<u>SOLUTIONS for Homework #6</u>

1. *a.* Outside the well, the wave function of a bound state describes the exponential penetration into the classically forbidden region,

$$\psi(x) = Be^{-\kappa x}, \quad \kappa = \sqrt{\frac{2m\epsilon}{\hbar^2}}, \tag{1}$$

where instead of negative energy E we use positive binding energy $\epsilon = -E$. The penetration length is

$$\frac{1}{\kappa} = \frac{\hbar}{\sqrt{2m\epsilon}} \approx 4.3\,\text{fm}, \tag{2}$$

where $m \approx m(\text{proton})/2 \approx 938$ MeV$/2c^2$ is the reduced mass for relative motion. Note that $\kappa^{-1} \gg a = 1.7$ fm.

b. The wave function inside the well, because of the boundary condition $\psi(0) = 0$ at the origin, is

$$\psi(x) = A\sin(kx), \quad k = \sqrt{\frac{2m[E-(-U_0)]}{\hbar^2}} = \sqrt{\frac{2m(U_0-\epsilon)}{\hbar^2}}. \tag{3}$$

The *critical* depth of the potential corresponds to the zero binding energy, $\epsilon \to 0$. The first opportunity to match continuously the inner function (3) with the outer function (1) arises when the sinusoidal function comes to the boundary $x = a$ horizontally, $(ka)_{crit} = \pi/2$. This determines the critical depth

$$U_0^{crit} = \frac{\hbar^2 k_{crit}^2}{2m} = \frac{\pi^2\hbar^2}{8ma^2} = 35.3 \text{ MeV}. \tag{4}$$

c. In dimensionless variables $\xi = ka$ and $\eta = \kappa a$, the matching conditions are

$$\xi^2 + \eta^2 = \frac{2mU_0}{\hbar^2}, \tag{5}$$

$$\eta = -\xi \cot\xi. \tag{6}$$

At the critical depth (4), $\epsilon = 0$ which corresponds to $\xi = \pi/2$ and $\eta = 0$. For a deeper well, $U_0 = U_0^{crit} + \delta U_0$ and $\xi = \pi/2 + \alpha$. We take the terms of the lowest nonvanishing order (linear in α). Then $\cot\xi = \cot(\pi/2+\alpha) = -\tan\alpha \approx -\alpha$, and it follows from (6) that $\eta \approx (\pi\alpha)/2$. In eq. (5) we can neglect η^2 as a quantity of the second order and obtain after that

$$\xi^2 = \left(\frac{\pi}{2} + \alpha\right)^2 \approx \frac{\pi^2}{4} + \pi\alpha = \frac{2m(U_0^{crit} + \delta U_0)a^2}{\hbar^2}. \tag{7}$$

Zero order terms cancel due to (4), and the first order terms determine

$$\alpha = \frac{2ma^2}{\pi\hbar^2}\delta U_0 = \frac{\pi}{4}\frac{\delta U_0}{U_0^{crit}} \tag{8}$$

where again eq. (4) was used. Now, with the definition of κ, eq.(1), we find for the binding energy

$$\epsilon = \frac{\hbar^2\kappa^2}{2m} = \frac{\hbar^2}{2ma^2}\eta^2 \approx \frac{\hbar^2}{2ma^2}\left(\frac{\pi\alpha}{2}\right)^2 = U_0^{crit}\alpha^2. \tag{9}$$

Using this value of α in (8), we come to

$$\delta U_0 = \frac{4}{\pi}U_0^{crit}\alpha = \frac{4}{\pi}\sqrt{\epsilon U_0^{crit}} \approx 11.2 \text{ MeV}. \tag{10}$$

The full depth of the well is, in this approximation, $U_0 \approx 46.5$ MeV.

d. The wave function of the problem is (we do not need the common normalization factor)

$$\psi(x) = \begin{cases} \sin kx, & x < a, \\ Be^{-\kappa x}, & x > a. \end{cases} \tag{11}$$

The matching condition is

$$B = \sin(ka)e^{\kappa a}. \tag{12}$$

The probability to be inside the well is proportional to the integral over the internal part of the wave function squared,

$$I_i = \int_0^a dx\psi^2 = \int_0^a dx \sin^2 kx = \frac{a}{2} - \frac{\sin(2ka)}{4k}. \tag{13}$$

