Quantum Dynamics, NWI-SM295, exercises week 6

Gerrit C. Groenenboom, June 8, 2019

Question 1: Elastic scattering in 3D

A plane wave traveling along the z-axis can be expanded in spherical waves:

$$e^{ikrz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(z), \tag{1}$$

where $z \equiv \cos\theta$, the position of the particle is given by the spherical coordinates (r, θ, ϕ), $j_l(kr)$ are spherical Bessel functions of the first kind, $P_l(z)$ are Legendre polynomials of order l, and the wave vector is $\boldsymbol{k} = k\boldsymbol{e}_z$.

The Legendre polynomials are defined by

$$P_0(z) = 1 \tag{2}$$

$$P_1(z) = z \tag{3}$$

$$P_{l+1}(z) = \frac{z(2l+1)P_l(z) - lP_{l-1}(z)}{l+1} \tag{4}$$

and they satisfy the orthogonality relations

$$\int_{-1}^{1} P_l(z) P_{l'}(z) dz = \frac{2}{2l+1} \delta_{ll'}.$$

1a. Use the orthogonality relation of the Legendre polynomials and the plane wave expansion to derive and explicit expression for $j_0(kr)$, i.e., project Eq. (1) onto $P_0(z)$.

Answer:

$$\int_{-1}^{1} P_0(z) e^{ikrz}\, dz = j_0(kr) \int_{-1}^{1} P_0(z)^2 dz = 2j_0(kr). \tag{5}$$

so

$$j_0(kr) = \frac{1}{2} \int_{-1}^{1} e^{ikrz} dz \tag{6}$$

$$= \frac{1}{2} \frac{1}{ikr} e^{ikrz} \Big|_{-1}^{1} \tag{7}$$

$$= \frac{1}{2} \frac{1}{ikr} \left(e^{ikr} - e^{-ikr} \right) \tag{8}$$

$$= \frac{\sin(kr)}{kr}. \tag{9}$$

1b. Also project Eq. (1) onto $P_1(z)$ to find the expression for $j_1(kr)$.

Answer:

$$\int_{-1}^{1} P_1(z) e^{ikrz} dz = 3i\, j_1(kr) \int_{-1}^{1} P_1(z)^2 dz = 2i\, j_1(kr). \tag{10}$$

so

$$j_1(kr) = \frac{1}{2i} \int_{-1}^{1} z\, e^{ikrz} dz \tag{11}$$

$$= \frac{1}{2i} \frac{1}{ikr} \int_{-1}^{1} z\, de^{ikrz} \tag{12}$$

$$= \frac{-1}{2kr} \left(z\, e^{ikrz} \Big|_{-1}^{1} - \int_{-1}^{1} e^{ikrz}\, dz \right) \tag{13}$$

$$= \frac{-1}{2kr} \left[\left(e^{ikr} + e^{-ikr} \right) - 2j_0(kr) \right] \tag{14}$$

$$= -\frac{\cos(kr)}{kr} + \frac{\sin(kr)}{(kr)^2}. \tag{15}$$

Equation 10.1.20 of A&S gives the following expression for the derivative of spherical Bessel function of the first kind:

$$(2l+1) \frac{\partial}{\partial x} j_l(x) = -(l+1) j_{l+1}(x) + l j_{l-1}(x). \tag{16}$$

1c. Show that this expression is consistent with the implicit definition of spherical Bessel functions in Eq. (1). Hint: define $x = kr$, then take the derivative of Eq.(1) with respect to x, project the equation by $P_l(z)$, and use the recursion relation of Legendre polynomials to rewrite $zP_l(z)$.

Answer: *Equation (1) with $x = kr$:*

$$e^{ixz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(x) P_l(z). \tag{17}$$

Its derivative with respect to x

$$ize^{ixz} = \sum_{l=0}^{\infty} i^l (2l+1) j_l'(x) P_l(z). \tag{18}$$

Project onto $P_l(z)$

$$\int_{-1}^{1} izP_l(z)e^{ixz}\, dz = i^l (2l+1) j_l'(x) \frac{2}{2l+1} \tag{19}$$

