## PHY522; Quantum Mechanics II, Problem Set 3

Due Wed 9 Feb 2007 at the beginning of class.

In the following scattering problems the incident particle wavevector is $\vec{k} = k\hat{z}$, the scattered wavevector is $\vec{k}'$, the scattering is elastic so $|\vec{k}| = |\vec{k}'| = k$, the momentum transfer wavevector is $\vec{q} = \vec{k}' - \vec{k}$, and $\theta$ is the scattering angle between $\vec{k}$ and $\vec{k}'$.

### 1. Scattering from a 3D square well.

Assume that a quantum mechanical system can be usefully approximated by a 3D attractive square-well potential, of depth $V_0 < 0$ and radius $R$,

$$V(r) = V_0\,\Theta(R - r)\ . \tag{1}$$

(A nucleus is an example of such a system.)
Since this is a radially symmetric potential, the Born-order scattering amplitude can be written as a 1D integral,

$$f = -\frac{2m}{\hbar^2} q^{-1} \int_0^\infty r\,V(r)\,\sin(qr)\,dr \tag{2}$$

where $q = |\vec{q}| = 2k\sin(\theta/2)$.

a) (*5 pts*) Evaluate this scattering amplitude, and show that the result is

$$f = -\frac{2mV_0R^3}{\hbar^2}\frac{j_1(qR)}{qR}. \tag{3}$$

b) (*5 pts*) The differential cross section $d\sigma/d\Omega = |f|^2 = W(\theta)$ is explicitly

$$\frac{d\sigma}{d\Omega} = \left(\frac{2mV_0R^3}{\hbar^2}\right)^2 \left[\frac{j_1(qR)}{qR}\right]^2 \tag{4}$$

where (again) $q = 2k\sin(\theta/2)$. Plot this differential cross section $W(\theta)$ numerically relative to the value at $\theta = 0$, $W(\theta)/W(0)$, for three choices of the incident particle's de Broglie wavelength $\lambda$ relative to the well size $R$; $\lambda = 10R$, $R$ and $0.1R$. (Note that $qR = 2kR\sin(\theta/2) = 4\pi(R/\lambda)\sin(\theta/2)$. Also, the physical range of scattering angle is $\theta \in [0, \pi]$.)

## 2. Scattering from linear point sources.

As a simplest possible finite crystal scattering problem, consider scattering of an incident beam of particles of mass $m$ from a pair of ions at $\vec{x}_1 = \vec{0}$ and $\vec{x}_2 = R\hat{z}$, thus aligned along the incident beam. Model the ions as point source potentials,

$$V(\vec{x}) = v_0 \left( \delta(\vec{x} - \vec{x}_1) + \delta(\vec{x} - \vec{x}_2) \right). \tag{5}$$

(The astute student will note that this is yet another delta-shell potential.)

a) (*2 pts*) Show that the Born-order scattering amplitude for two such ions at any $\vec{x}_1$ and $\vec{x}_2$ is given by

$$f = -\frac{mv_0}{2\pi\hbar^2} \left[ e^{-i\vec{q}\cdot\vec{x}_1} + e^{-i\vec{q}\cdot\vec{x}_2} \right] . \tag{6}$$

b) (*2 pts*) For the specific positions given this becomes

$$f = -\frac{mv_0}{2\pi\hbar^2} \left[ 1 + e^{-iq_z R} \right] . \tag{7}$$

Draw a $\vec{k}, \vec{k}', \vec{q}$ scattering diagram and convince yourself and the grader that

$$q_z = -2k \sin^2(\theta/2) . \tag{8}$$

c) (*3 pts*) Evaluate the differential cross section $d\sigma/d\Omega = |f|^2$ for the $f$ given above, and confirm that

$$\frac{d\sigma}{d\Omega} = \frac{1}{2} \left( \frac{mv_0}{\pi\hbar^2} \right)^2 \left[ 1 + \cos\left( 2kR \sin^2(\theta/2) \right) \right] . \tag{9}$$

d) (*3 pts*) As is traditional we may also call this differential cross section $W(\theta)$. Plot the scattered intensity versus $\theta$ relative to forward scattering,

$$\frac{W(\theta)}{W(0)} = \frac{1}{2} \left[ 1 + \cos\left( 2kR \sin^2(\theta/2) \right) \right] \tag{10}$$

for the three cases $kR = 1/4, 1, 4$.

## 3. Scattering from an infinite crystal.

Support we model a crystal by an infinite set of local atomic potential wells, so the total potential is

$$V_{tot.}(\vec{x}) = \sum_{i=1}^{N} v(\vec{x} - \vec{R}_i) \ , \tag{11}$$

where $v(\vec{x})$ is the potential due to a single atom, the $\{\vec{R}_i\}$ are atomic position vectors, and $N = \infty$ ($N \sim 10^{20-23}$ in practice) is the total number of atoms.

a) (*3 pts*) Using the first Born approximation, show that the scattering amplitude $f(\vec{q}; \vec{R}_i)$ from a single atom at $\vec{R}_i$ is related to the scattering amplitude $f_0(\vec{q})$ from an atom at the origin by

$$f(\vec{q}; \vec{R}_i) = f_0(\vec{q}) \, e^{-i\vec{q}\cdot\vec{R}_i} \ . \tag{12}$$

and hence the scattering amplitude from the entire crystal is

$$f_{tot.}(\vec{q}) = f_0(\vec{q}) \sum_{i=1}^{N} e^{-i\vec{q}\cdot\vec{R}_i} \ . \tag{13}$$

b) (*3 pts*) If the crystal is a regular periodic lattice, the atomic position vectors are integer multiples of three unit-cell vectors, $\vec{R}_i = m_a\vec{a} + m_b\vec{b} + m_c\vec{c}$, and the sum of phases above is of the form

$$\sum_{m_a, m_b, m_c} e^{-i(m_a\vec{q}\cdot\vec{a} + m_b\vec{q}\cdot\vec{b} + m_c\vec{q}\cdot\vec{c})} \ .$$

Given that there is no simple relation between the basis vectors $\vec{a}, \vec{b}, \vec{c}$ in general, show that the condition for maximum constructive interference in scattering from the crystal is $\vec{q}\cdot\vec{a} = 2\pi n_a$, $\vec{q}\cdot\vec{b} = 2\pi n_b$ and $\vec{q}\cdot\vec{c} = 2\pi n_c$. This is known as "Bragg scattering", and at each such $\vec{k}' = \vec{k} + \vec{q}_{n_a,n_b,n_c}$ in a scattering experiment one may often observe intense elastic "Bragg peaks".

c) (*4 pts*) The Bragg scattering condition

$$\vec{k}' = \vec{k} + \vec{q}_{n_a,n_b,n_c} \tag{14}$$

does not appear to automatically satisfy the elastic scattering (energy conservation) constraint $\vec{k}'^2 = \vec{k}^2$. Explain intuitively what this additional constraint tells you about the physical conditions under which Bragg scattering from a crystal takes place.