SOLUTIONS

PROBLEM 1. The Hamiltonian of the particle in the gravitational field can be written as

$$\hat{H} = \frac{\hat{p}^2}{2m} + U(x), \quad U(x) = \begin{cases} \infty, & x \leq 0, \\ mgx, & x > 0. \end{cases} \tag{1}$$

The simplest estimate comes from the uncertainty relation. If the ground state localization length is $\sim l$, the typical magnitude of the momentum is $\hbar/l$, and the expectation value of energy can be evaluated as

$$E(l) = \frac{\hbar^2}{2ml^2} + mgl. \tag{2}$$

This function has a minimum at

$$l = \left(\frac{\hbar^2}{m^2 g}\right)^{1/3}. \tag{3}$$

The corresponding energy equals

$$E = \frac{3}{2}(mg^2\hbar^2)^{1/3}. \tag{4}$$

A Bohr-Sommerfeld quantization would give a similar result with a slightly larger numerical coefficient, ≈ 1.8 instead of 1.5, in eq. (4). According to (3) and (4), $l \approx (2/3)(E/mg)$, the particle is localized inside the well. The average height (3) for the electron turns out to be $\sim 1\,\mathrm{mm}$ but it falls off for heavier particles $\sim m^{-2/3}$.

PROBLEM 2. a. If the particle has a bound state with energy $E = -\epsilon < 0$, the wave function has to decay to the right of the well,

$$\psi(x) = \begin{cases} A\sinh(\kappa x), & 0 \leq x \leq a, \\ Be^{-\kappa x}, & a \leq x < \infty. \end{cases} \tag{5}$$

Here the boundary condition at the infinite wall $\psi(a) = 0$ is taken into account, and

$$\kappa = \sqrt{\frac{2m\epsilon}{\hbar^2}} > 0. \tag{6}$$

The matching conditions at the well are the continuity of the function,

$$A\sinh(\kappa a) = Be^{-\kappa a}, \tag{7}$$

and the discontinuity of the derivative $(d\psi/dx) \equiv \psi'$,

$$\psi'(a+0) - \psi'(a-0) = -\frac{2m}{\hbar^2}g\psi(a) \equiv -t\psi(a), \tag{8}$$

which gives

$$-\kappa Be^{-\kappa a} - \kappa A\cosh(\kappa a) = -tA\sinh(\kappa a). \tag{9}$$

Eliminating B, we find the condition for κ which determines binding energy ϵ,

$$\tanh(\kappa a) = \frac{\kappa}{t-\kappa}. \tag{10}$$

The zero value of κ is not a solution since it gives $\psi \equiv 0$. The left hand side of eq. (10) as a function of κa starts at the origin with the slope 1 and asymptotically approaches the value 1 at large κa. The right hand side, $\kappa a/(ta - \kappa a)$, starts at the origin with the slope $1/(ta)$, then asymptotically approaches the vertical line $\kappa a = ta$. In order to have a second intercept with the curve $\tanh(\kappa a)$, the slope should be smaller than 1. This gives the condition

$$\frac{1}{ta} < 1, \quad \rightsquigarrow \quad \frac{2mga}{\hbar 2} > 1. \tag{11}$$

Under this condition we have one bound state; at $ta < 1$ the δ-well does not support any bound state; the difference with the case of a single δ-well with no wall comes from the boundary condition which forces the wave function to vanish at $x = 0$; this confinement pushes the value of energy up.

b. In the scattering problem energy E is positive,

$$\psi(x) = \begin{cases} A\sin(kx), & 0 \le x \le a, \\ B\sin(kx+\alpha), & x \ge a. \end{cases} \tag{12}$$