The external probability is proportional to

$$I_e = B^2 \int_a^\infty dx e^{-2\kappa x} = \frac{B^2}{2\kappa}e^{-2\kappa a} = \frac{\sin^2(ka)}{2\kappa}. \tag{14}$$

For the near-critical depth $ka \approx \pi/2$,

$$I_i \approx a/2, \quad I_e \approx \frac{1}{2\kappa}, \tag{15}$$

so that $I_e/I_e \approx 1/(\kappa R) \gg 1$. For the realistic values which have been found earlier, $I_e/I_i \approx 2.07/0.95 = 2.18$, or $I_e \approx 69\%$, $I_i \approx 31\%$.

2. The two-well potential

$$V(x) = -g[\delta(x-a) + \delta(x+a)] \tag{16}$$

is an even function of the coordinate, $V(x) = V(-x)$. The stationary states $\psi(x)$ in this case have certain parity,

$$\hat{\mathcal{P}}\psi^{(\pm)} = \pm\psi^{(\pm)}. \tag{17}$$

This facilitates our task since it is sufficient to satisfy the matching conditions at one singular point, let say $x = +a$, only. The conditions at the mirror point $x = -a$ will be satisfied automatically by an even, for $\psi^{(+)}$, or odd, for $\psi^{(-)}$, continuation from positive to negative values of x according to $\psi^{(\pm)}(-x) = \pm\psi^{(\pm)}(x)$. Thus, we have three distinct regions,

$$I.\, -\infty < x < -a; \quad II.\, -a < x < a; \quad III.\, a < x < \infty, \tag{18}$$

and we make the matching required at a point of a δ-function singularity at the right peak, $x = a$,

$$\psi_3^{(\pm)}(a) = \psi_2^{(\pm)}(a) \equiv \psi^{(\pm)}(a), \quad \psi_3^{(\pm)'}(a) - \psi_2^{(\pm)'}(a) = \frac{2m(-g)}{\hbar^2}\psi^{(\pm)}(a). \tag{19}$$

We are looking for a *bound* state solution with negative energy $E = -\epsilon$. In all three regions (18) the solutions are exponential,

$$\psi(x) \sim e^{\pm\kappa x}, \quad \kappa = \sqrt{\frac{2m\epsilon}{\hbar^2}} > 0. \tag{20}$$

In the region III only the decaying $\exp(-\kappa x)$ is admissible. In the middle region II the wave function is an even or odd superposition of the exponents (20), i.e. $\cosh(\kappa x)$ or $\sinh(\kappa x)$, respectively. Thus, the solutions have the form

$$\psi_1^{(\pm)}(x) = \pm A^{(\pm)} e^{\kappa x}, \tag{21}$$

$$\psi_2^{(+)}(x) = B^{(+)}\cosh(\kappa x), \quad \psi_2^{(-)}(x) = B^{(-)}\sinh(\kappa x), \tag{22}$$

$$\psi_3^{(\pm)}(x) = A^{(\pm)} e^{-\kappa x}. \tag{23}$$

For the matching conditions, eqs. (19), we find at $x = a$:

$$\psi^{(+)}(a) = A^{(+)}e^{-\kappa a} = B^{(+)}\cosh(\kappa a), \quad \psi^{(-)}(a) = A^{(-)}e^{-\kappa a} = B^{(-)}\sinh(\kappa a); \tag{24}$$

$$\left(\frac{2mg}{\hbar^2} - \kappa\right) A^{(+)}e^{-\kappa a} = \kappa B^{(+)}\sinh(\kappa a), \quad \left(\frac{2mg}{\hbar^2} - \kappa\right) A^{(-)}e^{-\kappa a} = \kappa B^{(-)}\cosh(\kappa a). \tag{25}$$

By division we can eliminate the coefficients $A^{(\pm)}$ and $B^{(\pm)}$ and obtain the transcendental equations for κ, or binding energy ϵ:

$$\frac{2mg}{\hbar^2} - \kappa = \kappa \tanh(\kappa a) \text{ (even)}, \quad \frac{1}{(2mg/\hbar^2) - \kappa} = \frac{1}{\kappa}\tanh(\kappa a) \text{ (odd)}. \tag{26}$$

