<u>SOLUTIONS for Homework #5</u>

1. The positive energy solution corresponds to the *scattering* of the wave generated by a source far away on the right hand side and reflected from the potential. The incident wave is ($x > a$, $V = 0$)

$$\psi_i = Ae^{-ikx}, \quad x > a, \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \tag{1}$$

with an arbitrary amplitude A. The reflected wave in the same region, $x > a$, describes the motion in the opposite direction but with the same absolute value of the wave vector k,

$$\psi_r = Be^{ikx}, \quad x > a. \tag{2}$$

Since the probability current in the positive direction of the x-axis,

$$j = \frac{\hbar k}{m}(|B|^2 - |A|^2), \tag{3}$$

is constant due to the continuity equation (in the one-dimensional case for a stationary situation $dj/dx = 0$), and the current vanishes at the infinite barrier at $x = 0$, we obtain $j = 0$ everywhere, the wave is totally reflected. Then the expression (3) shows that the amplitudes of the incident and reflected waves are equal, $|B| = |A|$. But the reflected wave, traveling to the wall and back, acquires an additional *energy-dependent phase* $\delta(E)$ (do not confuse with the delta-function!). We can always define

$$B = A\exp(2i\delta + i\pi). \tag{4}$$

With this definition of the reflection phase,

$$\psi = -A\left[e^{i(kx+2\delta)} - e^{-ikx}\right], \quad x > a. \tag{5}$$

Taking the factor $\exp(i\delta)$ outside the square bracket, we write down this solution in the convenient form,

$$\psi = D\sin(kx + \delta), \quad D = -2iAe^{i\delta}. \tag{6}$$

If experimentally one can observe only the reflected (scattered in three-dimensional geometry) wave, then the phase shift δ is the only observable quantity. After measuring $\delta(E)$ one can try to solve the *inverse scattering problem* and determine the potential which caused this phase shift.

To find the phase shift, we need to consider explicitly the wave function in the well region. With no well at $0 < x < a$, we would have the form (6) of the solution valid everywhere up to the origin. Then the boundary condition $\psi(0) = 0$ would lead to $\delta \equiv 0$ at any energy. This is easy to understand since in the absence of any distortion along the road the wave simply changes it sign by π at the reflection from an impenetrable wall, and this change is already accounted for by our definition (4) of the relation between B and A. The additional phase comes from the fact that the motion is distorted by the well at $0 < x < a$, where the wave vector is

$$k' = \sqrt{\frac{2m}{\hbar^2}\,(E + V_0)}. \tag{7}$$

Inside the well the solution is the superposition

$$\psi = A' e^{-ik'x} + B' e^{ik'x}, \quad 0 < x < a. \tag{8}$$

Because of the boundary condition $\psi(0) = 0$, we see that $B' = -A'$, and the solution is in fact

$$\psi = C \sin(k'x), \quad C = 2iA'. \tag{9}$$

Now we need to match the functions (6) and (9) as well as their derivatives at the well boundary $x = a$:

$$C \sin(k'a) = D \sin(ka + \delta), \quad Ck' \cos(k'a) = Dk \cos(ka + \delta). \tag{10}$$

As always in such problems, it is useful to eliminate the constants of normalization matching the *logarithmic derivative* ψ'/ψ:

$$k \tan(k'a) = k' \tan(ka + \delta). \tag{11}$$

This determines the scattering phase

$$\delta(k) = -ka + \tan^{-1}\left[\frac{k}{k'}\tan(k'a)\right]. \tag{12}$$

The first term here does not depend on the potential and has a pure kinematic origin: if the particle would not enter the region $0 < x < a$ of the potential at all, the phase of the wave function (5) would be smaller than for free motion by $2\delta = 2ka$, the phase of free motion from $x = a$ to the origin and back. Subtracting ka we add in (1) the phase induced by the motion inside the barrier.

