ADVANCED QUANTUM THEORY
EXERCISE SHEET 11

Markus Pawellek
markuspawellek@gmail.com

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Problem 18: Perturbation Theory

Let $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ be a separable Hilbert space which is modeling the perturbed and the unperturbed system. For the formal definition of both systems we will define $\mathcal{I}$ as a countable index set with the same cardinality as an orthonormal basis of $\mathcal{H}$.

The Hamiltonian $H\colon \mathcal{H} \to \mathcal{H}$ of the unperturbed system is assumed to have a discrete spectrum of real Energies.

$$\sigma(H) = \{E_n \mid n \in \mathcal{I}\} \subset \mathbb{R}$$

For all $n \in \mathcal{I}$ we denote $|n\rangle \in \mathcal{H}$ to be the unique normalized eigenstate of H with the eigenvalue E_n.

$$H\,|n\rangle = E_n\,|n\rangle\ , \qquad \langle n|n\rangle = 1$$

$$\forall m \in \mathcal{I}, m \neq n: \quad E_m \neq E_n$$

Based on this and due to the self-adjointness of the Hamiltonian H we can derive that H itself is non-degenerate and that the set $\{|n\rangle \mid n \in \mathcal{I}\}$ is building an orthonormal basis of the Hilbert space $\mathcal{H}$.

Further, we describe the perturbation of the system by the self-adjoint operator $V\colon \mathcal{H} \to \mathcal{H}$. For the application of V to H we will use an interaction strength parameter which is introduced by using a function $\tilde{H}$ as shown below.

$$\tilde{H}\colon [0,1] \to \mathrm{L}(\mathcal{H}, \mathcal{H})\ , \qquad \tilde{H}(\lambda) \coloneqq H + \lambda V$$

The continuous parameterization will enable us to analyze the solution of the perturbed system $\tilde{H}(\lambda)$ in form of a series expansion in terms of λ. Please note that $\tilde{H}(1)$ is describing the system under the full perturbation.

We will assume that the contribution of V is small and therefore not changes the essential properties. Hence, we choose $\lambda \in [0,1]$ to be arbitrary. $\tilde{H}(\lambda)$ has a discrete spectrum.

$$\sigma\left(\tilde{H}(\lambda)\right) = \{E_n(\lambda) \mid n \in \mathcal{I}\} \subset \mathbb{R}$$

$\tilde{H}(\lambda)$ is non-degenerate and we again assume its eigenstates to be normalized and therefore to build an orthonormal eigenbasis with respect to $\tilde{H}(\lambda)$ [1]. So for all $n \in \mathcal{I}$ it holds that

$$\tilde{H}(\lambda)\,|n(\lambda)\rangle = E_n(\lambda)\,|n(\lambda)\rangle$$

$$\forall m \in \mathcal{I}, m \neq n: \quad E_m(\lambda) \neq E_n(\lambda)$$

$$\langle n(\lambda)|n(\lambda)\rangle = 1$$

Additionally, we assume that we are able to expand $E_n(\lambda)$ and $|n(\lambda)\rangle$ in terms of λ for all $\lambda \in [0,1]$ for some constant coefficients.

$$\{E_{nk}\}_{k=0}^{\infty} \subset \mathbb{R}\ , \qquad E_n(\lambda) = \sum_{k=0}^{\infty} \lambda^k E_{nk}$$

$$\{|n_k\rangle\}_{k=0}^{\infty} \subset \mathcal{H}\ , \qquad |n(\lambda)\rangle = \sum_{k=0}^{\infty} \lambda^k\,|n_k\rangle$$

Taking the series expansions one can now derive inductive formulas for the coefficients. For that let $n \in \mathcal{I}$ and $\lambda \in [0,1]$ be arbitrary. We will start with the left-hand side of the eigenvalue equation.

$$\begin{aligned}
&\tilde{H}(\lambda)\,|n(\lambda)\rangle \\
&= (H + \lambda V) \sum_{k=0}^{\infty} \lambda^k\,|n_k\rangle \\
&= \sum_{k=0}^{\infty} \lambda^k H\,|n_k\rangle + \sum_{k=0}^{\infty} \lambda^{k+1} V\,|n_k\rangle
\end{aligned}$$

[1] The non-degeneracy of $\tilde{H}(\lambda)$ for all $\lambda \in [0,1]$ is not used explicitly. Therefore the derived formulas should be valid even if the perturbation described by V introduces degeneracies into the non-degenerate system described by H.

$$= \sum_{k=0}^{\infty} \lambda^k H \left|n_k\right\rangle + \sum_{k=1}^{\infty} \lambda^k V \left|n_{k-1}\right\rangle$$
$$= H \left|n_0\right\rangle + \sum_{k=1}^{\infty} \lambda^k \left(H \left|n_k\right\rangle + V \left|n_{k-1}\right\rangle\right)$$

For the right-hand side of the eigenvalue equation we do get the following.

