Markus Pawellek
144 645

Advanced Quantum Mechanics

exercise 1

We define the operators: $H_0 := \frac{p^2}{2m} - \frac{e^2}{r}$, $H' := \sqrt{m^2c^4 + p^2c^2} - \frac{e^2}{r}$

additionally: $x := \frac{p^2}{m^2c^2}$

$$\Rightarrow \sqrt{m^2c^4 + p^2c^2} = mc^2\sqrt{1 + \frac{p^2}{m^2c^2}} = mc^2\sqrt{1+x}$$

Now it makes sense to define $f : (-1, \infty) \to \mathbb{R}$, $f(x) := \sqrt{1+x}$ for all $x \in (-1,\infty)$ and expanding $f(x)$ for $x \in (-1,\infty)$ into a taylor series.

$$\Rightarrow f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(0)}{k!} x^k$$

(we assume that this series is absolut convergent for the given values)

$$\left.\begin{aligned} f^{(0)}(x) &= f(x) = \sqrt{1+x} \\ f'(x) &= \frac{1}{2\sqrt{1+x}} \\ f''(x) &= \frac{-1}{4(1+x)^{-3/2}} \end{aligned}\right\} \begin{aligned} &\Rightarrow f(0) = 1,\ f'(0) = \frac{1}{2},\ f''(0) = -\frac{1}{4} \\ &\Rightarrow f(x) = 1 + \frac{x}{2} - \frac{x^2}{8} + \sum_{k=3}^{\infty} \frac{f^{(k)}(0)}{k!} x^k \end{aligned}$$

We approximate f up to second order: $f(x) \approx 1 + \frac{x}{2} - \frac{x^2}{8}$

$$\Rightarrow f\left(\frac{p^2}{m^2c^2}\right) \approx 1 + \frac{p^2}{2m^2c^2} - \frac{p^4}{8m^4c^4}$$

$$\Rightarrow \sqrt{m^2c^4 + p^2c^2} \approx mc^2 + \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}$$ ✓

Then we neglect the constant term and define the new approximated Hamiltonian by

$$\tilde{H} := \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} - \frac{e^2}{r}$$

additionally we define a perturbation: $S := -\frac{p^4}{8m^3c^2}$

$$\Rightarrow \tilde{H} = H_0 + S$$

Now we are able to use first-order perturbation theory. We define $\tilde{H} : [0,1] \to L(\mathcal{H},\mathcal{H})$ where $\mathcal{H}$ is our used hilbert space and $L(\mathcal{H},\mathcal{H})$ is the set of operators. For all $\lambda \in [0,1]$ we say

$$\tilde{H}(\lambda) := H_0 + \lambda S$$

Further we define $|\varphi(\cdot)\rangle : [0,1] \to \mathcal{H}$, $E : [0,1] \to \mathbb{R}$ with

$$\tilde{H}(\lambda)\,|\varphi(\lambda)\rangle = E(\lambda)\,|\varphi(\lambda)\rangle \quad \text{for all } \lambda \in [0,1]$$

Now we assume that we can expand E and $|\varphi(\cdot)\rangle$ into series:

$$|\varphi(\lambda)\rangle = \sum_{k=0}^{\infty} \lambda^k |\varphi_k\rangle \quad , \quad E(\lambda) = \sum_{k=0}^{\infty} \lambda^k E_k$$

for all $\lambda \in [0,1]$ with $|\varphi_k\rangle \in \mathcal{H}$, $E_k \in \mathbb{R}$ for all $k \in \mathbb{N}_0$.