Here the wave vector is

$$k = \sqrt{\frac{2mE}{\hbar^2}} > 0. \tag{13}$$

The matching conditions are analogous to those in the previous version,

$$A\sin(ka) = B\sin(ka+\alpha), \tag{14}$$

$$kB\cos(ka+\alpha) - kA\cos(ka) = -tA\sin(ka). \tag{15}$$

Earlier the similar set of equations was used to determine binding energy; here, solving for the phase shift $\alpha(E)$, we obtain

$$\tan(ka+\alpha) = \frac{\tan(ka)}{1-(t/k)\tan(ka)}, \tag{16}$$

or

$$\tan\alpha = \frac{(t/k)\xi^2}{1-(t/k)\xi+\xi^2}. \quad \xi = \tan(ka). \tag{17}$$

Let us look at particular cases. Since α enters the answer only in the form of $\tan\alpha$, we can assume that α is defined in the interval from 0 to π. For $\xi = 0$, $ka = n\pi$, we have $\alpha = 0$ or π; in this case, the wave traveling from the well to the wall and back acquires the phase $2ka = 2n\pi$ and cannot be distinguished from the wave propagating with no δ-well. For $|\xi| \to \infty$, $ka = [n + (1/2)]\pi$, we find $\tan\alpha = t/k$, the phase falls off with energy, $\alpha \propto 1/\sqrt{E}$.

It is interesting to discuss the relation between the scattering problem and bound states. In the scattering problem, the wave on the right from the potential consists of the incident wave $\sim e^{-ikx}$ and the reflected (scattered) wave $\sim e^{ikx}$,

$$\sin(kx + \alpha) = \frac{1}{2i}\left[e^{i(kx+\alpha)} - e^{-i(kx+\alpha)}\right]. \tag{18}$$

Here α is the function of physical positive energy E or wave vector k which takes physically different values from 0 to π. Consider the *analytic continuation* of this function to negative values of energy, or imaginary wave vector, $k = i\kappa$, $\kappa > 0$,

$$\sin(kx + \alpha) \Rightarrow \frac{1}{2i}\left[e^{-\kappa x + i\alpha(i\kappa)} - e^{\kappa x - i\alpha(i\kappa)}\right]. \tag{19}$$

Now α becomes a complex function $\alpha(i\kappa)$. Assume that this function can go to $-i\infty$ at some value of κ. At this value of κ the second term in the square bracket (19), representing now the part of the wave function *increasing* at $x \to \infty$, vanishes, and only the *decaying* part $\propto \exp(-\kappa x)$ survives; in this term, originated from the reflected wave, the amplitude becomes infinitely large compared to that in the incident wave. But then the *analytically continued wave function of the scattering problem coincides with that for a bound state*. Indeed, let us rename $\alpha(i\kappa) = -i\beta(\kappa)$, where we are looking at the point κ where $\beta(\kappa) \to \infty$. At this point $\tan\alpha = -i\tanh(\beta) \to -i$. On the other hand, if we extend our definition of α in eq. (17) to complex values, it would give at this point

$$-i = \frac{(t/i\kappa)(-1)\tanh^2(\kappa a)}{1 - (t/i\kappa)i\tanh(\kappa a) - \tanh^2(\kappa a)}. \tag{20}$$

Using here the value

$$\tanh(ka) = \frac{\kappa}{t - \kappa} \tag{21}$$

which was obtained in eq. (10) for the bound state, we see that (20) is identically fulfilled. This result is of a very general character: the bound states can be related to the poles of the *scattering matrix*, in this case simply the amplitude of the reflected wave, with the help of the analytical continuation to negative energies or imaginary wave vectors.

PHY-851 QUANTUM MECHANICS I
Homework 8, 30=10+20 points
October 31 - November 7, 2001
One-dimensional motion; variational method; periodic potential.

Reading: *Merzbacher*, Chapter 8, sections 1, 2, 7; Chapter 6, section 5.

1. /10/ *Midterm, Problem 2.* The potential consists of an infinitely high wall at $x = 0$ and a narrow well $-g\delta(x - a)$; g and a are positive constants.

   a. Find the bound states of the particle of mass m in this potential and dependence of a number of such states on the parameters of the problem.

   b. For the scattering problem with the same potential find the solution that has the form $\sin(kx + \alpha)$ at distances $x > a$ and determine the phase shift α as a function of energy.

   c. Is it possible to find the bound states from the solution of the scattering problem? /*Consider the analytic continuation of the scattering wave function to complex values of the wave vector and assume that at some complex value $k = i\kappa$ the phase $\alpha(i\kappa) \to -i\infty$.*/

   Please write the solution of this problem separately from other problems; this will be considered as make-up for the midterm.