The scattering coefficient defined in the textbook,

$$|1 - e^{2i\delta}|^2 = 4\sin^2\delta, \tag{13}$$

exhibits *resonances* (equal to 1) at energies which correspond to

$$\delta = \pi\left(n + \frac{1}{2}\right), \quad n = 0, 1, ... \tag{14}$$

In the low-energy scattering, $ka \ll 1$ (the wavelength of the particle is much greater than the width of the well), the resonances appear as the well is made broader and deeper. The first resonance occurs when $k'a \approx \pi/2$; since $ka \ll 1$, this means that

$$k_0 a \approx \pi/2, \quad k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}. \tag{15}$$

This is the condition of the appearance of the first bound state in the well. Indeed, the sinusoidal wave function (9) with zero energy, $k' = k_0 = \pi/(2a)$, approaches the edge $x = a$ of the well with the zero derivative so that, in a little deeper well, the slope of the wave function at the boundary is getting negative, and the wave function would be able to match continuously the decreasing exponent as it is required for the bound state.

For a very narrow well, when $ka \ll 1$ *and* $k'a \ll 1$, the scattering phase will be small as well. In this case we can use the expansions

$$\tan z \approx z + \frac{z^3}{3}, \quad \tan^{-1} z \approx z - \frac{z^3}{3}, \tag{16}$$

and obtain from (12)

$$\delta = \frac{1}{3}\, a^3 k(k'^2 - k^2) = \frac{1}{3}(ka)\frac{2mV_0 a^2}{\hbar^2}. \tag{17}$$

This result corresponds to *perturbation* theory: it contains the interaction parameter $2mV_0a^2/\hbar^2$ (the ratio of potential energy V_0 to kinetic energy $\hbar^2/(2ma^2)$ required for localizing a particle interaction region) and the small low-energy parameter ka.

2. For energy higher than the height of the barrier, $E > V_0$, we proceed analogously to the previous problem. Let us consider the case of $E < V_0$. The general solution of the Schrödinger equation for the inner region under the barrier, $0 < x < a$, is a superposition of the two exponents,

$$\psi(x) = A\exp(\kappa x) + B\exp(-\kappa x), \quad \hbar^2\kappa^2 = 2m(V_0 - E). \tag{18}$$

The boundary condition $\psi(0) = 0$ selects the hyperbolic sine as a correct superposition,

$$\psi(x) = C\sinh(\kappa x), \quad 0 < x < a, \tag{19}$$

compare with the usual sine in the previous case, eq. (9). The scattering solution in the outer region of free motion is a superposition of the incident and reflected waves. Since at $x = 0$ we have, as in *Problem 1*, an impenetrable well, the total current vanishes, and the reflected and incident currents are to be equal. As a result, the outer wave function can always be written as in (6),

$$\psi(x) = D\sin(kx+\delta), \quad \hbar^2k^2 = 2mE, \quad x > a. \tag{20}$$

The common normalization D is arbitrary so that we have only one unknown coefficient C. Together with the phase shift δ, it is to be found from the continuity of the wave function and its derivative at $x = a$. For the amplitude C we find

$$C = \frac{\sin(ka+\delta)}{\sinh(\kappa a)}D. \tag{21}$$

The logarithmic derivative ψ'/ψ gives

$$\delta = -ka + \tan^{-1}\Big(\frac{k}{\kappa}\tanh(\kappa a)\Big). \tag{22}$$

In the low energy limit, $k/\kappa \ll 1$, $\tan^{-1}$ can be substituted by its argument,

$$\kappa a \approx \kappa_0 a \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}}, \tag{23}$$

and

$$\delta = -ka\Big[1 - \frac{\tanh(\kappa_0 a)}{\kappa_0 a}\Big]. \tag{24}$$

Here the phase shift is small (linear in k). For the infinite wall, $\kappa_0 \to \infty$ but $\tanh(\kappa_0 a)$ is finite changing in the interval from -1 to 1. Therefore, as agrees with the meaning of the phase shift,

$$\delta \to -ka, \quad V_0 \to +\infty, \tag{25}$$

the particle does not penetrate in the repulsion region, and the whole negative phase is originated by the size of the scatterer.

