Strongly correlated systems
in atomic and condensed matter physics

Lecture notes

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Chapter 10

Feshbach resonance

10.1 Scattering length, T-matrix, and scattering amplitude

Systems of ultracold atoms are also ultradilute. Interatomic distances ($n^{-1/3} \sim 5 \times 10^3 a_0$) are much larger than the range of interatomic interactions r_0 (Interactions between atoms are Van der Waals with a sharp short distance cut-off. See section 10.2.). Fine details of the short range potential should be unimportant for describing scattering processes. Said differently, colliding particles can not resolve detailed structure of the potential because they have small wavevectors. We should be able to characterize properties of collisions at low energies by the scattering length only.

We consider a collision between two particles of equal masses m (reduced mass $m_r = \frac{1}{2}m$). For the relative motion

$$\Psi(\vec{r}) = e^{ikz} + \Psi_{sc}(\vec{r}) \tag{10.1}$$

The first part on the right hand side describes the incoming particles. The second term describes scattered particles. Generally $\Psi_{sc}(\vec{r}) = f(\theta)e^{ikr}/r$. When only s-wave scattering is present, $k \to 0$, and we take the asymptotic form for $r \to \infty$

$$\Psi(\vec{r}) = e^{ikz} - \frac{a}{r} \tag{10.2}$$

The constant a is called the scattering length[12, 15].

In momentum space wavefunction (10.1) is given by

$$\Psi(\vec{k'}) = (2\pi)^3 \delta(\vec{k} - \vec{k'}) + \Psi_{sc}(\vec{k'}) \tag{10.3}$$

This wavefunction satisfies Schroedinger equation

$$(\frac{k^2}{m} - \frac{k'^2}{m})\Psi_{sc}(\vec{k'}) = U(\vec{k'}, \vec{k}) + \int \frac{d^3 k''}{(2\pi)^3} U(\vec{k'}, \vec{k''}) \Psi_{sc}(\vec{k''}) \tag{10.4}$$

Here V is the volume of the system and

$$U(\vec{k}', \vec{k}) = \int d^3\vec{r}\, d^3\vec{r}'\, U(\vec{r} - \vec{r}')\, e^{i\vec{k}\vec{r}}\, e^{-i\vec{k}'\vec{r}'} \tag{10.5}$$

Then

$$\Psi_{\mathrm{sc}}(\vec{k}') = (\frac{k^2}{m} - \frac{k'^2}{m} + i\delta)^{-1}\, [U(\vec{k}', \vec{k}) + \int \frac{d^3k''}{(2\pi)^3}\, U(\vec{k}', \vec{k}'')\, \Psi_{\mathrm{sc}}(\vec{k}'')] \tag{10.6}$$

In the last equation we added $i\delta$ to the denominator to ensure that we have outgoing waves only. Here is a brief reminder how to verify this. Consider

$$\int \frac{d^3k'}{(2\pi)^3} \frac{e^{i\vec{k}'\vec{r}}}{k^2 - k'^2 + i\delta} = \frac{1}{(2\pi)^3} \int_0^\infty k'^2 dk' \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\phi \frac{e^{ik'r\cos\theta}}{k^2 - k'^2 + i\delta}$$

$$= \frac{1}{2\pi^2} \int_0^\infty \frac{k'^2 dk'}{k^2 - k'^2 + i\delta} \frac{\sin k'r}{k'r} = \frac{-1}{4\pi^2 r\, i} \int_{-\infty}^{+\infty} \frac{e^{ik'r}\, k'}{k'^2 - k^2 - i\delta}$$

Since $r > 0$ we need to close the contour in the upper half-plane for k'. Hence we pick up the pole at $k' = |k| + i\delta$ and get

$$\int \frac{d^3k'}{(2\pi)^3} \frac{e^{i\vec{k}'\vec{r}}}{k^2 - k'^2 + i\delta} = -\frac{e^{i|k|r}}{4\pi\, r} \tag{10.7}$$

It is convenient to introduce

$$T(\vec{k}', \vec{k}, E) = U(\vec{k}', \vec{k}) + \int \frac{d^3k''}{(2\pi)^3} \frac{U(\vec{k}', \vec{k}'')}{(E - \frac{k''^2}{m} + i\delta)}\, T(\vec{k}'', \vec{k}, E) \tag{10.8}$$

Then $\Psi_{\mathrm{sc}}(\vec{k}')$ from equation (10.6) can be written as

$$\Psi(\vec{k}') = (\frac{k^2}{m} - \frac{k'^2}{m} + i\delta)^{-1}\, T(\vec{k}', \vec{k}, E = \frac{k^2}{m}) \tag{10.9}$$

Equation (10.8) is called the Lippman-Schwinger equation. When $k \to 0$ equation (10.9) gives

$$\Psi_{sc}(\vec{r}) = -\int \frac{d^3k'}{(2\pi)^3} \frac{m}{k'^2}\, T(0, k', 0)\, e^{i\vec{k}'\vec{r}} \tag{10.10}$$

The relevant values of k' are $1/r$, thus we can set $k' = 0$ inside $T(0, k', 0)$. Then

$$\Psi_{sc}(\vec{r}) = -\frac{m}{4\pi r}\, T(0, 0, 0) \tag{10.11}$$

Instead of the T matrix it is also convenient to use the scattering amplitude

$$f(k', k) = = -\frac{m}{4\pi\hbar^2}\, T(k', k, E = \frac{k^2}{m}) \tag{10.12}$$

Interactions between atoms are strong but they occur only when two atoms are close together. To avoid having to calculate short range correlations between atoms in detail, it is convenient to introduce the concept of an effective interaction. The idea of an effective interaction $\tilde{U}$ is that it is an effective interaction, which produces the correct scattering matrix, although it describes interactions between a limited set of states (low energy states).

