SOLUTIONS W. GRADING SCHEMES

Klausur 1
Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Aufgabe 1. Zwei harmonische Oszillatoren

Wir betrachten zwei harmonische Oszillatoren mit dem Hamiltonoperator

$$\hat{H} = \frac{\hat{p}_1^2 + \hat{p}_2^2}{2m} + \frac{m\omega^2}{2}(\hat{x}_1^2 + \hat{x}_2^2), \tag{1}$$

wobei $\hat{x}_i$ and $\hat{p}_i$ die kanonischen Vertauschungsrelationen erfüllen: $[\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0$ und $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$, mit $i, j = 1, 2$.

1. (**1.5 Punkte**) Mit Hilfe der Orts- und Impulsoperatoren $\hat{x}_i$, $\hat{p}_j$ definieren wir Erzeugungs- und Vernichtungsoperatoren $\hat{a}_i^\dagger$ sowie $\hat{a}_i$ wie folgt:

$$\hat{a}_i = \alpha\hat{x}_i + i\beta\hat{p}_i, \tag{2}$$
$$\hat{a}_i^\dagger = \alpha\hat{x}_i - i\beta\hat{p}_j \tag{3}$$

wobei α und β reelle Zahlen sind.

Bestimmen Sie α und β so, dass:

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}, \tag{4}$$
$$[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0, \tag{5}$$
$$\hat{H} = \sum_{j=1}^{2} \hbar\omega\left(\hat{n}_j + \frac{1}{2}\right) \tag{6}$$

wobei $\hat{n}_i = \hat{a}_i^\dagger\hat{a}_i$. Welches sind die Eigenwerte des Hamiltonoperators Gl. (1)?

2. (**1 Punkt**) Beweisen Sie die folgenden Identitäten:

$$[\hat{n}_i, \hat{a}_j] = -\hat{a}_j\delta_{ij}, \tag{7}$$
$$[\hat{n}_i, \hat{a}_j^\dagger] = \hat{a}_j^\dagger\delta_{ij}, \tag{8}$$
$$[\hat{n}_i, \hat{n}_j] = 0. \tag{9}$$

Betrachten wir nun, was passiert, wenn zwischen den beiden Oszillatoren eine zusätzliche Kopplung besteht:

$$\hat{H}' = \frac{\hat{p}_1^2 + \hat{p}_2^2}{2m} + \frac{m\omega^2}{2}(\hat{x}_1^2 + \hat{x}_2^2) + \gamma \hat{x}_1 \hat{x}_2 \tag{10}$$

mit $|\gamma| \leq m\omega^2$.

3. (**1 Punkt**) Drücken Sie den neuen Term (d.h. $\gamma\hat{x}_1\hat{x}_2$) durch die in Teil 2 erhaltenen a_i und $a_i^\dagger$ aus und zeigen Sie, dass der neue Hamiltonoperator in Bezug auf $\hat{a}_i$ und $\hat{a}_i^\dagger$ nicht die gleiche Form wie Gleichung (6) hat.

4. (**3 Punkte**) Um die Eigenzustände des Hamiltonoperators in Gl. (10) zu finden, führen Sie neue kanonische Operatoren ein, die aus $\hat{x}_i$ und $\hat{p}_i$ bestehen. Betrachten Sie dazu

$$\hat{X}_i = a_i\hat{x}_1 + b_i\hat{x}_2, \tag{11}$$
$$\hat{P}_i = c_i\hat{p}_1 + d_i\hat{p}_2, \tag{12}$$

die die folgenden Vertauschungsrelationen erfüllen

$$[\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}, \tag{13}$$
$$[\hat{X}_i, \hat{X}_j] = [\hat{P}_i, \hat{P}_j] = 0. \tag{14}$$

wobei $i = 1, 2$. Finden Sie die Koeffizienten a_i, b_i, c_i und d_i, so dass

$$\hat{H}' = \frac{\hat{P}_1^2}{2m_1} + \frac{\hat{P}_2^2}{2m_2} + \frac{1}{2}m_1\omega_1^2\hat{X}_1^2 + \frac{1}{2}m_2\omega_2^2\hat{X}_2^2 \tag{15}$$

und drücken Sie m_1, m_2, ω_1 und ω_2 durch m, ω und γ aus.

Was passiert wenn $|\gamma| > m\omega^2$?

