1.9: Example- Uniform Spherical Well in 3D

Let us test the Born series against a simple example, consisting of the scattering potential

$$V(\mathbf{r}) = \begin{cases} -U, & |\mathbf{r}| \le R \\ 0, & |\mathbf{r}| > 0. \end{cases} \tag{1.9.1}$$

We will assume that $U > 0$, so that the potential is attactive and describes a uniform spherically symmetric well of depth U and radius R, surrounded by empty space. For this potential, the scattering problem can be solved exactly, using the method of **partial wave analysis** described in Appendix A. The resulting scattering amplitudes are

$$\begin{aligned} f(\mathbf{k}_i \to \mathbf{k}_f) &= \frac{1}{2ik} \sum_{\ell=0}^{\infty} \left(e^{2i\delta_\ell} - 1\right)\left(2\ell+1\right) P_\ell(\hat{\mathbf{k}}_i \cdot \hat{\mathbf{k}}_f), \\ \text{where } \delta_\ell &= \frac{\pi}{2} + \arg\left[k h_\ell^{+\prime}(kR)\, j_\ell(qR) - q h_\ell^{+}(kR)\, j_\ell'(qR)\right], \\ q &= \sqrt{2m(E+U)/\hbar^2} \\ k &\equiv |\mathbf{k}_i| = |\mathbf{k}_f|. \end{aligned} \tag{1.9.2}$$

This solution is expressed in terms of various special functions; j_ℓ and h_ℓ are the spherical Bessel function of the first kind and spherical Hankel function, while P_ℓ is the Legendre polynomial (which appears in the definition of the spherical harmonic functions).

We will pit this exact solution against the results from the Born series:

$$f(\mathbf{k}_i \to \mathbf{k}_f) \approx -\frac{2m}{\hbar^2} \cdot 2\pi^2 \left[\langle \mathbf{k}_f | \hat{V} | \mathbf{k}_i \rangle + \langle \mathbf{k}_f | \hat{V}\hat{G}_0\hat{V} | \mathbf{k}_i \rangle + \cdots \right]. \tag{1.9.3}$$

The bra-kets can be evaluated in the position representation. Let us do this for just the first two terms in the series:

$$\begin{aligned} f(\mathbf{k}_i \to \mathbf{k}_f) \approx -\frac{2m}{\hbar^2}\, 2\pi^2 \Bigg[&\int d^3r_1\, \frac{\exp(-i\mathbf{k}_f \cdot \mathbf{r}_1)}{(2\pi)^{3/2}}\, V(\mathbf{r}_1)\, \frac{\exp(i\mathbf{k}_i \cdot \mathbf{r}_1)}{(2\pi)^{3/2}} \\ &+ \int d^3r_1 \int d^3r_2\, \frac{\exp(-i\mathbf{k}_f \cdot \mathbf{r}_2)}{(2\pi)^{3/2}}\, V(\mathbf{r}_2)\, \langle \mathbf{r}_2 | \hat{G}_0 | \mathbf{r}_1 \rangle\, V(\mathbf{r}_1)\, \frac{\exp(i\mathbf{k}_i \cdot \mathbf{r}_1)}{(2\pi)^{3/2}} \Bigg] \\ = \frac{1}{4\pi} \Bigg[&\frac{2mU}{\hbar^2} \int_{|\mathbf{r}_1| \le R} d^3r_1\; \exp[i(\mathbf{k}_i - \mathbf{k}_f) \cdot \mathbf{r}_1] \\ &+ \left(\frac{2mU}{\hbar^2}\right)^2 \int_{|\mathbf{r}_1| < R} d^3r_1 \int_{|\mathbf{r}_2| < R} d^3r_2\, \frac{\exp[i(k|\mathbf{r}_1 - \mathbf{r}_2| - \mathbf{k}_f \cdot \mathbf{r}_2 + \mathbf{k}_i \cdot \mathbf{r}_1)]}{4\pi|\mathbf{r}_1 - \mathbf{r}_2|} \Bigg]. \end{aligned} \tag{1.9.4}$$

If we use only the first term in the Born series, the result is called the "first Born approximation"; if we use two terms, the result is called the "second Born approximation". Higher-order Born approximations can be derived in a similar fashion.

