Quantentheorie II Übung 12

Besprechung: 2021WE28 (KW28)

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1. **Questions**

   (a) Give one or two simple arguments why the scattering amplitude is complex (as expressed by the order-l contribution of the form $e^{i\delta_l}\sin\delta_l$).

   (b) What is the ground state wave function of an electron in hydrogen atom?

   (c) What is the validity criterion for Born approximation?

2. **Scattering on central potential:** consider elastic scattering on a central potential

$$V(r) = \frac{c}{r^2}, \quad c > 0, \tag{1}$$

   where $2mc \ll 1$, and determine the scattering phases $\delta_l(k)$ and the scattering amplitude $f(\theta)$.

   (Hint1) By using the definition $\lambda(\lambda+1) \equiv l(l+1) + 2mc$, we can assume that the radial function $R_l(r)$ approximates to

$$R_l(kr) \to j_\lambda(kr). \tag{2}$$

   $R_l(kr)$ and $j_\lambda(kr)$ behave asymptotically as

$$R_l(kr) \to \frac{1}{kr}\sin\left(kr - \frac{l\pi}{2} + \delta_l\right)e^{i\delta_l}, \tag{3}$$

$$j_\lambda(kr) \to \frac{1}{kr}\sin\left(kr - \frac{\lambda\pi}{2}\right), \tag{4}$$

   when $kr \gg l$.
   (Hint 2) Use the formula

$$\sum_{l=0}^{\infty} P_l(\cos\theta) = \frac{1}{2\sin(\theta/2)}. \tag{5}$$

3. **Electron scattering on hydrogen atom (Born approximation):** we investigate scattering of electrons on neutral hydrogen atoms. We assume that each electron is scattered exactly on one hydrogen atom. The hydrogen atoms are in the ground state.

   (a) Formulate the scattering potential, and verify that it is a central potential.

   (b) Compute the scattering amplitude $f^{(1)}(\theta)$ in the first-order Born approximation and the differential cross section $\frac{d\sigma^{(1)}}{d\theta}$.

   (c) Compute the total cross section $\sigma^{(1)}$.

   (d) What is the condition for the validity of the Born approximation? Discuss it when $ka_B \ll 1$ and $ka_B \gg 1$ respectively.

1. **Questions**

(a) Give one or two simple arguments why the scattering amplitude is complex (as expressed by the order-l contribution of the form $e^{i\delta_l}\sin\delta_l$).

(b) What is the ground state wave function of an electron in hydrogen atom?

(c) What is the validity criterion for Born approximation?

a) $f = \sum_l \frac{2l+1}{k} e^{i\delta_l} \sin(\delta_l) \, P_l(\cos\theta)$

I $\quad \Psi = \Phi + f \frac{e^{ikr}}{r}$ $\quad$ Warum nicht?

II $\quad \sigma_{tot} = \frac{4\pi}{k} \operatorname{Im} f(0)$

III $\quad \delta_l \in \mathbb{R} \leftarrow V \in \mathbb{R}$

$H = H_0 + V$ $\quad H = H^{+} \rightsquigarrow e^{iHt}$

• elastisch

c)

The Born approximation is valid when $\underbrace{|\psi^{(1)}(\vec{r})|}_{V^{(1)}} \ll \underbrace{|\phi_k(\vec{r})|}_{V^{(0)}} = 1$, or equivalently (Ü11)

I
$$\frac{m}{2\pi}\left|\int d^3r' V(r') \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} e^{ikz'}\right| \ll 1 \quad \xrightarrow{r\to 0} \quad \left|\int_0^\infty dr V(r)(e^{2ikr}-1)\right| \ll \frac{k}{m},$$

II $\quad$ optisches Theorem $\rightsquigarrow$ Abschätzung Imaginärteil

III $\quad$ Unitaritätsschranke

$\sigma_l \leq \frac{4\pi}{k^2}(2l+1)$

2. **Scattering on central potential:** consider elastic scattering on a central potential

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where $2mc \ll 1$, and determine the scattering phases $\delta_l(k)$ and the scattering amplitude $f(\theta)$.