It is convenient to introduce the dimensionless energy $y^2 = \epsilon/\epsilon_0$ where $\epsilon_0 = \hbar^2/(2ma^2)$ is, by order of magnitude, the characteristic energy required according to the uncertainty relation for localizing the particle on a length $\sim a$. Then $\kappa a = y$. We use also the dimensionless parameter $\eta = 2mga/\hbar^2$ of the effective attraction strength. The resulting equations for y read

$$\frac{\eta - y}{y} = \tanh\, y \text{ (even)}, \qquad \frac{y}{\eta - y} = \tanh\, y \text{ (odd)}. \tag{27}$$

In the search for a solution, a graphical sketch of the two sides of eqs. (27) is useful. In the physical region of $y > 0$, we have $\tanh\, y$ changing from 0 to 1, and the asymptotic value of 1 is approached from below very fast when $y \geq 1$. This means that always $y < \eta$. For small $\eta < 1$, the derivative of the left hand side of the condition for the *odd* solution is $(d/dy)[y/(\eta - y)] = \eta/(\eta - y)^2 > 1/\eta > 1$. Therefore this function goes above $\tanh y$ and there is no bound odd solutions. The odd solution appears at $\eta = 1$, starting with zero binding energy. Near the critical point $\eta = 1$ the solution is small, $y \ll 1$, and we can expand $\tanh\, y \approx y - y^3/3$. In the vicinity of this point

$$\frac{y}{\eta - y} \approx \frac{1}{\eta}\left(1 + \frac{y}{\eta}\right) = y, \quad \rightsquigarrow \quad y \approx \eta(\eta - 1) \approx \eta - 1. \tag{28}$$

In other words, the odd solution becomes more and more bound as the attraction strength η grows beyond its critical value $\eta = 1$, $\epsilon \approx \epsilon_0(\eta - 1)^2$. For the *even* case, the solution exists always. Indeed, for small η, y is even smaller. Assuming $y < \eta \ll 1$, we obtain from (27

$$\frac{\eta}{y} - 1 \approx y \quad \rightsquigarrow \quad \eta(1 - \eta), \tag{29}$$

the value of binding energy increases as $y^2 \sim \eta^2$.

In the limit of large separation, $\eta \gg 1$, the wells only slightly perturb each other. Therefore two solutions should exist corresponding to the even and odd superposition of the solutions for the individual wells. Since $\tanh\, y$ rapidly approaches 1, it is clear that both solutions give $y \approx \eta/2$. To find their exponentially small splitting we need to use the expansion

$$\tanh\, y = \frac{e^y - e^{-y}}{e^y + e^{-y}} = \frac{1 - e^{-2y}}{1 + e^{-2y}} \approx 1 - 2e^{-2y}. \tag{30}$$

For the small deviation ξ from the asymptotic limit, $y = (\eta/2) + \xi$, and for the even solution, the equation (27) becomes

$$\frac{\eta}{y} - 1 \approx 1 - 4\frac{\xi}{\eta} = 1 - 2e^{-\eta} \quad \rightsquigarrow \quad \xi = \frac{1}{2}\eta e^{-\eta}. \tag{31}$$

In the same way we find for the odd solution

$$\frac{y}{\eta - y} \approx 1 + 4\frac{\xi}{\eta} = 1 - 2e^{-\eta} \quad \rightsquigarrow \quad \xi = -\frac{1}{2}\eta e^{-\eta}. \tag{32}$$

This gives the splitting between the excited, odd, and ground, even, energies

$$\Delta y = y^{(+)} - y^{(-)} = \eta e^{-\eta}, \tag{33}$$

or, in the normal energy scale ($E = -\epsilon = -\epsilon_0 y^2$),

$$\Delta E = E^{(-)} - E^{(+)} = \epsilon_0 2y\Delta y = \epsilon_0 \eta^2 e^{-\eta}. \tag{34}$$

This result can be also interpreted in terms of a small overlap of the individual unperturbed left- and right–localized functions which creates correct combinations of certain parity and splits their energies.