The most expedient way to calculate these integrals is to use Monte Carlo integration. To find an integral of the form

$$I = \int_{|\mathbf{r}| < R} d^3r\, F(\mathbf{r}), \tag{1.9.5}$$

we randomly sample N points within a cube of volume $(2R)^3$ centered around the origin, enclosing the desired sphere of radius R. For the n-th sampled point, $\mathbf{r}_n$, we compute

$$F_n = \begin{cases} F(\mathbf{r}_n), & |\mathbf{r}| < R \\ 0, & \text{otherwise.} \end{cases} \tag{1.9.6}$$

The F_n's give the values of the integrand at the sampling points, omitting the contribution from points outside the sphere. Then we estimate the integral as

$$I \approx (2R)^3 \langle F_n \rangle = \frac{(2R)^3}{N} \sum_{n=1}^{N} F_n. \tag{1.9.7}$$

The estimate converges to the true value as $N \to \infty$; in practice, $N \sim 10^4$ yields a good result for typical 3D integrals, and can be computed in around a second on a modern computer. Similarly, to calculate the double integral appearing in the second term of the Born series, we sample *pairs* of points; the volume factor $(2R)^3$ is then replaced by $(2R)^6$.

This method for calculating the Born series can be readily generalized to more complicated scattering potentials, including potentials for which there is no exact solution.

The figure below shows the results of the Born approximation for the uniform potential well, compared to the "exact" solution computed from partial wave analysis. It plots $|f|^2$ versus the scattering energy E, for the case of 90° scattering (i.e., $\mathbf{k}_f$ perpendicular to $\mathbf{k}_i$), with wells of different depth U and the same radius $R = 1$. We adopt computational units $\hbar = m = 1$, and each Monte Carlo integral is computed using 3×10^4 samples.

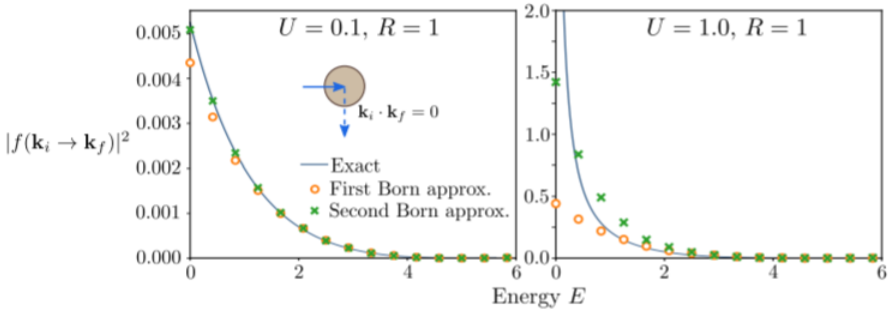

Figure 1.9.1

The first thing to notice in these results in that $|f|^2$ diminishes to zero for large E. This makes sense, since the scattering potential has some energy scale (U), so a incident particle that is too energetic ($E \gg U$) will just zoom through, with little chance of being deflected.

Looking more closely at the plots, we see that for the shallower well ($U = 0.1$), the first Born approximation agrees well with the exact results, and the second Born approximation is even better, particularly for small E. For the deeper well ($U = 1$), the Born approximations do not match the exact results. Roughly speaking, for the stronger scattering potential, an incident particle has a higher chance to undergo multiple-scattering (i.e., bouncing around the potential multiple times before escaping), which means that higher terms in the Born series become more important. In fact, if the potential is too strong, taking the Born approximation to higher orders might not even work, as the Born series itself can become non-convergent. In those cases, different methods must be brought to bear. We will see an example in the next chapter, in the form of phenomena known as "scattering resonances".