PHOT 301: Quantum Photonics

Example final exam questions and solutions

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General information on the exam

Grading: This final exam will count for 50% of your total grade. Together with the projects which count for 40%, and the midterm exam that counts for 10%, your total grade for the course will be determined.

Exam type: The final exam consists of 8 open questions/problems. The exam is a written exam and all questions can be answered using only pen and paper. Calculators, mobile phones, laptops are not needed, and are not allowed to be used during the exam. The last page of the exam contains some formulas which can be used to help solve the problems.

The duration of the final exam is 3 hours.

Exam questions

Please answer all questions listed below. Each of the questions is valued equally in the score calculation of the exam. If a question contains multiple part, each of the parts is valued equally within the score for the question.

Please tell if any question is unclear or ambiguous.

Question 1: Wave functions and expectation values

Consider the following 1D wave function defined with $x \in \mathbb{R}$:

$$\psi(x) = A \, \frac{1}{(x+i)^2}$$

with A a normalization constant.

(1/3) First calculate the normalization constant A of the wave function.
(2/3) Then calculate the expectation value for the position operator $\langle x \rangle \in \mathbb{R}$.
(3/3) Calculate the variance σ^2 (expectation value): $\sigma^2 = \left\langle \left(x - \langle x \rangle\right)^2 \right\rangle = \langle x^2 \rangle - \langle x \rangle^2$.

Solution (Q1)

The normalization factor $A = \sqrt{2/\pi}$ as can be seen from:

$$
\begin{aligned}
1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx &= |A|^2 \int_{-\infty}^{\infty} |\frac{1}{(x+i)^2}|^2 \, dx \\
&= |A|^2 \int_{-\infty}^{\infty} \frac{1}{(x-i)^2} \frac{1}{(x+i)^2} \, dx \\
&= |A|^2 \int_{-\infty}^{\infty} \frac{1}{(x^2+1)^2} \, dx \\
&= |A|^2 \frac{1}{2} \left(\arctan(x) + \frac{x}{x^2+1} \right) \Big|_{-\infty}^{+\infty} \\
&= |A|^2 \frac{1}{2} \left(\frac{\pi}{2} + \frac{\pi}{2} \right) = |A|^2 \frac{\pi}{2}
\end{aligned}
$$

The expectation value for the position $\langle x \rangle = 0$ can be derived as:

$$
\begin{aligned}
\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx &= |A|^2 \int_{-\infty}^{\infty} x |\frac{1}{(x+i)^2}|^2 \, dx \\
&= |A|^2 \int_{-\infty}^{\infty} \frac{x}{(x^2+1)^2} \, dx \\
&= -|A|^2 \frac{1}{2} \frac{1}{x^2+1} \Big|_{-\infty}^{+\infty} = 0
\end{aligned}
$$

The variance $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 = \langle x^2 \rangle - 0 = 1$ can be derived as:

$$
\begin{aligned}
\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx &= |A|^2 \int_{-\infty}^{\infty} x^2 |\frac{1}{(x+i)^2}|^2 \, dx \\
&= |A|^2 \int_{-\infty}^{\infty} \frac{x^2}{(x^2+1)^2} \, dx \\
&= |A|^2 \frac{1}{2} \left(\arctan(x) - \frac{x}{x^2+1} \right) \Big|_{-\infty}^{+\infty} \\
&= |A|^2 \frac{1}{2} \left(\frac{\pi}{2} + \frac{\pi}{2} \right) = |A|^2 \frac{\pi}{2} = 1
\end{aligned}
$$

Question 2: Infinite well eigenstate superposition

Consider the following two normalized superpositions (ϕ_a, ϕ_b) of 1D infinite well eigenstates $\psi_n(x)$:

$$\phi_a = \frac{1}{\sqrt{2}}(\psi_1 + \psi_3)$$
$$\phi_b = \frac{1}{\sqrt{2}}(\psi_1 + i\,\psi_3)$$

where the eigenstates of the infinite well (with width L) are given by:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}, \quad \text{with } n = 1, 2, 3, \ldots$$

(1/2) Calculate the expectation value of the position for the two superpositions: $\langle \hat{x} \rangle$

(2/2) Calculate the variance (expectation value) $\sigma^2 = \langle (\hat{x} - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$ for the two superpositions.

