1. intermediate exam (1. välikoe): 4 problems, 4 hours

1. As you remember, in the quantum mechanical description of elastic scattering, we aim at stationary wave functions which have the following asymptotic form

$$\psi_{\mathbf{k_i}}(\mathbf{r}) \overset{r\to\infty}{=} \frac{1}{(2\pi)^{3/2}} \left(e^{i\mathbf{k_i}\cdot\mathbf{r}} + \frac{e^{ikr}}{r} f_{\mathbf{k_i}}(\theta,\varphi) \right)$$

where $\mathbf{k_i} = k\hat{\mathbf{e}}_z$ and $k^2 = 2\mu E/\hbar^2$. We also recall that the implicit solution of the stationary Schrodinger equation for the potential scattering can be written as

$$\psi_{\mathbf{k_i}}(\mathbf{r}) = \Phi_{\mathbf{k_i}}(\mathbf{r}) + \int d^3r' G_{\mathbf{k_i}}(\mathbf{r}-\mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k_i}}(\mathbf{r}')$$

where

$$U(\mathbf{r}) = \frac{2\mu}{\hbar^2} V(\mathbf{r}), \quad \Phi_{\mathbf{k_i}}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k_i}\cdot\mathbf{r}}, \quad G_{\mathbf{k_i}}(\mathbf{r}) = -\frac{1}{4\pi}\frac{e^{ikr}}{r},$$

and where the potential $V(\mathbf{r})$ vanishes sufficiently quickly at large distances.

a) Using the information given above, show that the scattering amplitude becomes

$$f_{\mathbf{k_i}}(\theta,\varphi) = -2\pi^2 \int d^3r' \Phi^*_{\mathbf{k_f}}(\mathbf{r}') U(\mathbf{r}') \psi_{\mathbf{k_i}}(\mathbf{r}'),$$

where $\mathbf{k_f} = k\mathbf{r}/r = k\hat{\mathbf{e}}_r$.

b) Derive the Born series for the scattering amplitude and show that the Born approximation for the scattering amplitude is

$$f_B(\theta,\varphi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2} \int d^3r' e^{-i(\mathbf{k_f}-\mathbf{k_i})\cdot\mathbf{r}'} V(\mathbf{r}')$$

c) Compute the scattering amplitude $f_B(\theta,\varphi)$ in the Born approximation for the potential

$$V(r) = \begin{cases} V_0, & r \le a \\ 0, & r > a \end{cases}$$

where V_0 is a constant. In the end, write your result in a form which shows the dependence of the obtained scattering amplitude on the scattering angles and energy.

d) Compute $f_B(\theta,\varphi)$ for

* forward scattering at any energy
* backward scattering in the high-energy limit $ka \to \infty$

e) Compute the elastic total cross section in the low-energy limit ($ka \ll 1$).

2. Let's consider scattering off a radially symmetric potential in terms of the partial wave analysis. Let the potential be

$$V(r) = \begin{cases} \infty, & r \leq a \\ \alpha\delta(r-b), & r > a \end{cases}$$

where a, b ($b > a$) and α are constants. The scattering amplitude and the partial wave amplitudes are known to be

$$f_k(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta), \qquad f_l(k) = e^{i\delta_l(k)}\sin\delta_l(k).$$

Note also that the delta function above applies only to the radial distance r but not to the angles θ, φ.

a) Starting from the solutions of the stationary radial Schrödinger equation (see the collection of formulae), compute the s-wave phase shift $\delta_0(k)$ at the low-energy limit where $ka, kb \ll 1$. (*Note*: apply this limit already when considering the continuity conditions!)
Express your final result for $\tan\delta_0(k)$ in terms of k, a, b and the dimensionless variable $\beta \equiv \frac{2m\alpha b}{\hbar^2}$. You can use (without deriving it) the fact that the discontinuity of the 1st derivatives of $R(r)$ at $r = b$ is given by $R'(b+\epsilon) - R'(b-\epsilon) = \frac{\beta}{b}R(b)$, where $\epsilon \to 0_+$ and $R' \equiv \frac{dR(r)}{dr}$.

b) Let's then set $\alpha = 0$ for simplicity. Compute the s-wave contribution to the total cross section in the low-energy limit.

