_x, S_y and S_z satisfy the $\mathrm{SU}(2)$ algebra $[S_i, S_j] = \mathrm{i}\epsilon_{ijk} S_k$.

Optional Problem 5: Matrix multiplication [2]
Points: (a)[1](M); (b)[1](M)

Let A and B be $N \times N$ matrices with matrix elements $A^i{}_j = a_j \delta^i{}_m$ and $B^i{}_j = b_i \delta^i{}_j$, for a fixed choice of $m \in \{1, 2, \ldots, N\}$. *Remark:* Since the indices i and j are specified on the left, they are *not* summed over on the right even though in the expression for $B^i{}_j$ the index i appears twice on the right.

(a) For $N = 3$ and $m = 2$, write these matrices explicitly in the usual matrix representation and calculate the matrix product AB explicitly.

(b) Calculate the product AB for arbitrary $N \in \mathbb{N}$ and $1 \leq m \leq N$. [Check your result: the sum of the diagonal elements yields: $\sum_{i=1}^{N} (AB)^i{}_i = a_m b_m$.]

Optional Problem 6: Matrix multiplication [1]
Points: (a)[0.5](E); (b)[0.5](E)

Let A and B be $N \times N$ matrices with matrix elements $A^i{}_j = a_i \delta^i{}_{N+1-j}$ and $B^i{}_j = b_i \delta^i{}_j$. *Remark:* Since the indices i and j are specified on the left, they are *not* summed over on the right even though the index i appears twice in $B^i{}_j$ on the right.

(a) For $N = 3$ and $m = 2$, write these matrices explicitly in the usual matrix representation and calculate the matrix product AB explicitly.

(b) Calculate the product AB for arbitrary $N \in \mathbb{N}$ and $1 \leq m \leq N$. [Check your result: if N is odd, the sum of the diagonal elements yields: $\sum_{i=1}^{N} (AB)^i{}_i = a_{(N+1)/2} b_{(N+1)/2}$.]

[Total Points for Optional Problems: 15]