Solution (Q2)

In the following we will use that eigenstates $\psi_n(x)$ are real, and the substitution $x \longrightarrow u = g(x) = x/L$ for definite integrals:

$$\int_a^b f(g(x)) \frac{d\,g(x)}{dx}\, dx = \int_{g(a)}^{g(b)} f(u)\, du$$

where we will use it to convert to intervals such as for example:

$$\frac{2}{L} \int_0^L x^2 \sin^2(m\pi x/L)\, dx = 2L^2 \int_0^1 u^2 \sin^2(m\pi u)\, du$$

The expectation values for the position $\langle \hat{x} \rangle_a$ and $\langle \hat{x} \rangle_b$ for the superpositions ϕ_a and ϕ_b can be derived as follows.

$$\begin{aligned}
\langle x \rangle_a &= \int_0^L x |\phi_a|^2 dx \\
&= \frac{1}{2} \int_0^L x\,(\psi_1 + \psi_3)^2\, dx \\
&= \frac{1}{2} \int_0^L x\,\psi_1^2\, dx + \frac{1}{2} \int_0^L x\,\psi_3^2\, dx + \frac{1}{2} \int_0^L x\, 2\psi_1\psi_3\, dx \\
&= \frac{1}{L} \int_0^L x\, \sin^2(\pi x/L)\, dx + \frac{1}{L} \int_0^L x\, \sin^2(3\pi x/L)\, dx + \frac{1}{L} \int_0^L x\, 2\sin(\pi x/L) \sin(3\pi x)\, dx \\
&= L \int_0^1 x\, \sin^2(\pi x)\, dx + L \int_0^1 x\, \sin^2(3\pi x)\, dx + L \int_0^1 x\, 2\sin(\pi x) \sin(3\pi x)\, dx \\
&= \frac{L}{4} + \frac{L}{4} + 0 = \frac{L}{2}
\end{aligned}$$

The expectation value $\langle x\rangle_b$ of ϕ_b is obtained in the same way:

$$\begin{aligned}
\langle x\rangle_b &= \int_0^L x|\phi_b|^2 dx \\
&= \frac{1}{2}\int_0^L x\,(\psi_1^2+\psi_3^2)\,dx \\
&= \frac{1}{2}\int_0^L x\,\psi_1^2\,dx + \frac{1}{2}\int_0^L x\,\psi_3^2\,dx \\
&= \frac{1}{L}\int_0^L x\,\sin^2(\pi x/L)\,dx + \frac{1}{L}\int_0^L x\,\sin^2(3\pi x/L)\,dx \\
&= L\int_0^1 x\,\sin^2(\pi x)\,dx + L\int_0^1 x\,\sin^2(3\pi x)\,dx \\
&= \frac{L}{4}+\frac{L}{4}=\frac{L}{2}
\end{aligned}$$

For variance $\sigma^2 = \langle x^2\rangle - \langle x\rangle^2 = \langle x^2\rangle - \frac{L^2}{4}$ we calculate $\langle x^2\rangle$ and subtract then $\frac{L^2}{4}$:

$$\begin{aligned}
\langle x^2\rangle_a &= \int_0^L x^2|\phi_a|^2 dx \\
&= \frac{1}{2}\int_0^L x^2\,(\psi_1+\psi_3)^2\,dx \\
&= \frac{1}{2}\int_0^L x^2\,\psi_1^2\,dx + \frac{1}{2}\int_0^L x^2\,\psi_3^2\,dx + \frac{1}{2}\int_0^L x^2\,2\psi_1\psi_3\,dx \\
&= \frac{1}{L}\int_0^L x^2\,\sin^2(\pi x/L)\,dx + \frac{1}{L}\int_0^L x^2\,\sin^2(3\pi x/L)\,dx + \frac{1}{L}\int_0^L x^2\,2\sin(\pi x/L)\sin(3\pi x)\,dx \\
&= L^2\int_0^1 x^2\,\sin^2(\pi x)\,dx + L^2\int_0^1 x^2\,\sin^2(3\pi x)\,dx + L^2\int_0^1 x^2\,2\sin(\pi x)\sin(3\pi x)\,dx \\
&= L^2\left(\frac{1}{6}-\frac{1}{4\pi^2}+\frac{1}{6}-\frac{1}{9}\frac{1}{4\pi^2}+2\frac{3}{16\pi^2}\right) = L^2\left(\frac{1}{3}+\frac{7}{18\pi^2}\right) \\
\Longrightarrow \sigma_a^2 &= L^2\left(\frac{1}{12}+\frac{7}{18\pi^2}\right)
\end{aligned}$$

