# Bound state problems
# Mini-School on Few-Body Physics
# 6-10 October 2014

## 1 Weakly Bound States in 1D

(Landau and Lifshitz) Consider a particle with mass $m$ in one spatial dimension. The particle is subject to an attractive potential which is non-vanishing in a region of length $l$ and has strength $U < 0$. Assume that the strength is weak such that $|U| \ll \hbar^2/ml^2$.

1) Assume that the energy is $|E| \ll |U|$. Use the Schrödinger equation for the wave function of a weakly bound state, $\psi$, to show that

$$\left[\frac{d\psi}{dx}\right]_{-x_0}^{x_0} = \frac{2m}{\hbar^2}\int_{-\infty}^{\infty} U(x)dx, \tag{1}$$

where $l \ll x_0 \ll \kappa^{-1}$ and $\kappa = \sqrt{2m|E|/\hbar^2}$. Hint: You will need to assume that $\psi$ is constant inside the range of the potential.

**Solution:** Consider first $\psi$ as a constant and note that it solves the Schrödinger equation when we neglect the potential and set $E = 0$, so the constant wave function is the lowest order perturbative solution. Insert this as a lowest order guess in the potential term, neglect the energy term compared to the potential term and integrate once the kinetic term. Then you should arrive at the result. Since the integral over the potential is convergent (it is zero outside the range $l$) you can take the limits of that integral to infinity.

2) Use the fact that at large distance a bound state wave function has the form $\psi \propto e^{\pm\kappa x}$ to deduce that

$$|E| = \frac{m}{2\hbar^2}\left[\int_{-\infty}^{\infty} U(x)dx\right]^2, \tag{2}$$

i.e. weakly bound states will depend quadratically on the strength of the binding potential.

**Solution:** Evaluate the derivative of the wave function with the large distance asymptotic form given at some point outside the range of the potential but before you hit $x_0 = \kappa^{-1}$. Then you will get a factor of $\kappa$ from each of the terms with $\pm x_0$ but with opposite signs so the overall effect is $-2\kappa$. Now since you are also assuming that $x_0 \ll \kappa^{-1}$ the value of the wave function is still almost constant with values one, or more precisely $\psi = e^{\pm\kappa x} \sim 1 \pm \kappa x$ to linear order. Throw away the linear term and you have the result.

## 2 Weakly Bound States in 2D

(Landau and Lifshitz) Consider the same problem as above but now in two spatial dimensions. Assume that the integral $\int_{-\infty}^{\infty} \rho U(\rho)d\rho$ converges and that the potential has cylindrical symmetry.

1) Proceed as in the 1D case above and show that this time the Schrödinger equation gives us the relation

$$\left[\frac{d\psi}{d\rho}\right]_{\rho=\rho_0} = \frac{2m}{\hbar^2\rho_0}\int_0^\infty \rho U(\rho)d\rho, \tag{3}$$

where $l \ll \rho_0 \ll \kappa^{-1}$.

2) The asymptotic solution for a bound state is a Hankel function of the first kind, $\phi \propto H_0^{(1)}(i\kappa\rho)$, and the leading term goes like $\log(\kappa\rho)$. Take the logarithmic derivative, $\frac{d}{d\rho}\log(\psi)$, from inside and outside the potential and equate these expression to obtain

$$\frac{1}{l\log(\kappa l)} = \frac{2m}{\hbar^2 l}\int_0^\infty \rho U(\rho)d\rho, \tag{4}$$

to lowest order. Hint: Use Eq. (3) to get the logarithmic derivative from the inside (assuming that $\phi(l)$ is a constant) and use the leading asymptotic form $\log(\kappa\rho)$ to get the one from the outside.

3) Show that to lowest order in the strength of the potential we have

$$|E| = \frac{\hbar^2}{ml^2}\mathrm{Exp}(-\frac{m}{\hbar^2}\left|\int_0^\infty \rho U(\rho)d\rho\right|^{-1}), \tag{5}$$

thus in 2D weakly bound states have exponentially small binding energies! For this reason the 2D case is considered the borderline case and if you could analytically continue your equations in a parameter representing the dimension of space $d = 2 + \epsilon$ you would find powerlaw binding for $\epsilon < 0$ and no binding for sufficiently small strength for $\epsilon > 0$.