5. (**1 Punkt**) Finden Sie die Erzeugungs- und Vernichtungsoperatoren $\hat{A}_i$ und $\hat{A}_i^\dagger$, mit $i = 1, 2$ die folgendermassen gegeben sind

$$\hat{A}_i = \alpha_i\hat{X}_i + i\beta_i\hat{P}_i, \tag{16}$$
$$\hat{A}_i^\dagger = \alpha_i\hat{X}_i - i\beta_i\hat{P}_i \tag{17}$$

und die die folgende Beziehung erfüllen

$$[\hat{A}_i, \hat{A}_j^\dagger] = \delta_{ij}, \tag{18}$$
$$[\hat{A}_i, \hat{A}_j] = [\hat{A}_i^\dagger, \hat{A}_j^\dagger] = 0, \tag{19}$$
$$\hat{H}' = \sum_{j=1}^{2} \hbar\omega_j\left(\hat{N}_j + \frac{1}{2}\right). \tag{20}$$

Es gilt $\hat{N}_i = \hat{A}_i^\dagger\hat{A}_i$. Welches sind die Eigenwerte des Hamiltonoperators Gl. (10)?

Lösung 1

1.

$$[\hat{a}_i, \hat{a}_j] = [\alpha\hat{x}_i + i\beta\hat{p}_i, \alpha\hat{x}_j + i\beta\hat{p}_j] = i\alpha\beta([\hat{x}_i, \hat{p}_j] + [\hat{p}_j, \hat{x}_i]) = 0 \tag{21}$$
$$[\hat{a}_i^\dagger, \hat{a}_j^\dagger] = ([\hat{a}_j, \hat{a}_i])^\dagger = 0 \tag{22}$$
$$[\hat{a}_i, \hat{a}_j^\dagger] = [\alpha\hat{x}_i + i\beta\hat{p}_i, \alpha\hat{x}_j - i\beta\hat{p}_j] = -2i\alpha\beta[\hat{x}_i, \hat{p}_j] = 2\hbar\alpha\beta\delta_{ij} = \delta_{ij} \tag{23}$$

As a result, $\alpha\beta = \frac{1}{2\hbar}$. 0.5 P

$\hat{x}_i$ and $\hat{p}_i$ in terms of $\hat{a}_i$ and $\hat{a}_i^\dagger$ are given by

$$\hat{x}_i = \frac{\hat{a}_i + \hat{a}_i^\dagger}{2\alpha}, \tag{24}$$

$$\hat{p}_i = \frac{\hbar\alpha}{i}(\hat{a}_i^\dagger - \hat{a}_j^\dagger) \tag{25}$$

Plug this into the Hamiltonian:

$$\begin{aligned}
\hat{H} &= \sum_i^2 \Big[-\frac{\hbar^2\alpha^2}{2m}(\hat{a}_i - \hat{a}_i^\dagger)^2 + \frac{m\omega^2}{8\alpha^2}(\hat{a}_i + \hat{a}_i^\dagger)^2 \Big] \\
&= \sum_{i=1}^2 \Big[\Big(\frac{m\omega^2}{8\alpha^2} - \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i + \hat{a}_i^\dagger\hat{a}_i^\dagger) + \Big(\frac{m\omega^2}{8\alpha^2} + \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i^\dagger + \hat{a}_i^\dagger\hat{a}_i) \Big] \\
&= \sum_{i=1}^2 \Big[\Big(\frac{m\omega^2}{8\alpha^2} - \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i + \hat{a}_i^\dagger\hat{a}_i^\dagger) + \Big(\frac{m\omega^2}{8\alpha^2} + \frac{\hbar^2\alpha^2}{2m}\Big)(2\hat{a}_i^\dagger\hat{a}_i + 1) \Big] \\
&= \sum_{i=1}^2 \Big[\Big(\frac{m\omega^2}{8\alpha^2} - \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i\hat{a}_i + \hat{a}_i^\dagger\hat{a}_i^\dagger) + 2\Big(\frac{m\omega^2}{8\alpha^2} + \frac{\hbar^2\alpha^2}{2m}\Big)(\hat{a}_i^\dagger\hat{a}_i + 1/2) \Big] \stackrel{!}{=} \sum_{j=1}^2 \hbar\omega\Big[\hat{N}_j + 1/2\Big]
\end{aligned}$$

By comparison, we see that the following must apply

$$\frac{m\omega^2}{8\alpha^2} - \frac{\hbar\alpha^2}{2m} = 0 \Rightarrow \alpha = \sqrt{\frac{m\omega}{2\hbar}}. \quad 0.5p \tag{26}$$

Thus α has the dimensions of inverse length, and β of inverse momentum. Up to a factor, this could have also been derived by dimensional analysis.

