Quantentheorie II, 3. Übung, 9.11.2012

5) <u>Streuung an einem quaderförmigen Nanopartikel</u>

$$\vec{k} = (0,0,k)$$

$$V(x,y,z) = \begin{cases} V_0 > 0 & \text{wenn } |x| < L, |y| < L \text{ und } |z| < 2L \\ 0 & \text{sonst} \end{cases}$$

a) $$\vec{q} = \vec{k} - \vec{k}' = \begin{pmatrix} 0 \\ 0 \\ k \end{pmatrix} - \begin{pmatrix} k_x' \\ k_y' \\ k_z' \end{pmatrix} = \begin{pmatrix} -k_x' \\ -k_y' \\ k - k_z' \end{pmatrix}$$

mit
$$k_x' = k \cos\varphi \sin\theta$$
$$k_y' = k \sin\varphi \sin\theta$$
$$k_z' = k \cos\theta$$

$$\frac{d\sigma}{d\Omega} = |f(\theta,\varphi)|^2 \qquad f(\theta,\varphi) = -\frac{4m\pi^2}{\hbar^2} \langle \vec{k}' | V | \vec{k} \rangle$$

$$\langle \vec{k}' | V | \vec{k} \rangle = \frac{1}{(2\pi)^3} \int d^3r \, e^{i\vec{q}\cdot\vec{r}} V(\vec{r}) =$$

$$= \frac{1}{(2\pi)^3} \int_{-L}^{+L} dx \int_{-L}^{+L} dy \int_{-2L}^{+2L} dz \, e^{i(q_x \cdot x + q_y \cdot y + q_z \cdot z)} V(x,y,z) =$$

$$= \frac{V_0}{(2\pi)^3} \int_{-L}^{+L} dx \int_{-L}^{+L} dy \, e^{i(q_x \cdot x + q_y \cdot y)} \left[\frac{e^{iq_z \cdot z}}{iq_z} \right]_{-2L}^{+2L} =$$

$$= \frac{V_0}{(2\pi)^3} \int_{-L}^{L} dx \int_{-L}^{L} dy \, e^{i(q_x \cdot x + q_y \cdot y)} \frac{2\sin(2q_z L)}{q_z} =$$

$$= \frac{V_0}{(2\pi)^3} \cdot 2\frac{\sin(q_x L)}{q_x} \cdot 2\frac{\sin(q_y L)}{q_y} \cdot 2\frac{\sin(2q_z L)}{q_z}$$

$$f(\theta,\varphi) = -\frac{4m\cancel{\pi^2}}{\hbar^2} \cdot \frac{V_0}{\cancel{(2\pi)^3}} \cdot \cancel{2^3} \cdot L^3 \cdot 2 \, \frac{\sin(q_x L)}{q_x L} \cdot \frac{\sin(q_y L)}{q_y L} \cdot \frac{\sin(2q_z L)}{2q_z L}$$

b) $kL \ll 1$ mit $\lim\limits_{x\to 0} \frac{\sin x}{x} = \lim\limits_{x \to 0} \frac{\cos x}{1} = 1$ ergibt sich:

$$f(\theta,\varphi) = -\frac{8mV_0L^3}{\pi\hbar^2} \qquad \frac{d\sigma}{d\Omega} = \frac{64m^2V_0^2L^6}{\pi^2\hbar^4}$$

$$\sigma_{tot} = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi \cdot \frac{64m^2V_0^2L^6}{\pi^2\hbar^4}$$

6) Dichtematrix und reduzierte Dichtematrix

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 + i\,|\downarrow\rangle_1\right)$$

$$|\psi_2\rangle = \alpha\,|\uparrow\rangle_2 + \beta\,|\downarrow\rangle_2 \quad \text{mit} \quad |\alpha|^2 + |\beta|^2 = 1$$

$$H = \hbar g\left(|\uparrow\rangle_1\,{}_1\langle\uparrow| - |\downarrow\rangle_1\,{}_1\langle\downarrow|\right)\left(|\uparrow\rangle_2\,{}_2\langle\uparrow| - |\downarrow\rangle_2\,{}_2\langle\downarrow|\right)$$

a) $$|\psi(t=0)\rangle = |\psi_1\rangle\,|\psi_2\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 + i\,|\downarrow\rangle_1\right)\left(\alpha\,|\uparrow\rangle_2 + \beta\,|\downarrow\rangle_2\right) =$$