3. Suppose that the Hamilton operator in the Schrödinger picture is

$$\hat{H}_S(t) = \hat{H}_0 + \hat{V}_S(t),$$

where $\hat{H}_0$ does not depend on time but $\hat{V}_S$ does. In the interaction picture (I-picture), the states and operators are defined in terms of the Schrödinger picture as

$$|\psi(t)\rangle_I \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi(t)\rangle_S \qquad \hat{A}_I(t) \equiv e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_S(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}.$$

a) Derive the following equation of motion for the states in the I-picture:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle_I = \hat{V}_I(t)|\psi(t)\rangle_I.$$

b) Show next that the time-evolution operator $\hat{U}_I(t, t_0)$ in the I-picture has the following integral equation,

$$\hat{U}_I(t, t_0) = \hat{\mathbf{1}} - \frac{i}{\hbar}\int_{t_0}^{t} dt' V_I(t')\hat{U}_I(t', t_0).$$

c) Suppose then that the time-dependent potential $V_S(t)$ is a weak perturbation. Using the I-picture, derive the following lowest-order time-dependent perturbation theory result for the probability of a transition from an initial state $|\phi_i\rangle$ at t_0 to a state $|\phi_f\rangle$ at t:

$$P_{fi}(t, t_0) \equiv |\langle\phi_f|\psi(t)\rangle|^2 \approx \left|\delta_{fi} - \frac{i}{\hbar}\int_{t_0}^{t} dt_1\langle\phi_f|\hat{V}_S(t_1)|\phi_i\rangle e^{i(E_f - E_i)t_1/\hbar}\right|^2,$$

where the initial and final states are eigenstates of $\hat{H}_0$: $\hat{H}_0|\phi_f\rangle = E_f|\phi_f\rangle$ and $\hat{H}_0|\phi_i\rangle = E_i|\phi_i\rangle$.

4. Let's put a spinless hydrogen atom into a weak time-dependent perturbation potential

$$\hat{V}_S(t) = C\hat{y}^2\frac{e^{i\omega_{41}t} + e^{-i\omega_{41}t}}{t^2 - 2t\tau + 2\tau^2},$$

where C and $\tau > 0$ are real constants, and in terms of the eigenenergies of the unperturbed hydrogen atom $\omega_{41} = (E_4 - E_1)/\hbar$. Note that $\hat{y}$ above is the y-coordinate operator (and not a unit vector) and that $\hat{y}^2 = \hat{y}\hat{y}$.

a) Using lowest-order time-dependent perturbation theory, find the selection rules for n, l and m in transitions from the ground state $|1, 0, 0\rangle$ to any of the excited states. See the collection of formulae for help.

b) Calculate the probability of a transition from the ground state to the 3d-state $|3, 2, 2\rangle$ during an infinitely long period of time (set $t_0 \to -\infty$ and $t \to \infty$). In doing the residue integrals, explain why you choose the particular half-plane for closing the integration path. Express the final result in terms of the Bohr radius a, trigonometric and hyperbolic functions and $\omega_{31} \equiv (E_3 - E_1)/\hbar$, ω_{41} and τ. [*Note:* This is a rather lengthy exercise, so we suggest to leave it as the last one to answer. Don't panic if you seem to run out of time, just keep going as far as you can.]

Useful(?) formulas and equations, for any of the problems:

Spherical coordinates and spherical harmonics:

$$\mathbf{r} = (r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta) \qquad \nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) - \frac{1}{\hbar^2 r^2}\hat{L}^2$$

$$\int d^3r = \int_0^\infty drr^2 \int_{4\pi} d\Omega = \int_0^\infty drr^2 \int_0^\pi d\theta\sin\theta \int_0^{2\pi} d\varphi = \int_0^\infty drr^2 \int_{-1}^1 d(\cos\theta) \int_0^{2\pi} d\varphi$$

$$\hat{L}^2 Y_{lm}(\theta,\varphi) = \hbar^2 l(l+1) Y_{lm}(\theta,\varphi) \qquad \hat{L}_z Y_{lm}(\theta,\varphi) = \hbar m Y_{lm}(\theta,\varphi)$$