The energies are given by $E_{n_1,n_2} = \hbar\omega(n_1 + n_2 + 1)$ where $n_1,\, n_2 \in Z(\geq 0)$.

0.5p

2. We calculate

$$[\hat{N}_i, \hat{a}_j] = [\hat{a}_i^\dagger\hat{a}_i, \hat{a}_j] = \hat{a}_i^\dagger[\hat{a}_i, \hat{a}_j] + [\hat{a}_i^\dagger, \hat{a}_j]\hat{a}_i = -\delta_{ij}\hat{a}_i, \tag{27}$$

$$[\hat{N}_i, \hat{a}_j^\dagger] = (-[\hat{N}_i, \hat{a}_j])^\dagger = \delta_{ij}\hat{a}_i^\dagger, \tag{28}$$

$$[\hat{N}_i, \hat{N}_j] = [\hat{N}_i, \hat{a}_j^\dagger\hat{a}_j] = [\hat{N}_i, \hat{a}_j^\dagger]\hat{a}_j + \hat{a}_j^\dagger[\hat{N}_i, \hat{a}_j] = \delta_{ij}(\hat{N}_j - \hat{N}_j) = 0 \tag{29}$$

1p

3.

$$\gamma\hat{x}_1\hat{x}_2 = \frac{\gamma}{4\alpha^2}(\hat{a}_1 + \hat{a}_1^\dagger)(\hat{a}_2 + \hat{a}_2^\dagger) = \frac{\hbar\gamma}{2m\omega}(\hat{a}_1\hat{a}_2 + \hat{a}_1\hat{a}_2^\dagger + \hat{a}_1^\dagger\hat{a}_2 + \hat{a}_1^\dagger\hat{a}_2^\dagger) \tag{30}$$

$$\Rightarrow H' = \sum_i \hbar\omega(\hat{n}_i + 1/2) + \frac{\hbar\gamma}{2m\omega}(\hat{a}_1\hat{a}_2 + \hat{a}_1\hat{a}_2^\dagger + \hat{a}_1^\dagger\hat{a}_2 + \hat{a}_1^\dagger\hat{a}_2^\dagger). \tag{31}$$

1p

4. Recalling the center of mass formalism in the classical mechanics, we consider following Ansatz: (It is not a unique solution. Scaled values $X_i \to \frac{X_i}{\gamma}$ and $P_i \to \gamma P_i$ also satisfy the commutation relation and diagonalize the Hamiltonian.)

$$\left.\begin{aligned} \hat{X}_1 &= \frac{\hat{x}_1 + \hat{x}_2}{2},\ \hat{P}_1 = \hat{p}_1 + \hat{p}_2, \\ \hat{X}_2 &= \hat{x}_1 - \hat{x}_2,\ \hat{P}_2 = \frac{\hat{p}_1 - \hat{p}_2}{2}. \end{aligned}\right\} \quad 1p \tag{32, 33}$$

which results in $a_1 = b_1 = 1/2$, $c_1 = d_1 = 1$, $a_2 = -b_2 = 1$ and $c_2 = -d_2 = 1/2$.

$$[\hat{X}_i, \hat{X}_j] = [\hat{P}_i, \hat{P}_j] = 0 \; (\because [\hat{x}_i, \hat{x}_j] = [\hat{p}_i, \hat{p}_j] = 0), \tag{34}$$
$$[\hat{X}_1, \hat{P}_1] = \frac{1}{2}[\hat{x}_1 + \hat{x}_2, \hat{p}_1 + \hat{p}_2] = \frac{1}{2}(2i\hbar) = i\hbar, \tag{35}$$
$$[\hat{X}_1, \hat{P}_2] = \frac{1}{4}[\hat{x}_1 + \hat{x}_2, \hat{p}_1 - \hat{p}_2] = \frac{1}{4}[i\hbar - i\hbar] = 0, \tag{36}$$
$$[\hat{X}_2, \hat{P}_1] = [\hat{x}_1 - \hat{x}_2, \hat{p}_1 + \hat{p}_2] = i\hbar - i\hbar = 0, \tag{37}$$
$$[\hat{X}_2, \hat{P}_2] = \frac{1}{2}[\hat{x}_1 - \hat{x}_2, \hat{p}_1 - \hat{p}_2] = \frac{1}{2}[i\hbar + i\hbar] = i\hbar, \tag{38}$$
$$\therefore [\hat{X}_i, \hat{P}_j] = i\hbar\delta_{ij}. \tag{39}$$

