Leo Radzihovsky, Spring 2016

PHYS 5260: Quantum Mechanics - II

Homework Set 5

Issued March 14, 2016
Due April 11, 2016

Reading Assignment: Shankar, Ch.19; Sakurai, Ch 7.

1. (10 points) Compute the probability current density $\mathbf{j}$ for a state $\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\frac{e^{ikr}}{r}$. Argue that far away from a target (of interest in a scattering problem) and $\theta \neq 0$, many of the terms oscillate fast with θ and therefore average to zero, when integrated even over a narrow range of θ (physically corresponding to acceptance/resolution window of the detector). Thereby show that $\mathbf{j}$ reduces to $\mathbf{j} = \frac{\hbar\mathbf{k}}{m} + \frac{\hbar k}{m}\frac{|f(\theta)|^2}{r^2}\hat{\mathbf{r}}$, with the second contribution corresponding to the scattered current density.

2. (24 points) Diffraction from a crystal: Bragg scattering

   Within Born approximation, compute a scattering amplitude $f(\theta, \phi)$ and the corresponding differential scattering cross section $\frac{d\sigma}{d\Omega}$ for scattering from a large cubic crystal, i.e., from a periodic array of identical "blobs" (e.g., atoms) located at lattice sites $\mathbf{R_n} = an_1\hat{\mathbf{x}} + an_2\hat{\mathbf{y}} + an_3\hat{\mathbf{z}}$, with $-N \leq n_i \leq N$; $(2N)^3$ is the number of lattice sites.

   The scattering potential of the crystal is given by $V(\mathbf{r}) = \sum_{\mathbf{R_n}} v(|\mathbf{r} - \mathbf{R_n}|)$, where $v(r)$ is an isotropic potential characterizing an atom.

   (a) Work out the above scattering for
      i. $v(r) = v_0 a^3 \delta^3(\mathbf{r})$,
      ii. $v(r) = v_0 e^{-r^2/a^2}$,
      iii. $v(r) = v_0\theta(a - r)$, (where the theta-function $\theta(r)$ is of course not to be confused with the polar angle θ),

      where a models a finite radius of an atom.

   (b) What is the condition on $\mathbf{q}$ that determines the location of Bragg peaks that characterize the scattering amplitude (as you should discover)?

   (c) Show that the three cases of $v(r)$ above only differ in the form factors, that provide an envelope for the array of Bragg peaks.

(d) Show that the form factors for cases (ii) and (iii) become isotropic in the limit of low angle θ scattering, such that $ka \to 0$ and/or long wavelength and reduce in form to that of (i).

Hints:

(a) You should find our friend, Poisson summation formula

$$\sum_{n=-N}^{N} e^{iqn} = \frac{\sin q(N+1/2)}{\sin q/2}, \tag{1}$$

$$\overset{N\gg 1}{=} \sum_p 2N\delta_{q,2\pi p} \tag{2}$$

$$= \sum_p 2\pi\delta(q-2\pi p) \tag{3}$$

extremely useful.

(b) Your calculation of the scattering for the crystal should break up into computation of a scattering amplitude for an atom (giving you a so-called "form factor"), and a computation of coherent superposition from all atoms, with this second part independent of $v(r)$ and only determined by crystal structure (cubic here).

3. (20 points) Scattering amplitude properties

(a) Using the relation between scattering amplitude $f_\ell(k)$ for partial wave ℓ (angular momentum ℓ) and the scattering matrix S_ℓ, show that the unitarity of S_ℓ (particle conservation) implies that $f_\ell(k) = 1/(\tilde{F}_\ell(k) - ik)$, where $\tilde{F}_\ell(k)$ is a function of k (or equivalently energy $E = \hbar^2k^2/2m$), whose details are determined by the potential $V(r)$. Show that $\tilde{F}_\ell(k) = k/\tan\delta_\ell$, with δ_ℓ scattering phase shift in ℓth partial wave.

(b) By analyzing general properties of the Schrodinger's equation (that determine $\tilde{F}_\ell(k)$), it can be shown that $\tilde{F}_\ell(k) = F_\ell(k^2)/k^{2\ell}$, where $F_\ell(k^2)$ is another function that is analytic in k^2; you do not need to show this for a general case, but we will see examples of this for specific $V(r)$ below. Use this form of $f_\ell(k)$ to argue that generically low energy scattering is dominated by s-wave ($\ell = 0$) scattering, with other partial waves (channels) subdominant.

(c) At low energy $F_\ell(k^2)$ can be well approximated by its two lowest Taylor expansion terms, $F_\ell(k^2) \approx c_0 + \frac{1}{2}c_1k^2$. For the dominant s-wave scattering $c_0 \equiv -1/a$, $c_1 \equiv r_*$, with a the scattering length and r_* the effective range of the potential, giving

$$f_0(k) = \frac{1}{-a^{-1} + \frac{1}{2}r_*k^2 - ik}. \tag{4}$$

Hence show that at low energies the total cross section is generically given by $\sigma = 4\pi a^2$.