$$= \frac{1}{\sqrt{2}}\left(\alpha\,|\uparrow\rangle_1|\uparrow\rangle_2 + \beta\,|\uparrow\rangle_1|\downarrow\rangle_2 + i\alpha\,|\downarrow\rangle_1|\uparrow\rangle_2 + i\beta\,|\downarrow\rangle_1|\downarrow\rangle_2\right)$$

$$H\,|\uparrow\rangle_1|\uparrow\rangle_2 = \hbar g\,|\uparrow\rangle_1|\uparrow\rangle_2$$

$$H\,|\uparrow\rangle_1|\downarrow\rangle_2 = -\hbar g\,|\uparrow\rangle_1|\downarrow\rangle_2$$

$$H\,|\downarrow\rangle_1|\uparrow\rangle_2 = -\hbar g\,|\downarrow\rangle_1|\uparrow\rangle_2$$

$$H\,|\downarrow\rangle_1|\downarrow\rangle_2 = \hbar g\,|\downarrow\rangle_1|\downarrow\rangle_2$$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar}Ht}\,|\psi(t=0)\rangle$$

$$= \frac{1}{\sqrt{2}}\Big(\alpha\,e^{-igt}|\uparrow\rangle_1|\uparrow\rangle_2 + \beta\,e^{igt}|\uparrow\rangle_1|\downarrow\rangle_2 + i\alpha\,e^{igt}|\downarrow\rangle_1|\uparrow\rangle^2 + i\beta\,e^{-igt}|\downarrow\rangle_1|\downarrow\rangle_2\Big)$$

b) $$\rho = |\psi\rangle\langle\psi| = \sum_{\substack{m,n\\ m',n'}} \alpha_{mn}\,\alpha^*_{m'n'}\,|n\rangle_1\,|m\rangle_2\,{}_2\langle m|\,{}_1\langle n|$$

$$|\psi\rangle = \sum_{m,n} \alpha_{mn}\,|n\rangle_1|m\rangle_2$$

$$\begin{array}{cccc}
|\uparrow\rangle_1|\uparrow\rangle_2 & |\uparrow\rangle_1|\downarrow\rangle_2 & |\downarrow\rangle_1|\uparrow\rangle_2 & |\downarrow\rangle_1|\downarrow\rangle_2
\end{array}$$

$$\rho(t) = \frac{1}{2}\begin{pmatrix}
|\alpha|^2 & \alpha\beta^* e^{-2igt} & -i|\alpha|^2 e^{-2igt} & -i\alpha\beta^* \\
\alpha^*\beta\, e^{2igt} & |\beta|^2 & -i\alpha^*\beta & -i|\beta|^2 e^{2igt} \\
i|\alpha|^2 e^{2igt} & i\alpha\beta^* & |\alpha|^2 & \alpha\beta^* e^{2igt} \\
i\alpha^*\beta & i|\beta|^2 e^{-2igt} & \alpha^*\beta\, e^{-2igt} & |\beta|^2
\end{pmatrix}$$

$$\mathrm{Tr}(\rho) = \frac{1}{2}\Big(\underbrace{|\alpha|^2 + |\beta|^2}_{1} + \underbrace{|\alpha|^2 + |\beta|^2}_{1}\Big) = 1 \quad \checkmark$$

6) b)

$$\rho(t=0) = \begin{pmatrix} |\alpha|^2 & \alpha\beta^* & -i|\alpha|^2 & -i\alpha\beta^* \\ \alpha^*\beta & |\beta|^2 & -i\alpha^*\beta & -i|\beta|^2 \\ i|\alpha|^2 & i\alpha\beta^* & |\alpha|^2 & \alpha\beta^* \\ i\alpha^*\beta & i|\beta|^2 & \alpha^*\beta & |\beta|^2 \end{pmatrix}$$

c) $\rho_1 = \sum_{m,n,n'} \alpha_{mn}\alpha^*_{mn'} \, |n\rangle_1 \, {}_1\langle n|$

$$\rho_1(t) = \frac{1}{2} \begin{array}{c} \begin{array}{cc} |\uparrow\rangle_1 & \qquad\qquad\qquad |\downarrow\rangle_1 \end{array} \\ \begin{pmatrix} 1 & -i\left(|\alpha|^2 e^{-2igt} + |\beta|^2 e^{2igt}\right) \\ i\left(|\alpha|^2 e^{2igt} + |\beta|^2 e^{-2igt}\right) & 1 \end{pmatrix} \end{array}$$

