ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Quantenmechanik I
Lösung 12

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Prof. Gianni Blatter

Übung 1. Dichtematrix und Wahrscheinlichkeiten

(a) (i) $\rho = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$.

   (ii) $|\psi\rangle$ is a pure state. The density operator is the following:

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{2}\left(|0\rangle - i\,|1\rangle\right)\left(\langle 0| + i\,\langle 1|\right) \tag{L.1}$$

$$= \frac{1}{2}\left(|0\rangle\langle 0| + i|0\rangle\langle 1| - i|1\rangle\langle 0| + |1\rangle\langle 1|\right) \tag{L.2}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix}. \tag{L.3}$$

   (iii) $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$.

   (iv) We write ρ in the $|0\rangle, |1\rangle$ basis:

$$\rho = \frac{1}{2}|+\rangle\langle +| + \frac{1}{2}|-\rangle\langle -| \tag{L.4}$$

$$= \frac{1}{4}\left(|0\rangle + |1\rangle\right)\left(\langle 0| + \langle 1|\right) + \frac{1}{4}\left(|0\rangle - |1\rangle\right)\left(\langle 0| - \langle 1|\right) \tag{L.5}$$

$$= \frac{1}{4}\left(|0\rangle\langle 0| + |0\rangle\langle 1| + |1\rangle\langle 0| + |1\rangle\langle 1| + |0\rangle\langle 0| - |0\rangle\langle 1| - |1\rangle\langle 0| + |1\rangle\langle 1|\right) \tag{L.6}$$

$$= \frac{1}{2}\left(|0\rangle\langle 0| + |1\rangle\langle 1|\right) \tag{L.7}$$

$$= \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{L.8}$$

Note that the density matrix is identical to the density matrix from the previous item. In particular, this means that they evolve in time in the exact same way and result in the same measurement statistics.

   (v) Similar to the calculation in (ii), now we get $\rho = \frac{1}{4}\begin{pmatrix} 3 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$.

   (vi) After observing the state $|0\rangle$ in the measurement, the post measurement state is given by the pure state $|0\rangle$ ($|\phi\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle$ collapsed to $|0\rangle$). The density matrix is therefore $\rho = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$.

   (vii) When measuring $|\phi\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle$ in the basis $\{|0\rangle, |1\rangle\}$ we can get the state $|0\rangle$ with probability $\frac{3}{4}$ and the state $|1\rangle$ with probability $\frac{1}{4}$. If we do not know which of the results accrued then the post measurement state is the mixed state $\rho = \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}$.

Notice how the measurement procedure *decoheres* the state (i.e., its off-diagonal entries vanish compared to (v)). This happens for example in the Young slits experiment if one measures in which one of the two slits the particle has passed.

(viii) Again, after the measurement of $|\phi\rangle = \frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle$ in the basis $\{|+\rangle, |-\rangle\}$ we can get the state $|+\rangle$ with probability $|\langle+|\phi\rangle|^2$ and the state $|-\rangle$ with probability $|\langle-|\phi\rangle|^2$. So calculate the overlaps

$$|\langle\phi|+\rangle|^2 = \left|\frac{\sqrt{3}}{2}\langle+|0\rangle + \frac{1}{2}\langle+|1\rangle\right|^2 = \left|\frac{\sqrt{3}+1}{2\sqrt{2}}\right|^2 = \frac{2+\sqrt{3}}{4} \approx 0.93\ ; \qquad \text{(L.9)}$$

$$|\langle\phi|-\rangle|^2 = \left|\frac{\sqrt{3}}{2}\langle-|0\rangle + \frac{1}{2}\langle-|1\rangle\right|^2 = \left|\frac{\sqrt{3}-1}{2\sqrt{2}}\right|^2 = \frac{2-\sqrt{3}}{4} \approx 0.07, \qquad \text{(L.10)}$$