$$\begin{aligned} & E_n(\lambda) \left|n(\lambda)\right\rangle \\ &= \left(\sum_{k=0}^{\infty} \lambda^k E_{nk}\right) \left(\sum_{k=0}^{\infty} \lambda^k \left|n_k\right\rangle\right) \\ &= \sum_{p,q=0}^{\infty} \lambda^{p+q} E_{np} \left|n_q\right\rangle \\ &= \sum_{k=0}^{\infty} \lambda^k \sum_{p=0}^{k} E_{np} \left|n_{k-p}\right\rangle \end{aligned}$$

Looking at the eigenvalue equation as a whole we are now able to do a comparison of coefficients. This results in two equations. One for the starting values and one for all $k \in \mathbb{N}$.

$$H \left|n_0\right\rangle = E_{n0} \left|n_0\right\rangle$$
$$H \left|n_k\right\rangle + V \left|n_{k-1}\right\rangle = \sum_{p=0}^{k} E_{np} \left|n_{k-p}\right\rangle$$

After inserting the series expansions we can do something similar for the normalization condition.

$$\begin{aligned} 1 &= \langle n(\lambda) | n(\lambda) \rangle \\ &= \sum_{p,q=0}^{\infty} \lambda^{p+q} \langle n_p | n_q \rangle \\ &= \sum_{k=0}^{\infty} \lambda^k \sum_{p=0}^{k} \langle n_p | n_{k-p} \rangle \end{aligned}$$

Again we do comparison of coefficients and get two equations. One for the starting value and one for all $k \in \mathbb{N}$.

$$\langle n_0 | n_0 \rangle = 1$$

$$\begin{aligned} \langle n_0 | n_k \rangle + \langle n_k | n_0 \rangle &= 2\Re(\langle n_0 | n_k \rangle) \\ &= -\sum_{p=1}^{k-1} \langle n_p | n_{k-p} \rangle \end{aligned}$$

To make the second equation simpler consider that the overall phase is not determined in quantum mechanics. Hence, without loss of generality, we may assume $\langle n_0 | n_k \rangle = \Re(\langle n_0 | n_k \rangle) \in \mathbb{R}$ is purely real. For all $k \in \mathbb{N}$ the second equation becomes the following.

$$\langle n | n_k \rangle = -\frac{1}{2} \sum_{p=1}^{k-1} \langle n_p | n_{k-p} \rangle$$

After deriving these formulas we will first take a look at the starting value equations.

$$H \left|n_0\right\rangle = E_{n0} \left|n_0\right\rangle \ , \qquad \langle n_0 | n_0 \rangle = 1$$

We see that $\left|n_0\right\rangle$ is a normalized eigenfunction of H with the eigenvalue E_{n0}. Therefore we can state the following.

$$E_{n0} \in \sigma(H) \ , \qquad \left|n_0\right\rangle \in \{\left|m\right\rangle \mid m \in \mathcal{I}\}$$

We are free to choose the specific eigenfunction because this is the freedom of permuting the eigenstates. But for consistency we will use the straightforward definition.

$$\left|n_0\right\rangle \coloneqq \left|n\right\rangle \ , \qquad E_{n0} \coloneqq E_n$$

Now we take the inductive formula of the eigenvalue equation and insert the starting values to get an operator equation for $\left|n_k\right\rangle$ for all $k \in \mathbb{N}$.

$$\left(H - E_n\right) \left|n_k\right\rangle = -V \left|n_{k-1}\right\rangle + \sum_{p=1}^{k} E_{np} \left|n_{k-p}\right\rangle$$

But this equation gives us some information about the energy shift E_{nk} as well. For that we will apply $\langle n|$ on the equation for all $k \in \mathbb{N}$.

$$\begin{aligned} 0 &= \langle n | \left(H - E_n\right) \left|n_k\right\rangle \\ &= -\langle n | V \left|n_{k-1}\right\rangle + \sum_{p=1}^{k} E_{np} \langle n | n_{k-p} \rangle \end{aligned}$$

By solving the equation for E_{nk} one gets the following for all $k \in \mathbb{N}$.

$$E_{nk} = \langle n | V \left|n_{k-1}\right\rangle - \sum_{p=1}^{k-1} E_{np} \langle n | n_{k-p} \rangle$$

For the eigenstates $\left|n_k\right\rangle$ we basically have to invert the operator $H - E_n$. But due to its singularity this is not possible. For that reason we will first express $\left|n_k\right\rangle$ in terms of the orthonormal eigenbasis of $\mathcal{H}$ with respect to H.

$$\left|n_k\right\rangle = \sum_{m \in \mathcal{I}} \langle m | n_k \rangle \left|m\right\rangle$$

$$= \langle n|n_k\rangle |n\rangle + \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \langle m|n_k\rangle |m\rangle$$

Let now $m \in \mathcal{I}$ with $m \neq n$ be arbitrary as well and apply $\langle m|$ on the operator equation for $|n_k\rangle$ for all $k \in \mathbb{N}$.

$$\begin{aligned}
&\langle m| (H - E_n) |n_k\rangle \\
&= (E_m - E_n) \langle m|n_k\rangle \\
&= -\langle m| V |n_{k-1}\rangle + \sum_{p=1}^{k} E_{np} \langle m|n_{k-p}\rangle \\
&= -\langle m| V |n_{k-1}\rangle + \sum_{p=1}^{k-1} E_{np} \langle m|n_{k-p}\rangle
\end{aligned}$$