Here we only use first-order approximation.

$$\Longrightarrow \quad |\varphi(\lambda)\rangle \approx |\varphi_0\rangle + \lambda\,|\varphi_1\rangle \qquad \text{for all } \lambda \in [0,1]$$
$$E(\lambda) \approx E_0 + \lambda\, E_1 \qquad |\varphi_0\rangle, |\varphi_1\rangle \in \mathcal{H},\ E_0, E_1 \in \mathbb{R}$$

Using the definition of $\tilde{H}$, $|\varphi(\cdot)\rangle$, E we get

$$\tilde{H}(\lambda)\,|\varphi(\lambda)\rangle \approx (H_0 + \lambda S)(|\varphi_0\rangle + \lambda\,|\varphi_1\rangle)$$
$$= H_0|\varphi_0\rangle + \lambda\,(H_0|\varphi_1\rangle + S|\varphi_0\rangle) + \lambda^2 S|\varphi_1\rangle$$

$$\approx E(\lambda)\,|\varphi(\lambda)\rangle \approx (E_0 + \lambda E_1)(|\varphi_0\rangle + \lambda\,|\varphi_1\rangle)$$
$$= E_0|\varphi_0\rangle + \lambda(E_0|\varphi_1\rangle + E_1|\varphi_0\rangle) + \lambda^2 E_1|\varphi_1\rangle$$

Comparing the coefficients of λ^k for $k \in \{0,1,2\}$ this results in

(I) $H_0|\varphi_0\rangle = E_0|\varphi_0\rangle$

(II) $H_0|\varphi_1\rangle + S|\varphi_0\rangle = E_0|\varphi_1\rangle + E_1|\varphi_0\rangle$

(III) $E_1|\varphi_1\rangle = S|\varphi_1\rangle$ (this equation has no real meaning because we did only a first order approximation)

(I) says that $|\varphi_0\rangle$ and E_0 are eigenfunction and eigenvalue (energy) of the unperturbed system described by H_0

(II) shall be „multiplied" by $\langle\varphi_0|$ to get E_1:

$$\underbrace{\langle\varphi_0|H_0|\varphi_1\rangle}_{= E_0\langle\varphi_0|\varphi_1\rangle} + \langle\varphi_0|S|\varphi_0\rangle = \underbrace{\langle\varphi_0|E_0|\varphi_1\rangle}_{= E_0\langle\varphi_0|\varphi_1\rangle} + \underbrace{\langle\varphi_0|E_1|\varphi_0\rangle}_{= E_1}$$

$$\Longrightarrow \quad E_1 = \langle\varphi_0|S|\varphi_0\rangle$$

This means E_1 is the first-order energy-shift of a given system perturbed by S.

Now we write S in operator form: $S = -\frac{\hbar^4}{8m^3c^2}\Delta^2$

Then we rewrite Δ in sperical coordinates and use the knowledge that $|\varphi_0\rangle$ should be the ground state of an hydrogen atom.

Therefore we can omit the derivatives of angles.

$$\Rightarrow \quad \Delta = \frac{1}{r^2}\partial_r(r^2\partial_r) = \frac{2}{r}\partial_r + \partial_r^2 \qquad \text{(in case of } |\varphi_0\rangle)$$

$$\Rightarrow \quad \Delta^2 = \left(\frac{2}{r}\partial_r + \partial_r^2\right) = \frac{2}{r}\partial_r\left(\frac{2}{r}\partial_r\right) + \frac{2}{r}\partial_r^3 + \partial_r^2\left(\frac{2}{r}\partial_r\right) + \partial_r^4$$

$$= \frac{2}{r}\left(-\frac{2}{r^2}\partial_r + \frac{2}{r}\partial_r^2\right) + \frac{2}{r}\partial_r^3 + \left(\frac{4}{r^3}\partial_r + \frac{-2}{r^2}\partial_r^2 - \frac{2}{r^2}\partial_r^2 + \frac{2}{r}\partial_r^3\right) + \partial_r^4$$

$$= \partial_r^4 + \frac{4}{r}\partial_r^3 \quad \checkmark$$

The groundstate $|\varphi_0\rangle$ can be written as $\varphi_0(r) = Ae^{-ar}$ for constants $A \in \mathbb{R}$ and $a \in (0,\infty)$.