Rewrite the recursion relation Eq. (4)

$$z(2l+1)P_l(z) = (l+1)P_{l+1}(z) + lP_{l-1}(z) \tag{20}$$

and insert it into Eq. (19),

$$\int_{-1}^{1} i\left[(l+1)P_{l+1}(z) + lP_{l-1}(z)\right] e^{ixz}\, dz = 2i^l (2l+1) j_l'(x) \tag{21}$$

Projecting Eq. (17) onto $P_l(z)$ gives

$$\int_{-1}^{1} P_l(z)e^{ixz} dz = i^l (2l+1) j_l(x) \frac{2}{2l+1} \tag{22}$$

$$= 2i^l j_l(x) \tag{23}$$

Use this integral in Eq. (21)

$$i(l+1)2i^{l+1} j_{l+1}(x) + il2i^{l-1} j_{l-1}(x) = 2i^l (2l+1) j_l'(x) \tag{24}$$

Divide by $2i^l$ to recover Eq. (16)

$$-(l+1)j_{l+1}(x) + lj_{l-1}(x) = (2l+1)j_l'(x). \tag{25}$$

Question 2: Explicit expression for scattering amplitude

The boundary conditions for elastic scattering of a single particle are given by

$$\psi(\boldsymbol{r}) = e^{ikrz} + \frac{e^{ikr}}{r} f(\theta).$$

A nonzero potential will modify only the outgoing part of the plane wave [Eq. (1)]. For sufficiently large r the spherical Bessel functions of the first kind take the form

$$j_l(kr) = \frac{\sin(kr - l\frac{\pi}{2})}{kr}.$$

The sin function can be written as an incoming and an outgoing wave using

$$2i \sin x = -e^{-ix} + e^{ix}$$

and the effect of the potential is to modify the outgoing part:

$$-e^{-ix} + e^{ix} \Rightarrow -e^{-ix} + e^{ix} S.$$

The S may be different for each partial wave (each value of l), so the scattering amplitude $f(\theta)$ can be written as a sum involving “S-matrices” S_l.

2a. Derive the expression for the scattering amplitude $f(\theta)$ in terms of the S-matrixes S_l.

Answer: *The asymptotic form of the spherical Bessel functions of the the first kind is*

$$j_l(kr) = \frac{\sin(kr - l\frac{\pi}{2})}{kr} \tag{26}$$

$$= \frac{-e^{-i(kr-l\frac{\pi}{2})} + e^{i(kr-l\frac{\pi}{2})}}{2ikr}. \tag{27}$$

Modifying the outgoing part with a factor S_l *and substituting the result in the plane wave expansion Eq. (1) gives*

$$\sum_{l=0}^{\infty} i^l (2l+1) \frac{-e^{-i(kr-l\frac{\pi}{2})} + e^{i(kr-l\frac{\pi}{2})} S_l}{2ikr} P_l(z), \tag{28}$$

Collecting the spherically outgoing part that arises from terms where S_l *is not equal to one, i.e.,* $T_l = 1 - S_l$ *is nonzero:*

$$\frac{e^{ikr}}{r} \sum_{l=0}^{\infty} i^l (2l+1) \frac{ie^{-il\frac{\pi}{2}}}{2k} T_l P_l(z). \tag{29}$$

With $e^{-il\frac{\pi}{2}} = i^{-l}$ *we find for the scattering amplitude*

$$f(\theta) = \frac{i}{2k} \sum_{l=0}^{\infty} (2l+1) T_l P_l(\cos\theta). \tag{30}$$

Question 3: Differential and integral cross sections

The differential cross section is related to the scattering amplitude

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2.$$

The integral cross section is obtained by integrating over all scattering angles

$$\sigma = \int_0^{2\pi} d\phi \int_{-1}^{1} |f(\theta)|^2 \, d\cos\theta.$$

3a. Use the expression for $f(\theta)$ from the previous question and the orthogonality of the Legendre polynomials to find and explicit expression for the integral cross sections in terms of the S_l's.

Answer:

$$\sigma = 2\pi \int_{-1}^{1} \frac{1}{4k^2} \left| \sum_{l=0}^{\infty} (2l+1) T_l P_l(\cos\theta) \right|^2 d\cos\theta \tag{31}$$

$$= \frac{\pi}{2k^2} \sum_{l=0}^{\infty} (2l+1)^2 |T_l|^2 \frac{2}{2l+1} \tag{32}$$

$$= \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) |T_l|^2. \tag{33}$$