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right] \qquad \int d\Omega\, Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi) = \delta_{ll'}\delta_{mm'}$$

$$Y_{lm}(\theta,\varphi) = (-1)^{\frac{m+|m|}{2}}\sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-|m|)!}{(l+|m|)!}}P_l^{|m|}(\cos\theta)e^{im\varphi} \qquad Y_{l,-m}(\theta,\varphi) = (-1)^m Y^*_{l,m}(\theta,\varphi)$$

$$P_l^k(z) = (1-z^2)^{k/2}\frac{d^k}{dz^k}P_l(z) \qquad P_l(z) = \frac{1}{2^l l!}\frac{d^l}{dz^l}(z^2-1)^l$$

$$Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \qquad Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta \qquad Y_{1\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi}$$

$$Y_{20}(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta - 1\right) \qquad Y_{2\pm1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta e^{\pm i\varphi} \qquad Y_{2\pm2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm 2i\varphi}$$

Stationary Schrödinger equation, the radial part:

$$r^2\frac{d^2R(r)}{dr^2} + 2r\frac{dR(r)}{dr} + \left[(kr)^2 - l(l+1) - r^2\frac{2m}{\hbar^2}V(r)\right]R(r) = 0, \qquad k^2 = \frac{2mE}{\hbar^2}$$

Spherical Bessel & Neumann functions:

$$r^2\frac{d^2R(r)}{dr^2} + 2r\frac{dR(r)}{dr} + \left[(kr)^2 - l(l+1)\right]R(r) = 0 \to \qquad R(r) = Aj_l(kr) + Bn_l(kr)$$

$$j_l(x) = 2^l x^l\sum_{s=0}^\infty \frac{(-1)^s(s+l)!}{s!(2s+2l+1)!}x^{2s} \qquad n_l(x) = \frac{(-1)^{l+1}}{2^l x^{l+1}}\sum_{s=0}^\infty\frac{(-1)^s(s-l)!}{s!(2s-2l)!}x^{2s}$$

$$j_0(x) = \frac{\sin x}{x} \qquad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad n_0(x) = -\frac{\cos x}{x} \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

Trigonometric functions:

$$\cos 2x = \cos^2 x - \sin^2 x, \qquad \cos^2 x + \sin^2 x = 1, \qquad \sin 2x = 2\sin x\cos x$$

Euler: $e^{i\alpha} = \cos\alpha + i\sin\alpha$ $\qquad \cos\alpha = \frac{1}{2}(e^{i\alpha} + e^{-i\alpha})$ $\qquad \sin\alpha = \frac{1}{2i}(e^{i\alpha} - e^{-i\alpha})$

Hyperbolic functions:

$\sinh x = \frac{1}{2}(e^x - e^{-x})$ $\qquad \cosh x = \frac{1}{2}(e^x + e^{-x})$

See next page!

Power series, Taylor expansions:

$$e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!} \qquad \cos x = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{(2n)!} \qquad \sin x = \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n+1}}{(2n+1)!}$$

$$\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \ldots \qquad \ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 + \ldots$$

Hydrogen-like atom wave-functions:

$$\Psi_{nlm_l}(\mathbf{x}) = R_{nl}(r) Y_{lm_l}(\theta, \varphi) \qquad \kappa = \frac{Z}{na} \qquad a = \frac{4\pi\epsilon_0 \hbar^2}{\mu e^2} = \frac{\hbar}{\alpha \mu c}$$

$$R_{nl}(r) = \sqrt{(2\kappa)^3 \frac{(n-l-1)!}{2n(n+l)!}} (2\kappa r)^l e^{-\kappa r} L_{n-l-1}^{2l+1}(2\kappa r) \qquad L_p^q(x) = \sum_{k=0}^{p} (-1^k) \frac{(p+q)! x^k}{(p-k)!(q+k)!k!}$$