When solving (10.8) we introduce an intermediate energy scale ϵ_c and define

$$\tilde{U}(\vec{k}', \vec{k}, E) = U(\vec{k}', \vec{k}) + \int_{|\vec{k}''|>\epsilon_c} \frac{d^3k''}{(2\pi)^3} \frac{U(\vec{k}', \vec{k}'')}{(E - \frac{k''^2}{m} + i\delta)} \tilde{U}(\vec{k}'', \vec{k}, E) \quad (10.13)$$

The effective potential depends explicitely on the choice of the cut-off ϵ_c. We can rewrite equation (10.8) using $\tilde{U}$

$$T(\vec{k}', \vec{k}, E) = \tilde{U}(\vec{k}', \vec{k}) + \int_{|\vec{k}''|<\epsilon_c} \frac{d^3k'}{(2\pi)^3} \frac{\tilde{U}(\vec{k}', \vec{k}'')}{(E - \frac{k''^2}{m} + i\delta)} T(\vec{k}'', \vec{k}, E) \quad (10.14)$$

As the simplest effective potential one usually takes

$$V(r) = V_0 \, \delta^3(r) \quad (10.15)$$

with the energy cut-off $E_R = \frac{\hbar^2}{mR^2}$. Lippman-Schwinger equation for $f(\vec{k}', \vec{k})$:

$$f(\vec{k}', \vec{k}) = -\frac{mv(\vec{k}' - \vec{k})}{4\pi} + m \int \frac{d^3q}{(2\pi)^3} \frac{v(\vec{k}' - \vec{q})f(\vec{q}, \vec{k})}{k^2 - q^2 + i\delta} \quad (10.16)$$

Solving this equation requires the knowledge of $f(\vec{q}, \vec{k})$ even when $q^2 \neq k^2$ ("off the energy shell"). However the dominant contribution comes from $q^2 = k^2$ part. For low energy s-wave scattering we can change $f(\vec{q}, \vec{k}) \to f(k)$. Function $f(k)$ only depends on the magnitude of $\vec{k}$. With this approximation we can take $f(k)$ outside the integral in (10.16)

$$\frac{1}{f(k)} = -\frac{4\pi}{mv_0} + 4\pi \int_{|q|<\frac{1}{R}} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\delta} \quad (10.17)$$

We have

$$\int_{|q|<\frac{1}{R}} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\delta} = \frac{4\pi}{(2\pi)^3} \int_0^{|q|=\frac{1}{R}} dq \frac{q^2}{k^2 - q^2 + i\delta}$$

$$= \frac{1}{2\pi^2} [-\frac{1}{R} - \frac{k}{2} \log\left((-1)\frac{R^{-1} - k - i\delta}{R^{-1} + k + i\delta}\right)] \quad (10.18)$$

Assuming $kR << 1$

$$\int_{|q|<\frac{1}{R}} \frac{d^3q}{(2\pi)^3} \frac{1}{k^2 - q^2 + i\delta} = \frac{1}{2\pi^2} [-\frac{1}{R} - \frac{k}{2}(i\pi + \log(1 - 2kR))]$$

$$= \frac{1}{2\pi^2} [-\frac{1}{R} - \frac{i\pi k}{2} + k^2 R] \quad (10.19)$$

From the last equation

$$\frac{1}{f(k)} = -\frac{4\pi}{mv_0} - \frac{2}{\pi R} - ik + \frac{2R}{\pi}k^2 \tag{10.20}$$

We recall that $f(k \to 0) = -a$. Hence we have

$$f(k) = \frac{1}{-\frac{1}{a} + r_{eff}\frac{k^2}{2} - ik} \tag{10.21}$$

with

$$a = \frac{\pi}{2} \frac{R}{(1 + \frac{2\pi^2 R}{mv_0})} \tag{10.22}$$

Equation (10.21) is a generic form of the low energy form of the scattering amplitude[12]. Equation (10.22) is specific to the model interaction (10.15).

10.2   Simple model for interatomic interactions

The simplest model for interatomic interactions [15, 2]

$$U(r) = \{ \begin{array}{ll} -\frac{\alpha}{r^6} & \text{for } r > r_c \\ \infty & \text{for } r \le r_c \end{array} \tag{10.23}$$

The first part comes from the Van der Waals attraction. The hard core repulsion appears when electron wavefunctions begin to overlap. This simplified model captures essential aspects of atomic interactions when the potential has many bound states as in alkali atoms. For the radial part of the wavefunction of the relative motion of two atoms we have

$$\begin{aligned} \chi(r) &= rR(r) \\ \chi" &+ [k^2 - \frac{l(l+1)}{r^2} - mU(r)]\chi(r) = 0 \end{aligned} \tag{10.24}$$

We still use $m_r = \frac{1}{2}m$. We are interested in the $E \to 0$ limit so we can set $k = 0$ and $l = 0$ for s-wave sector. Then

$$\begin{aligned} \chi'' &+ \frac{m\alpha}{r^6}\chi = 0 & \text{for } r > r_c \\ \chi &= 0 & \text{for } r \le r_c \end{aligned} \tag{10.25}$$

We define

$$r_0 = \left(\frac{m\alpha}{\hbar^2}\right)^{1/4} \tag{10.26}$$

and measure distances in units of r_0, i.e. $x = r/r_0$. Then the last equation becomes

$$\frac{d^2\chi}{dx^2} + \frac{1}{x^6}\chi = 0 \tag{10.27}$$

We look for $\chi(x) = x^{1/2} g(\frac{1}{2x^2})$ and use $z = 1/2x^2$. Then

$$g''_{zz} + \frac{1}{z} g'_z + (1 - \frac{1}{16z^2})g = 0 \tag{10.28}$$

This is the familiar Bessel equation

$$g(z) = A J_{1/4}(z) + B J_{-1/4}(z) \tag{10.29}$$

here $z = r_0^2/2r^2$. From $\chi(r_c) = 0$ we obtain

$$\frac{A}{B} = -\frac{J_{-1/4}(r_0^2/2r_c^2)}{J_{1/4}(r_0^2/2r_c^2)} \tag{10.30}$$