$$\Rightarrow \quad E_1 = \langle\varphi_0|S|\varphi_0\rangle = \frac{-\hbar^4}{8m^3c^2}\int_0^\infty\int_0^\pi\int_0^{2\pi} \varphi_0^*(r)\left(\partial_r^4 + \frac{4}{r}\partial_r^3\right)\varphi_0(r)\, r^2\sin\vartheta \, d\varphi\, d\vartheta\, dr$$

$$= 4\pi A^2 \cdot \frac{-\hbar^4}{8m^3c^2} \cdot \int_0^\infty e^{-ar}\left(\partial_r^4 + \frac{4}{r}\partial_r^3\right)e^{-ar} \cdot r^2\, dr$$

$$= \frac{-4\pi A^2\hbar^4}{8m^3c^2}\int_0^\infty e^{-ar}\left(a^4 e^{-ar} + (-4a^3)\frac{e^{-ar}}{r}\right) r^2\, dr$$

$$= \frac{-4\pi A^2\hbar^4}{8m^3c^2}\int_0^\infty a^4 r^2 e^{-2ar} - 4a^3 r\, e^{-2ar}\, dr$$

$$\int_0^\infty r^2 e^{-2ar}\, dr = \frac{2}{(2a)^3} = \frac{1}{4a^3} \qquad \int_0^\infty r\, e^{-2ar}\, dr = \frac{1}{4a^2}$$

$$\Rightarrow \quad E_1 = \frac{-4\pi A^2\hbar^4}{8m^3c^2}\left(\frac{a^4}{4a^3} - \frac{4a^3}{4a^2}\right) = \underline{\underline{\frac{3\pi a A^2\hbar^4}{8m^3c^2}}} \quad \checkmark$$

ABER: $A = ?$ (-1.0)
$a = ?$

AUF 1: 3.0/4.0

Exercise 2

Let $(\mathcal{H}, \langle\cdot|\cdot\rangle)$ be a hilbert space. We define the unperturbed Hamiltonian $H_0 : \mathcal{H} \to \mathcal{H}$ as $H_0 := \frac{p^2}{2m} + \frac{m\omega^2}{2} x^2 = \hbar\omega(a^+a + \frac{1}{2})$.

For a small parameter $\lambda \in (0,\infty)$ we perturb the system with the following quartic potential operator $V : \mathcal{H} \to \mathcal{H}$, $V := \frac{1}{16 \mathcal{C}^4} (a+a^+)^4$ for $\mathcal{C} \in \mathbb{C}$ and $a, a^+ \in L(\mathcal{H}, \mathcal{H})$. Therefore the Hamiltonian H for the perturbed system can be defined as $H : \mathcal{H} \to \mathcal{H}$

$$H = H_0 + \lambda V$$

Determination of $\mathcal{C}$:

Let $A, B \in L(\mathcal{H}, \mathcal{H})$ be two operators. Then it holds that

$$(A + iB)(A - iB) = A^2 - iAB + iBA - i^2 B^2$$
$$= A^2 - i[A,B] + B^2 \quad \text{with } [A,B] := AB - BA$$

$$\Rightarrow A^2 + B^2 = (A + iB)(A - iB) + i[A,B]$$

Use this proposition for H_0:

$$\Rightarrow H_0 = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2} = \left(\sqrt{\frac{m\omega^2}{2}}\, x + i\sqrt{\frac{1}{2m}}\, p\right)\left(\sqrt{\frac{m\omega^2}{2}} - i\sqrt{\frac{1}{2m}}\, p\right)$$
$$+ i\left[\sqrt{\frac{m\omega^2}{2}}\, x, \sqrt{\frac{1}{2m}}\, p\right]$$

$$= \frac{m\omega^2}{2}\left(x + \frac{ip}{m\omega}\right)\left(x - \frac{ip}{m\omega}\right) + \frac{i\omega}{2}[x,p]$$

We already know: $[x,p] = i\hbar \mathbb{1}$ for the one-dimensional case.
Additionally it holds that $a^+a = aa^+ - 1$.