$$\begin{aligned}
\hat{H}' &= \frac{\hat{p}_1^2 + \hat{p}_2^2}{2m} + \frac{1}{2}m\omega^2(\hat{x}_1^2 + \hat{x}_2^2) + \gamma\hat{x}_1\hat{x}_2 \\
&= \frac{(\hat{p}_1 + \hat{p}_2)^2 + (\hat{p}_1 - \hat{p}_2^2)^2}{4m} + \frac{1}{2}m\omega^2\frac{(\hat{x}_1 + \hat{x}_2)^2 + (\hat{x}_1 - \hat{x}_2)^2}{2} + \gamma\frac{(\hat{x}_1 + \hat{x}_2)^2 - (\hat{x}_1 - \hat{x}_2)^2}{4} \\
&= \frac{\hat{P}_1^2 + 4\hat{P}_2^2}{4m} + (m\omega^2 + \gamma)\hat{X}_1^2 + \frac{1}{4}(m\omega^2 - \gamma)\hat{X}_2^2 \\
&= \frac{\hat{P}_1^2}{2(2m)} + \frac{\hat{P}_2^2}{2(m/2)} + \frac{1}{2}2m\frac{m\omega^2 + \gamma}{m}\hat{X}_1^2 + \frac{1}{2}\frac{m}{2}\frac{m\omega^2 - \gamma}{m}\hat{X}_2^2
\end{aligned} \tag{40}$$

1P

As a result, $m_1 = 2m$, $m_2 = m/2$, $\omega_1 = \sqrt{\frac{m\omega^2+\gamma}{m}}$ and $\omega_2 = \sqrt{\frac{m\omega^2-\gamma}{m}}$ (m_1 and m_2 can be changed by the scaling: $X_i \to \frac{X_i}{\gamma}$ and $P_i \to \gamma P_i$ but ω_i are unique).

1P If $|\gamma| > m\omega^2$, one of the terms $(m\omega^2 + \gamma)\hat{X}_1^2$ and $\frac{1}{4}(m\omega^2 - \gamma)\hat{X}_2^2$ becomes negative. So the ground state will be state with infinitely large $\langle\hat{X}_1\rangle$ or $\langle\hat{X}_2\rangle$.

5. We can use the results obtained in part 1. Then

$$\alpha_i = \sqrt{\frac{m_i\omega_i}{2\hbar}}, \quad \beta_i = \frac{1}{2\hbar}\sqrt{\frac{2\hbar}{m_i\omega_i}} \tag{41}$$

1P

Additionally, $\hat{A}_i$ and $\hat{A}_i^\dagger$ will satisfy the commutation relations:

$$[\hat{A}_i, \hat{A}_j^\dagger] = \delta_{ij}, \tag{42}$$
$$[\hat{A}_i, \hat{A}_j] = [\hat{A}_i^\dagger, \hat{A}_j^\dagger] = 0 \tag{43}$$

and the new Hamiltonian is given by

$$H' = \hbar\omega_1(\hat{N}_1 + 1/2) + \hbar\omega_2(\hat{N}_2 + 1/2). \tag{44}$$

The energies are given by $E'_{n_1,n_2} = \hbar\omega_1(n_1 + 1/2) + \hbar\omega_2(n_2 + 1/2)$ where $n_1, n_2 \in Z(\geq 0)$.

Aufgabe 2. Doppeltes Dirac-Delta-Potential

Betrachten Sie ein Teilchen der Masse m in einer Dimension im Potential

$$V(x) = -V_0\,\delta(x - L) - V_0\,\delta(x + L), \tag{45}$$

wobei $V_0 > 0$ sowie $L > 0$.

1. **(1 Punkt)** Welche Bedingung muss eine stationäre Wellenfunktion $\psi(x)$ bei $x = \pm L$ erfüllen, wenn sie die zeitunabhängige Schrödinger-Gleichung erfüllt?