3. The potential

$$U(x) = g[\delta(x-a) + \delta(x+a)] \tag{26}$$

consists of two delta-peaks and requires the matching of the wave functions in three regions. On the left of $x = -a$, considering that the wave of the unit amplitude comes from the left,

$$\psi_1(x) = e^{ikx} + De^{-ikx}, \quad x < -a. \tag{27}$$

In between the peaks it is convenient to start counting the phase from the point of the left peak $x = -a$,

$$\psi_2(x) = A\sin[k(x+a)] + B\cos[k(x+a)], \quad -a < x < a. \tag{28}$$

On the right of the right peak, where only the transmitted wave is possible,

$$\psi_3(x) = Ce^{ik(x-a)}. \tag{29}$$

The matching condition at the point $x = x_0$, where the delta-peak of intensity g is present in the potential, is that of continuity of the function and a jump of its derivative,

$$\psi_>(x_0) = \psi_<(x_0) \equiv \psi(x_0), \quad \psi'_>(x_0) - \psi'_<(x_0) = \frac{2mg}{\hbar^2}\psi(x_0). \tag{30}$$

In our case we obtain:

$$\psi_1(-a) = \psi_2(-a) \quad \rightsquigarrow \quad e^{-ika} + De^{ika} = B, \tag{31}$$

$$\psi_2(a) = \psi_3(a) \quad \rightsquigarrow \quad A\sin(2ka) + B\cos(2ka) = C, \tag{32}$$

$$\psi'_2(-a) - \psi'_1(-a) = \frac{2mg}{\hbar^2}\psi(-a) \quad \rightsquigarrow \quad A - i(e^{-ika} - De^{ika}) = \frac{2mg}{k\hbar^2}B, \tag{33}$$

$$\psi'_3(a) - \psi'_2(a) = \frac{2mg}{\hbar^2}\psi(a) \quad \rightsquigarrow \quad iC - A\cos(2ka) + B\sin(2ka) = \frac{2mg}{k\hbar^2}C. \tag{34}$$

Solving eqs. (32) and (34), we obtain

$$A = C[\sin(2ka) + (i-\alpha)\cos(2ka)], \quad B = C[\cos(2ka) - (i-\alpha)\sin(2ka)], \tag{35}$$

where the dimensionless parameter is introduced reflecting the relative strength of the delta-potential compared to kinetic energy,

$$\alpha = \frac{2mg}{k\hbar^2}. \tag{36}$$

Eliminating the reflection amplitude D from (31) and (33), we find

$$A = 2ie^{-ika} - (i-\alpha)B, \tag{37}$$

and comparing this result with (35),

$$C = \frac{2ie^{-ika}}{2\cos(2ka)(i-\alpha) + \sin(2ka)[1-(i-\alpha)^2]}; \tag{38}$$

the transmission coefficient is equal to

$$T(E) = |C|^2 = \frac{4}{4\alpha^2[\sin(2ka) - \cos(2ka)]^2 + [(2-\alpha^2)\sin(2ka) - 2\alpha\cos(2ka)]^2}. \tag{39}$$

The *transmission resonance* corresponds to the maximum value $T(E) = 1$. Then $R(E) = |D|^2 = 0$. The condition of vanishing coefficient D is equivalent to $B = e^{-ika}$. Comparing this with the expression (35) for B and equating two answers for C, we obtain the condition for resonance energies,

$$\tan(2ka) = -\frac{1}{\alpha} = -\frac{k\hbar^2}{2mg}. \tag{40}$$

The corresponding wave vectors k and energies E can be easily found graphically from the comparison of the two sides of eq. (40). High energy resonances, $n \gg mga/\hbar^2$, are almost equidistant in the wave vector scale, $k_n \approx (\pi/2a)(n + 1/2)$. These values correspond to quasibound states in the "box" between the delta-peaks.