2. /9/ *Merzbacher*, Exercises 8.1, 8.2, 8.3.

3. /5/ *Merzbacher*, Problem 5, p. 177.

4. /6/ *Merzbacher*, Exercise 8.29.

SOLUTIONS

1. See *Problem 2, Midterm.*

2. *Exercize 8.1.* The Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + g|x| \tag{22}$$

suggests that the ground state wave function should be even. Therefore the exponential choice for the trial function decreasing to $\pm\infty$ is

$$\psi(x) = \sqrt{\alpha}\, e^{-\alpha|x|}. \tag{23}$$

The preexponential factor in this function is chosen in such a way that the function is normalized,

$$\int_{-\infty}^{\infty} dx\, \psi^2(x) = 1. \tag{24}$$

The expectation value of the potential energy for this function is easily calculated,

$$\langle U \rangle = \alpha g \int_{-\infty}^{\infty} dx\, e^{-2\alpha|x|}|x| = 2\alpha g \int_{0}^{\infty} dx\, e^{-2\alpha x} x = \frac{2\alpha g}{4\alpha^2} = \frac{g}{2\alpha}. \tag{25}$$

The kinetic energy must be treated carefully because of the singularity of the trial wave function (23) at the origin. Indeed, this singularity brings a sign function after the differentiation:

$$\frac{d}{dx} e^{-\alpha|x|} = -\alpha\, \mathrm{sign}(x)\, e^{-\alpha|x|}, \quad \mathrm{sign}(x) = \frac{x}{|x|}, \tag{26}$$

$$\frac{d^2}{dx^2} e^{-\alpha|x|} = -\alpha \left\{ 2\delta(x) - \alpha[\mathrm{sign}(x)]^2 \right\} e^{-\alpha|x|}, \tag{27}$$

where we need to take into account that

$$\frac{d}{dx}\mathrm{sign}(x) = 2\delta(x), \quad [\mathrm{sign}(x)]^2 = 1. \tag{28}$$

Therefore

$$\langle K \rangle = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \psi(x) \frac{d^2}{dx^2} \psi(x) = \frac{\hbar^2}{2m}\, \alpha^2. \tag{29}$$

The variational problem reduces to finding the minimum of the expectation value

$$\langle H \rangle = \frac{\hbar^2}{2m}\, \alpha^2 + \frac{g}{2\alpha} \tag{30}$$

as a function of the variational parameter α. The function $\langle H(\alpha)\rangle$ has a parabolic minimum at

$$\alpha = \left(\frac{gm}{2\hbar^2}\right)^{1/3}. \tag{31}$$

The ground state energy in this approximation is equal to

$$\langle H\rangle = \left[\frac{1}{2^{5/3}} + \frac{1}{2^{2/3}}\right]\left(\frac{g^2\hbar^2}{m}\right)^{1/3}. \tag{32}$$

This value differs from the result of the variational calculation with the Gaussian function [*Merzbacher*, eqs. (8.12) and (8.15)] by the factor $(\pi/2)^{1/3} = 1.162$. The result is worse just because of the singularity of the exponential wave function at the origin. Here higher momentum component emerge which are absent in the actual case; the Gaussian approximation is more smooth and has no discontinuities in derivatives.