$$\lambda = -\frac{1}{2} \cancel{\pm} \sqrt{\underbrace{\frac{1}{4} + \ell(\ell+1)}_{(\ell+\frac{1}{2})^2} + 2mc}$$

$$\sqrt{b+x} \approx \sqrt{b} + \frac{x}{2}\frac{1}{\sqrt{b}} \qquad x=0$$

$$\lambda \hat{=} -\frac{1}{2} + (\ell+\tfrac{1}{2}) + \frac{mc}{\ell+1/2} = \ell + \frac{mc}{\ell+1/2}$$

$$\delta_\ell = \frac{\pi}{2}\left(-\frac{mc}{\ell+1/2}\right) = \frac{\pi}{2}(\ell-\lambda)$$

$$\sum_\ell P_\ell(\cos\theta) = \frac{1}{2\sin\theta/2}$$

$\ll 1$ da $2mc \ll 1$

$$f(\theta) = \sum_\ell \frac{2\ell+1}{k} \underbrace{e^{i\delta_\ell}\sin(\delta_\ell)}_{\approx\delta_\ell} P_\ell(\cos\theta)$$

$$= -\frac{\pi mc}{2k}\frac{1}{\sin\theta/2}$$

- $$\psi(r) = \sum_\ell R_\ell(r)\, \underline{P_\ell(\cos\theta)}, \qquad R_\ell(r) = \frac{u_\ell(r)}{r}$$

zentral $m=0$

$$\psi_{\ell m} \sim R(r)\, \underline{Y_{\ell m}(\theta,\varphi)}$$

$$Y_{\ell 0} \sim P_\ell(\cos\theta)$$

Schrödingergl. $(k^2+\Delta)\psi_\ell = 0$

$$\psi_\ell = R_\ell(r)\, Y_{\ell m}(\theta,\varphi)$$

Besselfunktion (1. Art) $j_\ell(x)$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial f}{\partial r}\right)=\underbrace{\frac{\partial^2 f}{\partial r^2}+\frac{2}{r}\frac{\partial f}{\partial r}=\frac{1}{r}\frac{\partial^2}{\partial r^2}\left(rf(r)\right)}_{\text{I}}$$

I $\quad \left(\frac{1}{x}\,\partial_x^2\, x\right) j_\ell(x) + \left[1-\frac{\ell(\ell+1)}{x^2}\right] j_\ell(x) = 0$

II $\quad \left(\partial_x^2 + \frac{2}{x}\,\partial_x\right) j_\ell(x) + \left[1-\frac{\ell(\ell+1)}{x^2}\right] j_\ell(x) = 0$

$x \gg 1: \qquad j_\ell(x) \hat{=} \dfrac{\sin\left(x-\frac{\pi}{2}\ell\right)}{x}$

Übergang $x = kr$

$\partial_x = \partial_r k^2$

$$\frac{1}{k^2}\left(\frac{1}{kr}\,\partial_r^2\, kr\right) j_\ell(kr) + \left[1-\frac{\ell(\ell+1)}{k^2r^2}\right] j_\ell(kr) = 0$$

$$\left(\frac{1}{r}\,\partial_r^2\, r\right) j_\ell(kr) + \left[k^2-\frac{\ell(\ell+1)}{r^2}\right] j_\ell(kr) = 0$$

$$-\frac{\hbar^2}{2m}u_l''(r)+\frac{\hbar^2 l(l+1)}{2mr^2}u_l(r)+V(r)\,u_l(r) = E\,u_l(r)$$
$$\Rightarrow\quad u_l''(r)+\left[k^2-v_{\text{eff}}(r)\right]u_l(r) = 0$$

$$k^2 := \frac{2mE}{\hbar^2},$$
$$v_{\text{eff}}(r) \equiv \frac{2m}{\hbar^2}V_{\text{eff}}(r) := \frac{2m}{\hbar^2}V(r)+\frac{l(l+1)}{r^2}.$$

TimmSkript

$\rightarrow u_\ell(r) = R_\ell(r)\cdot r$

$u' = r\cdot R' + R$

$u'' = r\cdot R'' + R' + R'$

$= r\cdot R'' + 2R'$

$r\cdot R'' + 2R' + \left[k^2 - v_{\text{eff}}\right] R\cdot r = 0$

$R'' + \frac{2}{r}R' + \left[k^2 - v_{\text{eff}}\right] R = 0$

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(a) Formulate the scattering potential, and verify that it is a central potential.

(b) Compute the scattering amplitude $f^{(1)}(\theta)$ in the first-order Born approximation and the differential cross section $\frac{d\sigma^{(1)}}{d\theta}$.

(c) Compute the total cross section $\sigma^{(1)}$.

