Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 9

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The problems whose solutions you need to upload are designated with stars.

⋆ Problem 1 ⋆ Particle in an electromagnetic field

In the presence of an external classical electromagnetic field, the Hamiltonian describing a charged particle is

$$\hat{H}(t) = \frac{[\hat{\boldsymbol{p}} - q\boldsymbol{A}(\boldsymbol{r},t)]^2}{2m} + q\varphi(\boldsymbol{r},t) + V(\boldsymbol{r}), \tag{1}$$

where $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\boldsymbol{\nabla}$, q is the charge, and φ and $\boldsymbol{A}$ are the scalar and vector potentials. We're in 3D and we shall use the position representation and SI units. Because we are treating the electromagnetic field classically, φ and $\boldsymbol{A}$ are real numbers, rather than operators, and their space and time-dependence is imposed externally.

1. If you are given a solution of the Schrödinger equation

$$\mathrm{i}\hbar\partial_t\Psi(\boldsymbol{r},t) = \hat{H}\Psi(\boldsymbol{r},t), \tag{2}$$

   what Schrödinger equation does the wavefunction $\Psi'(\boldsymbol{r},t) = \mathrm{e}^{-\mathrm{i}q\lambda(\boldsymbol{r},t)/\hbar}\Psi(\boldsymbol{r},t)$ satisfy? Absorb the changes into redefinitions of $\boldsymbol{A}$ and φ. What does this transformation from $(\Psi, \boldsymbol{A}, \varphi)$ to $(\Psi', \boldsymbol{A}', \varphi')$ represent physically?

2. Find the charge current $\boldsymbol{j}(\boldsymbol{r},t)$ that enters the charge conservation law

$$\partial_t\rho(\boldsymbol{r},t) + \boldsymbol{\nabla}\cdot\boldsymbol{j}(\boldsymbol{r},t) = 0, \tag{3}$$

   where $\rho(\boldsymbol{r},t) = q\,|\Psi(\boldsymbol{r},t)|^2$.

3. How do $\rho(\boldsymbol{r},t)$ and $\boldsymbol{j}(\boldsymbol{r},t)$ transform under the transformation of part 1 of this problem?

⋆ Problem 2 ⋆ Spin precession

Consider a spin-$\frac{1}{2}$ particle coupled to the magnetic field:

$$\hat{H} = -\hat{\boldsymbol{\mu}}\cdot\boldsymbol{B} = -(\hat{\mu}_x B_x + \hat{\mu}_y B_y + \hat{\mu}_z B_z), \tag{4}$$

where $\hat{\boldsymbol{\mu}} = -\gamma\hat{\boldsymbol{S}}$ is the magnetic dipole moment, γ is the gyromagnetic ratio, $\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}$ is a vector of spin operators, and $\boldsymbol{B}$ is the magnetic field. (Note that $\hat{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z) \equiv \hat{\boldsymbol{x}}\sigma_x + \hat{\boldsymbol{y}}\sigma_y + \hat{\boldsymbol{z}}\sigma_z$ is a convenient shorthand for a vector whose components are operators, in this case 2×2 Pauli matrices, similarly to how the momentum $\hat{\boldsymbol{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z) \equiv \hat{\boldsymbol{x}}\hat{p}_x + \hat{\boldsymbol{y}}\hat{p}_y + \hat{\boldsymbol{z}}\hat{p}_z$ is vector composed of differentiation operators.)

1. Diagonalize this Hamiltonian for an arbitrary magnetic field $\boldsymbol{B} = B_0\hat{\boldsymbol{n}}$, where $\hat{\boldsymbol{n}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ is a unit vector whose direction is oriented along an arbitrary direction.

2. Write down the Ehrenfest equation for the spin expectation value $\left\langle \hat{\boldsymbol{S}}(t) \right\rangle$.

3. If $\boldsymbol{B} = B_0\hat{\boldsymbol{z}}$ points along z, and $\left\langle \hat{\boldsymbol{S}}(t=0) \right\rangle = \frac{\hbar}{2}\hat{\boldsymbol{x}}$, find $\left\langle \hat{\boldsymbol{S}}(t) \right\rangle$ by solving the Ehrenfest equation.

4. Now assume that $\boldsymbol{B} = B_0\hat{\boldsymbol{z}}$ and that the wavefunction initially equals $|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$. Calculate $|\Psi(t)\rangle$ by solving the Schrödinger equations and then calculate $\left\langle \Psi(t) \middle| \hat{\boldsymbol{S}} \middle| \Psi(t) \right\rangle$. Compare with the previous part of this problem.

Problem 3 Singlet and triplet states

Consider two spin-$\frac{1}{2}$ particles.

Formally, the total Hilbert space describing two particles is given by the *tensor product* of the Hilbert spaces describing the particles individually. In this case, the individual Hilbert spaces are $\mathbb{C}^2$ and $\mathbb{C}^2$, and their tensor product is $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^{2\times 2} = \mathbb{C}^4$. The tensor product of two 2-component vectors

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \qquad u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \tag{5}$$

is the 4-component vector

$$v \otimes u = \begin{pmatrix} v_1 u_1 \\ v_1 u_2 \\ v_2 u_1 \\ v_2 u_2 \end{pmatrix}. \tag{6}$$

The tensor product of two 2×2 matrices

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \qquad B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \tag{7}$$

is defined as the 4×4 matrix

$$A \otimes B = \left(\begin{array}{cc|cc} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ \hline A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{array}\right), \tag{8}$$

where the horizontal and vertical lines were added for readability only. Notice how the tensor product is linear in both of its arguments and how it is not commutative, $A \otimes B \neq B \otimes A$.

If the spin operator of an individual particle is given by $\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}}$, where $\hat{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$ are Pauli matrices, then the spin operators of the first and second particles are $\hat{\boldsymbol{S}}_1 = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}} \otimes \mathbb{1}$ and $\hat{\boldsymbol{S}}_2 = \frac{\hbar}{2}\mathbb{1} \otimes \hat{\boldsymbol{\sigma}}$ in the basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ of the total Hilbert space; here $\mathbb{1}$ is the 2×2 identity matrix.

1. Write down the matrices for $\hat{S}_{1,x}$ and $\hat{S}_{2,y}$ in the $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ basis.

2. Show that $[\hat{S}_{1,i}, \hat{S}_{2,j}] = 0$. (Hint: do this abstractly using $(A \otimes B)(C \otimes D) = (AB) \otimes (CD)$.)

3. Introduce $\hat{\boldsymbol{\Sigma}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$. Calculate $[\hat{\Sigma}_i, \hat{\Sigma}_j]$ and find the matrices for $\hat{\boldsymbol{\Sigma}}^2$ and $\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$.

4. Diagonalize the total spin $\hat{\boldsymbol{\Sigma}}^2$ simultaneously with the total spin along z $\hat{\Sigma}_z$. Make sure that the phases of the different eigenvectors are properly related through raising and lower operations $\hat{\Sigma}_\pm$. What spin values do you find?