$$\Rightarrow \hbar\omega(a^+a + \tfrac{1}{2}) = \hbar\omega(aa^+ - 1 + \tfrac{1}{2}) = \hbar\omega(aa^+ - \tfrac{1}{2}) = H_0$$

$$\Rightarrow aa^+ - \frac{1}{2} = \frac{m\omega}{2\hbar}\left(x + \frac{ip}{m\omega}\right)\left(x - \frac{ip}{m\omega}\right) - \frac{1}{2}$$

$$\Rightarrow aa^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \cdot \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

$$\Rightarrow a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right), \quad a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right)$$

It was given that: $16\mathcal{C}^4 x^4 = (a+a^+)^4 \Rightarrow 2\mathcal{C}x = a + a^+$

$$a + a^+ = \sqrt{\frac{m\omega}{2\hbar}}\, 2x = \sqrt{\frac{2m\omega}{\hbar}}\, x \Rightarrow \underline{\underline{\mathcal{C} = \frac{1}{2}\sqrt{\frac{2m\omega}{\hbar}} = \sqrt{\frac{m\omega}{2\hbar}}}} \quad ✓$$

Determination of terms P_1 and P_2:

$$(a+a^+)^4 = [(a+a^+)^2]^2 = [aa + aa^+ + a^+a + a^+a^+]^2$$

$$= [aa + (N+1) + N + a^+a^+]^2 = [aa + a^+a^+ + 2N+1]^2$$

$$= \underline{aaaa} + aaa^+a^+ + aa(2N+1)$$
$$+ a^+a^+aa + \underline{a^+a^+a^+a^+} + a^+a^+(2N+1)$$
$$+ (2N+1)aa + (2N+1)a^+a^+ + (2N+1)(2N+1)$$

$$= a^4 + a^{+4} + [aa(2N+1) + (2N+1)aa]$$
$$+ [a^+a^+(2N+1) + (2N+1)a^+a^+]$$
$$+ a^+a^+aa + aaa^+a^+ + (2N+1)(2N+1)$$

(I) $$[a,N] = aN - Na = aa^+a - Na = (aa^+ - N)a$$
$$= (N+1-N)a = a$$
$$\Rightarrow \quad aN = Na + [a,N] = (N+1)a$$
$$\Rightarrow \quad Na = aN - [a,N] = a(N-1)$$

(II) $$[a^+,N] = a^+N - Na^+ = a^+N - a^+aa^+ = a^+(N - aa^+) = -a^+$$
$$\Rightarrow \quad a^+N = Na^+ + [a^+,N] = (N-1)a^+$$
$$\Rightarrow \quad Na^+ = a^+N - [a^+,N] = a^+(N+1)$$

$$\Rightarrow \quad a^+a^+aa = a^+(N)a \overset{(II)}{=} (N-1)a^+a = (N-1)N = N^2 - N$$
$$\Rightarrow \quad aaa^+a^+ = a(N+1)a^+ \overset{(I)}{=} (N+2)aa^+ = (N+2)(N+1) = N^2+N+2N+2$$
$$(2N+1)(2N+1) = 4N^2 + 2N + 2N + 1$$

$$\Rightarrow \quad a^+a^+aa + aaa^+a^+ + (2N+1)(2N+1) = 6N^2 + 6N + 3 = 3(2N^2+2N+1)$$

$$aa(2N+1) \overset{(I)}{=} a[2(N+1)+1]a = a(2N+3)a$$
$$(2N+1)aa \overset{(I)}{=} a[2(N-1)+1]a = a(2N-1)a$$

$$\Rightarrow \quad aa(2N+1) + (2N+1)aa = a(4N+2)a = a[2(2N+1)]a$$
$$\Rightarrow \quad a^+a^+(2N+1) + (2N+1)a^+a^+ \overset{(II)}{=} a^+[(2N-1)+(2N+3)]a^+ = a^+[2(2N+1)]a^+$$

$$\Rightarrow \quad \Delta = a^4 + a^{+4} + a[2(2N+1)]a + a^+[2(2N+1)]a^+ + 3(2N^2+2N+1)$$

$$\Rightarrow \quad \underline{\underline{P_1(N) = 3(2N^2+2N+1), \quad P_2(N) = 2(2N+1)}}$$ ✓

Computation of energy shift in first-order perturbation theory:

We already know: $a|\varphi_n\rangle = \sqrt{n}\,|\varphi_{n-1}\rangle$ for all $n \in \mathbb{N}$, $a|\varphi_0\rangle = 0$

$a^+|\varphi_n\rangle = \sqrt{n+1}\,|\varphi_{n+1}\rangle$ for all $n \in \mathbb{N}_0$

with $|\varphi_n\rangle \in \mathcal{H}$ for all $n \in \mathbb{N}_0$ as the eigenstates of H_0.

