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 $r \to 0$.

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

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

where the energy E is

$$E = \frac{p^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu} \tag{2}$$

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

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

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

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

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

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

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

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

where

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

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

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

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

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

$$\int_{0}^{1} \left(1-x^2\right)^m dx = \frac{(2m)!!}{(2m+1)!!} \tag{12}$$

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

The last line follows because $\left(1-x^2\right)^m$ 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.

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

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

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

$$j_l \underset{\rho\to 0}{\longrightarrow} \frac{\rho^l}{(2l+1)!!} \tag{16}$$

We thus have

$$\int_{-1}^{1} P_a(x)\, e^{ikrx} dx \underset{r\to 0}{=\longrightarrow} \frac{2}{2a+1}\frac{k^a r^a}{(2a+1)!!} C_a \tag{17}$$

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 $l = 0, \ldots, a-1$. Because of 9, this means that

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

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

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

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

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

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

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

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

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

We can integrate by parts repeatedly until the derivative in the integrand disappears. Note that the nth derivative of $\left(1-x^2\right)^a$ will always contain a factor of $\left(1-x^2\right)$ 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 $\frac{d^a\left(1-x^2\right)^a}{dx^a}$ (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

$$\int_{-1}^{1} x^a P_a(x)\,dx = \frac{(-1)^{2a}}{2^a a!} a! \int_{-1}^{1} \left(1-x^2\right)^a dx \tag{24}$$

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

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

$$\begin{aligned} (2a)!! &= (2a)(2a-2)\ldots(4)(2) &(26)\\ &= 2^a a(a-1)\ldots(2)(1) &(27)\\ &= 2^a a! &(28) \end{aligned}$$

We therefore have

$$\begin{aligned} \int_{-1}^{1} x^a P_a(x)\,dx &= \frac{1}{2^a} \frac{2\times 2^a a!}{(2a+1)!!} &(29)\\ &= \frac{2a!}{(2a+1)!!} &(30) \end{aligned}$$

Plugging this back into 22 we have

$$C_a = i^a (2a+1) \tag{31}$$

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

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