SOLUTIONS for Homework #8

1. See *Problem 2, Midterm.*

2. *Exercize 8.1.* The Hamiltonian
$$\hat{H} = \frac{\hat{p}^2}{2m} + g|x| \tag{1}$$
suggests that the ground state wave function should be even. Therefore the exponential choice for the trial function decreasing to $\pm\infty$ is
$$\psi(x) = \sqrt{\alpha}\, e^{-\alpha|x|}. \tag{2}$$
The preexponential factor in this function is chosen in such a way that the function is normalized,
$$\int_{-\infty}^{\infty} dx\, \psi^2(x) = 1. \tag{3}$$
The expectation value of the potential energy for this function is easily calculated,
$$\langle U \rangle = \alpha g \int_{-\infty}^{\infty} dx\, e^{-2\alpha|x|}|x| = 2\alpha g \int_{0}^{\infty} dx\, e^{-2\alpha x} x = \frac{2\alpha g}{4\alpha^2} = \frac{g}{2\alpha}. \tag{4}$$
The kinetic energy must be treated carefully because of the singularity of the trial wave function (2) at the origin. Indeed, this singularity brings a sign function after the differentiation:
$$\frac{d}{dx} e^{-\alpha|x|} = -\alpha\, \mathrm{sign}(x)\, e^{-\alpha|x|}, \quad \mathrm{sign}(x) = \frac{x}{|x|}, \tag{5}$$
$$\frac{d^2}{dx^2} e^{-\alpha|x|} = -\alpha \left\{ 2\delta(x) - \alpha[\mathrm{sign}(x)]^2 \right\} e^{-\alpha|x|}, \tag{6}$$
where we need to take into account that
$$\frac{d}{dx}\mathrm{sign}(x) = 2\delta(x), \quad [\mathrm{sign}(x)]^2 = 1. \tag{7}$$
Therefore
$$\langle K \rangle = -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \psi(x) \frac{d^2}{dx^2} \psi(x) = \frac{\hbar^2}{2m}\, \alpha^2. \tag{8}$$
The variational problem reduces to finding the minimum of the expectation value
$$\langle H \rangle = \frac{\hbar^2}{2m}\, \alpha^2 + \frac{g}{2\alpha} \tag{9}$$

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

$$\alpha = \left(\frac{gm}{2\hbar^2}\right)^{1/3}. \tag{10}$$

The ground state energy in this approximation is equal to

$$\langle H\rangle = \left[\frac{1}{2^{5/3}} + \frac{1}{2^{2/3}}\right]\left(\frac{g^2\hbar^2}{m}\right)^{1/3}. \tag{11}$$

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 (8) to the equivalent form [compare *Merzbacher*, eq. (8.2)]

$$\langle K\rangle = \frac{1}{2m}\int_{-\infty}^{\infty} dx\, |\hat{p}\psi(x)|^2. \tag{12}$$

This immediately gives

$$\langle K\rangle = \frac{\alpha}{2m}\int_{-\infty}^{\infty} dx\, |i\hbar\alpha e^{-\alpha|x|}\mathrm{sign}(x)|^2 = \frac{\alpha}{2m}\hbar^2\alpha^2\int_{-\infty}^{\infty} dx\, e^{-2\alpha|x|} = \frac{\hbar^2\alpha^2}{2m}. \tag{13}$$

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

$$C^2\int_{-\alpha}^{\alpha} dx\,(\alpha - |x|)^2 = 1 \quad \rightsquigarrow \quad C = \sqrt{\frac{3}{2\alpha^3}}. \tag{14}$$

Using (12) we find

$$\langle K\rangle = \frac{C^2}{2m}\int_{-\alpha}^{\alpha} dx\, \left|-\hat{p}|x|\right|^2 = \frac{C^2\hbar^2}{m}\alpha, \tag{15}$$

and

$$\langle U\rangle = C^2 g\int_{-\alpha}^{\alpha} dx\, |x|(\alpha - |x|)^2 = \frac{1}{6}C^2 g\alpha^4. \tag{16}$$

With the normalization (14), the function to minimize becomes

$$\langle H\rangle = \frac{3\hbar^2}{2m\alpha^2} + \frac{1}{4}g\alpha. \tag{17}$$

The minimum corresponds to

$$\alpha = \left(12\frac{\hbar^2}{mg}\right)^{1/3}, \quad \langle H\rangle = \frac{5}{4}\left(\frac{3}{2}\right)^{1/3}\left(\frac{g^2\hbar^2}{m}\right)^{1/3} = 1.431\left(\frac{g^2\hbar^2}{m}\right)^{1/3}. \tag{18}$$