Now we show that the solution can be significantly simplified if we start not with the differential Schrödinger equation but with the equivalent *integral* equation for bound states,

$$\psi(x) = -\frac{m}{\hbar^2\kappa}\int dx'\, e^{-\kappa|x-x'|}U(x')\psi(x'). \tag{35}$$

With our two-well δ-functional potential (16), this equation acquires the form

$$\psi(x) = \frac{mg}{\hbar^2\kappa}\left[e^{-\kappa|x-a|}\psi(a) + e^{-\kappa|x+a|}\psi(-a)\right]. \tag{36}$$

This is in fact an explicit solution as a function of x and two constants, values of the function at the singular points $\pm a$. Taking here $x = \pm a$, we obtain a set of two coupled equations for $\psi(\pm a)$:

$$\psi(a) = t\left[\psi(a) + e^{-2\kappa a}\psi(-a)\right], \quad \psi(-a) = t\left[\psi(-a) + e^{-2\kappa a}\psi(a)\right], \tag{37}$$

where the new dimensionless constant t is a combination of the parameters,

$$t = \frac{mg}{\hbar^2\kappa} = \frac{\eta}{2y}. \tag{38}$$

It is clear from the original symmetry reflected in the symmetry of these equations that there can be two types of solutions: even, $\psi(a) = \psi(-a)$, and odd, $\psi(a) = -\psi(-a)$. The nontrivial solutions of eq. (37) are possible if the determinant of this set of equations vanishes,

$$(1-t)^2 - t^2 e^{-4\kappa a} = \left(1 - t - te^{-2\kappa a}\right)\left(1 - t + te^{-2\kappa a}\right) = 0. \tag{39}$$

Introducing

$$z = 1/t, \quad 2\kappa a = \frac{2mga}{\hbar^2}\, z \equiv \eta z, \tag{40}$$

we obtain two separate equations for $z \propto \kappa \propto \sqrt{\epsilon}$:

$$z - 1 = e^{-\eta z} \quad \text{(even)}, \quad 1 - z = e^{-\eta z} \quad \text{(odd)}. \tag{41}$$

A simple graphical construction shows that there is always a solution $z > 0$ for the even case while in the odd case the derivative of the exponent at $z = 0$ should satisfy the condition which we have seen earlier, $\eta > 1$. In the case of well separated wells, $\kappa a \gg 1$, the two solutions exist, and they both are close to $z = 1$, being greater (smaller) than 1 in the even (odd) case. This means, in accordance with general regularities, that the ground state is an even (nodeless) function, the even level is deeper than the odd one. At $\kappa a \gg 1$, the splitting is exponentially small. It can be easily found with the help of expansion of our equations (41) near $z = 1$:

$$z_{\text{even}} = 1 + e^{-\eta}, \quad z_{\text{odd}} = 1 - e^{-\eta}, \tag{42}$$

in agreement with what has been found in a direct method.

3. *a.* We need to transform the Schrödinger equation from the coordinate representation,

$$\frac{\hat{p}^2}{2m}\psi(x) + U(x)\psi(x) = E\psi(x), \tag{43}$$

to the momentum representation. We multiply all terms of (43) by $\exp[-(i/\hbar)px]$, where p is the variable of the wave function (not an operator!) and integrate over x. The right hand side gives $E\phi(p)$. The kinetic energy term gives

$$\int dx\, e^{(-i/\hbar)px}\frac{\hat{p}^2}{2m}\psi(x) = \int dx\, \left(\frac{\hat{p}^2}{2m}e^{(i/\hbar)px}\right)^* \psi(x) = \frac{p^2}{2m}\phi(p), \tag{44}$$

where he used the Hermiticity of the momentum operator. As it should be, the momentum operator $\hat{p}$ becomes that of the multiplication, p, acting on $\phi(p)$. The potential term gives

$$\int dx\, e^{-(i/\hbar)px}U(x)\psi(x) = \int dx\, e^{-(i/\hbar)px}U(x)\int \frac{dp'}{2\pi\hbar}e^{(i/\hbar)p'x}\phi(p'). \tag{45}$$