$$
\begin{aligned}
\langle x^2\rangle_b &= \int_0^L x^2 |\phi_b|^2 dx \\
&= \frac{1}{2}\int_0^L x^2\left(\psi_1^2+\psi_3^2\right)dx \\
&= \frac{1}{2}\int_0^L x^2\,\psi_1^2\,dx + \frac{1}{2}\int_0^L x^2\,\psi_3^2\,dx \\
&\quad \text{same integrals as above without 3rd term} \\
&= L^2\left(\frac{1}{6}-\frac{1}{4\pi^2}+\frac{1}{6}-\frac{1}{9}\frac{1}{4\pi^2}\right) = L^2\left(\frac{1}{3}-\frac{5}{18\pi^2}\right) \\
\Longrightarrow \sigma_b^2 &= L^2\left(\frac{1}{12}-\frac{5}{18\pi^2}\right)
\end{aligned}
$$

Question 3: Oscillations of eigenstates

Consider a Hydrogen atom in a superposition state $\Psi(\vec{r},t)$ of a $1S$ and a $2P_z$ orbital (ignore spin):

$$
\Psi(\vec{r},t) = \frac{1}{\sqrt{2}}\left(\psi_{100}(\vec{r})\,e^{-iE_1t/\hbar} + \psi_{210}(\vec{r})\,e^{-iE_2t/\hbar}\right).
$$

where the eigenstates ψ_{nlm} for the hydrogen orbitals (without spin) $\psi_{100}(\vec{r})$ and $\psi_{210}(\vec{r})$ and their eigenenergies are given by

$$
\begin{aligned}
\psi_{100}(\vec{r}) &= \frac{1}{\sqrt{\pi a_0^3}}e^{-r}, & E_1 &= -\mathrm{Ry} \\
\psi_{210}(\vec{r}) &= \frac{1}{\sqrt{32\pi a_0^3}}e^{-r/2}\,r\cos\theta = \frac{1}{\sqrt{32\pi a_0^3}}e^{-r/2}\,z, & E_2 &= -\frac{\mathrm{Ry}}{4}
\end{aligned}
$$

with r in units of the Bohr radius a_0.

(1/1) Calculate the expectation value for the position along the z-axis $\langle \hat{z}\rangle$ as a function of time and show that it oscillates (in time) around zero.

Solution (Q3)

As shorthand notation we rename real-valued eigenstates $\psi_{100},\ \psi_{210} \longrightarrow \psi_1,\ \psi_2$ and define $\omega_1 = E_1/\hbar,\ \omega_2 = E_2/\hbar$ and $\Delta\omega = \omega_1 - \omega_2$. We also simply use the notation $\int_V dV$ for the integral over the whole space. The expection value for z:

$$
\begin{aligned}
\langle z\rangle &= \frac{1}{2}\int_V z\,\left(\psi_1\,e^{i\omega_1 t}+\psi_2\,e^{i\omega_2 t}\right)\,\left(\psi_1\,e^{-i\omega_1 t}+\psi_2\,e^{-i\omega_2 t}\right)\,dV \\
&= \frac{1}{2}\int_V z\,\left(\psi_1^2+\psi_2^2+2\psi_1\psi_2\cos(\Delta\omega t)\right)dV \\
&\quad |\psi_1|^2 \text{ and } |\psi_1|^2 \text{ are symmetric under } z\longrightarrow -z \\
&= 0+0+\cos(\Delta\omega t)\int_V z\,\psi_1\psi_2 dV \\
&\quad \text{Integration in spherical coordinates with } z=r\cos\theta \\
&= \frac{1}{\sqrt{32\pi a_0^3}}\cos(\Delta\omega t)\int_0^\infty dr\int_0^\pi d\theta\int_0^{2\pi} d\phi\, r^2\cos^2\theta\, e^{-\frac{3r}{2}}r^2\sin\theta \\
&= \frac{1}{\sqrt{32\pi a_0^3}}\cos(\Delta\omega t)\int_0^{2\pi} d\phi\times\int_0^\infty r^4\,e^{-\frac{3r}{2}}dr\times\int_0^\pi \cos^2\theta\,\sin\theta d\theta \\
&= \frac{1}{\sqrt{8a_0^3}}\cos(\Delta\omega t)\frac{4!\,2^5}{3^5}\times\frac{2}{3} \\
&= \frac{1}{\sqrt{2a_0^3}}\,\frac{256}{243}\,\cos(\Delta\omega t)
\end{aligned}
$$