Solving this for $\langle m|n_k\rangle$ for all $k \in \mathbb{N}$ gives us the following equations.

$$\langle m|n_k\rangle = -\frac{\langle m| V |n_{k-1}\rangle}{E_m - E_n} + \sum_{p=1}^{k-1} \frac{E_{np} \langle m|n_{k-p}\rangle}{E_m - E_n}$$

Inserting now the equations for $\langle n|n_k\rangle$ and $\langle m|n_k\rangle$ into the expansion with respect to the eigenbasis yields the following for all $k \in \mathbb{N}$.

$$\begin{aligned}
|n_k\rangle = &-\frac{1}{2} \sum_{p=1}^{k-1} \langle n_p|n_{k-p}\rangle |n\rangle \\
&+ \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \left[-\frac{\langle m| V |n_{k-1}\rangle}{E_m - E_n} \right. \\
&\qquad \left. + \sum_{p=1}^{k-1} \frac{E_{np} \langle m|n_{k-p}\rangle}{E_m - E_n} \right] |m\rangle
\end{aligned}$$

With this last equation we now have obtained explicit inductive formulas with their respective starting values for E_{nk} and $|n_k\rangle$ for all $k \in \mathbb{N}$. Through an iterative procedure beginning by $k = 1$ one can now directly obtain the formulas for the energy and state shifts.

$$E_{n1} = \langle n| V |n\rangle$$

$$|n_1\rangle = -\sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \frac{\langle m| V |n\rangle}{E_m - E_n} |m\rangle$$

The same formulas will be used for $k = 2$. But this time we will directly insert the equations for E_{n1} and $|n_1\rangle$ obtained above.

$$\begin{aligned}
E_{n2} &= \langle n| V |n_1\rangle - E_{n1} \langle n|n_1\rangle \\
&= -\sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \frac{\langle m| V |n\rangle}{E_m - E_n} \langle n| V |m\rangle
\end{aligned}$$

$$\begin{aligned}
|n_2\rangle = &-\frac{1}{2} \langle n_1|n_1\rangle |n\rangle \\
&+ \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \left[-\frac{\langle m| V |n_1\rangle}{E_m - E_n} \right. \\
&\qquad \left. + \frac{E_{n1} \langle m|n_1\rangle}{E_m - E_n} \right] |m\rangle \\
&= -\frac{1}{2} \sum_{\substack{m,k\in\mathcal{I}\\ m,k\neq n}} \frac{\langle n| V |m\rangle}{E_m - E_n} \frac{\langle k| V |n\rangle}{E_k - E_n} \langle m|k\rangle |n\rangle \\
&+ \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \left[\sum_{\substack{k\in\mathcal{I}\\ k\neq n}} \frac{\langle k| V |n\rangle}{E_k - E_n} \frac{\langle m| V |k\rangle}{E_m - E_n} \right. \\
&\qquad \left. - \sum_{\substack{k\in\mathcal{I}\\ k\neq n}} \frac{\langle k| V |n\rangle}{E_k - E_n} \frac{\langle n| V |n\rangle \langle m|k\rangle}{E_m - E_n} \right] |m\rangle \\
&= -\frac{1}{2} \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \frac{|\langle m| V |n\rangle|^2}{(E_m - E_n)^2} |n\rangle \\
&+ \sum_{\substack{m,k\in\mathcal{I}\\ m,k\neq n}} \frac{\langle k| V |n\rangle \langle m| V |k\rangle}{(E_k - E_n)(E_m - E_n)} |m\rangle \\
&- \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \frac{\langle n| V |n\rangle \langle m| V |n\rangle}{(E_m - E_n)^2} |m\rangle
\end{aligned}$$

This proves the proposition. □

Problem 19: Scattering off a Radial Potential

Preliminaries: Let $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ be the separable Hilbert space of three-dimensional square-integrable functions with Lebesgue-measure λ and the typical scalar product which models the scattering of a nonrelativistic particle of mass $m \in \mathbb{R}^+$.

$$\mathcal{H} = \left\{ \varphi \colon \mathbb{R}^3 \to \mathbb{C} \;\middle|\; \int_{\mathbb{R}^3} |\varphi|^2 \,\mathrm{d}\lambda < \infty \right\}$$

$$\langle\cdot|\cdot\rangle : \mathcal{H} \to \mathcal{H} \,, \qquad \langle\varphi|\psi\rangle \coloneqq \int_{\mathbb{R}^3} \bar{\varphi}\psi \,\mathrm{d}\lambda$$

Let $V \in \mathcal{H}$ be the spherically symmetric potential of the given system. We will use the spherical standard parameterization (M, μ) of $\mathbb{R}^3$.

$$M \coloneqq \mathbb{R}^+ \times [0, \pi] \times [0, 2\pi)$$

$$\mu \colon M \to \mathbb{R}^3 \,, \qquad \mu(r, \vartheta, \varphi) \coloneqq \begin{pmatrix} r \sin\vartheta \cos\varphi \\ r \sin\vartheta \sin\varphi \\ r \cos\vartheta \end{pmatrix}$$

The potential V can be rewritten in form of a scaled radial potential U.