2. **(4 Punkte)** Finden Sie alle gebundenen Zustände dieses Potentials. Die gebundenen Zustände müssen nicht normiert werden. Lösen Sie die dabei auftretende transzendente Gleichung grafisch. Wie viele gebundene Zustände gibt es?

3. **(1.5 Punkte)** Bestimmen Sie explizit die Energie des am wenigsten stark gebundenen Zustands zur niedrigsten Ordnung in δ, mit der Annahme, dass

$$\frac{2mV_0}{\hbar^2}L = 1 + \delta \tag{46}$$

mit kleinem δ. (Der am wenigsten stark gebunde Zustand ist der gebundene Zustand mit der höchsten Energie. Die Taylorentwicklung $(1 + \coth s)s \approx 1 + s$ ist dabei hilfreich.)

4. **(1.5 Punkte)** Betrachten Sie eine kleine Störung des Potentials der Form

$$V(x) \to V(x) + v(x), \tag{47}$$

wobei $v(x)$ eine glatte Funktion ist. Schreiben Sie innerhalb des Unterraums aller gebundenen Zustände die Integrale auf, deren Werte die Korrekturen erster und zweiter Ordnung der Energien bestimmen. Für welches $v(x)$ verschwindet die Energiekorrektur erster Ordnung? Und für welches $v(x)$ verschwindet die Energiekorrektur zweiter Ordnung? Welche Symmetrie ist dafür verantwortlich? Berücksichtigen Sie auch hier nur den Unterraum aller gebundenen Zustände.

Lösung 2

1. By integrating the stationary Schrödinger equation

$$\frac{-\hbar^2}{2m}\partial_x^2\psi(x) - V_0\,\delta(x-L)\psi(x) - V_0\,\delta(x+L)\psi(x) = E\psi(x)$$ 0.5

around $x = \pm L$, we obtain

$$\frac{-\hbar^2}{2m}\left[\psi'(-L+\epsilon) - \psi'(-L-\epsilon)\right] = V_0\psi(-L),$$
$$\frac{-\hbar^2}{2m}\left[\psi'(L+\epsilon) - \psi'(L-\epsilon)\right] = V_0\psi(L)$$ 0.5

for infinitesimal $\epsilon > 0$.

2. For $x \neq \pm L$, the solutions of the stationary Schrödinger equation have the form of exponentials:

$$\psi(x) = \begin{cases} Ae^{\kappa(x+L)}, & \text{for } x < -L, \\ B\cosh(\kappa x) + C\sinh(\kappa x), & \text{for } -L < x < L, \\ De^{-\kappa(x-L)}, & \text{for } L < x, \end{cases}$$ 1

where the solutions which exponentially diverge at infinity have been dropped (they aren't localized/bounded). Here

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}.$$

The wavefunction must be continuous at $x = \pm L$. Hence

$$A = B\cosh(\kappa L) - C\sinh(\kappa L),$$
$$D = B\cosh(\kappa L) + C\sinh(\kappa L),$$

The $x = \pm L$ conditions in addition give:

$$(\lambda - \kappa)A = \kappa[B\sinh(\kappa L) - C\cosh(\kappa L)],$$
$$(\lambda - \kappa)D = \kappa[B\sinh(\kappa L) + C\cosh(\kappa L)],$$

where

$$\lambda = \frac{2mV_0}{\hbar^2}.$$

By dividing the two sets of equations

$$\lambda - \kappa = \kappa\frac{B\sinh(\kappa L) - C\cosh(\kappa L)}{B\cosh(\kappa L) - C\sinh(\kappa L)} = \kappa\frac{B\sinh(\kappa L) + C\cosh(\kappa L)}{B\cosh(\kappa L) + C\sinh(\kappa L)}$$