4) How would you proceed if $\int_0^\infty \rho U(\rho)d\rho = 0$? Hint: Have a look at A.G. Volosniev *et al.*, Phys. Rev. Lett. **106**, 250401 (2011).

## 3 Weakly Bound States in 3D

Finally consider three spatial dimensions.

1) Take the spherically symmetric finite square well with length parameter $l$ and depth $U < 0$. Show that there is a critical strength, $U_c$, such that if $U > U_c$ then there is no bound states in the well.

**Solution:** Reduce the problem to a radial equation for the reduced wave function $u(r) = r\psi(r)$ with boundary condition $u(0) = 0$. Look for a solution that is a $Sin(kr)$ inside and $e^{-\kappa r}$ outside where as usual $\kappa = \sqrt{2m|E|/\hbar^2}$. Match the wave functions and derivatives at $l$ and deduce an equation connection $k$ and $\kappa$. Show that this equation cannot have solutions when $|U| \to 0$.

# 4 Scattering length and bound states in 3D

Consider a particle scattering on a potential, $U(r)$, in three spatial dimensions. We will assume that the potential is spherically symmetric (depend only on $r$) and that the scattering is only significant for states with zero angular momentum, also called $s$-wave states. The Schrödinger equation for the reduced wave function $u = r\psi(r)$ has the form

$$\frac{d^2u(r)}{dr^2} + \left(k^2 - \frac{2m}{\hbar^2}U(r)\right)u(r) = 0, \tag{6}$$

where $E = \hbar^2k^2/2m$.

1) Assume that the potential $U(r)$ vanishes for $r > R$. Show that a solution of the Schrödinger equation for $r > R$ is $u(r) = A\sin(kr + \delta(k))$, where $A$ is a constant. The quantity $\delta(k)$ is called the scattering phase shift. Explain why this name makes sense.

2) Consider the limit of very low-energy scattering, i.e. $k \to 0$. Argue that $u(r) = B(r - a)$ is a solution of the scattering problem outside the range of the potential. Here $B$ is some other constant. Comparing this particular solution to the general solution, show that

$$\frac{u'(r)}{u(r)} = k\cot\left[k\left(r + \frac{\delta(k)}{k}\right)\right] \to \frac{1}{r-a}, \text{ for } k \to 0. \tag{7}$$

3) Assume that $R \ll |a|$ and set $r = 0$ in the formula from 2) to obtain the low-energy relation between $a$ and the scattering phase shift in the form

$$k\cot\delta(k) = -\frac{1}{a}. \tag{8}$$

4) To gain some intuition for the meaning of $a$, consider an attractive box potential with some finite range. Draw the potential and sketch how you would match the inside and outside solutions for the cases where $a < 0$ and for $a > 0$. Hint: Use the solution $r - a$ for the outside region and match it to something reasonable from the inside keeping in mind that $u(0) = 0$.

5) Argue that in the limit $k \to 0$, the solution inside the box is essentially the same irrespective of whether $k \to 0^+$ (scattering) or $k \to 0^-$ (bound state). A

bound state wave function has the form $\psi(r) \propto e^{-\kappa r}$. Equate the logarithmic derivatives of the $k \to 0$ solutions on the bound and the scattering side of $k = 0$ and show that for $R \ll a$ we find

$$\kappa = \frac{1}{a}, \tag{9}$$

and that we may thus relate the bound state energy and the scattering length by

$$E_B = -\frac{\hbar^2}{2ma^2}. \tag{10}$$

6) Argue that when $a < 0$ there is no low-energy bound state.

7) Show that the expectation value of the squared radius in the bound state is $\langle r^2 \rangle = a^2/2$.

# 5 Three-Body States in BO limit

Consider two heavy particles of mass $M$ in 3D that are localized a distance $R$. The two heavy particles interact with a light particle of mass $m$. We assume $m \ll M$. This is the Born-Oppenheimer limit that applies to molecules and/or ions like for instance $H_2^-$ with $M$ the proton and $m$ the electron mass.