Changing the order of integration and introducing the Fourier-components U_q of the potential according to

$$U_q = \int dx\, e^{-(i/\hbar)qx}U(x), \tag{46}$$

we rewrite eq. (45) as a convolution of the Fourier-components,

$$\int dx\, e^{-(i/\hbar)px}U(x)\psi(x) = \int \frac{dp'}{2\pi\hbar}U_{p-p'}\phi(p'). \tag{47}$$

Thus, a differential wave equation in the coordinate representation is converted into an integral equation in the momentum representation,

$$\frac{p^2}{2m}\phi(p) + \int \frac{dp'}{2\pi\hbar} U_{p-p'}\phi(p') = E\phi(p). \tag{48}$$

b. In the case of the δ-potential, all Fourier-components are equal,

$$U_q = \int dx\, e^{-(i/\hbar)qx}(-g)\delta(x) = -g. \tag{49}$$

The equation to solve takes the form

$$\frac{p^2}{2m}\phi(p) - g\int \frac{dp'}{2\pi\hbar}\phi(p') = E\phi(p). \tag{50}$$

The integral here is just a number

$$\int \frac{dp'}{2\pi\hbar}\phi(p') = A. \tag{51}$$

Now we can solve the resulting algebraic equation:

$$\phi(p) = \frac{2mgA}{p^2 - 2mE} = \frac{2mgA}{p^2 + 2m\epsilon}, \tag{52}$$

where we specified that we are interested in a bound state with binding energy $\epsilon = -E > 0$. (The continuous spectrum of states with positive energy E can be also found.) Integrating both parts of eq. (52) and comparing with (51) we obtain the self-consistency condition for $A \neq 0$:

$$\frac{gm}{\pi\hbar}\int \frac{dp}{p^2 + 2m\epsilon} = 1. \tag{53}$$

For $g > 0$ the condition can be fulfilled. This integral gives

$$1 = \frac{g}{\hbar}\sqrt{\frac{m}{2\epsilon}} \quad \rightsquigarrow E = -\epsilon = -\frac{mg^2}{2\hbar^2}. \tag{54}$$

We have found the unique bound state which exists for an attractive δ-potential of arbitrary strength $g > 0$. The normalization condition

$$\int \frac{dp}{2\pi\hbar}\phi^2(p) = 1 \tag{55}$$

determines the remaining constant,

$$A^2 = \frac{\hbar(2m\epsilon)^{3/2}}{m^2g^2} = \frac{mg}{\hbar^2}. \tag{56}$$

4. The problem can be solved in full but we are interested here in a partial problem only - if the well can support a bound state. The limiting case corresponds to energy equal to the lower barrier, $E = U_2$. For such energy the solution which does not unphysically grow at $x \to \pm\infty$ can be written as

$$\psi(x) = \begin{cases} Ae^{\kappa x}, & x < 0, \quad \kappa = \sqrt{\frac{2m(U_1-U_2)}{\hbar^2}}, \\ B\cos(kx+\alpha), & 0 < x < a, \quad k = \sqrt{\frac{2mU_2}{\hbar^2}}, \\ C, & x > a. \end{cases} \tag{57}$$

The matching conditions are

$$A = B\cos\alpha, \quad \kappa A = -kB\sin\alpha, \quad B\cos(ka+\alpha) = C, \quad kB\sin(ka+\alpha) = 0. \tag{58}$$

They lead to

$$\alpha = -ka, \quad B = C, \quad \kappa = k\tan(ka). \tag{59}$$

The level becomes bound after $\tan(ka)$ increases slightly beyond the value determined by the last equation (59). Thus, the condition of existence of a bound state is

$$\sqrt{\frac{2ma^2U_2}{\hbar^2}} \geq \tan^{-1}\left(\sqrt{\frac{U_1-U_2}{U_2}}\right). \tag{60}$$

This gives for an infinite left barrier, $U_1 \to \infty$, the correct condition $U_2 \geq \pi^2\hbar^2/8ma^2$, while eq. (60) is always fulfilled for $U_2 = U_1$, i.e. there is a bound state in a symmetric well.