which is oscillating in time with frequency $\Delta\omega/2\pi$.

Question 4: Perturbation: the anharmonic oscillator

Consider the 1D harmonic oscillator perturbed by a perturbation part: $\hat{H}_p = \beta x^4$ with β a small number:

$$
\begin{aligned}
\hat{H} &= \frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2x^2+\beta x^4 \\
&= \hat{H}_0+\hat{H}_p
\end{aligned}
$$

where the unperturbed Hamiltonian $\hat{H}_0$ has eigenenergies $E_m^{(0)}$, that is:

$$
\hat{H}_0\psi_m(x)=E_m^{(0)}\psi_m(x), \quad \text{and ground state: } \psi_0=\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\,e^{-\frac{m\omega}{2\hbar}x^2}, \quad E_0^{(0)}=\frac{1}{2}\hbar\omega
$$

(1/1) Calculate the value of the energy of the perturbed ground state E_0 within first order perturbation theory approximation.

Hint: The energy E_m of eigenstate ψ_m up to first order in perturbation theory is given by:

$$
E_m = E_m^{(0)} + \langle\psi_m^{(0)}|\hat{H}_p|\psi_m^{(0)}\rangle
$$

Solution (Q4)

The energy up to first order perturbation for the ground state is given by:

$$\begin{aligned}
E_0 &= E_0^{(0)} + \langle \psi_0^{(0)} | \hat{H}_p | \psi_0^{(0)} \rangle \\
&= \frac{1}{2}\hbar\omega + \beta \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} x^4 e^{-\frac{m\omega}{\hbar} x^2}\, dx \\
&= \frac{1}{2}\hbar\omega + \beta \sqrt{\frac{m\omega}{\pi\hbar}} \frac{3\sqrt{\pi}(\sqrt{\hbar})^5}{4(\sqrt{m\omega})^5} \\
&= \frac{1}{2}\hbar\omega + \beta\, \frac{3\hbar^2}{4m^2\omega^2}
\end{aligned}$$

Question 5: Spin projection operators

Consider a particle with spin with the following orthonormal basis of eigenstates:

$$|u\rangle = |\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |d\rangle = |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Consider further the left and right spin states:

$$\begin{aligned}
|l\rangle = |\leftarrow\rangle &= \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \\
|r\rangle = |\rightarrow\rangle &= \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}
\end{aligned}$$

and projection operators derived from them: $\hat{P}_u = |u\rangle\langle u|$ and $\hat{P}_l = |l\rangle\langle l|$.

(1/1) Perform the following projections:

$$\hat{P}_u \hat{P}_l |u\rangle = ?$$

Solution (Q5)

$$\begin{aligned}
\hat{P}_u \hat{P}_l |u\rangle &= |u\rangle\langle u|\, |l\rangle\langle l|\, |u\rangle = |u\rangle\langle u|l\rangle\langle l|u\rangle \\
&= \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \times \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \\
&= \frac{1}{2}|u\rangle
\end{aligned}$$

Question 6: Spin evolution in a magnetic field

Look at the evolution of the spin in time under a B-field oriented along the x-axis: $\vec{B} = (B, 0, 0)$. That is, consider the following Schrodinger equation:

$$\mu_B B \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_u \\ c_d \end{pmatrix} = E \begin{pmatrix} c_u \\ c_d \end{pmatrix}$$

where $\mu_B = \frac{e\hbar}{2m_0}$ is the Bohr magneton.