We can note that the calculation of the kinetic contribution would be simpler if we would use the Hermiticity of the momentum operator $\hat{p}$ and transform (29) to the equivalent form [compare *Merzbacher*, eq. (8.2)]

$$\langle K\rangle = \frac{1}{2m}\int_{-\infty}^{\infty} dx\, |\hat{p}\psi(x)|^2. \tag{33}$$

This immediately gives

$$\langle K\rangle = \frac{\alpha}{2m}\int_{-\infty}^{\infty} dx\, |i\hbar\alpha e^{-\alpha|x|}\mathrm{sign}(x)|^2 = \frac{\alpha}{2m}\hbar^2\alpha^2\int_{-\infty}^{\infty} dx\, e^{-2\alpha|x|} = \frac{\hbar^2\alpha^2}{2m}. \tag{34}$$

Exercise 8.2. We act as in the previous case. First we normalize the wave function:

$$C^2\int_{-\alpha}^{\alpha} dx\,(\alpha - |x|)^2 = 1 \quad \rightsquigarrow \quad C = \sqrt{\frac{3}{2\alpha^3}}. \tag{35}$$

Using (33) we find

$$\langle K\rangle = \frac{C^2}{2m}\int_{-\alpha}^{\alpha} dx\, \left|-\hat{p}|x|\right|^2 = \frac{C^2\hbar^2}{m}\alpha, \tag{36}$$

and

$$\langle U\rangle = C^2 g\int_{-\alpha}^{\alpha} dx\, |x|(\alpha - |x|)^2 = \frac{1}{6}C^2 g\alpha^4. \tag{37}$$

With the normalization (35), the function to minimize becomes

$$\langle H\rangle = \frac{3\hbar^2}{2m\alpha^2} + \frac{1}{4}g\alpha. \tag{38}$$

The minimum corresponds to

$$\alpha = \left(12\frac{\hbar^2}{mg}\right)^{1/3}, \quad \langle H \rangle = \frac{5}{4}\left(\frac{3}{2}\right)^{1/3}\left(\frac{g^2\hbar^2}{m}\right)^{1/3} = 1.431\left(\frac{g^2\hbar^2}{m}\right)^{1/3}. \tag{39}$$

Thus, this trial function is worse than both Gaussian and exponential. Here one still has a singularity of the derivative in the middle and the wings of the function are cut off which means too strong localization,

Exercise 8.3. A possible choice of an even function could be for example

$$\psi(x) = \begin{cases} A(a^2 - x^2), & |x| \leq a, \\ 0, & |x| > a. \end{cases} \tag{40}$$

The normalization determines $A = \sqrt{15}/(4a^{5/2})$. Then the expectation value of the Hamiltonian is

$$\langle H(\alpha) \rangle = \frac{5\hbar^2}{4ma^2} + \frac{5}{16}ga. \tag{41}$$

The minimization determines

$$a = 2\left(\frac{\hbar^2}{mg}\right)^{1/3} \tag{42}$$

and the corresponding expectation value of the ground state energy

$$\langle H \rangle = \frac{15}{16}\left(\frac{g^2\hbar^2}{m}\right)^{1/3} = 0.9375\left(\frac{g^2\hbar^2}{m}\right)^{1/3} \tag{43}$$

This result is better than the previous one because there is no singularity in the middle but the discontinuities on the edges are still present.

For an odd function with one node, we can use

$$\psi(x) = \begin{cases} Ax(a^2 - x^2), & |x| \leq a, \\ 0, & |x| > a. \end{cases} \tag{44}$$

The standard calculation gives

$$\langle H \rangle = 2.1966\left(\frac{g^2\hbar^2}{m}\right)^{1/3}. \tag{45}$$

The exact value for the first excited state is, in the same units, 1.8588. Again the Gaussian approximation would be better.

The procedure can be continued with the choice of new trial functions orthogonal to all previous ones; a number of nodes increases each time.

