Applications of Quantum Mechanics: Example Sheet 4

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1. For classical scattering with a repulsive potential $V(r) = K/r^2$ show that the orbits of particles with energy E are given by

$$\frac{1}{r} = A \sin\alpha\,(\pi - \theta) \quad \text{with} \quad \alpha^2 = 1 + \frac{K}{Eb^2}\,,$$

where b is the impact parameter and θ is measured counterclockwise, with $\theta = 0$ aligned with the positive x-axis. Hence show that the scattering angle is given by $\theta_\infty = \pi(1 - 1/\alpha)$.

2. A particle of mass m and energy $\hbar^2k^2/2m$ scatters off a hard sphere of radius a. Show that the phase shifts δ_l obey

$$\tan\delta_l = \frac{j_l(ka)}{n_l(ka)}$$

3. A particle of mass m and energy $\hbar^2k^2/2m$ scatters off the attractive potential

$$V(r) = \begin{cases} -\hbar^2\gamma^2/2m & \text{if } r < a \\ 0 & \text{if } r \geq a \end{cases}$$

Show that the phase shifts obey

$$\tan\delta_l = \frac{q\, j_l(ka) j_l'(qa) - k\, j_l'(ka) j_l(qa)}{q\, n_l(ka) j_l'(qa) - k\, n_l'(ka) j_l(qa)}$$

where $q^2 = k^2 + \gamma^2$. Hence show that, as $k \to 0$, $\delta_l \sim (ka)^{2l+1}$.

[*Hint:* You will require the small x behaviours of $j_l(x)$ and $n_l(x)$ given in the handout. To answer the first part, consider the requirements of regularity of the wavefunction at $r = 0$.]

4. Consider a particle of essentially zero energy scattering off a repulsive spherical potential

$$V(r) = \begin{cases} +\hbar^2\gamma^2/2m & \text{if } r < a \\ 0 & \text{if } r \geq a \end{cases}$$

From the linear behaviour of the s-wave wavefunction $r\psi(r)$ for $r \geq a$, show that the scattering length is positive.

Consider now the attractive potential from Question 3. Show that for a sufficiently small the scattering length is negative. Show further that as a increases to a critical value a_0, the scattering length becomes infinite. What occurs for $a > a_0$?

5. Consider the spherical shell of delta-functions,

$$V(r) = \frac{\hbar^2\lambda}{2m}\delta(r-a)$$

Show that the phase shifts are given by

$$\tan\delta_l = -\frac{k\lambda a^2[j_l(ka)]^2}{1 - k\lambda a^2 j_l(ka) n_l(ka)}$$

[*Hint*: The δ-function leads to two continuity conditions at $r = a$. Either take appropriate ratios of these conditions, or arrange them as two linear equations for the unknown amplitudes and recognise that the determinant of coefficients must vanish. You will need the Wronskian condition that $x^2(j_l(x)n_l'(x) - j_l'(x)n_l(x)) = 1$.]

For λ large, show that δ_l is close to the result given in Question 2 *unless* $k \simeq k_0$ where $j_l(k_0 a) = 0$. In the latter case, show that we can write $\tan\delta_l \approx -A/(k - k_0')$ where $k_0' = k_0 + \mathcal{O}(\lambda^{-1})$ and $A = \mathcal{O}(\lambda^{-2})$. What is the interpretation of this result?

6. The s-wave wavefunction $\psi_k(r) = \chi_k(r)/r$ obeys the Schrödinger equation

$$-\frac{d^2\chi_k}{dr^2} + V(r)\chi_k = k^2\chi_k\,,$$

with $k \in \mathbf{C}$ and where $\chi_k(r)$ satisfies the boundary conditions $\chi_k(0) = 0$ and $\chi_k'(0) = 1$. Show that

$$\chi_k(r) = \chi_{-k}(r) \quad \text{and} \quad [\chi_k(r)]^* = \chi_{k^*}(r)$$

For large r

$$\chi_k(r) \sim \frac{i}{2k}\left[f(k)\,e^{ikr} - f(-k)\,e^{-ikr}\right]\,.$$

Identify the S-matrix element $S(k)$ for scattering in the $l = 0$ sector in terms of $f(k)$. What conditions do $S(k)$ obey?

7. Show that the S-matrix in the $l = 0$ sector can be written as

$$S(k) = e^{2i\delta_0(k)} = \frac{\cot\delta_0(k) + i}{\cot\delta_0(k) - i}\,.$$

Suppose that, for k small,

$$\cot\delta_0(k) \simeq -\frac{1}{a_s k} + \frac{1}{2} r_0 k$$

with a_s positive and r_0 small and positive. Verify that $S(k)$ satisfies the expected symmetry and reality conditions. Deduce from the form of $S(k)$ that there is a bound state, and find its energy.