$$U \colon \mathbb{R}^+ \to \mathbb{R}$$

$$\forall x \in \mathbb{R}^3 : \quad U(\|x\|) \coloneqq \frac{2m}{\hbar^2} V(x)$$

Hence, the typical Hamilton operator is given by the expression below.

$$H \colon \mathcal{H} \to \mathcal{H} \,, \qquad H \coloneqq -\frac{\hbar^2}{2m}\Delta + V$$

Expansion: Let $k \in \mathbb{R}^+$ be arbitrary and let $|\psi_k\rangle \in \mathcal{H}$ be a solution of the Schrödinger equation with eigenvalue $E(k)$.

$$H\,|\psi_k\rangle = E(k)\,|\psi_k\rangle \;, \qquad E(k) \coloneqq \frac{\hbar^2 k^2}{2m}$$

By inserting the definitions and multiplying with $2m\hbar^{-2}$ this equation takes on the following form.

$$\left(\Delta - U \circ \|\cdot\| + k^2\right) |\psi_k\rangle = 0$$

To model the scattering of a particle, we assume the particle to be a plane wave in z-direction. Because of that and due to the radial potential the wave function should not depend on the azimuth angle. So for all $(r, \vartheta, \varphi) \in M$ we can reformulate the wave function as follows.

$$\tilde{\psi}_k(r, \vartheta) \coloneqq \psi_k \circ \mu(r, \vartheta, \varphi)$$

Thanks to the spherically symmetric potential, we can expand $|\psi_k\rangle$ in terms of radial functions $A_l \colon \mathbb{R}^+ \to \mathbb{C}$ and spherical harmonics $\mathcal{Y}_{l0}$ with coefficients $c_l \in \mathbb{C}$ for all $l \in \mathbb{N}_0$ and $r \in \mathbb{R}^+$. Therefore, we get the following for all $(r, \vartheta, \varphi) \in M$.

$$\begin{aligned} \tilde{\psi}_k(r, \vartheta) &= \sum_{l=0}^{\infty} c_l A_l(r) \mathcal{Y}_{l0}(\vartheta) \\ &= \sum_{l=0}^{\infty} \tilde{c}_l A_l(r) P_l(\cos\vartheta) \end{aligned}$$

Here P_l are the Legendre polynomials and $\tilde{c}_l \in \mathbb{C}$ for all $l \in \mathbb{N}_0$. For the expansion to be valid, the radial functions A_l have to fulfill the radial Schrödinger equation for all $l \in \mathbb{N}_0$ and $r \in \mathbb{R}^+$.

$$\begin{aligned} 0 = {} & r^2 A_l''(r) + 2r A_l'(r) \\ & + \left[\left(k^2 - U(r)\right) r^2 - l(l+1)\right] A_l(r) \end{aligned}$$

This equation can be simplified by defining a variant of the radial function for all $l \in \mathbb{N}_0$ and $r \in \mathbb{R}^+$.

$$u_l \colon \mathbb{R}^+ \to \mathbb{C} \,, \qquad u_l(r) \coloneqq r A_l(r)$$

Then for all $l \in \mathbb{N}_0$ the variants u_l fulfill the following differential equation for all $r \in \mathbb{R}^+$.

$$u_l''(r) + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right] u_l(r) = 0$$

Differential Equation: In the expansion of the final-state wave function of the scattered particle ψ_k takes on the following form for all $r \in \mathbb{R}^+$ and $\vartheta \in [0, \pi]$.

$$\psi_k(r, \vartheta) = \sum_{l=0}^{\infty} i^l (2l+1) P_l(\cos\vartheta) \frac{e^{i\delta_l}}{kr} g_l(r)$$

Here $\delta_l \in [0, 2\pi]$ is the phase shift and $g_l \colon \mathbb{R}^+ \to \mathbb{C}$ another radial function for all $l \in \mathbb{N}_0$. Comparing this expression with the former wave expansion we find a proportional relation for all $l \in \mathbb{N}_0$ and $r \in \mathbb{R}^+$.

$$\frac{g_l(r)}{r} \propto A_l(r) \quad \Longrightarrow \quad g_l(r) \propto u_l(r)$$

For any $l \in \mathbb{N}_0$ both differential equations for A_l and for u_l are linear homogeneous differential equations of second order. Hence, any solution of these equations multiplied by any constant is also a solution. As a result g_l has to fulfill the same differential equation as the variants u_l for all $l \in \mathbb{N}_0$ and $r \in \mathbb{R}^+$.

$$g_l''(r) + \left[k^2 - U(r) - \frac{l(l+1)}{r^2}\right] g_l(r) = 0$$

Asymptotic Behavior: Let $l \in \mathbb{N}_0$ be arbitrary. To get a general idea of what is happening near infinity we will first look at the asymptotic behavior of the differential equation fulfilled by g_l. We will assume that $U(r) \xrightarrow{r\to\infty} 0$ which leads us to the following equation. Choose $r \in \mathbb{R}^+$ to be near infinity.

$$g_l''(r) + k^2 g_l(r) = 0$$

This is the differential equation of the classical harmonic oscillator and can be solved easily for constants $A, B \in \mathbb{C}$.

$$g_l(r) = Ae^{ikr} + Be^{-ikr}$$

Therefore the variants of the radial functions will asymptotically behave the same way as a spherical wave. To determine the values A and B we will use another more detailed approach based on the scattering amplitude.