(d) What is the condition for the validity of the Born approximation? Discuss it when $ka_B \ll 1$ and $ka_B \gg 1$ respectively.

$$\alpha = \frac{e^2}{4\pi\varepsilon_0}$$

$\varepsilon_0 = 1$

b) $$V(r) = -\alpha e^{-2r/a}\left(\frac{1}{a} + \frac{1}{r}\right)$$

$$\tilde{V}(q) = \int d^3x \, e^{-i\vec{q}\vec{x}} \, V(\vec{x})$$

Zentralp. $\omega \neq 0$

$$\tilde{V}(q) = \frac{4\pi}{q}\int dr \left[V(r)\, r \sin(qr)\right]$$

$$= -\frac{4\pi}{q}\alpha\left[\frac{1}{a}\int dr \frac{1}{2i}\left(e^{-(2/a - iq)r} - c.c.\right)r + \int \frac{1}{2i} dr \left(e^{-(2/a - iq)r} - c.c.\right)\right]$$

$$\int_0^\infty x e^{ax} = \frac{1}{a^2}$$

$$= -\frac{4\pi}{q}\alpha\frac{1}{2i}\left(\frac{1}{a}\frac{8ia^3q}{(4+a^2q^2)^2} + \frac{2ia^2q}{4+a^2q^2}\right)$$

$$\hat{V}(q) = -\frac{4\pi}{\cancel{q}}\alpha\frac{1}{\cancel{2i}}\frac{\cancel{2i}a^2\cancel{q}(8+a^2q^2)}{(4+a^2q^2)^2}$$

$$f = -\frac{m}{2\pi}\hat{V}(q) = \frac{2a(8+a^2q^2)}{(4+a^2q^2)^2}$$

$$a_B = \frac{1}{\alpha m}$$

c) $\sigma^{(1)} = \int d\Omega \, |f(\Theta)|^2 = 2\pi \int d\cos\Theta \, |f(\Theta)|^2$

$$q^2 = 4k^2 \sin\theta/2 = 2k^2 (1-\cos\Theta)$$

$$dq^2 = -2k^2 \, d\cos\Theta$$

$$\hookrightarrow \int_{-1}^{1} d\cos\Theta \ldots = -\int_{4k^2}^{0} \frac{dq^2}{2k^2} \ldots = \int_0^{4k^2} \frac{dq^2}{2k^2} \ldots$$

$$\sigma = \frac{2\pi}{k} \int_0^{4k^2} dq^2 \left(\frac{2a\,(8+q^2a^2)}{(4+q^2a^2)^2} \right)^2$$

$x = q^2a^2$
$$= \frac{\pi}{k^2} \, 4 \int_0^{4k^2a^2} dx \, \underbrace{\left(\frac{8+x}{(4+x)^2}\right)^2}_{I}$$

Partialbruchzer.

$$I = \frac{A}{4+x} + \frac{B}{(4+x)^2} + \frac{C}{(4+x)^3} + \frac{D}{(4+x)^4}$$

$A=0 \quad B=1 \quad C=8 \quad D=16$

$$\sigma = \underbrace{\pi a^2}_{\text{geometr. Fläche}} \frac{12+18k^2a^2+\boxed{7k^4a^4}}{3\boxed{(1+k^2a^2)^3}}$$

d) $\beta = ka$

1. $\beta \ll 1 \qquad \sigma \simeq 4\pi a^2$ (s-Wellenstr.)

2. $\beta \gg 1 \qquad \sigma \simeq \pi a^2 \frac{7}{3} \frac{1}{k^2a^2} = \frac{7}{3}\frac{\pi}{k^2}$

$$\sigma_\ell \leq \frac{4\pi}{k}(2\ell+1) \qquad \frac{7}{3} < 4$$

$\ell = 0$

Nr 2) $V = \frac{c}{r^2}$ $\quad \psi = \sum R_\ell P_\ell(\cos\theta)$

$$(-2m\Delta + q^2)\,\psi = \Sigma\,\psi \qquad R_\ell = \frac{u_\ell}{r}$$

$$(\partial_r^2 + q^2)\,u_\ell = V_{eff}\,u_\ell(r) \qquad V_{eff} = V(r) + \frac{\ell(\ell+1)}{r^2} = \frac{1}{r^2}\left(2mc + \ell(\ell+1)\right)$$

$$\Delta f = \frac{1}{\rho}\frac{\partial f}{\partial \rho} + \frac{\partial f}{\partial \rho^2} - \frac{c^2}{r^2}$$

$$\left[\frac{\partial}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + q^2 - \frac{1}{r^2}\left(\ell(\ell+1) + 2mc\right)\right] R_\ell(q\cdot r) = 0 \qquad \text{Teu geteilt}$$

$$\lambda(\lambda+1) = \ell(\ell+1) + 2mc$$

$$\rho = q\cdot r$$

$$\left[\frac{\partial}{\partial \rho^2} + \frac{2}{\rho}\frac{\partial}{\partial \rho} + 1 - \frac{\lambda(\lambda+1)}{\rho^2}\right] R_\ell(\rho) = 0$$

