Exercise 11.1 Free-particle Green's function and propagator (2 points)

Green's functions for the time-independent Schrödinger equation are defined by

$$G^{\pm}(E, \vec{x}, \vec{x}') = \langle \vec{x} | (E - \hat{H} \pm i0)^{-1} | \vec{x}' \rangle, \qquad (1)$$

where \hat{H} is the (time-independent) Hamilton operator of the system. From $G^{\pm}(E, \vec{x}, \vec{x}')$, Green's functions for the forward/backward evolution in time, the so-called retarded/ad-vanced "propagators", are obtained as

$$G^{\pm}(\vec{x},t;\vec{x}',t') = i \int_{-\infty}^{\infty} \frac{dE}{2\pi} e^{-iE(t-t')/\hbar} G^{\pm}(E,\vec{x},\vec{x}').$$
(2)

For the motion of a free particle (mass M) in three dimensions, calculate $G_0^{\pm}(\vec{x}, t; \vec{x}', t')$ from

$$G_0^{\pm}(E, \vec{x}, \vec{x}') = \frac{\mathrm{i}}{(2\pi)^2 |\vec{x} - \vec{x}'|} \int_{-\infty}^{\infty} \mathrm{d}k \, \frac{k \mathrm{e}^{-\mathrm{i}k|\vec{x} - \vec{x}'|}}{E - \frac{\hbar^2 k^2}{2M} \pm \mathrm{i}0}$$
$$= -\frac{M \mathrm{e}^{\pm \mathrm{i}k_E |\vec{x} - \vec{x}'|}}{2\pi \hbar^2 |\vec{x} - \vec{x}'|}, \qquad k_E = \sqrt{2M(E \pm \mathrm{i}0)}/\hbar_E$$

which was derived in the lecture.

Hint: Perform the integration over E first, so that the integration over k can be done with the Fresnel integral $\int_{-\infty}^{\infty} dx e^{iax^2} = \sqrt{\frac{i\pi}{a}}$ for $a \in \mathbb{R}$.

Please turn over!

Exercise 11.2 Spread of free wave packets (3 points)

Consider the one-dimensional propagation of a free wave packet of mass m which is described by any normalised wave function $\psi(x, t)$.

- a) Show that the momentum expectation value $\langle \hat{p} \rangle$ and momentum uncertainty $\Delta p \equiv \sqrt{\langle (\hat{p} \langle \hat{p} \rangle)^2 \rangle}$ are constant in time. How does the position expectation value $\langle \hat{x} \rangle$ develop in t?
- b) Prove that the uncertainties Δx and Δp of position and momentum are related by

$$\Delta x^2 = \frac{\Delta p^2 t^2}{m^2} + at + \Delta x_0^2,\tag{3}$$

where Δx_0 is the spread at t = 0 and a is a constant. Interpret the leading term for large times t.

c) Derive a bound on |a| from Heisenberg's uncertainty principle. Which values can be taken by a if Δx_0 is minimal?

Exercise 11.3 Free-particle wave functions with quantum numbers l, m (3 points)

We consider the separation of the time-independent Schrödinger equation for a free particle of mass M in polar coordinates with the ansatz $\phi_{klm}(r, \theta, \varphi) = R_l(kr)Y_{lm}(\theta, \varphi)$ for the wave function. This leads to the differential equation

$$D^{(l)}R_l(\rho) \equiv \left(\frac{1}{\rho^2}\frac{\mathrm{d}}{\mathrm{d}\rho}\rho^2\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{l(l+1)}{\rho^2} + 1\right)R_l(\rho) = 0 \tag{4}$$

for the radial function $R_l(\rho) = R_l(kr)$, where $k \ge 0$ is related to the energy eigenvalue by $E(k) = \hbar^2 k^2/(2M)$. As an ordinary 2nd-order differential equation, Eq. (4) possesses two linearly independent solutions for each value of $l = 0, 1, 2, \ldots$

a) Show that the two independent solutions of Eq. (4) are given by

$$j_{l}(\rho) = (-\rho)^{l} \left(\frac{1}{\rho} \frac{\mathrm{d}}{\mathrm{d}\rho}\right)^{l} j_{0}(\rho), \qquad j_{0}(\rho) = \frac{\sin\rho}{\rho},$$
$$n_{l}(\rho) = (-\rho)^{l} \left(\frac{1}{\rho} \frac{\mathrm{d}}{\mathrm{d}\rho}\right)^{l} n_{0}(\rho), \qquad n_{0}(\rho) = -\frac{\cos\rho}{\rho}, \qquad l = 0, 1, \dots,$$

where j_l and n_l are the spherical Bessel and Neumann functions, respectively.

Hint: A simple way is based on induction using $R_{l+1}(\rho) = -\rho^l \frac{\mathrm{d}}{\mathrm{d}\rho} \rho^{-l} R_l(\rho)$ and evaluating the commutator of the differential operator $D^{(l+1)}$, as defined in Eq. (4), and the operator $\rho^l \frac{\mathrm{d}}{\mathrm{d}\rho} \rho^{-l}$.

- b) Derive series expansions for j_l and n_l about $\rho = 0$, making use of the series for $\sin \rho$ and $\cos \rho$. Give the leading asymptotic behaviour of j_l and n_l for $\rho \to 0$.
- c) Show that the leading asymptotic behaviour of j_l and n_l for $\rho \to \infty$ is given by

$$j_l(\rho) \sim_{\rho \to \infty} \frac{1}{\rho} \sin\left(\rho - \frac{l\pi}{2}\right), \qquad n_l(\rho) \sim_{\rho \to \infty} -\frac{1}{\rho} \cos\left(\rho - \frac{l\pi}{2}\right).$$
 (5)