The scattering amplitude $f_k\colon [0,\pi] \to \mathbb{C}$ in its partial wave expansion with partial-wave amplitudes $f_{kl} \in \mathbb{C}$ for $l \in \mathbb{N}_0$ can be written as follows for all $\vartheta \in [0,\pi]$.

$$f_k(\vartheta) = \sum_{l=0}^{\infty} (2l+1) f_{kl} P_l(\cos\vartheta)$$

Applying this formula on the wave function of the scattered particle we get the following.

$$\begin{aligned}\psi_k(r) \longrightarrow \sum_{l=0}^{\infty} &(2l+1) P_l(\cos\vartheta) \\ &\cdot \frac{1}{2ik}\left[\left(1 + 2ikf_{kl}\right)\frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right]\end{aligned}$$

By definition, the partial-wave amplitudes are related to the phase shifts.

$$1 + 2ikf_{kl} = e^{2i\delta_l}$$

Taking this equation and comparing the partial-wave expansion based on the scattering amplitude to the already given expansion we can now conclude the following.

$$\begin{aligned} i^l e^{i\delta_l}\frac{g_l(r)}{kr} &\longrightarrow \frac{1}{2ik}\left[e^{2i\delta_l}\frac{e^{ikr}}{r} - \frac{e^{-i(kr-l\pi)}}{r}\right] \\ &= \frac{e^{i\left(\delta_l + \frac{\pi}{2}l\right)}}{2ikr}\left[e^{i\left(kr - \frac{\pi}{2}l + \delta_l\right)} - e^{-i\left(kr - \frac{\pi}{2}l + \delta_l\right)}\right] \\ &= e^{il\frac{\pi}{2}}\frac{e^{i\delta_l}}{kr}\sin\left(kr - \frac{\pi}{2}l + \delta_l\right) \\ &= i^l\frac{e^{i\delta_l}}{kr}\sin\left(kr - \frac{\pi}{2}l + \delta_l\right)\end{aligned}$$

The detailed asymptotic behavior of g_l is explicitly be described below.

$$g_l(r) \longrightarrow \sin\left(kr - \frac{\pi}{2}l + \delta_l\right)$$

Wronskian Determinant: Let V_1 and V_2 be potentials with the same properties as V and define U_1, $\delta_l^{(1)}$ and U_2, $\delta_l^{(2)}$ analog to U and δ_l. Let $g_l, h_l\colon \mathbb{R}^+ \to \mathbb{C}$ be radial functions such that they fulfill the following differential equations for all $r \in \mathbb{R}^+$.

$$g_l''(r) + \left[k^2 - U_1(r) - \frac{l(l+1)}{r^2}\right] g_l(r) = 0$$

$$h_l''(r) + \left[k^2 - U_2(r) - \frac{l(l+1)}{r^2}\right] h_l(r) = 0$$

For twice continuously differentiable functions $f, g\colon \mathbb{R}^+ \to \mathbb{C}$ we define the Wronskian determinant.

$$W(f,g) \coloneqq \begin{vmatrix} f & g \\ f' & g' \end{vmatrix} = fg' - gf'$$

Then the derivative of this functional determinant is given by the following expression.

$$\begin{aligned}\mathrm{D}\,W(f,g) &= f'g' + fg'' - g'f' - gf'' \\ &= fg'' - gf''\end{aligned}$$

Inserting now g_l and h_l we can prove the proposition.

$$\begin{aligned}&\mathrm{D}W(g_l,h_l)(r) \\ &\quad= g_l(r)h_l''(r) - h_l(r)g_l''(r) \\ &\quad= g_l(r)h_l(r)\left[U_2(r) + \frac{l(l+1)}{r^2} - k^2\right] \\ &\qquad - h_l(r)g_l(r)\left[U_1(r) + \frac{l(l+1)}{r^2} - k^2\right] \\ &\quad= g_l(r)h_l(r)\left[U_2(r) - U_1(r)\right]\end{aligned}$$

□

Phase Shift Difference: The integral for the phase shift difference can be computed straightforward by using the results above and the fundamental theorem of calculus.

$$\begin{aligned}
&-\frac{2m}{\hbar^2 k}\int_0^\infty g_l(r)h_l(r)\left[V_2(r)-V_1(r)\right]\,\mathrm{d}r \\
&\quad=-\frac{1}{k}\int_0^\infty g_l(r)h_l(r)\left[U_2(r)-U_1(r)\right]\,\mathrm{d}r \\
&\quad=-\frac{1}{k}\int_0^\infty \mathrm{D}\,W(g_l,h_l)(r)\,\mathrm{d}r \\
&\quad=-\frac{1}{k}\,W(g_l,h_l)(r)|_{r=0}^{\infty} \\
&\quad=-\frac{1}{k}\,\left[g_l(r)h_l'(r)-h_l(r)g_l'(r)\right]|_{r=0}^{\infty}
\end{aligned}$$