We assume that the heavy and light particles interact via a zero-range interaction. To model this we take the following potential as seen by the light particle

$$V(\boldsymbol{r}) = V_0 \left[\delta(\boldsymbol{r} - \boldsymbol{R}/2) + \delta(\boldsymbol{r} + \boldsymbol{R}/2)\right], \tag{11}$$

where we assume that the two heave particles are located at $\pm\boldsymbol{R}/2$. This potential needs to be regularized since as it stands it leads to an ultraviolet divergence. We return to this point below. Now we consider the Schrödinger equation for the particle of mass $m$ in this potential

$$H\phi = E_L\phi, \tag{12}$$

where $E_L$ is the energy and $\phi$ the wave function. Since $V(\boldsymbol{r})$ contains delta-functions, it is convenient to work in momentum-space. For the sake of clarity, we use the following convention for the 3D Fourier transforms

$$\phi(\boldsymbol{r}) = \tfrac{1}{(2\pi)^3} \int d^3k e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} \phi(\boldsymbol{k}), \tag{13}$$

$$\phi(\boldsymbol{k}) = \int d^3r e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \phi(\boldsymbol{r}). \tag{14}$$

1) Show that the Schrödinger equation in momentum-space can then be written

$$\epsilon_{\boldsymbol{k}}\phi(\boldsymbol{k}) + \frac{1}{(2\pi)^3}\int d^3k' \phi(\boldsymbol{k}')V(\boldsymbol{k} - \boldsymbol{k}') = E_L\phi(\boldsymbol{k}). \tag{15}$$

with $\epsilon_{\boldsymbol{k}} = \hbar^2 k^2/2m$ and $V(\boldsymbol{q}) = \int d^3 r V(\boldsymbol{r}) e^{i\boldsymbol{q}\cdot\boldsymbol{r}}$.

2) Show that for the case at hand we have

$$V(\boldsymbol{q}) = 2V_0 \cos\left(\boldsymbol{q}\cdot\frac{\boldsymbol{R}}{2}\right), \tag{16}$$

and therefore we get

$$(\epsilon_{\boldsymbol{k}} - E_L)\,\phi(\boldsymbol{k}) = \frac{-2V_0}{(2\pi)^3}\int d^3k' \cos\left(\frac{(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}{2}\right)\phi(\boldsymbol{k}'). \tag{17}$$

3) Now show that

$$\phi(\boldsymbol{k}) = \frac{-2V_0}{(2\pi)^3}\frac{1}{\epsilon_{\boldsymbol{k}} - E_L}\int d^3k' \left[\cos(\frac{\boldsymbol{k}\cdot\boldsymbol{R}}{2})\cos(\frac{\boldsymbol{k}'\cdot\boldsymbol{R}}{2}) + \sin(\frac{\boldsymbol{k}\cdot\boldsymbol{R}}{2})\sin(\frac{\boldsymbol{k}'\cdot\boldsymbol{R}}{2})\right]\phi(\boldsymbol{k}'). \tag{18}$$

4) Since we are looking for the ground state we may assume that $\phi(\boldsymbol{k}) = \phi(-\boldsymbol{k})$. Multiply by $\cos(\frac{\boldsymbol{k}\cdot\boldsymbol{R}}{2})$, integrate over $\boldsymbol{k}$, and use this to show that

$$1 = -\frac{2V_0}{(2\pi)^3}\int d^3k \frac{\cos^2\left(\frac{\boldsymbol{k}\cdot\boldsymbol{R}}{2}\right)}{\epsilon_{\boldsymbol{k}} - E_L}. \tag{19}$$

Show that this can be rewritten into

$$1 = -\frac{V_0}{(2\pi)^3}\int d^3k \frac{1}{\epsilon_{\boldsymbol{k}} - E_L} - \frac{V_0}{(2\pi)^3}\int d^3k \frac{\cos(\boldsymbol{k}\cdot\boldsymbol{R})}{\epsilon_{\boldsymbol{k}} - E_L}. \tag{20}$$

The time has now come to relate $V_0$ and the scattering length of the interaction between the heavy and the light particle, $a$. From the Lippmann-Schwinger equation for the heavy-light scattering we have

$$\frac{1}{V_0} = \frac{\mu}{2\pi a \hbar^2} - \frac{1}{(2\pi)^3}\int d^3k \frac{1}{\epsilon^{\mu}_{\boldsymbol{k}}}, \tag{21}$$

where $\mu = mM/(m+M)$ and $\epsilon^{\mu}_{\boldsymbol{k}} = \hbar^2 k^2/2\mu$ are reduced mass and energy. Since we assume $m \ll M$, we can safely use $\epsilon^{\mu}_{\boldsymbol{k}} = \epsilon_{\boldsymbol{k}}$ and $\mu = m$.