($\{|\varphi_n\rangle \mid n \in \mathbb{N}_0\}$ forms an orthonormal basis of $\mathcal{H}$)

Additionally we know from exercise 1: $E_n^{(1)} = \langle \varphi_n^{(0)} | V | \varphi_n^{(0)} \rangle$

where $|\varphi_n^{(0)}\rangle := |\varphi_n\rangle$ for all $n \in \mathbb{N}_0$ and $E_n^{(1)}$ is the first-order energy shift of the state with quantum number $n \in \mathbb{N}_0$ in perturbation theory.

$$\Rightarrow E_n^{(1)} = \frac{1}{16\,\xi^4} \langle \varphi_n^{(0)} | \Delta | \varphi_n^{(0)} \rangle = \frac{4\hbar^2}{16 m^2\omega^2} \langle \varphi_n | \Delta | \varphi_n \rangle = \hbar\omega \cdot \frac{\hbar}{4m^2\omega^3} \langle \varphi_n | \Delta | \varphi_n \rangle$$

$$= \hbar\omega \cdot \frac{\hbar}{4m^2\omega^3} \langle \varphi_n | \Big(P_1(N)|\varphi_n\rangle + a P_2(N) a |\varphi_n\rangle + a^+ P_2(N) a^+ |\varphi_n\rangle + a^4|\varphi_n\rangle + a^{+4}|\varphi_n\rangle \Big) \quad \text{for all } n \in \mathbb{N}_0$$

$$a^{+4}|\varphi_n\rangle = \sqrt{\frac{(n+4)!}{n!}}\,|\varphi_{n+4}\rangle, \quad a^4|\varphi_n\rangle = \begin{cases} 0 & : n < 4 \\ \sqrt{\frac{n!}{(n-4)!}}\,|\varphi_{n-4}\rangle & : \text{else} \end{cases}$$

$$a^+ P_2(N) a^+ |\varphi_n\rangle = P_2(n+1)\sqrt{\frac{(n+2)!}{n!}}\,|\varphi_{n+2}\rangle$$

$$a P_2(N) a |\varphi_n\rangle = \begin{cases} 0 & : n < 2 \\ P_2(n-1)\sqrt{\frac{n!}{(n-2)!}}\,|\varphi_{n-2}\rangle & : \text{else} \end{cases}$$

$$P_1(N)|\varphi_n\rangle = P_1(n)\,|\varphi_n\rangle$$

for all $n \in \mathbb{N}_0$; here $P_1(N)$ and $P_2(N)$ mean operators and $P_1(n)$, $P_2(n)$ mean polynoms on $\mathbb{N}_0$ with the same coefficients

$$\Rightarrow E_n^{(1)} = \hbar\omega \cdot \frac{\hbar}{4m^2\omega^3} P_1(n) \quad \text{for all } n \in \mathbb{N}_0$$

(use $\langle \varphi_n | \varphi_m \rangle = \delta_{nm}$ for all $n, m \in \mathbb{N}_0$)

$\Rightarrow$ first-order perturbation energy levels: (with $E_n^{(0)}$ as energy levels of unperturbed system for all $n \in \mathbb{N}_0$)

$$\tilde{E}_n = E_n^{(0)} + \lambda E_n^{(1)}$$

$$= \hbar\omega \left(\frac{1}{2} + n + \frac{\hbar\lambda}{4m^2\omega^3}\, 3(2n^2 + 2n + 1) \right) \quad \text{for all } n \in \mathbb{N}_0$$

AUF 2: 6.0/6.0