Because the radial functions have to be regular at the origin, we are assuming the following conditions.

$$g_l(0)=h_l(0)=0$$

We already know about the asymptotic behavior of g_l and h_l. Choose $r\in\mathbb{R}^+$ to be near infinity.

$$g_l(r)\longrightarrow \sin\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right)$$

$$h_l(r)\longrightarrow \sin\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right)$$

Therefore we can derive the asymptotic behavior of h_l' and g_l' as well by computing the derivative of the asymptotic function.

$$g_l'(r)\longrightarrow k\cos\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right)$$

$$h_l'(r)\longrightarrow k\cos\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right)$$

We will now insert these ideas into the calculation of the integral. Additionally, we use an addition theorem to finish the proof.

$$\begin{aligned}
&-\frac{2m}{\hbar^2 k}\int_0^\infty g_l(r)h_l(r)\left[V_2(r)-V_1(r)\right]\,\mathrm{d}r \\
&\quad=-\frac{1}{k}\lim_{r\to\infty}\left[g_l(r)h_l'(r)-h_l(r)g_l'(r)\right] \\
&\quad=-\frac{1}{k}\lim_{r\to\infty}\Big[\sin\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right) \\
&\qquad\qquad\cdot k\cos\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right) \\
&\qquad\qquad-\sin\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right) \\
&\qquad\qquad\cdot k\cos\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right)\Big] \\
&\quad=\lim_{r\to\infty}\Big[\sin\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right) \\
&\qquad\qquad\cdot\cos\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right) \\
&\qquad\qquad-\sin\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right) \\
&\qquad\qquad\cdot\cos\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right)\Big] \\
&\quad=\lim_{r\to\infty}\sin\Big[\left(kr-\frac{\pi}{2}l+\delta_l^{(2)}\right) \\
&\qquad\qquad-\left(kr-\frac{\pi}{2}l+\delta_l^{(1)}\right)\Big] \\
&\quad=\lim_{r\to\infty}\sin\left(\delta_l^{(2)}-\delta_l^{(1)}\right) \\
&\quad=\sin\left(\delta_l^{(2)}-\delta_l^{(1)}\right)
\end{aligned}$$

□

Problem 20: Identical Particles in an Infinite Well

Preliminaries: Let $\mathcal{L}^2(\mathbb{R})$ be the space of square-integrable functions with domain $\mathbb{R}$ and Lebesgue-measure λ.

$$\mathcal{L}^2(\mathbb{R}) \coloneqq \left\{ f \colon \mathbb{R} \to \mathbb{C} \;\middle|\; \int_{\mathbb{R}} |f|^2 \,\mathrm{d}\lambda < \infty \right\}$$

We define the typical scalar product for such a space as follows.

$$\langle \cdot | \cdot \rangle : \mathcal{L}^2 \times \mathcal{L}^2 \to \mathbb{C}\,, \qquad \langle f | g \rangle \coloneqq \int_{\mathbb{R}} \bar{f} g \,\mathrm{d}\lambda$$

The Hilbert space for a single particle with mass $m \in \mathbb{R}^+$ in an infinite potential well with size $a \in \mathbb{R}^+$ centered at the origin is described by $\left(\mathcal{L}^2(\mathbb{R}), \langle \cdot | \cdot \rangle\right)$. For convenience, we define the following constants.

$$\omega \coloneqq \frac{\pi}{2a}\,, \qquad \varepsilon \coloneqq \frac{\hbar^2 \omega^2}{2m}\,, \qquad z \coloneqq \frac{1}{\sqrt{a}}$$

With $|n\rangle \in \mathcal{L}^2(\mathbb{R})$, we denote the eigenstates of the Hamiltonian $H \colon \mathcal{L}^2(\mathbb{R}) \to \mathcal{L}^2(\mathbb{R})$ with eigenvalues E_n for all $n \in \mathbb{N}$.

$$|n\rangle \coloneqq \begin{cases} z\cos(n\omega\cdot) & : n = 2k-1 \quad \text{for } k \in \mathbb{N} \\ z\sin(n\omega\cdot) & : n = 2k \quad \text{for } k \in \mathbb{N} \end{cases}$$

$$E_n \coloneqq \varepsilon n^2$$

Hilbert Space: For three identical particles the following space $\mathcal{H}$ builds a superset of the Hilbert space for these particles.

$$\mathcal{H} \coloneqq \mathcal{L}^2(\mathbb{R}) \otimes \mathcal{L}^2(\mathbb{R}) \otimes \mathcal{L}^2(\mathbb{R}) \cong \mathcal{L}^2\left(\mathbb{R}^3\right)$$

To define the scalar product for this space we first define the product state for all $|\varphi_1\rangle, |\varphi_2\rangle, |\varphi_3\rangle \in \mathcal{L}^2(\mathbb{R})$.

$$|\varphi_1\varphi_2\varphi_3\rangle \coloneqq |\varphi_1\rangle \otimes |\varphi_2\rangle \otimes |\varphi_3\rangle$$

Please note, that for convenience we will use function overloading to define the scalar product.

$$\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$$

$$\langle \varphi_1\varphi_2\varphi_3 | \vartheta_1\vartheta_2\vartheta_3 \rangle \coloneqq \langle \varphi_1 | \vartheta_1 \rangle \langle \varphi_2 | \vartheta_2 \rangle \langle \varphi_3 | \vartheta_3 \rangle$$

This scalar product will also be used for the Hilbert space of the three identical particles, which is possible because its a subset of $\mathcal{H}$.