For alkali atoms $r_c \leq 10a_0$ and $r_0 \sim 100a_0$. Hence we can use asymptotic form of Bessel functions

$$J_p(z) \simeq \sqrt{\frac{2}{\pi z}} \cos(z - (p + \frac{1}{2})\frac{\pi}{2}) \tag{10.31}$$

Hence

$$\frac{A}{B} = -\frac{\cos(r_0^2/2r_c^2 - \pi/8)}{\cos(r_0^2/2r_c^2 - 3\pi/8)} \tag{10.32}$$

To determine the scattering length we need to examine the wavefunction for $r \gg r_0$, i.e. for $z \ll 1$. In this limit

$$J_p(z) \simeq \frac{z^p}{2^p \Gamma(1 + p)} \tag{10.33}$$

Then using $z = r_0^2/2r^2$ we obtain

$$\chi(r) = \left(\frac{r}{r_0}\right)^{1/2} g = \frac{A}{\sqrt{2}\Gamma(\frac{5}{4})} + B \frac{\sqrt{2}}{\Gamma(\frac{3}{4})}$$

$$R(r) = \frac{\chi(r)}{r} = B \frac{\sqrt{2}}{\Gamma(\frac{3}{4})} \frac{1}{r_0} + A \frac{1}{\sqrt{2}\Gamma(\frac{5}{4})} \frac{1}{r} \tag{10.34}$$

From comparison with (10.2) we find

$$a = \frac{A}{B} \frac{r_0}{2} \frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{5}{4})}$$

$$\simeq \frac{r_0}{2} \frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{5}{4})} \frac{\cos(\frac{r_0^2}{2r_c^2} - \frac{\pi}{8})}{\cos(\frac{r_0^2}{2r_c^2} - \frac{3\pi}{8})} \tag{10.35}$$

The scale of a is set by r_0. The scattering length canbe either positive or negative depending on the short-range part of interactions. A bound state appears whenever a tends to minus infinity[12]. Thus the number of bound states is given by the integer part of $\frac{r_0^2}{2\pi r_c^2}$. For a more detailed discussion see references [15, 2].
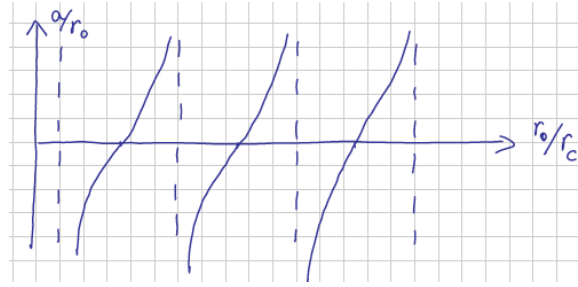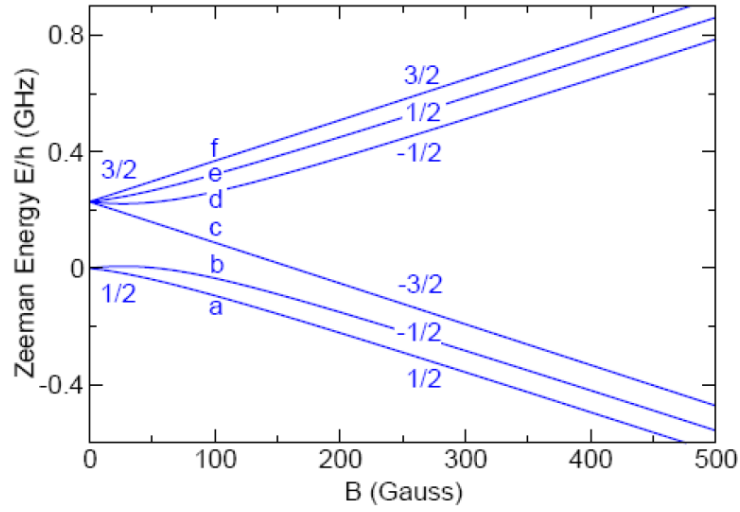
Figure 10.1: Scattering length for the model potential (10.23).

Figure 10.2: Atomic energy levels of the ^{6}Li, which has $S = 1/2$, $I = 1$, and $F = 1/2$ and 3/2. The figure shows both m_z and the alphabetic shorthand notation used in the text. Figure taken from [3].

10.3   Multichannel model

We consider a specific example of fermionic ^{6}Li atoms, which have electronic spin $s = 1/2$ and nuclear spin $I = 1$. Hyperfine structure of individual atoms needs to be found from

$$\mathcal{H}_{\text{HF+Zeeman}} = A_{\text{HFS}}\vec{I}\vec{S} + (2\mu_B S_z - \mu_n I_z)B \qquad (10.36)$$

The only operator that commutes with $\mathcal{H}_{\text{HF+Zeeman}}$ is $F_z = S_z + I_z$. So we can only label states by $m_f = m_s + m_I$. Figure 10.2 shows single particle levels of ^{6}Li. When $B >> A_{\text{HFS}}/\mu_B = 30$ G in ^{6}Li the energy is primarily determined
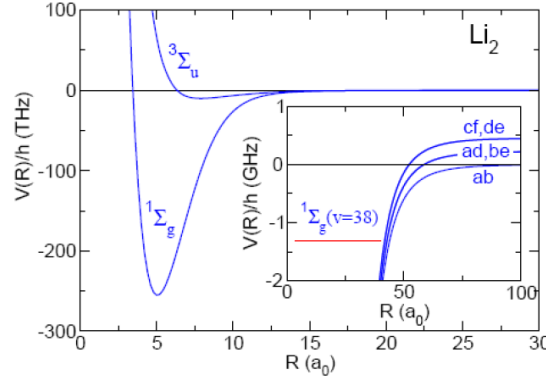
Figure 10.3: Molecular potentials $V(R)$ vs R of the two electronic states of Li_2. The inset shows the long range s-wave potential of ^6Li at $B = 0$, indicating hyperfine states of the separated atoms. The inset also shows the last degenerate bound state, corresponding to the $v = 38$ vibrational level of $^1\Sigma_g^+$ potential. Figure taken from [3].