$$R_\ell(\rho) \to j_\lambda(\rho)$$

$$R_\ell(\rho) \to \frac{1}{\rho}\sin\left(\rho - \frac{\ell\pi}{2} + \delta_\ell\right)\underbrace{e^{i\delta_\ell}}_{\approx 1} \to \frac{1}{\rho}\sin\left(\rho - \frac{\lambda\pi}{2}\right)$$

$$\frac{1}{\rho}\sin\left(\rho - \frac{\ell\pi}{2} + \delta_\ell\right) = \frac{1}{\rho}\sin\left(\rho - \frac{\lambda\pi}{2}\right)$$

$$\rho - \frac{\ell\pi}{2} + \delta_\ell = \rho - \frac{\lambda\pi}{2}$$

$$\delta_\ell = \frac{\pi}{2}(\ell - \lambda)$$

$$\lambda^2 + \lambda = \ell^2 + \ell + 2mc$$

$$\lambda = -\frac{1}{2} \pm \sqrt{\frac{1}{4} + \ell^2 + \ell + 2mc}$$

Neselfunktion Positiv

$$\left(\ell + \frac{1}{2}\right)^2$$

$$\sqrt{a+x} \approx \sqrt{a} + \frac{x}{2}\frac{1}{\sqrt{a}} \qquad \lambda = -\frac{1}{2} + \left(\ell + \frac{1}{2}\right) + \frac{mc}{\ell + \frac{1}{2}} = \ell + \frac{mc}{\ell + \frac{1}{2}}$$

$$\downarrow$$

$$x = 0$$

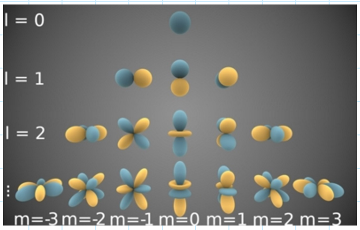
$$\delta_\ell = \frac{\pi}{2}\left(-\frac{2mc}{\ell+\frac{1}{2}}\right)$$

$\ll 1$ da $2mc \ll 1$

$$f(\vartheta) = \sum \frac{2\ell+1}{k}\underbrace{e^{i\delta_\ell}\sin(\delta_\ell)}_{\sin(x)\approx x} P_\ell(\cos\vartheta) = -\frac{i\pi m c}{2k}\,\frac{1}{\sin\left(\frac{\vartheta}{2}\right)}$$

$$\sum_\ell P_\ell \cos\vartheta = \frac{1}{2\sin\frac{\vartheta}{2}}$$

Nr 3) $\psi_{n\ell m}$: Tabellen



$l = 0$:	$Y_{00}(\vartheta,\varphi)$	$\equiv \frac{1}{\sqrt{4\pi}}$,	(5.108)
$l = 1$:	$Y_{10}(\vartheta,\varphi)$	$= \sqrt{\frac{3}{4\pi}}\cos\vartheta$,	(5.109)
	$Y_{1\pm1}(\vartheta,\varphi)$	$= \mp\sqrt{\frac{3}{8\pi}}\sin\vartheta\, e^{\pm i\varphi}$,	(5.110)

$$V_e = \frac{e^2}{4\pi\varepsilon_0}\int \frac{|\psi_{100}|^2}{|r-r_0|}\,d^3r$$

$$V_K = -\frac{e^2}{4\pi\varepsilon_0 r_0}$$

$$R_{10}(r) = 2\left(\frac{Z}{a_B}\right)^{3/2} e^{-Zr/a_B} , \quad (6.60)$$

$$R_{20}(r) = 2\left(\frac{Z}{2a_B}\right)^{3/2}\left(1-\frac{Zr}{2a_B}\right) e^{-Zr/2a_B} , \quad (6.61)$$

$$R_{21}(r) = \frac{1}{\sqrt{3}}\left(\frac{Z}{2a_B}\right)^{3/2}\frac{Zr}{a_B} e^{-Zr/2a_B} , \quad (6.62)$$

$$R_{30}(r) = 2\left(\frac{Z}{3a_B}\right)^{3/2}\left(1-\frac{2Zr}{3a_B}+\frac{2(Zr)^2}{27a_B^2}\right) e^{-Zr/3a_B} , \quad (6.63)$$

$$R_{31}(r) = \frac{4\sqrt{2}}{3}\left(\frac{Z}{3a_B}\right)^{3/2}\frac{Zr}{a_B}\left(1-\frac{Zr}{6a_B}\right) e^{-Zr/3a_B} , \quad (6.64)$$

$$R_{32}(r) = \frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{Z}{3a_B}\right)^{3/2}\left(\frac{Zr}{a_B}\right)^2 e^{-Zr/3a_B} . \quad (6.65)$$