5) Use the Lippmann-Schwinger relation to show that

$$\frac{m}{2\pi a \hbar^2} = -\frac{1}{(2\pi)^3}\int d^3k \left[\frac{1}{\epsilon_{\boldsymbol{k}} - E_L} - \frac{1}{\epsilon_{\boldsymbol{k}}}\right] - \frac{1}{(2\pi)^3}\int d^3k \frac{\cos(\boldsymbol{k}\cdot\boldsymbol{R})}{\epsilon_{\boldsymbol{k}} - E_L}. \tag{22}$$

6) Show that the first term on the right-hand side is

$$\frac{1}{(2\pi)^3}\int d^3k \left[\frac{1}{\epsilon_{\boldsymbol{k}} - E_L} - \frac{1}{\epsilon_{\boldsymbol{k}}}\right] = -\frac{m}{\pi^2\hbar^2}\int_0^\infty dk \frac{\alpha^2}{k^2+\alpha^2} = -\frac{m\alpha}{2\pi\hbar^2}, \tag{23}$$

where $\alpha^2 = -2mE_L/\hbar^2 > 0$ since we are looking for bound states here. A perfectly convergent results due to the subtraction via the Lippmann-Schwinger equation.

7) Show that the second integral becomes

$$\frac{1}{(2\pi)^3}\int d^3k \frac{\cos(\boldsymbol{k}\cdot\boldsymbol{R})}{\epsilon_{\boldsymbol{k}} - E_L} = \frac{m}{\pi^2\hbar^2 R}\int_0^\infty dk \frac{k\sin(kR)}{k^2+\alpha^2} = \frac{m}{2\pi^2\hbar^2 R}\mathrm{Im}\left\{\int_{-\infty}^{\infty} dk \frac{ke^{ikR}}{(k+i\alpha)(k-i\alpha)}\right\}. \tag{24}$$

8) Perform the final integral via contour integration and show that we finally arrive at

$$\alpha R = \frac{R}{a} + e^{-\alpha R}, \tag{25}$$

which determines $E_L(R)$.

9) At unitarity, $|a| \to \infty$, we have the simpler equation, $\alpha R = e^{-\alpha R}$. Use a non-linear equation solver to show that $x_0 = e^{-x_0}$ is solved by $x_0 \sim 0.567$.

10) Let us do a perturbative expansion around unitarity, i.e. we assume that $R/a$ is very small, or put another way, we are considering the potential at distances much smaller than $a$. Writing $\alpha R = x_0 + \epsilon$, show that $\epsilon = (R/a)/(1 + e^{-x_0})$. Use this to show that

$$E_L = -\frac{\hbar^2 x_0^2}{2mR^2}\left[1 + \frac{1}{x_0^2(1+e^{x_0})}\frac{R}{a}\right]. \tag{26}$$

11) Another interesting limit, is $R \gg a$. Show that in this case we find

$$E_L = -\frac{\hbar^2}{2ma^2}. \tag{27}$$

Argue that this *only* works for $a > 0$. This energy is the usual energy of a particle of mass $m$ in the delta-function potential of a much heavier particle of mass $M \gg m$ (i.e. a fixed potential center). The physical interpretation is that the small mass particle forms a bound state with one of the heavy particles.

Following the Born-Oppenheimer description, this energy is now an effective potential for the two heavy particles as function of their distance $R$. So we have the heavy-heavy Schrödinger equation

$$\left[-\frac{\hbar^2}{M}\nabla^2_{\boldsymbol{R}} + E_L(\boldsymbol{R})\right]\Phi(\boldsymbol{R}) = E\Phi(\boldsymbol{R}), \tag{28}$$

where the kinetic energy is missing a factor of 2 in the denominator since the reduced mass in the heavy-heavy system is $M/2$. Here $E$ is the total energy of the system of light-heavy-heavy type.