(use $\langle\pm|0\rangle = 1/\sqrt{2}$ and $\langle\pm|1\rangle = \pm 1/\sqrt{2}$) and then

$$\rho = |\langle\phi|+\rangle|^2|+\rangle\langle+| \ + \ |\langle\phi|-\rangle|^2|-\rangle\langle-| = |\langle\phi|+\rangle|^2 \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} + |\langle\phi|-\rangle|^2 \begin{pmatrix} 1/2 & -1/2 \\ -1/2 & 1/2 \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2}|\langle\phi|+\rangle|^2 + \frac{1}{2}|\langle\phi|-\rangle|^2 & \frac{1}{2}|\langle\phi|+\rangle|^2 - \frac{1}{2}|\langle\phi|-\rangle|^2 \\ \frac{1}{2}|\langle\phi|+\rangle|^2 - \frac{1}{2}|\langle\phi|-\rangle|^2 & \frac{1}{2}|\langle\phi|+\rangle|^2 + \frac{1}{2}|\langle\phi|-\rangle|^2 \end{pmatrix} = \begin{pmatrix} 1/2 & \sqrt{3}/4 \\ \sqrt{3}/4 & 1/2 \end{pmatrix} \approx \begin{pmatrix} 0.5 & 0.43 \\ 0.43 & 0.5 \end{pmatrix}$$
$$\text{(L.11)}$$

Here, the system has only slightly decohered. It is no longer pure (it doesn't have rank 1), yet it still has off-diagonal terms. However, in the $\{|\pm\rangle\}$ basis, ρ has competely decohered (the off-diagonal elements have vanished in that basis).

In systems (i), (ii), (v) and (vi) the density matrix is pure so we trivially have its spectral decomposition; in all these cases the density matrix is not diagonal in the $\{|\pm\rangle\}$ basis. In systems (iii) and (iv) the state is maximally mixed (=proportional to the identity matrix), so it is diagonal in every basis. In system (vii) ρ is diagonal in the $\{|0\rangle, |1\rangle\}$ basis by construction, and has different eigenvalues, so it is not diagonal in the $\{|\pm\rangle\}$ basis. In (viii) ρ is diagonal in the $\{|\pm\rangle\}$ basis by construction.

(b) (i) To see that $\text{Tr}\,\rho = 1$ first note that the trace function is "similarity-invariant", i.e., it is independent of the choice of basis in which we write ρ. Therefore, write ρ in its diagonal basis. ρ can then be understood as a mixture of the different eigenstates $|\varphi_i\rangle$, each with probability corresponding to its eigenvalue λ_i. We therefore have $\text{Tr}\,\rho = \sum_i \lambda_i = 1$.

Alternatively, see the calculation in page 197 in the script.

(ii) For all states $|\varphi\rangle$, $\langle\varphi|\rho|\varphi\rangle = \sum_k p_k|\langle\varphi|\psi_k\rangle|^2 \geq 0$.

(iii) If the system is in state $|\psi_k\rangle$, then the probability of obtaining the measurement result a_i is $\text{Pr}[a_i|\psi_k] = \langle\psi_k|P_i|\psi_k\rangle = \text{Tr}\,[|\psi_k\rangle\langle\psi_k|\,P_i]$.[1] Using the basic rules of probability,

$$\text{Pr}[a_i] = p_1\,\text{Pr}[a_i|\psi_1] + p_2\,\text{Pr}[a_i|\psi_2] + \ldots = \sum_k p_k\,\text{Tr}\,[|\psi_k\rangle\langle\psi_k|\,P_i] = \text{Tr}\,(\rho\,P_i)\,. \qquad \text{(L.12)}$$

(iv) If the system is in state $|\psi_k\rangle$, and the outcome a_i is observed, then the system will be left in the state $|\psi_k'\rangle = P_i|\psi_k\rangle/\sqrt{\text{Pr}[a_i|\psi_k]}$. Consider the event tree in Fig. 1: we see that in general the probability to end up in the state $|\psi_k'\rangle$ is $\text{Pr}[a_i|\psi_k]\,p_k$. However these probabilities don't add up to one, because they take into accout the cases where we didn't observe the outcome a_i. If we condition on indeed observing a_i, we need to