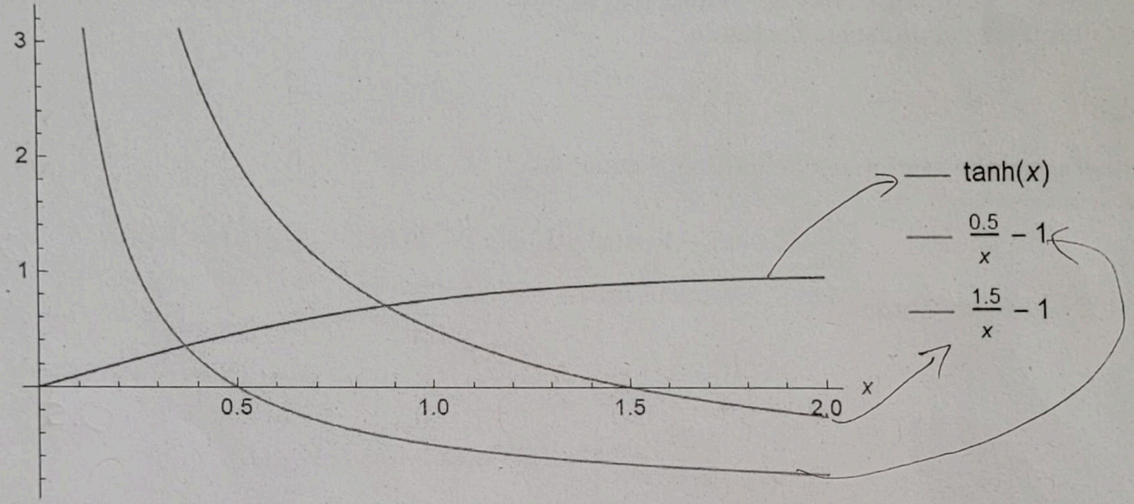
which implies that

$$BC = 0.$$

So either $C = 0$, in which case we have an even solution, or $B = 0$, in which case we have an odd solution. The even-parity solution has $A = B\cosh(\kappa L) = D$ and its energy is found by solving the transcedental equation

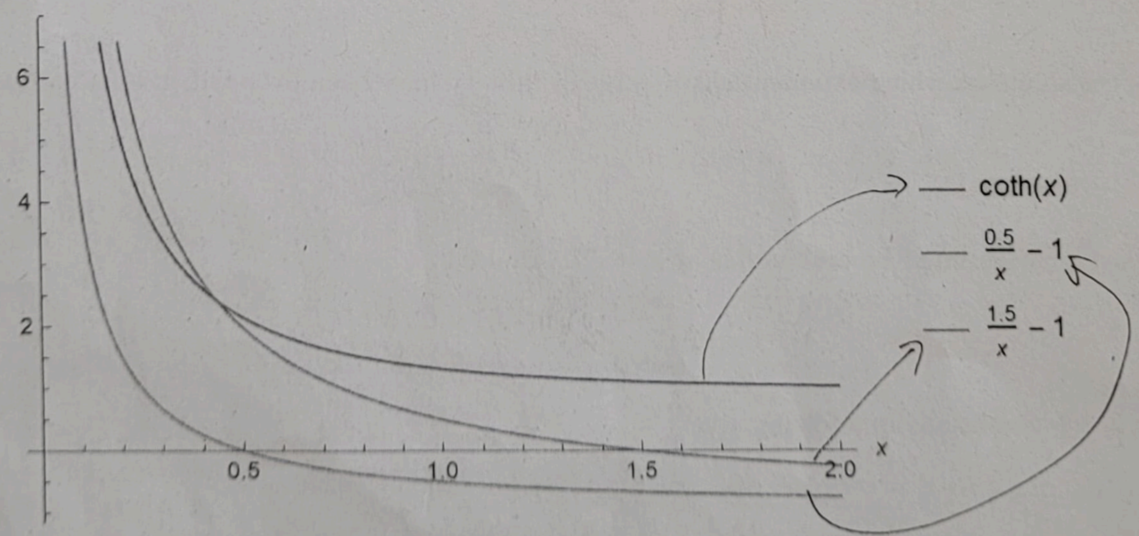
$$\tanh\kappa_+ L = \frac{\lambda L}{\kappa_+ L} - 1 \qquad\qquad \Longrightarrow\ E = -\frac{\hbar^2}{2m}\kappa_+^2.$$

Graphical solution:



The odd-parity solution has $-A = C\sinh(\kappa L) = D$ and its energy is found by solving

$$\coth\kappa_- L = \frac{\lambda L}{\kappa_- L} - 1 \qquad\qquad \Longrightarrow\ E = -\frac{\hbar^2}{2m}\kappa_-^2.$$



By inspection, one sees that there is no odd-parity solution when $\lambda L < 1$. Hence there is only one bound state for $\lambda L < 1$ and two bound states for $\lambda L > 1$. 1

