ADVANCED QUANTUM THEORY
EXERCISE SHEET 11

Markus Pawellek
markuspawellek@gmail.com

January 27, 2019

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.

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

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.

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

[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.

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

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

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 $k \in \mathbb{N}$.

$$H\,|n_0\rangle = E_{n0}\,|n_0\rangle$$

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

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

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

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.

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

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

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

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.

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

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

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

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 $k \in \mathbb{N}$.

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

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

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

For the eigenstates $|n_k\rangle$ 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 $|n_k\rangle$ in terms of the orthonormal eigenbasis of $\mathcal{H}$ with respect to H.

$$\begin{aligned} |n_k\rangle &= \sum_{m\in\mathcal{I}} \langle m|n_k\rangle\,|m\rangle \\ &= \langle n|n_k\rangle\,|n\rangle + \sum_{\substack{m\in\mathcal{I}\\ m\neq n}} \langle m|n_k\rangle\,|m\rangle \end{aligned}$$

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 $k \in \mathbb{N}$.

$$\langle m|\,(H - E_n)\,|n_k\rangle$$

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

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 $k \in \mathbb{N}$.

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

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.

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

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

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.

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

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

This proves the proposition. $\square$