by m_s. Consider a collision between states $|a\rangle$ and $|b\rangle$

$$|a\rangle = |m_s = -\frac{1}{2}; m_I = 1\rangle + \text{small admixture of } |m_s = \frac{1}{2}; m_I = 0\rangle$$

$$|b\rangle = |m_s = -\frac{1}{2}; m_I = 0\rangle + \text{small admixture of } |m_s = \frac{1}{2}; m_I = -1\rangle \quad (10.37)$$

Interaction during the collision depends on the *electron spins* (not the full hyperfine spin). There is stronger repulsion at short distances for the triplet configuration of electron spins (see fig. 10.3).

$$V(r) = \frac{1}{4} \left(3V_t(r) + V_s(r) \right) + \vec{S}_1 \vec{S}_2 \left(V_t(r) - V_s(r) \right) \quad (10.38)$$

The initial state $|a, b\rangle$ (see figure 10.2) is not a purely triplet state and spins can evolve during the collision. The spin state $|a, b\rangle$ may be coupled to other scattering states $|c, f\rangle$, provided that the z-projection of the total spin, $m_f = m_s + m_I$, is conserved ($m_{fa} + m_{fb} = m_{fc} + m_{ff}$). When atoms are far apart, the energy of the $|c, f\rangle$ state is a sum of single particle energies of $|c\rangle$ and $|f\rangle$. It exceeds the energy of the $|a, b\rangle$ state by an energy that is of the order of the hyperfine energy or the Zeeman energy of electrons. So the channel $|c, f\rangle$ is closed and the atoms always emerge from the collision in the open channel state $|a, b\rangle$. However due to strong coupling of $|a, b\rangle$ to $|c, f\rangle$ the effective scattering amplitude in the open channel can be strongly modified. A Feshbach resonance occurs when the incoming state in the open channel is resonant with a bound state in the closed channel. The two states have different magnetic moments, so the energy difference between the incoming and the Feshbach bound state can be tuned via applied magnetic field.

We consider a simple model of the Feshbach resonance in which there is only one important bound state[11]. We denote the continuum of plane waves of relative momentum $\vec{k}$ in the incoming open channel as $|\vec{k}\rangle$. The bound state is $|m\rangle$. In the absence of coupling

$$
\begin{aligned}
\mathcal{H}_0 \,|\vec{k}\rangle &= 2\epsilon_k \,|\vec{k}\rangle \\
\mathcal{H}_0 \,|m\rangle &= \delta \,|m\rangle
\end{aligned}
\tag{10.39}
$$

Here δ is energy of the molecular state, which can be controlled by the magnetic field. We neglect interactions in the incoming channel, which do not originate from $|m\rangle$. We define

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + V \\
\langle m|V|\vec{k}\rangle &= \frac{g_k}{\sqrt{V}}
\end{aligned}
\tag{10.40}
$$

From the Schroedinger equation

$$
\begin{aligned}
\mathcal{H}|\phi\rangle &= E|\phi\rangle \\
|\phi\rangle &= \alpha|m\rangle + \sum_k c_k|\vec{k}\rangle
\end{aligned}
\tag{10.41}
$$

we obtain coupled equations

$$
\begin{aligned}
(E - 2\epsilon_k)c_k &= \frac{g_k}{\sqrt{V}}\alpha \\
(E - \delta)\alpha &= \frac{1}{\sqrt{V}}\sum_k g_k c_k = \frac{\alpha}{V}\sum_k \frac{g_k^2}{(E - 2\epsilon_k)}
\end{aligned}
\tag{10.42}
$$

Thus energy eigenvalues of the system can be found from equation

$$
E - \delta = \frac{1}{V}\sum_k \frac{g_k^2}{(E - 2\epsilon_k)}
\tag{10.43}
$$

We assume that the range of potential $r_0 \ll 1/k$. The closed channel molecular state $|m\rangle$ has a size R of the order of r_0, which the colliding atoms can not resolve. Thus the couplings g_k should not vary vary much for $k \ll 1/R$. Thus we can take $g_k \approx g_0$ to be constant, up to a natural cut-off $E_R = 1/mR^2$ and $g_k = 0$ beyond. Then equation (10.43) simplifies to

$$
E - \delta = g_0^2 \int_k \frac{d^3k}{(2\pi)^3}\frac{1}{(E - 2\epsilon_k)}
\tag{10.44}
$$

We look for bound states with $E < 0$

$$
|E| + \delta = g_0^2 \int_{|k|<R^{-1}} \frac{d^3k}{(2\pi)^3}\frac{1}{(|E| + 2\epsilon_k)}
\tag{10.45}
$$

We define

$$
\begin{aligned}
E_0^{1/2} &= \frac{g_0^2}{2\pi}\left(\frac{m}{2}\right)^{3/2} \\
\delta_0 &= \frac{4}{\pi}\sqrt{E_0\,E_R}
\end{aligned}
\tag{10.46}
$$

For $|E| >> E_R$ we have using (10.45)

$$
|E| + \delta = \frac{2}{3}\,\delta_0\,\frac{E_R}{|E|}
\tag{10.47}
$$

so $E = -\delta$.