8. Resonance scattering in the $l = 0$ sector is modelled by an S-matrix

$$S(k) = \frac{k - K_0 - i\gamma}{k - K_0 + i\gamma}$$

with $K_0 \gg \gamma > 0$. For k real, $S(k) = e^{2i\delta_0(k)}$. Show that

$$\tan\delta_0(k) = \frac{\gamma}{K_0 - k} \quad \text{and} \quad \sigma \simeq \frac{4\pi\gamma^2}{K_0^2}\frac{1}{(K_0 - k)^2 + \gamma^2}\,.$$

Show that for $k = K_0 - i\gamma$, the magnitude of the complex wavefunction has an exponential growth for large r at fixed t and, including the time-dependent factor $e^{-iEt/\hbar}$, that it decays with time at fixed r.

9. Calculate, in the Born approximation, the differential cross-section $d\sigma/d\Omega$ for a particle of mass m scattering off the potential

$$V(r) = \frac{Ae^{-\mu r}}{r}$$

as a function of the momentum transfer. Express this as a function of energy E and scattering angle θ, and show that, for large E, $d\sigma/d\Omega$ is proportional to E^{-2} at fixed $\theta \neq 0$. Show that $d\sigma/d\Omega$ is independent of E at $\theta = 0$. Show that the total cross section σ is proportional to E^{-1} for large E.

10. Calculate the Born approximation to the differential cross-section for the following potentials:

$$-V_0\, e^{-\lambda^2 r^2} \quad , \quad \frac{V_0}{r^2} \quad , \quad V_0\,\delta(r - a) \quad , \quad V(r) = \begin{cases} V_0, & r < a \\ 0\,, & r > a\,. \end{cases}$$

[*Note*: $\int_0^\infty (\sin x/x)\, dx = \pi/2$.]

11. For an atom at the origin, the elastic scattering amplitude for incident waves with wavevector $\mathbf{k}$ and outgoing waves with wavevector $\mathbf{k}' = k\hat{\mathbf{r}}$ is $f(\hat{\mathbf{r}})$. Show that the scattering amplitude for an atom at $\mathbf{d}$ is

$$e^{i\mathbf{q}\cdot\mathbf{d}} f(\hat{\mathbf{r}}) \quad \text{with} \quad \mathbf{q} = \mathbf{k} - \mathbf{k}'$$

A crystal has n atoms in each unit cell, located relative to the origin of the unit cell at $\mathbf{d}_j$, for which the scattering amplitudes are f_j, $j = 1, \ldots, n$. Show that the scattering amplitude due to the whole crystal is

$$\Delta(\mathbf{q}) \sum_{j=1}^{n} e^{i\mathbf{q}\cdot\mathbf{d}_j} f_j(\hat{\mathbf{r}})$$

with $|\Delta(\mathbf{q})|$ sharply peaked where $\mathbf{q}$ is equal to a reciprocal lattice vector.

12. A diamond is a lattice of identical carbon atoms located at $\mathbf{r} = \sum_i n_i \mathbf{a}_i$ and $\mathbf{r} = \sum_i n_i \mathbf{a}_i + \mathbf{d}$, $n_i \in \mathbf{Z}$ where

$$\mathbf{a}_1 = \frac{a}{2}(0,1,1), \quad \mathbf{a}_2 = \frac{a}{2}(1,0,1), \quad \mathbf{a}_3 = \frac{a}{2}(1,1,0), \quad \mathbf{d} = \frac{a}{4}(1,1,1).$$

In Question 3 of Example Sheet 2, you showed that the nearest neighbours of each atom form a regular tetrahedron and that there are two atoms in each unit cell.

The reciprocal lattice vectors $\{\mathbf{b}\}$ are defined by $\mathbf{b}\cdot\mathbf{r} \in 2\pi\mathbf{Z}$ for any $\mathbf{r} = \sum_i n_i \mathbf{a}_i$ with $n_i \in \mathbf{Z}$. Show that the scattering amplitude for scattering of waves on a diamond is proportional to

$$(1 + e^{i\mathbf{q}\cdot\mathbf{d}})\Delta(\mathbf{q})$$

where $\Delta(\mathbf{q})$ is strongly peaked on the reciprocal lattice. Determine the four lowest values of $|\mathbf{q}|$ for which there is non-zero scattering.