

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

$$(0.1) \quad \psi_E(x, y, z) = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$$

where the energy E is

$$(0.2) \quad E = \frac{p^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu}$$

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

$$(0.3) \quad \psi_E(r, \theta, \phi) = \frac{1}{(2\pi\hbar)^{3/2}} e^{ikr\cos\theta}$$

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

$$(0.4) \quad e^{ikr\cos\theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^l C_l^m j_l(kr) Y_l^m(\theta, \phi)$$

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

$$(0.5) \quad e^{ikr \cos \theta} = \sum_{l=0}^{\infty} C_l^0 j_l(kr) Y_l^0(\theta, \phi)$$

$$(0.6) \quad = \sum_{l=0}^{\infty} \sqrt{\frac{2l+1}{4\pi}} C_l^0 j_l(kr) P_l(\cos \theta)$$

$$(0.7) \quad = \sum_{l=0}^{\infty} C_l j_l(kr) P_l(\cos \theta)$$

where

$$(0.8) \quad C_l \equiv \sqrt{\frac{2l+1}{4\pi}} C_l^0$$

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

$$(0.9) \quad \int_{-1}^1 P_l(x) P_{l'}(x) dx = \frac{2\delta_{ll'}}{2l+1}$$

$$(0.10) \quad P_l(x) = \frac{1}{2^l l!} \frac{d^l (x^2 - 1)^l}{dx^l}$$

$$(0.11) \quad = \frac{(-1)^l}{2^l l!} \frac{d^l (1 - x^2)^l}{dx^l}$$

$$(0.12) \quad \int_0^1 (1 - x^2)^m dx = \frac{(2m)!!}{(2m+1)!!}$$

$$(0.13) \quad \int_{-1}^1 (1 - x^2)^m dx = \frac{2(2m)!!}{(2m+1)!!}$$

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 0.9.

$$(0.14) \quad \int_{-1}^1 P_a(x) e^{ikrx} dx = \sum_{l=0}^{\infty} C_l j_l(kr) \int_{-1}^1 P_a(x) P_l(x) dx$$

$$(0.15) \quad = \frac{2}{2a+1} C_a j_a(kr)$$

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

$$(0.16) \quad j_l \xrightarrow{\rho \rightarrow 0} \frac{\rho^l}{(2l+1)!!}$$

We thus have

$$(0.17) \quad \int_{-1}^1 P_a(x) e^{ikrx} dx \xrightarrow{r \rightarrow 0} \frac{2}{2a+1} \frac{k^a r^a}{(2a+1)!!} C_a$$

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 0.9, this means that

$$(0.18) \quad \int_{-1}^1 x^l P_a(x) dx = 0 \text{ if } l < a$$

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

$$(0.19) \quad \int_{-1}^1 P_a(x) e^{ikrx} dx = \int_{-1}^1 P_a(x) \left(1 + ikrx + \frac{(ikrx)^2}{2!} + \dots \right) dx$$

$$(0.20) \quad = \int_{-1}^1 P_a(x) \left(\frac{(ikrx)^a}{a!} + \dots \right) dx$$

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

$$(0.21) \quad \frac{(ikr)^a}{a!} \int_{-1}^1 x^a P_a(x) dx = \frac{2}{2a+1} \frac{k^a r^a}{(2a+1)!!} C_a$$

$$(0.22) \quad C_a = \frac{i^a (2a+1) (2a+1)!!}{2a!} \int_{-1}^1 x^a P_a(x) dx$$

Now consider the integral in the last line. Using 0.11 we have

$$(0.23) \quad \int_{-1}^1 x^a P_a(x) dx = \frac{(-1)^a}{2^a a!} \int_{-1}^1 x^a \frac{d^a (1-x^2)^a}{dx^a} dx$$

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

$$(0.24) \quad \int_{-1}^1 x^a P_a(x) dx = \frac{(-1)^{2a}}{2^a a!} a! \int_{-1}^1 (1-x^2)^a dx$$

$$(0.25) \quad = \frac{1}{2^a} \frac{2(2a)!!}{(2a+1)!!}$$

where we used 0.13 in the last line. The double factorial in the numerator can be written as

$$(0.26) \quad (2a)!! = (2a)(2a-2)\dots(4)(2)$$

$$(0.27) \quad = 2^a a(a-1)\dots(2)(1)$$

$$(0.28) \quad = 2^a a!$$

We therefore have

$$(0.29) \quad \int_{-1}^1 x^a P_a(x) dx = \frac{1}{2^a} \frac{2 \times 2^a a!}{(2a+1)!!}$$

$$(0.30) \quad = \frac{2a!}{(2a+1)!!}$$

Plugging this back into 0.22 we have

$$(0.31) \quad C_a = i^a (2a+1)$$

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

$$(0.32) \quad \psi_E(r, \theta, \phi) = \frac{1}{(2\pi\hbar)^{3/2}} \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr) P_l(\cos \theta)$$