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[1] Note that in general for an operator A and a normalized ket $|\phi\rangle$ it holds that $\langle\phi|A|\phi\rangle = \text{Tr}\,[A|\phi\rangle\langle\phi|]$. To see this, evaluate the trace in a basis containing the vector $|\phi\rangle$.
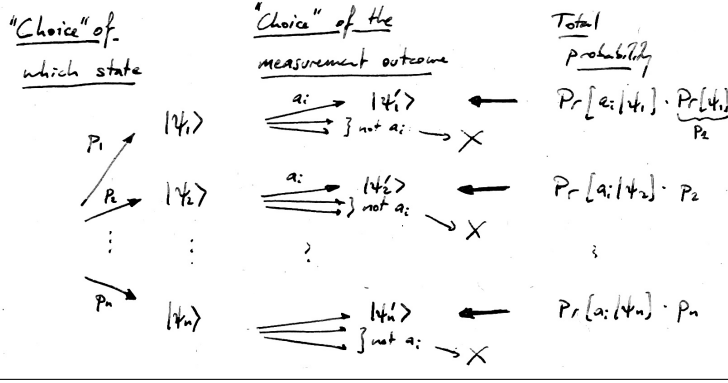
Fig. 1: Tree of possible events. The actual state of the system is in either one of the $|\psi_k\rangle$ with probability p_k. In each case: a measurement of A might give the outcome a_i, resulting in the collapsed state $|\psi_k'\rangle$, with probability $\Pr[a_i|\psi_k] = \langle\psi_k|P_i|\psi_k\rangle$, or another outcome, which we don't care about for now.

divide by the total probability $\Pr[a_i]$ of observing a_i; we thus get a new, normalized ensemble:

$$\rho_i = \sum_k \frac{\Pr[a_i|\psi_k]\,p_k}{\Pr[a_i]} \cdot |\psi_k'\rangle\langle\psi_k'| = \frac{1}{\Pr[a_i]} \sum_k p_k \cdot P_i|\psi_k\rangle\langle\psi_k|P_i = \frac{P_i\,\rho\,P_i}{\operatorname{Tr}(\rho\,P_i)}, \quad \text{(L.13)}$$

as we have seen before that $\Pr[a_i] = \operatorname{Tr}(\rho\,P_i)$.

(c) Now ρ is a classical probability distribution, i.e. diagonal in the predetermined eigenbasis $\{|\psi_k\rangle\}$. We can think of the system as a classical register which can be in one of the states $k = 1, 2, \ldots n$. To fix some notation, let's say $\rho = \sum q_k|\psi_k\rangle\langle\psi_k|$ with some eigenvalues q_k. We have for the properties in (b):

  (i) The condition $\operatorname{Tr}\rho = 1$ implies that $\sum q_k = 1$ (take the trace in the $\{|\psi_k\rangle\}$ basis), thus recovering the *normalization condition* of classical probability distributions.

  (ii) The property $\rho \geqslant 0$ implies that all the eigenvalues of ρ must be positive, i.e. $q_k \geqslant 0$ for all k. This corresponds to the postulate that *probabilities must be non-negative*.

  (iii) In classical probability theory, a measurement simply corresponds to *observing* the actual value of a random variable, or, equivalently, which of a set of possible mutually exclusive events took place. For example, if I throw a die, a possible measurement would correspond to look at the value shown by the die (6 outcomes). Another example of a measurement would be to look at whether the value shown on the die is even or odd (2 outcomes).

  Thus if we measure A (also taken diagonal in the basis $\{|\psi_k\rangle\}$) and observe a_i, this corresponds to testing whether the system is in the state $k \in I_i$, where I_i is an index set designating all k's for which $|\psi_k\rangle$ is in the eigenspace spanned by P_i.

  The value $\operatorname{Tr}(\rho\,P_i)$ can then be written as $\operatorname{Tr}(\rho\,P_i) = \sum_{k \in I_i} q_k$, i.e. the probability of being in one of the states in I_i.