12) Define $u(\boldsymbol{R}) = R\Phi(\boldsymbol{R})$, $\kappa^2 = -ME/\hbar^2 > 0$ (we are looking for bound states with $E < 0$), and $z = \kappa R$, and show that the heavy-heavy Schrödinger equation becomes

$$\frac{d^2u(z)}{dz^2} - u(z) + \frac{\beta(a,z)^2}{z^2}u(z) = 0, \tag{29}$$

where

$$\beta(a,z)^2 = \frac{x_0^2}{2}\frac{M}{m}\left[1 + \frac{1}{x_0^2(1+e^{x_0})}\frac{R}{a}\right], \tag{30}$$

is still a function of $z$.

If we consider $z \ll \kappa a$ ($R \ll a$) or $|a| \to \infty$, we can drop the second term and get a constant $\beta$. In this case, the solution to Eq. (29) which has the correct boundary condition at $z \to \infty$ (exponentially decreasing, $e^{-z}$) contains a modified Bessel of the second kind, $K_n(z)$. However, the order has to be imaginary, i.e. $n \to i(\beta^2 - 1/4)$, and we arrive at $u(z) = \sqrt{z}K_{i(\beta^2-1/4)}(z)$ (not normalized). In our case, $M \gg m$, so $\beta^2 \gg 1$, i.e. it is always a positive imaginary order.

13) Show that the wave function $u(z)$ has the following behavior at small $z$

$$u(z) \propto \sqrt{z}\cos\left(s_0\log(z)\right), \tag{31}$$

where $s_0 = \sqrt{\beta^2 - 1/4}$. This is the origin of the log-periodic behavior of the states found by Efimov when $|a| \to \infty$.

14) Show that Eq. (28) has an interesting scaling invariance, i.e. show that $\Phi(\lambda\boldsymbol{R})$ solves the Schrödinger equation with energy $\lambda^2 E$ when $|a| \to \infty$ for $\lambda$ a real number.

15) However, Eq. (31) further contrains the choice of $\lambda$. Using $z = \kappa R$, we have

$$\Phi(\boldsymbol{R}) \propto \sqrt{\kappa R}\cos\left(s_0\log(\frac{R}{R_0})\right), \tag{32}$$

where $R_0$ is a necessary short-distance cut-off which comes from the repulsive cores of atoms at short distance. Show that in order to preserve the $\lambda$ scaling, we need to require $s_0\log(\lambda) = n\pi$, where $n$ is an integer.

16) Show that this implies that there is an infinitude of three-body bound states with energies

$$E_n = E_0 e^{-2\pi n/s_0}, \tag{33}$$

which is the famous Efimov effect.

The ground state is related to $R_0$ since $E_0 \sim -\hbar^2/2MR_0^2$ (up to constants of order 1 that we have neglected for simplicity). For $M \gg m$, $s_0$ will be large and will therefore in turn lead to a small scale factor $e^{-2\pi n/s_0}$, which means that the spectrum of three-body bound states is quite dense, there are many three-body bound states around!

17) Argue that for finite $a$, it the above considerations are good up to $R \sim |a|$, and that the number of bound states is approximately $N \sim s_0 \log(|a|/R_0)/\pi$ and increases with $s_0$, i.e. with $\sqrt{M/m}$.

# 6 Efimov Physics in a Many-body Background

The Efimov states we observe in Nature are most often embedded in some larger systems so that one could suspect that many-body effects will influence these few-body bound states in certain regimes of for instance higher density.

1) Consider the Born-Oppenheimer solution of the previous problem. How would you modify the equations if the light particle is a fermion that has a Fermi sea background? Assume for simplicity that the Fermi sea is inert, i.e. there are no particle-hole pairs in the Fermi sea. (This has been considered recently by MacNeill and Zhou, Phys. Rev. Lett. **106** (2011) 145301.)

2) Consider now the case where the light particle is part of a condensate. How would you now modify the Born-Oppenheimer equations for the three-body bound states? (This has been considered recently by Zinner, see Europhysics Letters **101** 60009 (2013) and Eur. Phys. J. D **68**, 261 (2014).)