(d) A weakly attractive potential $V(r)$ is characterized by a negative scattering length. However, as its depth V is made sufficiently deep at some point V_c, the potential will admit a bound state. Around this point generically $a(V) \sim 1/(V - V_c)$, diverges to negative infinity, changes sign and comes back to a finite value from a positive infinity.

Recalling that poles of the scattering amplitude (and matrix) give bound states of $V(r)$, show that as this shallow bound state develops, its energy is given by $E_b = -\frac{\hbar^2}{2ma^2}$. By thinking about the form of the scattered part of the wavefunction, argue that the pole corresponds to a true bound state only for $a > 0$, i.e., a pole for $a < 0$ is unphysical, at least for $|a| \gg r_*$.

4. (23 points) Hard sphere scattering

Consider scattering from a hard (infinitely massive) sphere characterized by potential $V(r < r_0) = \infty$ and $V(r > r_0) = 0$.

(a) For low energy scattering, $kr_0 \ll 1$, focussing on the leading order contribution of the $\ell = 0, 1$ (s- and p-wave) partial waves, compute the corresponding (i) scattering phase shifts $\delta_{0,1}(k)$, (ii) scattering amplitudes $f_{0,1}(k)$, and (iii) total cross section $\sigma(k)$ to lowest nontrivial order in kr_0. Extract from (ii) the scattering length a and the effective range r_*, characterizing $\ell = 0$ case.

(b) For high energy scattering, $kr_0 \gg 1$, argue on physical grounds why many partial waves ℓ upto $\ell_{max} \approx kr_0$ need to be included.

Hint: Think of the range of the potential, impact parameter and the corresponding angular momentum.

(c) For high energy scattering, $kr_0 \gg 1$, verify above expectation by computing the scattering phase shifts δ_ℓ, focussing separately on high $\ell \gg kr_0$ and and low $\ell \ll kr_0$ partial waves.

Hint: You will find asymptotic forms of spherical Bessel and Neumann functions (given in Shankar) very useful.

(d) After obtaining the phase shifts, δ_ℓ, in the limit $kr_0 \gg 1$, compute approximately the scattering matrix S_ℓ and show that the total cross section is given by $\sigma \approx 2\pi r_0^2$.

Hint: In this high energy limit, one can replace sum over ℓ by integral and approximate an fast oscillating function by its mean.

5. (23 points) Scattering from a soft sphere: square-well and square barrier

Consider scattering from a potential $V(r) = -V_0\theta(r_0 - r)$.

(a) Recalling that the general radial solution is given by a linear combination of spherical Bessel and Neumann functions, $\psi_\ell(r) = B_\ell j_\ell(kr) + C_\ell n_\ell(kr)$, requiring that the function is well behaved everywhere in the physical region, and matching the inner and outer solutions at $r = r_0$, show that

$$\tan \delta_\ell(k) = \frac{k j'_\ell(kr_0) j_\ell(\kappa r_0) - \kappa j_\ell(kr_0) j'_\ell(\kappa r_0)}{k n'_\ell(kr_0) j_\ell(\kappa r_0) - \kappa n_\ell(kr_0) j'_\ell(\kappa r_0)}, \tag{5}$$

where κ, k are inner and outer wavevectors, respectively.

(b) Show that at low energies the scattering amplitude $f_\ell(k)$ is indeed characterized by a function $\tilde{F}_\ell(k) = F_\ell(k^2)/k^{2\ell}$, as asserted on general grounds in problem 3, above.

(c) Since, as discussed above, the low energy scattering is dominated by s-wave amplitude, show that above expression reduces to (it is actually more convenient to rederive this result from scratch, focussing on $\ell = 0$ from the start) $\tan(kr_0 + \delta_0) = \frac{k}{\kappa} \tan \kappa r_0$ that gives:

$$\tan \delta_0 = \frac{k \tan \kappa r_0 - \kappa \tan kr_0}{\kappa + k \tan kr_0 \tan \kappa r_0} \tag{6}$$

(d) Use this to show that at low energies $kr_0 \ll 1$, the s-wave scattering amplitude for the attractive case of $V_0 > 0$ is given by $f_0(k) \approx (\tan \kappa r_0 - \kappa r_0)/\kappa$, and that for strongly repulsive case $V_0 < 0$ ($|V_0| > \hbar^2 k^2/2m$) it is given by $f_0(k) \approx (\tanh \kappa r_0 - \kappa r_0)/\kappa$.

(e) Extract the corresponding scattering lengths a and effective ranges r_*, characterizing low energy scattering for above two cases.

(f) Show that for a weak potential $|V_0| \ll \hbar^2/mr_0^2$ both attractive and repulsive cases give Born scattering cross section $\sigma \approx (4\pi r_0^2/9)(\kappa r_0)^4$, and in the strongly repulsive case $f_0 \approx -r_0$ and $\sigma \approx 4\pi r_0^2$, as expected.