When $|E| << E_R$ we find from (10.45)

$$
|E| + \delta = \delta_0 - \sqrt{2\,E_0\,|\,E\,|}
\tag{10.48}
$$

For $\delta < \delta_0$ we find bound states with $E < 0$. Solving quadratic equation we obtain (see also figure 10.4)

$$
E = -E_0 + \delta - \delta_0 + \sqrt{(E_0 - \delta + \delta_0)^2 - (\delta - \delta_0)^2}
\tag{10.49}
$$

Close to the resonance, $\delta_0 - \delta < E_0$, we obtain

$$
E_{\text{bound}} = -\frac{1}{2}\frac{(\delta_0 - \delta)^2}{E_0}
\tag{10.50}
$$

Note that E_{bound} depends quadratically on $(\delta_0 - \delta)$. Far from the resonance $|\delta| >> \delta_0$, E_R we find

$$
E_{\text{bound}} = \delta
\tag{10.51}
$$

This is the original bound state.

Let us now discuss the scattering amplitude. Going back to equations (10.42) we find

$$
(E - 2\epsilon_k)c_k = \frac{g_k}{\sqrt{V}}\alpha = \frac{g_k}{V}\sum_q \frac{g_q c_q}{E - \delta} = \frac{1}{V}V_{\text{eff}}(k, q)c_q
\tag{10.52}
$$

The molecular state causes an effective interaction V_{eff} that corresponds to two atoms collidingand forming a molecule (matrix element $g_k/\sqrt{V}$), spending small amount of time (of order $\hbar/(E - \delta)$) in the molecular state, and exiting again as two unbound atoms (matrix element $g_k/\sqrt{V}$).

In equation (10.17) we need to replace $v_0 \to \frac{g_0^2}{E - \delta}$

$$
\frac{1}{f(k)} = -\frac{4\pi}{mg_0^2}(E - \delta) + 4\pi\int_{|q| < \frac{1}{R}}\frac{d^3q}{(2\pi)^3}\frac{1}{k^2 - q^2 + i\delta}
\tag{10.53}
$$

We take $E \to k^2/m$ and express g_0 using E_0 and obtain

$$
\frac{1}{f(k)} = -\left(\frac{m}{2E_0}\right)^{1/2}(\delta_0 - \delta) - \frac{1}{2}\left(\frac{2}{mE_0}\right)^{1/2}k^2 - ik
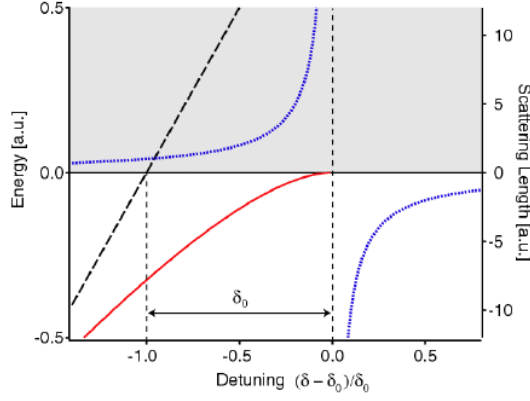\tag{10.54}
$$

Figure 10.4: Bare, uncoupled molecular state (dashed line), coupled, bound molecular state (solid line) and scattering length (dotted line) close to a Feshbach resonance. The continuum of scattered states with $E > 0$ is marked by the shaded area. Figure taken from [11]

So we can read off

$$\begin{aligned}
a &= \left(\frac{2E_0}{m}\right)^{1/2}\frac{1}{(\delta_0 - \delta)} \\
r_{\text{eff}} &= -\left(\frac{2}{mE_0}\right)^{1/2}
\end{aligned} \tag{10.55}$$

Note a universal relation between the scattering length and the energy of the bound state when $E_{\text{bound}} << E_R$

$$E_{\text{bound}} = -\frac{1}{ma^2} \tag{10.56}$$

Resonance is called broad when $E_0 >> E_R$. In this case the bound state oeys universal behavior already when $k_F a \approx 1$.

10.4   Three body recombination

Three body recombination is a process in which two atoms for a bound state and a third once carries away the energy equal to to the binding energy of a molecule. In the dilute atomic limit (size of the molecule much smaller than interatomic distances) we can estimate the rate of three body recombinations using the following argument. We start with the case of bosons. For atoms of equal mass momentum of the scattered atom $k_A \sim 1/a$. Recombination to a weakly bound state occurs in a collision between two atoms, when a third atoms is located inside a sphere of radius $l \sim a$ around the colliding pair. For such locations of the third atom (statistical weigth $\sim nl^3$) a molecule is formed with
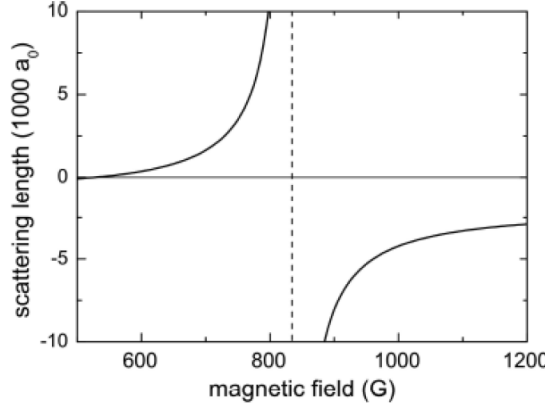
Figure 10.5: Magnetic field dependence of the scattering length between the two lowest magnetic sub-states of ^{6}Li with a Feshbach resonance at $B_0 = 834$G. The background scattering length is exceptionally large in this case. Figure taken from [3].

probability of the order of unity. The number of recombinations per unit time and unit volume

$$\nu_{\text{rec}} \sim n^2 \sigma v (nl^3) \tag{10.57}$$

Take the scattering cross section $\sigma \sim 8\pi a^2$ and $v \sim \hbar k_A / m$. We find $\nu_{rec} = \alpha_{\text{rec}} n^3$ with $\alpha \sim \frac{8\pi\hbar}{m} a^4$ [8].