(1/2) Calculate the eigenvalues and corresponding eigenstates of the system.

(2/2) Start in the spin up state $\Psi(t=0) = |u\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ at time $t = 0$. After what time will the system returns back to the spin up state?

Solution (Q6)

The eigenenergies of this eigenvalue equation can be derived as follows:

$$\det\left(\mu_B B \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - E\mathbb{1}\right) = \det\left(\begin{pmatrix} -E & \mu_B B \\ \mu_B B & -E \end{pmatrix}\right) = E^2 - (\mu_B B)^2 = 0$$

$$\Rightarrow \quad E_\pm = \pm\mu_B B$$

Corresponding eigenstates $\psi_\pm$ can be found by inserting the eigenenergies in the original equation:

$$\mu_B B \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} c_u \\ c_d \end{pmatrix} = \pm\mu_B B \begin{pmatrix} c_u \\ c_d \end{pmatrix}$$

$$\Rightarrow \quad \mu_B B c_d = \pm\mu_B B c_u \quad \Rightarrow \quad c_d = \pm c_u \quad \Rightarrow \quad \psi_\pm \propto \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

Normalizing the eigenstates $\psi_\pm$ we obtain:

$$\psi_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

If we start in the spin-up state, we can expand this state in the eigenstates $\psi_\pm$ where the coefficients of the expansion can be seen to be:

$$\Psi(t=0) = \frac{1}{\sqrt{2}}(\psi_+ + \psi_-)$$

Adding the time-dependency factors for the eigenstates with energies $E_{\pm}$:

$$\Psi(t>0) = \frac{1}{\sqrt{2}}\left(\psi_+ e^{-i\mu_B Bt/\hbar} + \psi_- e^{i\mu_B Bt/\hbar}\right) = \frac{1}{2}\begin{pmatrix} e^{-i\mu_B Bt/\hbar} + e^{i\mu_B Bt/\hbar} \\ e^{-i\mu_B Bt/\hbar} - e^{i\mu_B Bt/\hbar} \end{pmatrix}$$
$$= \frac{1}{2}\begin{pmatrix} 2\cos(\mu_B Bt/\hbar) \\ -2i\sin(\mu_B Bt/\hbar) \end{pmatrix}$$

Therefore the first occurence that the wave function gets into the same spin-up state:

$$\Psi(t>0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \Leftrightarrow \quad \cos(\mu_B Bt/\hbar) = 1 \quad \& \quad \sin(\mu_B Bt/\hbar) = 0$$

Therefore $\mu_B Bt/\hbar = 2\pi$ and $t = \frac{2\pi\hbar}{\mu_B B}$. ($\pi$ instead of 2π as alternative is also accepted as *probability* for the spin-up state is one).

Question 7: Periodic systems

Assume a 1D periodic system of equi-distant δ-function potential barriers. A single unit cell has length L and contains a single potential barrier with strength α, that is $V(x) =$ (x). The relation between the coefficients (A, B) before at $x = 0$ and (C, D) after the barrier at $x = L$ can be written as:

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{ka}\begin{pmatrix} (ka-i)e^{ikL} & -ie^{ikL} \\ ie^{-ikL} & (ka+i)e^{-ikL} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix}$$

where the wave vector is $k = \sqrt{2mE}/\hbar$ and $a = \frac{\hbar^2}{m\alpha}$. According to the Bloch theorem we can write

$$\begin{pmatrix} C \\ D \end{pmatrix} = e^{i\beta L}\begin{pmatrix} A \\ B \end{pmatrix}$$

with β the Bloch wave vector which provides the slowly varying phase of the envelope function.