All particles are Bosons because of their spin which is equal to zero. Therefore $\mathcal{H}$ has to be symmetrized such that all possible wave functions are symmetric. We call $(\mathcal{H}_\mathrm{S}, \langle \cdot | \cdot \rangle)$ the Hilbert space of these three identical Bosons.

$$\mathcal{H}_\mathrm{S} \coloneqq \{ |\varphi\rangle \in \mathcal{H} \mid \forall \pi \in \mathrm{S}_3 : \; P(\pi) |\varphi\rangle = |\varphi\rangle \} \subset \mathcal{H}$$

Here, S_3 is the three-dimensional permutation group and $P(\pi)$ the related permutation operator for $\pi \in \mathrm{S}_3$.

Eigenbasis: The three particles do not interact. Hence, the Hamiltonian $H_\mathrm{S} \colon \mathcal{H}_\mathrm{S} \to \mathcal{H}_\mathrm{S}$ for $\mathcal{H}_\mathrm{S}$ can be stated as follows.

$$H_\mathrm{S} \coloneqq H \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes H \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes H$$

We can now conclude that for all $n_1, n_2, n_3 \in \mathbb{N}$ the states $|n_1 n_2 n_3\rangle$ are eigenstates of $H_\mathrm{S}|_\mathcal{H}$ with eigenvalue $E_{n_1 n_2 n_3}$.

$$\begin{aligned} H_\mathrm{S} |n_1 n_2 n_3\rangle &= H |n_1\rangle \otimes |n_2\rangle \otimes |n_3\rangle \\ &\quad + |n_1\rangle \otimes H |n_2\rangle \otimes |n_3\rangle \\ &\quad + |n_1\rangle \otimes |n_2\rangle \otimes H |n_3\rangle \\ &= (E_{n_1} + E_{n_2} + E_{n_3}) |n_1 n_2 n_3\rangle \end{aligned}$$

$$E_{n_1 n_2 n_3} \coloneqq E_{n_1} + E_{n_2} + E_{n_3}$$

Additionally, for all $m_1, m_2, m_3 \in \mathbb{N}$ the following equation shows that the states are orthonormal and consequently are building an orthonormal basis of $\mathcal{H}$.

$$\begin{aligned} &\langle m_1 m_2 m_3 | n_1 n_2 n_3 \rangle \\ &= \langle m_1 | n_1 \rangle \langle m_2 | n_2 \rangle \langle m_3 | n_3 \rangle \\ &= \delta_{m_1 n_1} \delta_{m_2 n_2} \delta_{m_3 n_3} \end{aligned}$$

But these states are in general not symmetric and may not lie in $\mathcal{H}_\mathrm{S}$ which would violate the condition that the system consists of three identical Bosons. Like $\mathcal{H}$ had to be symmetrized, the states also have to be symmetrized. For all $n_1, n_2, n_3 \in \mathbb{N}$ we define the symmetric states as follows.

$$|n_1 n_2 n_3\rangle_\mathrm{S} \coloneqq \sum_{\sigma \in \mathrm{S}_3} \left| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle$$

Due to the linear combination and the permutation we are now making sure that the states are building a symmetric eigenbasis of $\mathcal{H}_\mathrm{S}$ with respect to H_S. Of course,

these symmetric states are not normalized. To normalize the states, we choose $n_1, n_2, n_3 \in \mathbb{N}$ to be arbitrary.

$$\begin{aligned}
&{}_{\mathrm{S}}\langle n_1 n_2 n_3 | n_1 n_2 n_3 \rangle_{\mathrm{S}} \\
&= \sum_{\pi,\sigma \in \mathrm{S}_3} \left\langle n_{\pi(1)} n_{\pi(2)} n_{\pi(3)} \middle| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle \\
&= \sum_{\pi,\sigma \in \mathrm{S}_3} \delta_{n_{\pi(1)} n_{\sigma(1)}} \delta_{n_{\pi(2)} n_{\sigma(2)}} \delta_{n_{\pi(3)} n_{\sigma(3)}}
\end{aligned}$$

We have to sum over $3! \cdot 3! = 36$ terms and at least six of them will be one because the permutations σ and π can be the same.