3. First we normalize the wave function, compare (35),

$$C^2 = \frac{3}{2a}. \tag{46}$$

Similarly to (36),

$$\langle K \rangle = C^2 \frac{\hbar^2}{ma} = \frac{3\hbar^2}{2ma^2}; \tag{47}$$

the potential contribution is

$$\langle U \rangle = C^2 \frac{1}{2} m\omega^2 \int_{-a}^{a} dx\, x^2 \left(1 - \frac{|x|}{a}\right)^2 = C^2 \frac{1}{30} m\omega^2 a^3 = \frac{1}{20} m\omega^2 a^2. \tag{48}$$

The minimization of full energy gives

$$a^2 = \sqrt{30} \frac{\hbar}{m\omega}, \quad \langle H \rangle = \frac{\hbar\omega}{2} \frac{6}{\sqrt{30}} = 1.095 \frac{\hbar\omega}{2}. \tag{49}$$

4. Consider, for example, the case of $E > 0$. The equation for allowed energies $E = E(k)$ reads, in notations used in class,

$$\cos(kl) = \cos(qa)\cos(q'b) - \frac{q^2 + q'^2}{2qq'} \sin(qa)\sin(q'b), \tag{50}$$

where

$$q = \sqrt{\frac{2mE}{\hbar^2}}, \quad q' = \sqrt{\frac{2m(E - U_0)}{\hbar^2}}, \tag{51}$$

the bottom of the well is put at $E = 0$, the height of the barrier is U_0, and their widths are a and b, respectively ($a + b = l$). The quasimomentum k labeling the stationary state changes between $-\pi/l$ and π/l. The limiting transition to the sequence of δ-functions, the *Kronig-Penney model*, goes as

$$U_0 \to \infty, \quad b \to 0, \quad U_0 b \to \text{const} = g, \quad a \to l, \quad q'^2 \to -\frac{2mU_0}{\hbar^2}. \tag{52}$$

When $U_0 \to \infty$, we can neglect q^2 compared to q'^2. The argument $q'b$ is small in this limit, $\sim g/\sqrt{U_0}$. Thus we have $\cos(q'b) \to 0$, $\sin(q'b) \to q'b$, and the main equation (50) takes the form

$$\cos(kl) = \cos(ql) + \frac{t}{q}\sin(ql), \quad t = \frac{mg}{\hbar^2}. \tag{53}$$

Recall that here q characterizes energy while k is a label (quantum number) of the wave function. The allowed and forbidden energy bands $E(k)$ follow from the fact that the left hand side is bounded by $|\cos(kl)| \le 1$.

Without any potential $t \to 0$, and we have free motion, which allows to identify q and k.

There are various ways to analyze the result (53). We can introduce an angle $\varphi = \tan^{-1}(t/q)$ so that

$$\tan\varphi = \frac{t}{q}, \quad \sin\varphi = \frac{t}{\sqrt{t^2+q^2}}, \quad \cos\varphi = \frac{q}{\sqrt{t^2+q^2}}. \tag{54}$$

Then

$$\cos(ql) + \frac{t}{q}\sin(kl) = \cos(ql) + \tan\varphi\sin(ql) = \frac{\cos(ql-\varphi)}{\cos\varphi} \tag{55}$$

and we find from eq. (53):

$$\cos(kl) = \frac{\cos(ql-\varphi)}{\cos\varphi}. \tag{56}$$

The boundaries of the energy bands, $\cos(kl) = (-)^n$, are determined by

$$\cos(ql-\varphi) = (-)^n\cos(\varphi), \tag{57}$$

where an integer n labels the bands. The solutions of (57) are

$$ql = n\pi \quad \text{or} \quad ql = n\pi + 2\varphi; \tag{58}$$

Forbidden bands are located between these values for any n. The width of the n^{th} forbidden band is determined by $2\varphi = 2\tan^{-1}(t/q)$. At high energies, $q \gg t$, this gives $\varphi \approx t/q \ll 1$. In this case the forbidden zone is very narrow and located, according to (58), around $ql = n\pi$. This means that the width of narrow bands, $n \gg 1$, can be estimated as

$$\Delta_n(ql) = 2\varphi \approx 2\frac{tl}{n\pi}, \tag{59}$$

or, in energy units, see (51),

$$\frac{\Delta_n(E)}{E} = \sqrt{\frac{2\hbar^2}{mE}}\,\frac{2t}{n\pi}. \tag{60}$$