4. *a.* Consider the asymptotic form of the wave function with energy $E > U_0$ far away from the barrier:

$$\psi(x \to -\infty) = Ae^{ikx} + Be^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} > 0, \tag{41}$$

$$\psi(x \to \infty) = Ce^{ik'x}, \quad k' = \sqrt{\frac{2m(E - U_0)}{\hbar^2}} > 0. \tag{42}$$

The reflection and transmission coefficients are equal to

$$R = \frac{j_r}{j_i} = \frac{|B|^2}{|A|^2}, \quad T = \frac{j_t}{j_i} = \frac{k'}{k}\frac{|C|^2}{|A|^2}. \tag{43}$$

The probability current is conserved,

$$j = j_i - j_r = j_t \quad \rightsquigarrow \quad k|A|^2(1 - R) = k|A|^2 T. \tag{44}$$

This is equivalent to

$$R + T = 1. \tag{45}$$

If energy $E < U_0$, the transmitted part of the wave function asymptotically is a falling exponent,

$$\psi(x \to \infty) = Ce^{-\kappa x}, \quad \kappa = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}} > 0. \tag{46}$$

In this case $j_t = 0$, $T = 0$, $R = 1$, $|A| = |B|$.

b. Consider two arbitrary solutions ψ_l and ψ_r of the Schrödinger equation for a given potential $U(x)$ and the same energy E,

$$\psi''_{l,r} + k^2(x)\psi_{l,r} = 0, \quad k(x) = \sqrt{\frac{2m[E - U(x)]}{\hbar^2}}. \tag{47}$$

Multiplying the equation for ψ_l by ψ_r and subtracting the equation for ψ_r multiplied by ψ_l we see that the terms with the wave vector $k(x)$ cancel, and we come, similarly to the derivation of the continuity equation, to

$$\psi_r\psi_l'' - \psi_l\psi_r'' = 0. \tag{48}$$

This means the conservation (x-independence) of the *Wronskian*

$$W(\psi_r, \psi_l) \equiv W_{rl}(x) = \psi_r\psi_l' - \psi_l\psi_r', \tag{49}$$

$$\frac{dW_{rl}}{dx} = 0, \quad \rightsquigarrow \quad W_{rl} = \text{ const.} \tag{50}$$

The wave vector of the problem has the following asymptotic form:

$$k(x) = \sqrt{\frac{2mE}{\hbar^2}} \equiv k, \quad x \to -\infty, \tag{51}$$

and

$$k(x) = \sqrt{\frac{2m(E-U_0)}{\hbar^2}} \equiv k', \quad x \to \infty. \tag{52}$$

We select as our pair of solutions ψ_l generated by the unit source on the far left,

$$\psi_l(x) = \begin{cases} e^{ikx} + Be^{-ikx}, & x \to -\infty, \\ Ae^{ik'x}, & x \to \infty, \end{cases} \tag{53}$$

and ψ_r generated by the unit source on the far right,

$$\psi_r(x) = \begin{cases} Ce^{-ikx}, & x \to -\infty, \\ e^{-ik'x} + De^{ik'x}, & x \to \infty. \end{cases} \tag{54}$$

We are interested in comparing two transmission coefficients,

$$T_r = \frac{k}{k'}|C|^2, \quad T_l = \frac{k'}{k}|A|^2. \tag{55}$$

To do this comparison, we calculate the same Wronskian (49) in the far left region and in the far right region,

$$W_{rl}(x \to -\infty) = 2ikC, \quad W_{rl}(x \to \infty) = 2ik'A. \tag{56}$$

Since $W_{rl} =$const, this implies

$$kC = k'A \quad \rightsquigarrow \quad T_r = T_l. \tag{57}$$