$$\rho_1(t=0) = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \qquad \mathrm{Tr}(\rho_1) = 1 \ \checkmark$$

d) reiner Zustand: $\mathrm{Tr}(\rho^2) = 1$

gemischter Zustand: $\mathrm{Tr}(\rho^2) < 1$

$$\rho^2 = \frac{1}{2}\begin{pmatrix} |\alpha|^4 + |\alpha|^2|\beta|^2 & \cdot & \cdot & \cdot \\ \cdot & |\beta|^4 + |\alpha|^2|\beta|^2 & \cdot & \cdot \\ \cdot & \cdot & |\alpha|^4 + |\alpha|^2|\beta|^2 & \cdot \\ \cdot & \cdot & \cdot & |\beta|^4 + |\alpha|^2|\beta|^2 \end{pmatrix}$$

$$\mathrm{Tr}(\rho^2) = |\alpha|^4 + 2|\alpha|^2|\beta|^2 + |\beta|^4 = \left(|\alpha|^2 + |\beta|^2\right)^2 = 1^2 = 1$$

$\Rightarrow$ Das Gesamtsystem ist zu jeder Zeit t in einem reinen Zustand.

$$\rho_1^2(t) = \frac{1}{4}\begin{pmatrix} 1 + \underbrace{\left(|\alpha|^2 e^{-2igt} + |\beta|^2 e^{2igt}\right)\left(|\alpha|^2 e^{2igt} + |\beta|^2 e^{-2igt}\right)}_{\gamma} & \shortparallel \\ \shortparallel & 1+\gamma \end{pmatrix}$$

$$\mathrm{Tr}\left(\rho_1^2(t)\right) = \frac{1}{4}\, 2\cdot\left(1 + \left(|\alpha|^2 e^{-2igt} + |\beta|^2 e^{2igt}\right)\left(|\alpha|^2 e^{2igt} + |\beta|^2 e^{-2igt}\right)\right) =$$

$$= \frac{1}{2}\left(1 + |\alpha|^4 + |\beta|^4 + |\alpha|^2|\beta|^2 \underbrace{\left(e^{4igt} + e^{-4igt}\right)}_{2\cos(4gt)}\right) = \Rightarrow$$

$$\mathrm{Tr}\left(\rho_1^2(t)\right) = \frac{1}{2}\left(1 + |\alpha|^4 + |\beta|^4 + 2|\alpha|^2|\beta|^2\cos 4gt\right) \leqslant$$

$$\leqslant \frac{1}{2}\left(1 + \big(\underbrace{|\alpha|^2+|\beta|^2}_{1}\big)^2\right) = \frac{1}{2}(1+1) = 1$$

also $\mathrm{Tr}\left(\rho_1^2(t)\right) \leqslant 1$

Gleichheit genau dann, wenn $\cos 4gt = 1$, also $t=0$ oder $t = n\cdot\frac{\pi}{2g}$ mit $n \in \mathbb{N}$.

Wir haben also für $t=0$ oder $t = n\cdot\frac{\pi}{2g}$ einen reinen Zustand, für alle anderen Zeiten einen gemischten.

e) $$\bar{\rho}_1 = \lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, \rho_1(t)$$

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt\, {}_1\langle\uparrow|\rho_1(t)|\downarrow\rangle_1 = \lim_{T\to\infty} \frac{(-i)}{T}\int_0^T dt\left(|\alpha|^2 e^{-2igt} + |\beta|^2 e^{2igt}\right) =$$

$$= \lim_{T\to\infty} \frac{(-i)}{T}\left[-|\alpha|^2 e^{-2igt} + |\beta|^2 e^{2igt}\right]_0^T =$$

$$= \lim_{T\to\infty} \frac{1}{T}\,\frac{|\alpha|^2 e^{-2igT} - |\beta|^2 e^{2igT} - |\alpha|^2 + |\beta|^2}{2g} =$$

$$= \lim_{T\to\infty} \frac{1}{T}\,\frac{|\alpha|^2(\cos 2gT - i\sin 2gT) - |\beta|^2(\cos 2gT + i\sin 2gT) - |\alpha|^2 + |\beta|^2}{2g}$$

$$= 0$$

$$\bar{\rho}_1 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$