

FREE PARTICLE MOVING IN THE Z DIRECTION

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Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.10.

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The radial function for a free particle can be either a spherical Bessel function j_l or a spherical Neumann function n_l . If the solution space includes the origin, then only j_l is acceptable since the n_l functions diverge as $r \rightarrow 0$.

In rectangular coordinates, a free particle wave function has the form

$$\psi_E(x, y, z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar} \quad (1)$$

where the energy E is

$$E = \frac{p^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu} \quad (2)$$

For a free particle travelling in the z direction, this becomes

$$\psi_E(r, \theta, \phi) = \frac{1}{(2\pi\hbar)^{3/2}} e^{ikr \cos \theta} \quad (3)$$

since $z = r \cos \theta$.

Since the solutions of the free-particle Schrödinger equation in spherical coordinations form a complete set, we must be able to express this wave function as a linear combination of these solutions, so that

$$e^{ikr \cos \theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^l C_l^m j_l(kr) Y_l^m(\theta, \phi) \quad (4)$$

where the C_l^m are constants. Because we're looking at motion in the z direction, there is no angular momentum about the z axis, which is reflected in the fact that ψ_E does not depend on ϕ . Thus $L_z = m\hbar = 0$ and $m = 0$. We therefore have

$$e^{ikr \cos \theta} = \sum_{l=0}^{\infty} C_l^0 j_l(kr) Y_l^0(\theta, \phi) \quad (5)$$

$$= \sum_{l=0}^{\infty} \sqrt{\frac{2l+1}{4\pi}} C_l^0 j_l(kr) P_l(\cos \theta) \quad (6)$$

$$= \sum_{l=0}^{\infty} C_l j_l(kr) P_l(\cos \theta) \quad (7)$$

where

$$C_l \equiv \sqrt{\frac{2l+1}{4\pi}} C_l^0 \quad (8)$$

The problem, of course, is to find these constants. We can do this using the identities given by Shankar in his problem 12.6.10, which are

$$\int_{-1}^1 P_l(x) P_{l'}(x) dx = \frac{2\delta_{ll'}}{2l+1} \quad (9)$$

$$P_l(x) = \frac{1}{2^l l!} \frac{d^l (x^2 - 1)^l}{dx^l} \quad (10)$$

$$= \frac{(-1)^l}{2^l l!} \frac{d^l (1 - x^2)^l}{dx^l} \quad (11)$$

$$\int_0^1 (1 - x^2)^m dx = \frac{(2m)!!}{(2m+1)!!} \quad (12)$$

$$\int_{-1}^1 (1 - x^2)^m dx = \frac{2(2m)!!}{(2m+1)!!} \quad (13)$$

The last line follows because $(1 - x^2)^m$ is an even function and is therefore symmetric about $x = 0$.

We can use the standard procedure for isolating C_l by multiplying both sides by C_a and using 9.

$$\int_{-1}^1 P_a(x) e^{ikrx} dx = \sum_{l=0}^{\infty} C_l j_l(kr) \int_{-1}^1 P_a(x) P_l(x) dx \quad (14)$$

$$= \frac{2}{2a+1} C_a j_a(kr) \quad (15)$$

This relation must be true for all values of r , so we can look at the limit of small (but not zero, since both sides are then zero) r . We have the asymptotic relation for the spherical Bessel functions

$$j_l \xrightarrow{\rho \rightarrow 0} \frac{\rho^l}{(2l+1)!!} \quad (16)$$

We thus have

$$\int_{-1}^1 P_a(x) e^{ikrx} dx \xrightarrow{r \rightarrow 0} \frac{2}{2a+1} \frac{k^a r^a}{(2a+1)!!} C_a \quad (17)$$

We can then look at the integral on the LHS and hope that, when we expand the exponential, that the terms in $(kr)^n$ for $n < a$ vanish. We can then match the coefficients of $(kr)^a$ on both sides to find C_a .

We can see that this will work because the Legendre polynomials P_l are a complete set of functions, and the polynomial P_l has degree l . This means that *any* polynomial of degree $a-1$ can be written as a linear combination of the P_l , where $l = 0, \dots, a-1$. Because of 9, this means that

$$\int_{-1}^1 x^l P_a(x) dx = 0 \text{ if } l < a \quad (18)$$

Therefore, when we expand e^{ikrx} in a power series, we have

$$\int_{-1}^1 P_a(x) e^{ikrx} dx = \int_{-1}^1 P_a(x) \left(1 + ikrx + \frac{(ikrx)^2}{2!} + \dots \right) dx \quad (19)$$

$$= \int_{-1}^1 P_a(x) \left(\frac{(ikrx)^a}{a!} + \dots \right) dx \quad (20)$$

In the limit of small r , higher order terms in the sum on the RHS can be ignored, so we get

$$\frac{(ikr)^a}{a!} \int_{-1}^1 x^a P_a(x) dx = \frac{2}{2a+1} \frac{k^a r^a}{(2a+1)!!} C_a \quad (21)$$

$$C_a = \frac{i^a (2a+1) (2a+1)!!}{2a!} \int_{-1}^1 x^a P_a(x) dx \quad (22)$$

Now consider the integral in the last line. Using 11 we have

$$\int_{-1}^1 x^a P_a(x) dx = \frac{(-1)^a}{2^a a!} \int_{-1}^1 x^a \frac{d^a (1-x^2)^a}{dx^a} dx \quad (23)$$

We can integrate by parts repeatedly until the derivative in the integrand disappears. Note that the n th derivative of $(1-x^2)^a$ will always contain a factor of $(1-x^2)$ to some power for any $n < a$, and thus is zero at both limits of integration. Since the integrated term in the integration by parts

always contains such a derivative, all integrated terms are zero at both limits. We therefore integrate $\frac{d^a(1-x^2)^a}{dx^a}$ (a times) and differentiate x^a (a times) and keep only the residual integral after each iteration. The differentiation of x^a (a times) introduces a factor of $a!$. Since the sign of the residual integral alternates as we perform each integration by parts, the final result is

$$\int_{-1}^1 x^a P_a(x) dx = \frac{(-1)^{2a}}{2^a a!} a! \int_{-1}^1 (1-x^2)^a dx \quad (24)$$

$$= \frac{1}{2^a} \frac{2(2a)!!}{(2a+1)!!} \quad (25)$$

where we used 13 in the last line. The double factorial in the numerator can be written as

$$(2a)!! = (2a)(2a-2)\dots(4)(2) \quad (26)$$

$$= 2^a a(a-1)\dots(2)(1) \quad (27)$$

$$= 2^a a! \quad (28)$$

We therefore have

$$\int_{-1}^1 x^a P_a(x) dx = \frac{1}{2^a} \frac{2 \times 2^a a!}{(2a+1)!!} \quad (29)$$

$$= \frac{2a!}{(2a+1)!!} \quad (30)$$

Plugging this back into 22 we have

$$C_a = i^a (2a+1) \quad (31)$$

The wave function for a free particle moving in the z direction is therefore

$$\psi_E(r, \theta, \phi) = \frac{1}{(2\pi\hbar)^{3/2}} \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos\theta) \quad (32)$$