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

$$\psi(x) = \begin{cases} A(a^2 - x^2), & |x| \le a, \\ 0, & |x| > a. \end{cases} \tag{19}$$

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

$$\langle H(\alpha)\rangle = \frac{5\hbar^2}{4ma^2} + \frac{5}{16}ga. \tag{20}$$

The minimization determines

$$a = 2\left(\frac{\hbar^2}{mg}\right)^{1/3} \tag{21}$$

and the corresponding expectation value of the ground state energy

$$\langle H\rangle = \frac{15}{16}\left(\frac{g^2\hbar^2}{m}\right)^{1/3} = 0.9375\left(\frac{g^2\hbar^2}{m}\right)^{1/3} \tag{22}$$

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

$$\psi(x) = \begin{cases} Ax(a^2 - x^2), & |x| \le a, \\ 0, & |x| > a. \end{cases} \tag{23}$$

The standard calculation gives

$$\langle H\rangle = 2.1966\left(\frac{g^2\hbar^2}{m}\right)^{1/3}. \tag{24}$$

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 (14),
$$C^2 = \frac{3}{2a}. \tag{25}$$
Similarly to (15),
$$\langle K \rangle = C^2 \frac{\hbar^2}{ma} = \frac{3\hbar^2}{2ma^2}; \tag{26}$$
the potential contribution is
$$\langle U \rangle = C^2 \frac{1}{2} m\omega^2 \int_{-a}^{a} dx\, x^2 \left(1 - \frac{|x|}{a}\right)^2 = C^2 \frac{1}{30}\, m\omega^2 a^3 = \frac{1}{20}\, m\omega^2 a^2. \tag{27}$$
The minimization of full energy gives
$$a^2 = \sqrt{30}\frac{\hbar}{m\omega}, \quad \langle H \rangle = \frac{\hbar\omega}{2} \frac{6}{\sqrt{30}} = 1.095\, \frac{\hbar\omega}{2}. \tag{28}$$

4. Consider, for example, the case of $E > 0$. The equation for allowed energies $E = E(k)$ reads, in notations used in class,
$$\cos(kl) = \cos(qa)\cos(q'b) - \frac{q^2 + q'^2}{2qq'} \sin(qa)\sin(q'b), \tag{29}$$
where
$$q = \sqrt{\frac{2mE}{\hbar^2}}, \quad q' = \sqrt{\frac{2m(E - U_0)}{\hbar^2}}, \tag{30}$$
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
$$U_0 \to \infty, \quad b \to 0, \quad U_0 b \to \text{const} = g, \quad a \to l, \quad q'^2 \to -\frac{2mU_0}{\hbar^2}. \tag{31}$$
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 (29) takes the form
$$\cos(kl) = \cos(ql) + \frac{t}{q}\sin(ql), \quad t = \frac{mg}{\hbar^2}. \tag{32}$$
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 (32). We can introduce an angle $\varphi = \tan^{-1}(t/q)$ so that

$$\tan\varphi = \frac{t}{q}, \quad \sin\varphi = \frac{t}{\sqrt{t^2+q^2}}, \quad \cos\varphi = \frac{q}{\sqrt{t^2+q^2}}. \tag{33}$$

Then

$$\cos(ql) + \frac{t}{q}\sin(kl) = \cos(ql) + \tan\varphi\sin(ql) = \frac{\cos(ql-\varphi)}{\cos\varphi} \tag{34}$$

and we find from eq. (32):

$$\cos(kl) = \frac{\cos(ql-\varphi)}{\cos\varphi}. \tag{35}$$

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

$$\cos(ql-\varphi) = (-)^n\cos(\varphi), \tag{36}$$

where an integer n labels the bands. The solutions of (36) are

$$ql = n\pi \quad \text{or} \quad ql = n\pi + 2\varphi; \tag{37}$$

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 (37), around $ql = n\pi$. This means that the width of narrow bands, $n \gg 1$, can be estimated as

$$\Delta_n(ql) = 2\varphi \approx 2\frac{tl}{n\pi}, \tag{38}$$

or, in energy units, see (30),

$$\frac{\Delta_n(E)}{E} = \sqrt{\frac{2\hbar^2}{mE}}\,\frac{2t}{n\pi}. \tag{39}$$