  (iv) The collapsed state after such a measurement is then according to above

$$\rho_i = \frac{P_i\,\rho\,P_i}{\operatorname{Tr}(\rho\,P_i)} = \sum_{k \in I_i} \frac{q_k}{\Pr[a_i]}\,|\psi_k\rangle\langle\psi_k|, \quad \text{(L.14)}$$

which is again a "classical" density operator (i.e., diagonal in the predefined fixed basis) with the distribution corresponding to the *probability distribution conditioned on the event* that $k \in I_i$. We recover the rule in probability theory, where if we condition on a set of outcomes, the conditioned probability is set to zero for outcomes which are not included in the conditioning event, while we rescale the outcomes that we keep while preserving the relative probabilities.

Übung 2.   Free particle in the Heisenberg picture

The Hamiltonian of a free particle is $H = \frac{P^2}{2m}$.

Let $X_H(0)$ be the position operator at time $t = 0$. Using Equation (7.31) in the script, $X_H(t)$ satisfies the following equation:

$$i\hbar \frac{d}{dt} X_H(t) = [X_H(t), H_H(t)] + (\partial_t X)_H = [X_H(t), H], \tag{L.15}$$

where we used $\partial_t X = 0$ and $H_H(t) = H$ as the Hamiltonian is independent of the time. Plugging

$$[X_H(t), H] = \left[X_H(t), \frac{P^2}{2m} \right] = i\hbar \frac{P}{m} \tag{L.16}$$

into Equation (L.15) we get

$$\frac{d}{dt} X_H(t) = \frac{P}{m}, \tag{L.17}$$

which means

$$X_H(t) = \frac{P}{m} t + X_H(0). \tag{L.18}$$

Note that in all the above equations P is just the momentum operator in the Schrödinger picture, as $H_H(t) = H$.

We can now use Equation (L.18) to calculate the commutator of $X_H(0)$ with $X_H(t)$:

$$[X_H(0), X_H(t)] = \left[X_H(0), \frac{P}{m} t + X_H(0) \right] = \frac{t}{m} [X_H(0), P] + [X_H(0), X_H(0)] = \frac{i\hbar t}{m}. \tag{L.19}$$

Using the uncertainty relation (see Serie 6 Übung 2) we get,

$$\Delta X_H(0) \cdot \Delta X_H(t) \geq \frac{1}{2} |\langle i[X_H(0), X_H(t)] \rangle| = \frac{\hbar t}{2m}. \tag{L.20}$$

Übung 3.   Das Helium Atom

(a) Das Zustand Ψ_0 ist wohl normiert (siehe Vorlesungsskript). Es gilt dann

$$\int d^3 \boldsymbol{r}_1 d^3 \boldsymbol{r}_2 \, \Psi^* (\boldsymbol{r}_1, \boldsymbol{r}_2) \Psi (\boldsymbol{r}_1, \boldsymbol{r}_2) = \alpha^6 \int d^3 \boldsymbol{r}_1 d^3 \boldsymbol{r}_2 \, \Psi_0^* (\alpha \boldsymbol{r}_1) \Psi_0^* (\alpha \boldsymbol{r}_2) \Psi_0 (\alpha \boldsymbol{r}_1) \Psi_0 (\alpha \boldsymbol{r}_2)$$

$$= \int d^3 (\alpha \boldsymbol{r}_1) \, \Psi_0^* (\alpha \boldsymbol{r}_1) \Psi_0 (\alpha \boldsymbol{r}_1) \int d^3 (\alpha \boldsymbol{r}_2) \, \Psi_0^* (\alpha \boldsymbol{r}_2) \Psi_0 (\alpha \boldsymbol{r}_2) = 1. \tag{L.21}$$