3. The odd-parity solution is always the one that has the highest energy. For small κL, we find that

$$\lambda L = (1 + \coth \kappa_* L)\kappa_* L = 1 + \kappa_* L + \cdots .$$

1

Hence the odd-parity solution has the energy

$$E = -\frac{\hbar^2}{2mL^2}\delta^2 + \mathcal{O}(\delta^3).$$

0.5

4. From the previous parts we know the even and odd eigenstates:

$$\psi_+(x) = \mathcal{N}_+ \begin{cases} \cosh(\kappa_+ L)\mathrm{e}^{\kappa_+(x+L)}, & \text{for } x < -L, \\ \cosh(\kappa_+ x), & \text{for } -L < x < L, , \\ \cosh(\kappa_+ L)\mathrm{e}^{-\kappa_+(x-L)}, & \text{for } L < x, \end{cases}$$

$$\psi_-(x) = \mathcal{N}_+ \begin{cases} -\sinh(\kappa_- L)\mathrm{e}^{\kappa_-(x+L)}, & \text{for } x < -L, \\ \sinh(\kappa_- x), & \text{for } -L < x < L, . \\ \sinh(\kappa_- L)\mathrm{e}^{-\kappa_-(x-L)}, & \text{for } L < x. \end{cases}$$

Non-degenerate perturbation theory performed within the subspace of bound states tells us that

$$E_\pm = E_\pm^{(0)} + \mathcal{I}_\pm \pm \frac{|\mathcal{J}|^2}{E_+^{(0)} - E_-^{(0)}} + \cdots \quad . \tag{48}$$

0.5

where

$$\mathcal{I}_\pm = \int \mathrm{d}x \, |\psi_\pm(x)|^2 \, v(x), \tag{49}$$

0.5

$$\mathcal{J} = \int \mathrm{d}x \, \psi_+^*(x)\psi_-(x)v(x). \tag{50}$$

The second-order correction vanishes when $\mathcal{J} = 0$. Since $\psi_+^*(x)\psi_-(x) = -\psi_+^*(-x)\psi_-(-x)$ is an odd function overall, the only way to guarantee that $\mathcal{J} = 0$ generically holds (without fine-tuning) is to make $v(x) = +v(-x)$ and even function. Hence even $v(x)$ yield vanishing second-order corrections. The explanation for this is parity: the initial $V(x)$ respect parity so if $v(x)$ is even as well, then there cannot be mixing between even and odd eigenstates.

0.5

Aufgabe 3. Spin-Triplett-Zustand mit Störung

Betrachten Sie zwei lokalisierte Spin-$\frac{1}{2}$ Teilchen mit den Spinoperatoren des ersten und zweiten Teilchens $\hat{\boldsymbol{S}}_1 = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}} \otimes \mathbb{1}$ bzw. $\hat{\boldsymbol{S}}_2 = \frac{\hbar}{2}\mathbb{1} \otimes \hat{\boldsymbol{\sigma}}$, wobei $\hat{\boldsymbol{\sigma}} = (\sigma_x, \sigma_y, \sigma_z)$ die Pauli-Matrizen sind, wobei

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{51}$$

$\mathbb{1}$ ist die 2×2-Einheitsmatrix. Die Operatoren $\hat{\boldsymbol{S}}_1$ und $\hat{\boldsymbol{S}}_2$ wirken in der Basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ des gesamten Hilbert-Raums.

1. **(1.5 Punkte)** Schreiben Sie die Matrizen für $\hat{S}_{1,x}$ und $\hat{S}_{2,y}$ in der Basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$ auf.
2. **(3 Punkte)** Führen Sie $\hat{\boldsymbol{\Sigma}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$ ein. Berechnen Sie $[\hat{\Sigma}_i, \hat{\Sigma}_j]$ und finden Sie die Matrizen für $\hat{\boldsymbol{\Sigma}}^2$ und $\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2$.

Betrachten wir nun den folgenden Spin-Hamiltonoperator:

$$H = J\hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 \qquad (J > 0). \tag{52}$$

3. (**1 Punkt**) Finden Sie mithilfe der Ergebnisse aus Teil 2 die Eigenzustände und Eigenwerte des Hamiltonoperators H. (Tipp: Verwenden Sie die Eigenwerte des gesamten $\hat{\Sigma}^z = \hat{S}_1^z + \hat{S}_2^z$.)
4. (**1 Punkt**) Bestimmen Sie den Dichteoperator $\hat{\rho} = |\Psi\rangle\langle\Psi|$, wobei $|\Psi\rangle$ der Grundzustand ist.
5. (**1.5 Punkte**) Bestimmen Sie die reduzierte Dichtematrix $\hat{\rho}_1 = \mathrm{tr}_2(\hat{\rho})$ und ihre Eigenwerte. Bestimmen Sie mithilfe dieser Eigenwerte ($\{\lambda_i\}$) die Verschränkungsentropie des Grundzustands.

