Advanced Quantum Theory
Exercise Sheet 11

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January 26, 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 eigenfunction 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 H, for all $n, m \in \mathcal{I}$ with $n \neq m$ we can derive that $|m\rangle$ and $|n\rangle$ are orthogonal.

$$\langle m| H |n\rangle = E_n \langle m|n\rangle = E_m \langle m|n\rangle$$

$$\implies (E_n - E_m)\langle m|n\rangle = 0$$

$$\implies \langle m|n\rangle = 0$$

Hence, for all $n, m \in \mathcal{I}$ we can state the following.

$$\langle m|n\rangle = \delta_{mn}$$

H is therefore non-degenerate and $\{|n\rangle \mid n \in \mathcal{I}\}$ is building an orthonormal basis of $\mathcal{H}$.

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 of non-degeneracy and that of a discrete spectrum of $\tilde{H}(\lambda)$ for all $\lambda \in [0,1]$.

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

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

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

$$\langle m(\lambda)|n(\lambda)\rangle = \delta_{mn}$$

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

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

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

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 left-hand side of the eigenvalue equation.

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

$$= (H + \lambda V)\sum_{k=0}^{\infty} \lambda^k |n_k\rangle$$

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

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 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 equations 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.

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

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 will 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 also information about the energy shift E_{nk}. 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.

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

Let now $m \in \mathfrak{I}$ 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 $k \in \mathbb{N}$.

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

With this we now have inductive explicit 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.

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

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.

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

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

This proves the proposition. $\square$