(b) Wir versuchen, den Ausdruck $\langle \Psi | H_{\text{kin}} | \Psi \rangle$ als funktion von E_0^{kin} zu schreiben:

$$\int d^3 \boldsymbol{r}_1 \, d^3 \boldsymbol{r}_2 \, \Psi^* (\boldsymbol{r}_1) H_{\text{kin}} \Psi (\boldsymbol{r}_2)$$

$$= \alpha^6 \int d^3 \boldsymbol{r}_1 \, d^3 \boldsymbol{r}_2 \left[\Psi_0^* (\alpha \boldsymbol{r}_1) \left(\frac{-\hbar^2}{2m} \Delta_{\boldsymbol{r}_1} \right) \Psi_0 (\alpha \boldsymbol{r}_1) \, \Psi_0^* (\alpha \boldsymbol{r}_2) \Psi_0 (\alpha \boldsymbol{r}_2) \right.$$

$$\left. + \Psi_0^* (\alpha \boldsymbol{r}_1) \Psi_0 (\alpha \boldsymbol{r}_1) \, \Psi_0^* (\alpha \boldsymbol{r}_2) \left(\frac{-\hbar^2}{2m} \Delta_{\boldsymbol{r}_2} \right) \Psi_0 (\alpha \boldsymbol{r}_2) \right]$$

$$= 2 \alpha^2 \int d^3 (\alpha \boldsymbol{r}_1) \left[\Psi_0^* (\alpha \boldsymbol{r}_1) \left(\frac{-\hbar^2}{2m} \Delta_{\alpha \boldsymbol{r}_1} \right) \Psi_0 (\alpha \boldsymbol{r}_1) \right] = 2\alpha^2 \, E_0^{\text{kin}}, \tag{L.22}$$

wobei die zwei Termen im grossen Klammer unter $\boldsymbol{r}_1 \leftrightarrow \boldsymbol{r}_2$ gleich sind, den Zustand Ψ_0 normiert ist, und $\Delta_{\alpha\boldsymbol{r}_1} = (1/\alpha^2)\Delta_{\boldsymbol{r}_1}$. Im letzten Ausdruck erkennen wir die kinetische Energie des Grundzustands des Wasserstoffatoms.[2] Es folgt $E^{\mathrm{kin}} = 2\alpha^2 E_0^{\mathrm{kin}} = e^2\alpha^2/a_B$.

Ebenso untersuchen wir $E^{\mathrm{pot}} = \langle\Psi|H_{\mathrm{pot}}|\Psi\rangle$:

$$E^{\mathrm{pot}} = \alpha^6 \int d^3\boldsymbol{r}_1\, d^3\boldsymbol{r}_2 \Big[\Psi_0^*(\alpha\boldsymbol{r}_1)\left(\frac{-2e^2}{r_1}\right)\Psi_0(\alpha\boldsymbol{r}_1)\ \Psi_0^*(\alpha\boldsymbol{r}_2)\,\Psi_0(\alpha\boldsymbol{r}_2)$$

$$+\ \Psi_0^*(\alpha\boldsymbol{r}_1)\,\Psi_0(\alpha\boldsymbol{r}_1)\ \Psi_0^*(\alpha\boldsymbol{r}_2)\left(\frac{-2e^2}{r_2}\right)\Psi_0(\alpha\boldsymbol{r}_2)\Big]$$

$$= 4\,\alpha \int d^3(\alpha\boldsymbol{r}_1)\left[\Psi_0^*(\alpha\boldsymbol{r}_1)\left(\frac{-e^2}{(\alpha r_1)}\right)\Psi_0(\alpha\boldsymbol{r}_1)\right] = 4\alpha\, E_0^{\mathrm{pot}}. \tag{L.23}$$

Daraus schliessen wir $E^{\mathrm{pot}} = 4\alpha\, E_0^{\mathrm{pot}} = -4e^2\alpha/a_B$.

Das term E^{WW} können wir nicht zum Wasserstoffatomfall zurückziehen, da es im Wasserstoffatom trivialerweise keine Elektronenwechselwirkung stattfindet. Dann rechnen wir explizit $E^{\mathrm{WW}} = \langle\Psi|H_{\mathrm{WW}}|\Psi\rangle$, indem wir $1/|\boldsymbol{r}_1-\boldsymbol{r}_2|$ in der Fourierdarstellung ausdrucken:

$$E^{\mathrm{WW}} = \left(\frac{\alpha^3}{\pi a_B^3}\right)^2 \int d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2\, \frac{e^2}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\,\exp\left\{-2\alpha\frac{r_1+r_2}{a_B}\right\}$$