5 Quantentheorie des Drehimpulses

$l = 2$:	$Y_{20}(\vartheta,\varphi)$	$= \sqrt{\frac{5}{16\pi}}\left(3\cos^2\vartheta - 1\right)$,	(5.111)
	$Y_{2\pm1}(\vartheta,\varphi)$	$= \mp\sqrt{\frac{15}{8\pi}}\sin\vartheta\cos\vartheta\, e^{\pm i\varphi}$,	(5.112)
	$Y_{2\pm2}(\vartheta,\varphi)$	$= \sqrt{\frac{15}{32\pi}}\sin^2\vartheta\, e^{\pm i2\varphi}$.	(5.113)

$$\psi_{100} = \frac{2}{\sqrt{4\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Z\frac{r}{a_0}} = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-\frac{r}{a_0}}$$

$$\frac{2\pi}{\pi a_0^3}\int_0^\infty\int_0^\pi \frac{e^{-\frac{2r}{a_0}}}{\sqrt{r^2+r_0^2-2rr_0\cos\vartheta}}\, r^2\sin\vartheta\, dr\, d\vartheta$$

$x = \cos\vartheta$

$$= \frac{2}{a_0^3}\int dr\, r^2 e^{-\frac{2r}{a_0}}\int_{-1}^{1} dx\left(r^2+r_0^2-2rr_0x\right)^{-\frac{1}{2}}$$

$$\int du\,\frac{1}{\sqrt{a+\alpha u}} = \frac{2}{\alpha}\sqrt{a+\alpha u}$$

$$= \frac{2}{a_0}\int r^2 e^{-\frac{2r}{a_0}}\,\frac{2}{2r_0r}\left(\sqrt{r^2+r_0^2+2rr_0}-\sqrt{r^2+r_0^2-2rr_0}\right)dr$$

$$\sqrt{(r+r')^2}-\sqrt{(r-r')^2} = r+r'-|r-r'| = \begin{cases} 2r' & r>r' \\ 2r & r\le r'\end{cases} = \begin{cases}\frac{2}{r} \\ \frac{2}{r'}\end{cases}$$

$$= \frac{2}{a_0^3}\left[\frac{2}{r_0}\int_0^{r_0} r^2 e^{-\frac{2r}{a_0}}\,dr + 2\int_{r_0}^{\infty} r\, e^{-\frac{2r}{a_0}}\,dr\right]$$

$$V_e(\mathbf{r}_0) = \frac{e^2}{\pi\,\varepsilon_0\,a_B^3}\left[\frac{1}{r_0}\,\frac{2}{(2/a_B)^3}\left(1 - e^{-\frac{2r_0}{a_B}}\left(1 + \frac{2r_0}{a_B} + \frac{2r_0^2}{a_B^2}\right)\right) + \frac{1}{(2/a_B)^2}\,e^{-2r_0/a_B}\left(1 + \frac{2r_0}{a_B}\right)\right]$$

$$= \frac{e^2}{\pi\,\varepsilon_0\,a_B^3}\left[\frac{a_B^3}{4r_0} + e^{-2r_0/a_B}\left(\frac{a_B^2}{4} + \frac{a_B\,r_0}{2} - \frac{a_B^3}{4r_0} - \frac{a_B^2}{2} - \frac{a_B\,r_0}{2}\right)\right]$$

$$= \frac{e^2}{4\pi\,\varepsilon_0\,a_B}\left[\frac{a_B}{r_0} - e^{-2r_0/a_B}\left(1 + \frac{a_B}{r_0}\right)\right].$$

$$\int_0^{x_0} dx\, e^{-\alpha x}\, x^n = \frac{n!}{\alpha^{n+1}}\left(1 - e^{-\alpha x_0}\sum_{\nu=0}^{n}\frac{(\alpha\, x_0)^\nu}{\nu!}\right),$$

$$\int_{x_0}^{\infty} dx\, e^{-\alpha x}\, x^n = \frac{n!}{\alpha^{n+1}}\, e^{-\alpha x_0}\sum_{\nu=0}^{n}\frac{(\alpha\, x_0)^\nu}{\nu!}.$$

$$= \frac{1}{a_0}\left[\frac{a_0}{r_0} - e^{-\frac{2r_0}{a_0}}\left(1 + \frac{a_0}{r_0}\right)\right]$$

$r_0 \to r$

$$V(r) = -\frac{e^2}{4\pi\varepsilon_0}\, e^{-\frac{2r}{a_0}}\left(\frac{1}{a_0} + \frac{1}{r}\right)$$