In the case of fermionic atoms relaxation requires the presence of at least three fermions close to each other. As two of them are necessarily identical, due to the Pauli exclusion principle, the relaxation probability is strongly suppressed [16].

10.5   T-matrix revisited and geometrical resonances

10.5.1   Motivation

Atoms can be confined into one dimensional traps using optical potentials [13, 18, 4] or microtraps[7, 9]. To have a truly one dimensional system we need to have transverse confinement frequency to be higher than the chemical potential of the 1d system. We expect that a collision of two particles can also be described using a purely one dimensional problem. For we want to have an effective model of the type

$$\mathcal{H}_{1d} = \int dx \, \left\{ \frac{\hbar^2}{2m} |\nabla_x \Psi|^2 + \frac{g_{1d}}{2} \, \Psi^\dagger(x) \, \Psi^\dagger(x) \, \Psi(x) \, \Psi(x) - \mu \, \Psi^\dagger(x) \, \Psi(x) \right\} \tag{10.58}$$
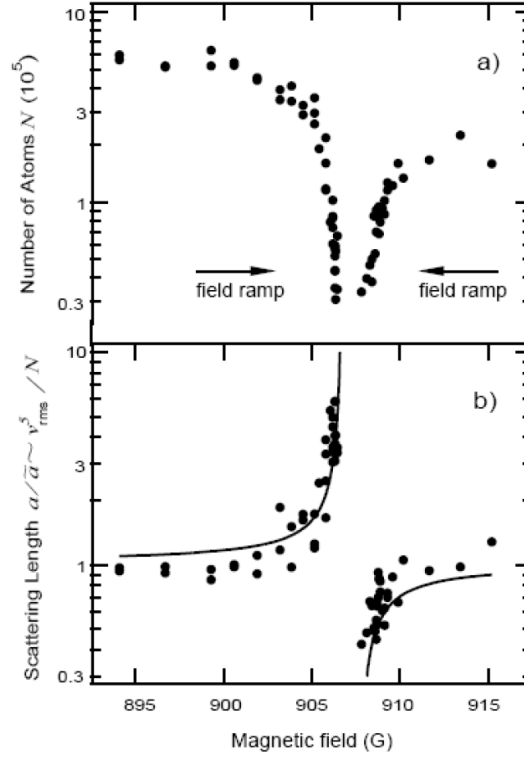
Figure 10.6: Observation of a magnetically tuned Feshbach resonance in an optically trapped BEC of Na atoms. The upper panel shows a strong loss of atoms near the resonance due to three body recombination. Figure taken from [6].

The question we address is how to relate g_{1d} to the scattering length in three dimensions. The simplest idea is to assume that particles are always in the oscillator ground state in the transverse direction

$$
\begin{aligned}
\Psi(r_\perp, z) &= \Psi_0(r_\perp)\Psi(z) \\
\Psi_0(r_\perp) &= \left(\frac{1}{\pi l}\right)^{1/2} e^{-\frac{r_\perp^2}{2l^2}} \\
l &= \left(\frac{\hbar}{m\omega}\right)^{1/2}
\end{aligned} \tag{10.59}
$$

Then we find that

$$
g_{1d} \sim \frac{g_{3d}}{l^2} \sim \frac{a_{3d}}{l^2} \tag{10.60}
$$

However this analysis becomes unreliable when we discuss systems close to Feshbach resonance [14, 1, 13, 5]. When interactions are strong virtual excita-

tions into excited transverse states become important [14, 1]. This is what we will analyze now.

Let us now formulate the problem more precisely. We consider a problem of scattering of two identical particles in a system in which parabolic potential is applied in $d_\perp$ transverse directions and motion is free in $d_\parallel = 3 - d_\perp$ directions. The full Hamiltonian of particles $i = 1, 2$ is given by

$$\mathcal{H} = -\frac{1}{m} \sum_{i=1,2;\, \alpha=1\ldots(d_\parallel+d_\perp)} \nabla_{i\alpha}^2 + \frac{m\omega^2}{2} \sum_{i=1,2;\, \alpha=1\ldots d_\perp} x_{i\alpha}^2 + V(r_1 - r_2) \quad (10.61)$$

Here $x_{i\alpha=1\ldots d_\perp}$ correspond to transverse components of particles i. We assume that delta function in the interaction term has a cutoff at energy $E_R = 1/mR^2$.

The center of mass and relative coordinates parts of the Hamiltonian separate (this is special to parabolic confinement) For the COM motion we find simple harmonic oscillator Hamiltonian

$$
\begin{aligned}
X_\alpha &= \frac{x_{1\alpha} + x_{2\alpha}}{2} & P_\alpha = p_{1\alpha} + p_{2\alpha} \\
\mathcal{H}_{CM} &= \frac{1}{4m} \sum_\alpha P_\alpha^2 + \frac{2m}{2}\omega^2 \sum_\alpha X_\alpha^2 & (10.62)
\end{aligned}
$$

The relative motion is described by the Hamiltonian

$$
\begin{aligned}
x_\alpha &= x_{1\alpha} - x_{2\alpha} & p_\alpha = \frac{1}{2}(x_{1\alpha} - x_{2\alpha}) \\
\mathcal{H}_{rel} &= \frac{1}{m}\sum_\alpha p_\alpha^2 + \frac{m\omega^2}{4}\sum_{\alpha=1\ldots d_\perp} x_\alpha^2 + V(r) & (10.63)
\end{aligned}
$$

From now one we will only be concerned with the relative motion.