# 7 Two fermions in a 1D harmonic oscillator with strong interparticle interactions

Consider the following Hamiltonian in one dimension for two particles in a harmonic oscillator potential

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 + g\delta(x_1 - x_2) = H_1 + H_2 + g\delta(x_1 - x_2), \tag{34}$$

where $x_1$ and $x_2$ are the coordinates of the particles, $p_1$ and $p_2$ the momenta, $m$ is the mass, and $\omega$ is the angular frequency of the oscillator trap. The interaction between the particles is given by a zero-range Dirac delta-function with strength $g$.

1) First consider the non-interacting case, $g = 0$. Sketch the potential and the eigenenergies for a single particle on the same plot. What are the wave functions for a single particle in the ground state and in the first excited state?

2) What is the ground-state energy if you have two identical bosons? What is the ground state energy for two identical fermions? What is the ground state for fermions with two opposite spin states (spin up and spin down)?

3) What does the $g = 0$ wave function look like for two identical fermions? Make a sketch of it using relative coodinates $x = x_1 - x_2$. What changes when we have $g \neq 0$?

4) Consider instead two fermions with different spin states, i.e. an up and a down spin pair. Write down the wave function for $g = 0$. Change to relative coordinates, $x = x_1 - x_2$ and $X = (x_1 + x_2)/2$, throw away the center-of-mass $X$ coordinate (we have to worry about that for interactions), and sketch the wave function as a function of relative coordinate, $x$.

5) Now consider repulsive interactions, $g > 0$, and the case of two fermions with opposite spins. What happens to the energy of the state consider in **4)**? Make a sketch of the energy.

6) Argue that for a Dirac delta function interaction $g\delta(x_1 - x_2)$, the wave function is continuous but the derivative is not.

7) What is the energy of a state with one spin up in the ground state and one spin down in the first excited state? Compare this energy to the energy of two identical fermions from **2)**.

8) Combining your knowledge from **3)**, **5)** and **6)**, make a sketch of the energy of two identical fermions and of two fermions with opposite spins as the strength of the interaction goes from $g = 0$ to $g = +\infty$.

You now know what people mean when they say fermionization of two fermions with opposite spin states. This has been explored experimentally in G. Zürn *et al.*, Phys. Rev. Lett. **108**, 075303 (2012). What remains is to figure out what the wave function looks like at $g = +\infty$ for the two fermions with different spins.

9) The Hamiltonian conserves parity and we can thus classify state as even or odd under parity. What is the parity of the wave function in **3)**? What is the parity of the wave function in **4)**?

10) The wave function must be a solution of the non-interacting ($g = 0$) Hamiltonian expect when $x = x_1 - x_2 = 0$ where the delta function contributes. Argue that for $g = +\infty$, the wave function at $x = 0$ has to vanish.

11) Use conservation of parity to argue that the ground state wave function for two fermions with opposite spins at $g = \infty$ must have even parity.

12) Combine non-interacting wave functions for $x < 0$ and $x > 0$ for two fermions with different spins into an even parity solution that vanishes at $x = 0$.

# 8 Exact Two-Body Solutions in a Harmonic Trap

For two equal mass particles in a harmonic trap interacting via a zero-range interaction, it turns out that one can solve the problem exactly. For simplicity we will consider the 1D case in this problem. The Hamiltonian for the system is

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega^2 x_1^2 + \frac{1}{2}m\omega^2 x_2^2 + g\delta(x_1 - x_2), \tag{35}$$

where $x_1, x_2$ are the coordinates while $p_1, p_2$ are the momenta of the two particles. The strength of the interaction is $g$.

1) Show that the Hamiltonian is seperable in relative, $x = (x_1 - x_2)/\sqrt{2}$, and center-of-mass coordinates $X = (x_1 + x_2)/\sqrt{2}$ and that we may thus forget about the center-of-mass part when looking for the solution of the interacting problem.

2) **HARD!** Find an equation that relates the energy eigenvalues to $g$ for general $g$. Hint: Expand a general solution of the problem in the well-known basis of harmonic oscillator energy eigenstates. Find relations for the coefficients of such an expansion. From there one needs to use different mathematical properties of the solutions of the oscillator to advance.