Case $n_1 \neq n_2 \neq n_3 \neq n_1$: Then it is clear that only these six terms can contribute to the actual sum because for every permutation $\pi \in \mathrm{S}_3$ we compute the result below.

$$\begin{aligned}
&\sum_{\sigma \in \mathrm{S}_3} \left\langle n_{\pi(1)} n_{\pi(2)} n_{\pi(3)} \middle| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle \\
&= \sum_{\sigma \in \mathrm{S}_3} \delta_{\pi(1)\sigma(1)} \delta_{\pi(2)\sigma(2)} \delta_{\pi(3)\sigma(3)} = 1
\end{aligned}$$

The normalization in this case is straightforward.

$$|n_1 n_2 n_3\rangle_{\tilde{\mathrm{S}}} \coloneqq \frac{1}{\sqrt{3!}} |n_1 n_2 n_3\rangle_{\mathrm{S}}$$

Case $n_1 \neq n_2 = n_3$: If two values are the same then a permutation interchanging those values will not change the actual state. This can be stated as follows for all permutations $\pi \in \mathrm{S}_3$.

$$\begin{aligned}
&\sum_{\sigma \in \mathrm{S}_3} \left\langle n_{\pi(1)} n_{\pi(2)} n_{\pi(3)} \middle| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle \\
&= \sum_{\sigma \in \mathrm{S}_3} \left(\delta_{\pi(1)\sigma(1)} \delta_{\pi(2)\sigma(2)} \delta_{\pi(3)\sigma(3)} \right. \\
&\qquad \left. + \delta_{\pi(1)\sigma(1)} \delta_{\pi(2)\sigma(3)} \delta_{\pi(3)\sigma(2)} \right) \\
&= 2
\end{aligned}$$

In this case the normalization factor changes and the normalized state is defined below.

$$|n_1 n_2 n_3\rangle_{\tilde{\mathrm{S}}} \coloneqq \frac{1}{\sqrt{3! \cdot 2!}} |n_1 n_2 n_3\rangle_{\mathrm{S}}$$

Case $n_1 = n_2 = n_3$: If all of these three values are the same then every term in the sum has to be one because for every permutation $\pi \in \mathrm{S}_3$ we can conclude the following.

$$\begin{aligned}
&\sum_{\sigma \in \mathrm{S}_3} \left\langle n_{\pi(1)} n_{\pi(2)} n_{\pi(3)} \middle| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle \\
&= \sum_{\sigma \in \mathrm{S}_3} \sum_{\kappa \in \mathrm{S}_3} \delta_{\pi(1)\sigma(\kappa(1))} \delta_{\pi(2)\sigma(\kappa(2))} \delta_{\pi(3)\sigma(\kappa(3))} \\
&= 6
\end{aligned}$$

Of course, this is a direct consequence of the following equation for all $\sigma \in \mathrm{S}_3$.

$$|n_1 n_2 n_3\rangle = \left| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle$$

Hence, the normalization in this case can formulated as follows.

$$|n_1 n_2 n_3\rangle_{\tilde{\mathrm{S}}} \coloneqq \frac{1}{\sqrt{3! \cdot 3!}} |n_1 n_2 n_3\rangle_{\mathrm{S}}$$

General Normalization: The results obtained here can be generalized. Define $p_n \in \mathbb{N}_0$ to be the count of particles in the state $|n\rangle$ for all $n \in \mathbb{N}$. Because we have three particles the following equation is fulfilled.

$$\sum_{n \in \mathbb{N}} p_n = 3$$

Particles in the same state can be interchanged. There are $p_n!$ possible permutations for every $n \in \mathbb{N}$ such that the state is not changed. Thus, for every permutation $\pi \in \mathrm{S}_3$ the following holds.

$$\sum_{\sigma \in \mathrm{S}_3} \left\langle n_{\pi(1)} n_{\pi(2)} n_{\pi(3)} \middle| n_{\sigma(1)} n_{\sigma(2)} n_{\sigma(3)} \right\rangle = \prod_{n \in \mathbb{N}} p_n!$$

With this we could have also defined the following general normalization rule.

$$|n_1 n_2 n_3\rangle_{\tilde{\mathrm{S}}} \coloneqq \frac{1}{\sqrt{3! \prod_{n \in \mathbb{N}} p_n!}} |n_1 n_2 n_3\rangle_{\mathrm{S}}$$

The set $\{|n_1 n_2 n_3\rangle_{\tilde{\mathrm{S}}} \mid n_1, n_2, n_3 \in \mathbb{N}\}$ is therefore building an orthonormal eigenbasis of $\mathcal{H}_{\mathrm{S}}$ with respect to H_{S}. Please note, that the states are symmetric and therefore the order of n_1, n_2 and n_3 can be ignored. It suffices to describe the symmetric state by the numbers $(p_n)_{n \in \mathbb{N}}$.

Lowest Energy States: As shown above for a normalized eigenstate $|n_1 n_2 n_3\rangle_{\tilde{\mathrm{S}}}$ of the Hamiltonian H_{S} with have the energy $E_{n_1 n_2 n_3}$ as an eigenvalue for all $n_1, n_2, n_3 \in \mathbb{N}$. Therefore we can find the five states with the lowest energy by direct computation.

$$\begin{aligned}
|111\rangle_{\tilde{\mathrm{S}}} &: \qquad E_{111} = 3\varepsilon \\
|112\rangle_{\tilde{\mathrm{S}}} &: \qquad E_{112} = 6\varepsilon \\
|122\rangle_{\tilde{\mathrm{S}}} &: \qquad E_{122} = 9\varepsilon \\
|113\rangle_{\tilde{\mathrm{S}}} &: \qquad E_{113} = 11\varepsilon \\
|222\rangle_{\tilde{\mathrm{S}}} &: \qquad E_{222} = 12\varepsilon
\end{aligned}$$