$$R_{10} = 2\left(\frac{Z}{a}\right)^{3/2} e^{-Zr/a} \qquad R_{20} = \frac{1}{\sqrt{2}}\left(\frac{Z}{a}\right)^{3/2} \left(1 - \frac{Zr}{2a}\right) e^{-Zr/2a} \qquad R_{21} = \frac{1}{2\sqrt{6}}\left(\frac{Z}{a}\right)^{5/2} r e^{-Zr/2a}$$

$$R_{30} = \frac{2}{3\sqrt{3}}\left(\frac{Z}{a}\right)^{3/2} \left(1 - \frac{2Zr}{3a} + \frac{2}{27}(\frac{Zr}{3a})^2\right) e^{-Zr/3a} \qquad R_{31} = \frac{8}{27\sqrt{6}}\left(\frac{Z}{a}\right)^{5/2} r \left(1 - \frac{Zr}{6a}\right) e^{-Zr/3a}$$

$$R_{32} = \frac{4}{81\sqrt{30}}\left(\frac{Z}{a}\right)^{7/2} r^2 e^{-Zr/3a}$$

Spherical spinors : $\quad (\mathcal{Y}_{ljm}(\Omega))_{m_s} = \langle \Omega, m_s | l, s = \frac{1}{2}, j, m \rangle_c$

$$\begin{aligned} |l, s = \frac{1}{2}, j = l \pm \frac{1}{2}, m\rangle_c &= \pm\sqrt{\frac{l \pm m + \frac{1}{2}}{2l+1}} |l, s = \frac{1}{2}, m_l = m - \frac{1}{2}, m_s = \frac{1}{2}\rangle_u \\ &+ \sqrt{\frac{l \mp m + \frac{1}{2}}{2l+1}} |l, s = \frac{1}{2}, m_l = m + \frac{1}{2}, m_s = -\frac{1}{2}\rangle_u \end{aligned}$$

$$\int d\Omega \mathcal{Y}_{ljm}(\Omega)^\dagger \mathcal{Y}_{l'j'm'}(\Omega) = \delta_{ll'} \delta_{jj'} \delta_{mm'}$$

For integrations in the complex plane:

$$\mathrm{Res} f(z)\big|_{z=z_0} = \lim_{z \to z_0} \frac{1}{(n-1)!} (\frac{d}{dz})^{n-1} [(z-z_0)^n f(z)] \qquad \oint_C dz f(z) = 2\pi i \sum_{j=1}^{n} \mathrm{Res} f(z)\big|_{z=z_j}.$$

For integrations:

$$\int_0^\infty dx x^n e^{-x} = n! \qquad \int_0^\infty dx x^n e^{-ax} = \frac{n!}{a^{n+1}}$$

Generalized angular momentum:

$$[\hat{J}_i, \hat{J}_j] = i\hbar \sum_{k=1}^{3} \epsilon_{ijk} \hat{J}_k, \qquad [\hat{\mathbf{J}}^2, \hat{J}_i] = 0, \qquad \hat{\mathbf{J}}^2 |j, m\rangle = \hbar^2 j(j+1)|j, m\rangle, \qquad \hat{J}_z |j, m\rangle = \hbar m |j, m\rangle$$

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y, \qquad \hat{J}_\pm |j, m\rangle = \hbar\sqrt{(j \mp m)(j \pm m + 1)}|j, m \pm 1\rangle$$

Pauli spin-matrix identities:

$$(\vec{\sigma} \cdot \mathbf{A})(\vec{\sigma} \cdot \mathbf{B}) = (\mathbf{A} \cdot \mathbf{B})\mathbf{I}_2 + i(\mathbf{A} \times \mathbf{B}) \cdot \vec{\sigma}$$

$$\sigma_j \sigma_k = \delta_{jk} \mathbf{I}_2 + i\epsilon_{jkl}\sigma_l \qquad [\sigma_j, \sigma_k] = 2i\epsilon_{jkl}\sigma_l \qquad \vec{\sigma} \times \vec{\sigma} = 2i\vec{\sigma}$$

Vector and Levi-Civita identities:

$$(\mathbf{a} \times \mathbf{b})_i = \epsilon_{ijk} a_j b_k \qquad \epsilon_{ijk}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$$