$$S = -\sum_i \lambda_i \log \lambda_i. \tag{53}$$

Lösung 3

1. They are

$$\hat{S}_{1,x} = \frac{\hbar}{2}\begin{pmatrix} & & 1 & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{pmatrix}, \qquad \hat{S}_{2,y} = \frac{\hbar}{2}\begin{pmatrix} & -\mathrm{i} & & \\ \mathrm{i} & & & \\ & & & -\mathrm{i} \\ & & \mathrm{i} & \end{pmatrix}.$$

2. We have:

$$\begin{aligned}[\hat{\Sigma}_i, \hat{\Sigma}_j] &= [\hat{S}_{1,i} + \hat{S}_{2,i}, \hat{S}_{1,j} + \hat{S}_{2,j}] = [\hat{S}_{1,i}, \hat{S}_{1,j}] + [\hat{S}_{2,i}, \hat{S}_{2,j}] \\ &= \mathrm{i}\hbar \sum_k (\hat{S}_{1,k} + \hat{S}_{2,k}) = \mathrm{i}\hbar \sum_k \hat{\Sigma}_k.\end{aligned}$$

Moreover

$$\begin{aligned}\hat{\boldsymbol{\Sigma}}^2 &= (\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 = \hat{\boldsymbol{S}}_1^2 + \hat{\boldsymbol{S}}_2^2 + \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 + \hat{\boldsymbol{S}}_2 \cdot \hat{\boldsymbol{S}}_1 \\ &= \frac{\hbar^2}{4}\sum_i \sigma_i^2 \otimes \mathbb{1} + \frac{\hbar^2}{4}\sum_i \sigma_i^2 \otimes \mathbb{1} + 2\frac{\hbar^2}{4}\sum_i \sigma_i \otimes \sigma_i \\ &= \frac{3\hbar^2}{2}\mathbb{1} \otimes \mathbb{1} + \frac{\hbar^2}{2}\sum_i \sigma_i \otimes \sigma_i, \\ \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 &= \frac{\hbar^2}{4}\sum_i \sigma_i \otimes \sigma_i.\end{aligned}$$

where

$$\sum_i \sigma_i \otimes \sigma_i = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Hence

$$\hat{\mathbf{\Sigma}}^2 = \hbar^2 \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix},$$

$$\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 = \frac{\hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

3. Since

$$\hat{S}_z = \hbar \begin{pmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{pmatrix},$$

the singlet state is

$$|s=0, m=0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} = \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}},$$

and the triplet states are

$$|s=1, m=1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = |\uparrow\uparrow\rangle\,,$$

$$|s=1, m=0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}},$$

$$|s=1, m=-1\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = |\downarrow\downarrow\rangle\,.$$

By applying H Eq. (52) to the above singlet and triplet states, you can easily find that they are eigenstates of the Hamiltonian with eigenvalues: $-J\frac{3\hbar^2}{4}$ for the singlet state and $\frac{J\hbar^2}{4}$ for the triplet states.

4. The ground state is the singlet state and its density operator is given by

$$\begin{aligned} \hat{\rho} &= \frac{1}{2}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)(\langle\uparrow\downarrow| - \langle\downarrow\uparrow|) \\ &= \frac{1}{2}(|\uparrow\rangle\langle\uparrow| \otimes |\downarrow\rangle\langle\downarrow| - |\uparrow\rangle\langle\downarrow| \otimes |\downarrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\uparrow| \otimes |\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\downarrow| \otimes |\uparrow\rangle\langle\uparrow|) \end{aligned} \tag{54}$$

5. The reduece density operator is given by

$$\begin{aligned} \hat{\rho}_1 = Tr_2(\hat{\rho}) &= \sum_{\sigma} \langle\sigma|_2 \hat{\rho} |\sigma\rangle_2 \\ &= \frac{1}{2}(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) \end{aligned} \tag{55}$$

Eigenvalues of $\hat{\rho}_1$ are $\frac{1}{2}$. As a result,

$$S = \ln 2. \tag{56}$$