$$= \left(\frac{\alpha^3}{\pi a_B^3}\right)^2 4\pi e^2 \int d^3\boldsymbol{r}_1 d^3\boldsymbol{r}_2\frac{d^3\boldsymbol{k}}{(2\pi)^3}\frac{1}{k^2}\exp\left\{i\boldsymbol{k}(\boldsymbol{r}_1-\boldsymbol{r}_2) - 2\alpha\frac{r_1+r_2}{a_B}\right\}$$

$$= \frac{\alpha^6 e^2}{2\pi^4 a_B^6}\int\frac{d^3\boldsymbol{k}}{k^2}\underbrace{\int d^3\boldsymbol{r}_1\exp\left\{i\boldsymbol{k}\boldsymbol{r}_1 - 2\alpha\frac{r_1}{a_B}\right\}}_{I}\underbrace{\int d^3\boldsymbol{r}_2\exp\left\{-i\boldsymbol{k}\boldsymbol{r}_2 - 2\alpha\frac{r_2}{a_B}\right\}}_{=I,\ \mathrm{mit}\ \boldsymbol{r}_2\to-\boldsymbol{r}_2,\, r_2\to r_2} \tag{L.24}$$

Wir berechnen jetzt das innere Integral I in sphärischen Koordinaten:

$$I = \int d\phi \int dr\, r^2 e^{-2\alpha\frac{r}{a_B}}\int_{-1}^{+1} d(\cos\theta)\, e^{ikr\cos\theta} = 2\pi\int dr\, r^2 e^{-\alpha\frac{r}{a_B}}\frac{1}{ikr}\left[e^{ikr}-e^{-ikr}\right]$$

$$= \frac{4\pi}{k}\int dr\, r\, e^{-2\alpha\frac{r}{a_B}}\,\mathrm{Im}\left[e^{ikr}\right] = \frac{4\pi}{k}\int dr\, r\,\mathrm{Im}\left[e^{\left(ik-\frac{2\alpha}{a_B}\right)r}\right] \qquad\qquad \wr\ x = -ik + \frac{2\alpha}{a_B}$$

$$= \frac{4\pi}{k}\mathrm{Im}\left[-\int_0^\infty dr\,\frac{\partial}{\partial x}\,e^{-xr}\right] = \frac{4\pi}{k}\mathrm{Im}\left[-\frac{\partial}{\partial x}\left[0 + \frac{1}{x}\right]\right] = \frac{4\pi}{k}\mathrm{Im}\left[\frac{1}{x^2}\right]. \tag{L.25}$$

Mit $x^{-1} = \frac{a_B}{2\alpha - ika_B} = a_B\frac{2\alpha+ika_B}{4\alpha^2+k^2a_B^2}$ erhalten wir

$$(\mathrm{L.25}) = \frac{4\pi}{k}\mathrm{Im}\left[a_B^2\frac{2\cdot 2\alpha\cdot ika_B + (...)}{(4\alpha^2+k^2a_B^2)^2}\right] = \frac{4\pi}{k}\cdot\frac{4\alpha\, k\, a_B^3}{(4\alpha^2+k^2a_B^2)^2} = \frac{16\pi\alpha/a_B}{\left(\frac{4\alpha^2}{a_B^2}+k^2\right)^2}. \tag{L.26}$$

Setzt man dieser Ausdruck in (L.24) zweimal wieder ein, so bekommt man

$$E^{\mathrm{WW}} = \frac{\alpha^6 e^2}{2\pi^4 a_B^6}\int\frac{d^3\boldsymbol{k}}{k^2}\left(\frac{16\pi\alpha/a_B}{\left(k^2+\frac{4\alpha^2}{a_B^2}\right)^2}\right)^2 = \frac{\alpha^6 e^2}{2\pi^4 a_B^6}\frac{(16\pi\alpha)^2}{a_B^2}\int d\Omega\, dk\,\frac{1}{\left(k^2+\frac{4\alpha^2}{a_B^2}\right)^4}$$