10.5.2   T-matrix

We define a more general equation for the T-matrix in the operator form

$$\hat{T} = \hat{V} + \hat{V}\frac{1}{(E - \hat{\mathcal{H}}_0 + i0)}\hat{T} \quad (10.64)$$

When there is no transverse confinement we can define

$$
\begin{aligned}
V_{k',k} &= \langle k'|\hat{V}|k\rangle \\
T_{k',k} &= \langle k'|\hat{T}|k\rangle
\end{aligned}
\quad (10.65)
$$

This gives us the same equation for the T-matrix that we introduced before

$$T_{k',k} = V_{k',k} + \int \frac{d^3q}{(2\pi)^3}\frac{V_{k'q}T_{qk}}{E - \frac{q^2}{m} + i0} \quad (10.66)$$

We now consider contact interaction, assuming that delta function in the interaction term has a cutoff at energy $E_R = 1/mR^2$. We have

$$\langle r|\hat{V}|r'\rangle = V_0\delta(r)\delta(r') \tag{10.67}$$

This implies

$$\langle r|\hat{T}|r'\rangle = T\delta(r)\delta(r') \tag{10.68}$$

Note that T is a function of energy. We obtain

$$T = V_0 + V_0\langle 0|\frac{1}{(E - \hat{\mathcal{H}}_0 + i0)}|0\rangle T \tag{10.69}$$

We can take a set of basis states that are plane wave in free directions and harmonic oscillator eigenstates in the transverse directions.

$$\phi(x_\alpha) = \prod_{\alpha=1\ldots d_\parallel}\frac{e^{ik_\alpha x_\alpha}}{\sqrt{L}}\prod_{\alpha'=1\ldots d_\perp}\phi_n(x_{\alpha'}) \tag{10.70}$$

where L is the system size for each of the free directions and $\vec{n} = n_1, n_2, \ldots, n_{d_\perp}$ labels oscillator quantum numbers in the transverse directions. Then equation (10.69) can be written

$$T^{-1} = V_0^{-1} - \sum_{\vec{n}}\int\frac{d^{d_\parallel}k}{(2\pi)_\parallel^d}\frac{|\phi_{\vec{n}}(0)|^2}{E - \frac{k^2}{m} - (n_1 + \ldots n_{d_\perp} + d_\perp/2)\omega + i0} \tag{10.71}$$

To analyze equation (10.71) we need to introduce cut-offs in momentum integration and summation over transverse bands. We will explore an alternative approach. We have

$$-\langle 0|\frac{1}{(E - \hat{\mathcal{H}}_0 + i0)}|0\rangle = \int_0^\infty d\tau\langle 0|e^{(E-\hat{\mathcal{H}}_0+i0)\tau}|0\rangle \tag{10.72}$$

In writing the last equation we assumed $E < 0$. For positive E we can change limits of integration and arrive at the same result. We can combine equations (10.69) and (10.72) to write

$$T^{-1} = V_0^{-1} + \int_0^\infty d\tau\langle 0|e^{(E-\hat{\mathcal{H}}_0+i0)\tau}|0\rangle \tag{10.73}$$

For a harmonic oscillator expression inside the integral can be computed

$$\langle 0|e^{(E-\hat{\mathcal{H}}_0+i0)\tau}|0\rangle = \left(\frac{m\omega}{4\pi\sinh\omega\tau}\right)^{d_\perp/2}\left(\frac{m}{4\pi\tau}\right)^{d_\parallel/2} \tag{10.74}$$

Hence we find

$$T^{-1} = V_0^{-1} + \int_0^\infty d\tau\left(\frac{m\omega}{4\pi\sinh\omega\tau}\right)^{d_\perp/2}\left(\frac{m}{4\pi\tau}\right)^{d_\parallel/2} \tag{10.75}$$

The last equation has ultraviolet divergencies which appear as divergencies for $\tau \to 0$. These are the usual divergencies of the delta-function interaction. We will now discuss a way of working with equation (10.75) without introducing cut-offs explicitly.

When $d_\perp = 0$ and $d_\parallel = 3$, we know that the the $E \to 0$ limit of the T-matrix should be of the form $\frac{m}{4\pi a}$. Hence we can write

$$V_0^{-1} + \int_0^\infty d\tau \left(\frac{m}{4\pi\tau}\right)^{3/2} = \frac{m}{4\pi a} \tag{10.76}$$

Hence for the general case we have

$$T^{-1} = \frac{m}{4\pi a} + \int_0^\infty d\tau [e^{(E+i0)\tau} \left(\frac{m\omega}{4\pi \sinh \omega\tau}\right)^{d_\perp/2} \left(\frac{m}{4\pi\tau}\right)^{d_\parallel/2} - \left(\frac{m}{4\pi\tau}\right)^{3/2}] \tag{10.77}$$

The last expression is divergence free. We introduce $\epsilon = \frac{E}{\omega} - \frac{d_\perp}{2}$

$$T^{-1} = \frac{m}{4\pi a} + \frac{m}{4\pi}\sqrt{\frac{m\omega}{2}} \int_0^\infty \frac{dx}{\sqrt{2\pi}x^{3/2}} [e^{(\epsilon+i0)x} \left(\frac{2x}{1-e^{-2x}}\right)^{d_\perp/2} - 1] \tag{10.78}$$

10.5.3 Analysis of bound states

When $d_\perp = 0$ we have

$$T^{-1} = \frac{m}{4\pi a} - \frac{m}{4\pi}\sqrt{-mE - i0} \tag{10.79}$$

We observe that for $a > 0$ the T-matrix has a pole at $E = -\frac{1}{ma^2}$. This is the molecular bound state that we discussed before.