(1/1): Show that the Bloch theorem leads to the following characteristic equation (which defines the band structure $E(\beta)$):

$$\cos(\beta L) = \cos(kL) + \frac{1}{ka}\sin(kL)$$

Solution (Q7)

We use the Bloch condition $e^{i\beta L}\begin{pmatrix}A\\B\end{pmatrix} = \begin{pmatrix}C\\D\end{pmatrix}$ to eliminate coefficients A and B:

$$e^{-i\beta L}\begin{pmatrix}C\\D\end{pmatrix} = \frac{1}{ka}\begin{pmatrix}(ka-i)e^{ikL} & -ie^{ikL}\\ ie^{-ikL} & (ka+i)e^{-ikL}\end{pmatrix}\begin{pmatrix}C\\D\end{pmatrix}$$

$$\Rightarrow \quad \left[\frac{1}{ka}\begin{pmatrix}(ka-i)e^{ikL} & -ie^{ikL}\\ ie^{-ikL} & (ka+i)e^{-ikL}\end{pmatrix} - \begin{pmatrix}e^{-i\beta L} & 0\\ 0 & e^{-i\beta L}\end{pmatrix}\right]\begin{pmatrix}C\\D\end{pmatrix} = \begin{pmatrix}0\\0\end{pmatrix}$$

This means the determinant of the matrix should be zero:

$$\det\left[\frac{1}{ka}\begin{pmatrix}(ka-i)e^{ikL} & -ie^{ikL}\\ ie^{-ikL} & (ka+i)e^{-ikL}\end{pmatrix} - \begin{pmatrix}e^{-i\beta L} & 0\\ 0 & e^{-i\beta L}\end{pmatrix}\right] = 0$$

We derive the characteristic equation by writing out the determinant:

$$\begin{aligned}
0 &= \frac{1}{(ka)^2}\left[(ka)^2 + 1 + (ka)^2 e^{-i2\beta L} - ka(ka-i)e^{ikL}e^{-i\beta L} - ka(ka+i)e^{-ikL}e^{-i\beta L} - 1\right]\\
&= \frac{e^{-i\beta L}}{(ka)^2}\left[(ka)^2 e^{i\beta L} + (ka)^2 e^{-i\beta L} - ka(ka-i)e^{ikL} - ka(ka+i)e^{-ikL}\right]\\
&= \frac{2e^{-i\beta L}}{(ka)^2}\left[(ka)^2(e^{i\beta L}+e^{-i\beta L}) - (ka)^2(e^{ikL}+e^{-ikL}) + ika(e^{ikL}-e^{-ikL})\right]\\
&= 2e^{-i\beta L}\left[\cos(\beta L) - \cos(kL) - \frac{1}{ka}\sin(kL)\right]
\end{aligned}$$

$$\Rightarrow \quad \cos(\beta L) = \cos(kL) + \frac{1}{ka}\sin(kL)$$

Question 8: two particles in an infinite well

Consider the 1D infinite well with two particles. Assume that the particles are not interacting and ignore exchange energy:

(1/1) Assume that the particles are bosons and both are in the ground state: what is the energy of the system?

Hint: For an infinite square well with width L the solutions for a single particle can be written in the form:

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right), \qquad E_n = \frac{\hbar^2\pi^2 n^2}{2mL^2}, \quad \text{with } n = 1, 2, 3, \ldots$$

Solution (Q8)

For two bosons the wave function is the symmetric sum: $\psi(x_1, x_2) \propto \psi_1(x_1)\psi_1(x_2) + \psi_1(x_2)\psi_1(x_1)$. Since the particles are not interacting the Hamiltonian is decoupled:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_2^2}$$

The symmetric wave function for both single-particle wave functions in the ground state:

$$\psi(x_1, x_2) \propto \psi_1(x_1)\psi_1(x_2) + \psi_1(x_2)\psi_1(x_1) \propto \psi_1(x_1)\psi_1(x_2)$$

where normalization leads to $\psi(x_1, x_2) = \psi_1(x_1)\psi_1(x_2)$. Using this wave function and the Hamiltonian above we obtain the expectation value for the energy $\langle\hat{H}\rangle$:

$$\begin{aligned}
\langle\hat{H}\rangle &= \int_0^L dx_1 \int_0^L dx_2 \psi^*(x_1, x_2)\hat{H}\psi(x_1, x_2) \\
&= \int_0^L dx_1 \int_0^L dx_2 \psi(x_1, x_2)(\hat{H}_1 + \hat{H}_2)\psi(x_1, x_2) \\
&= \int_0^L dx_1 \int_0^L dx_2 \psi_1(x_1)\psi_1(x_2)\hat{H}_1\psi_1(x_1)\psi_1(x_2) + \int_0^L dx_1 \int_0^L dx_2 \psi_1(x_1)\psi_1(x_2)\hat{H}_2\psi_1(x_1)\psi_1(x_2) \\
&= \int_0^L dx_2 \psi_1^2(x_2) \int_0^L dx_1[\psi_1(x_1)\hat{H}_1\psi_1(x_1)] + \int_0^L dx_1 \psi_1^2(x_1) \int_0^L dx_2[\psi_1(x_2)\hat{H}_2\psi_1(x_2)] \\
&= E_1 \int_0^L dx_2 \psi_1^2(x_2) + E_1 \int_0^L dx_1 \psi_1^2(x_1) \\
&= 2\,E_1 = \frac{2\hbar^2\pi^2}{2mL^2}
\end{aligned}$$

Formulas

In the following formulas parameters n, m are integers and $0 < a \in \mathbb{R}$ and $b \in \mathbb{R}_0$:

Anti-derivatives (indefinite integrals)

$$\int \frac{1}{(x^2+1)^2}\,dx = \frac{1}{2}\left(\arctan(x) + \frac{x}{x^2+1}\right)$$

$$\int \frac{x}{(x^2+1)^2}\,dx = -\frac{1}{2}\frac{1}{x^2+1}$$

$$\int \frac{x^2}{(x^2+1)^2}\,dx = \frac{1}{2}\left(\arctan(x) - \frac{x}{x^2+1}\right)$$

$$\int \frac{x^3}{(x^2+1)^2}\,dx = \frac{1}{2}\left(\frac{1}{x^2+1} + \log(x^2+1)\right)$$

$$\int \cos^n(ax)\sin(ax)\,dx = -\frac{1}{a(n+1)}\cos^{n+1}(ax)$$

$$\int \cos(ax)\sin^n(ax)\,dx = \frac{1}{a(n+1)}\sin^{n+1}(ax)$$

Definite integrals

$$\int_0^\infty x^n e^{-ax}\,dx = \frac{n!}{a^{n+1}}$$

$$\int_0^\infty e^{-ax^2}\,dx = \frac{\sqrt{\pi}}{2\sqrt{a}}$$

$$\int_0^\infty x^2 e^{-ax^2}\,dx = \frac{\sqrt{\pi}}{4a^{3/2}}$$

$$\int_0^\infty x^4 e^{-ax^2}\,dx = \frac{3\sqrt{\pi}}{8a^{5/2}}$$

Definite integrals

$$\int_0^1 \sin(m\pi x)\sin(n\pi x)\,dx = \frac{1}{2}\delta_{mn}$$

$$\int_0^1 x\sin^2(m\pi x)\,dx = \frac{1}{4}$$

$$\int_0^1 x^2\sin^2(m\pi x)\,dx = \frac{1}{6} - \frac{1}{4\pi^2 m^2}$$

$$\int_0^1 x\sin(\pi x)\sin(3\pi x)\,dx = 0$$

$$\int_0^1 x^2\sin(\pi x)\sin(3\pi x)\,dx = \frac{3}{16\pi^2}$$

$$\int_0^1 x^3\sin(\pi x)\sin(3\pi x)\,dx = \frac{9}{32\pi^2}$$

$$\int_{-\infty}^\infty e^{-ax^2}\,dx = \frac{\sqrt{\pi}}{\sqrt{a}}$$

$$\int_{-\infty}^\infty x^2 e^{-ax^2}\,dx = \frac{\sqrt{\pi}}{2a^{3/2}}$$

$$\int_{-\infty}^\infty x^4 e^{-ax^2}\,dx = \frac{3\sqrt{\pi}}{4a^{5/2}}$$

Integration in spherical coordinates:

$$\int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dz\, f(x,y,z) = \int_0^\infty d\rho \int_0^\pi d\theta \int_0^{2\pi} d\phi\, \rho^2 \sin\theta\; F(\rho,\theta,\phi)$$

where volume element $dx\,dy\,dz = \rho^2 \sin\theta\, d\theta\, d\phi\, d\rho$

$x = \rho\sin(\theta)\cos(\phi),\ \ y = \rho\sin(\theta)\sin(\phi),\ \ z = \rho\cos(\theta)$