$$= \frac{2^9\,\alpha^8 e^2}{\pi a_B^8}\int dk\,\frac{1}{\left(\frac{4\alpha^2}{a_B^2}\right)^4}\cdot\frac{1}{\left(1+\frac{a_B^2 k^2}{4\alpha^2}\right)^4} = \frac{2^9\,\alpha^8 e^2}{\pi a_B^8}\cdot\frac{a_B^8}{2^8\alpha^8}\cdot\frac{2\alpha}{a_B}\int dk'\,\frac{1}{(1+k'^2)^4}$$

$$= \frac{4e^2\alpha}{\pi a_B}\cdot\frac{5\pi}{32} = \frac{5e^2\alpha}{8a_B}, \tag{L.27}$$

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[2] Die Werten E_0^{kin} und E_0^{pot} für das Wasserstoffatom folgen aus dem Virialsatz, der die relative Verhaltung zwischen potentielle und kinetische Energie beschreibt. Sie können auch sonst explizit berechnet werden.

wobei wir $k' = a_B k/2\alpha$ definieren und das im Übungsblatt gegebene Integral benutzen. (Dieses Integral könnte man z.B. mit dem Residuensatz lösen.)

Der Term E^{kin} ist minimal, wenn das Teilchen maximal delokalisiert ist, i.e. wenn $\alpha \to 0$. Dies versteht man aus der Fourierdarstellung: in dieser Fall ist die Zustandswellenfunction im Impulsraum um $k = 0$ gepeakt und ist somit eine Superposition von Zuständen, die wenig kinetische Energie haben. Wird α grösser, dann wird das Teilchen mehr lokalisiert und wächst E^{kin}. Der Term E^{pot} kämpft dagegen, indem die potentielle Energie minimiert wird, wenn das Teilchen maximal bei $r = 0$ lokalisiert wird ($\alpha \to \infty$). Es ist dann offenbar aus dem Ausdruck dieser Energien, dass die totale Energie wohl ein Minimum für ein $\alpha > 0$ aufweisen wird.

Der Term E^{WW} ist eine Korrektur dazu, indem wir die Abstossung zwischen den Elektronen eingerechnet haben; der Term verhält sich auch linear in α wie E^{pot}, weil er die gleiche Art von Kraft (Coulomb-Kraft) entspricht, jedoch mit dem anderen Vorzeichen. So wird den Minimum in α verschoben: der Grundzustand wird wegen Abstossung der Elektronen mehr delokalisiert werden.

(c) Die totale mittele Energie ist dann

$$E = \langle \Psi | H | \Psi \rangle = \frac{e^2 \alpha^2}{a_B} - \frac{4e^2 \alpha}{a_B} + \frac{5\,\alpha e^2}{8\,a_B}. \tag{L.28}$$

Die Ableitung dieses Ausdrucks verschwindet genau dann, wenn $2\alpha - (4 - {}^5\!/\!{}_8) = 0 \Leftrightarrow \alpha = 27/16$. Für diese α ist dann $E \approx -2.85\ e^2/a_B$, was eine richtig gute Schätzung des experimentellen Wertes ist.

Bemerkung 1: Für das Wasserstoffatomproblem, wenn $Z \neq 1$, dann ändert sich die Lösung durch eine Ausdehnung der Wellenfunktion, d.h. wie $\Psi_0\,(Z\,\boldsymbol{r})$ (siehe im Skript (5.73), mit $\kappa \propto Z$). Man könnte dann hier $\alpha = 2$ erwartet haben, denn für das Helium-Atom $Z = 2$ gilt. Es ist jedoch wegen Elektronenwechselwirkung nicht exakt so.

Bemerkung 2: Die Präsenz eines anderen Elektrons ändert die effektive Ladung des Kernes, die ein Elektron fühlt. Wir siehen, dass effektiv jede Elektron die Kernladung für das andere Elektron mit einer effektiven Ladung 5/16 abschrimt, sodass jede Elektron nur eine Kernladung von $27/16 = 2 - 5/16$ spürt. Die Anwesenheit der zweiten negativen Ladung schirmt die Kernladung 2 um c.a. 1/3 ab.