When $d_\perp = 2$ and $d_\parallel = 1$ and $|\epsilon| << 1$ we find

$$T^{-1} = \frac{m}{4\pi a} + \frac{m}{4\pi}\sqrt{\frac{m\omega}{2}}[\sqrt{\frac{2}{-\epsilon - i0}} - A + O(\epsilon)] \tag{10.80}$$

Here $A = -\zeta(1/2) \approx 1.036$. We observe that we can find a bound state even with a large negative scattering length. Introducing the oscillator length as $l = (m\omega)^{-1/2}$ we have

$$\epsilon = -\left(\frac{|a|}{l}\right)^2 \tag{10.81}$$

For positive a that is much smaller than l, the bound state energy in (10.78) approaches its 3d limit. This is natural since the relative motion of atoms no longer "sees" the parabolic confining potential. Comparison of the bound state energy computed in the model with contact interaction and more elaborate microscopic models is given in fig. 10.7.

When $d_\perp = 1$ and $d_\parallel = 2$ and $|\epsilon| << 1$ we find

$$T^{-1} = \frac{m}{4\pi a} + \frac{m}{4\pi}\sqrt{\frac{m\omega}{2}}\{-\frac{1}{\sqrt{\pi}} \log\left[C\left(-\epsilon - i0\right) + O(\epsilon)\right]\} \tag{10.82}$$
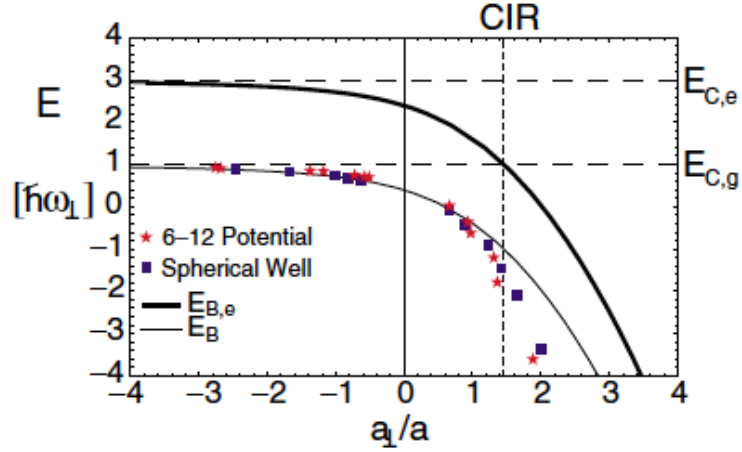
Figure 10.7: Energies of bound states in 1d computed with three types of potential: 6-12, spherical well, and delta-dunction with a cut-off. Figure taken from [1].

10.5.4 Effective Interaction Strength

For the Hamiltonian (10.58) we consider a scattering process

$$\Psi_{1d}(z) = e^{ikz} + \Psi_{sc}(z) \tag{10.83}$$

Note that we have a reduced mass $m_r = \frac{m}{2}$. For the scattered part of the wavefunction in momentum space we have the usual Schroedinger equation

$$\left(\frac{k^2}{m} - \frac{k'^2}{m}\right) \Psi_{1d}(k') = U_{1d}(k', k) + g_{1d} \int \frac{dk''}{2\pi} U_{1d}(k', k'') \Psi_{1d}(k'') \tag{10.84}$$

For contact interaction $U_{1d}(k', k) = g_{1d}$. We can define the T-matrix by analogy with the 3-dimensional problem

$$T_{1d}(k', k, E) = g_{1d} + g_{1d} \int \frac{dk''}{2\pi} \frac{T_{1d}(k'', k, E)}{\left(\frac{k^2}{m} - \frac{k''^2}{m} + i\delta\right)} \tag{10.85}$$

The right hand side of the last equation does not depend on k', so $T(k', k, E = \frac{k^2}{m})$ depends on k only. Also note that we no longer have UV divergence in (10.85), so we can take integration limits in k' from minus to plus infinity We set $T_{1d}(k) = T(k', k, E = \frac{k^2}{m})$ and obtain

$$T_{1d}(k) = g_{1d} + \frac{g_{1d} T_{1d}(k) m}{2(i\,k)}$$

$$\frac{2}{m} \frac{1}{T_{1d}(k)} = \frac{2}{m} \frac{1}{g_{1d}(k)} + \frac{i}{k} \tag{10.86}$$
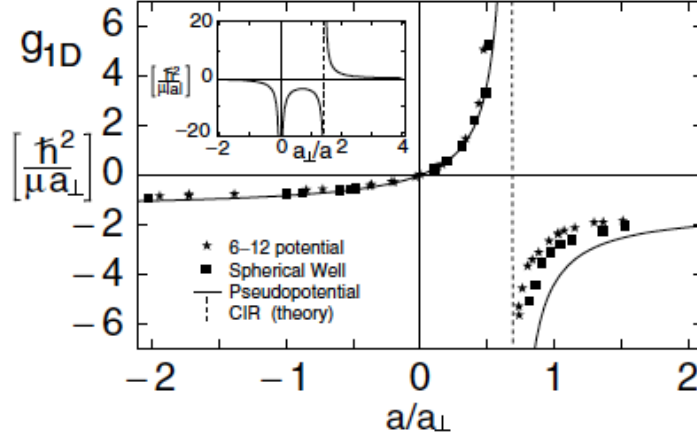
Figure 10.8: Effective 1d interaction computed with three types of potential: 6-12, spherical well, and delta-dunction with a cut-off. Figure taken from [1].

From comparing to (10.80) we observe that

$$\frac{2}{m} \frac{1}{g_{1d}} = \frac{l^2}{a} - \frac{A\,l}{2\sqrt{2}}$$
(10.87)

This expression was first derived in [14, 1] and comparison to more elaborate models of interatomic interactions are shown in fig. 10.8.

From equation (10.87) we observe that only when $a_{3d} << l$ we have $g_{1d} \sim a_{3d}/l^2$. When g_{1d} becomes comparable to l there are important corrections. One implication of this is that effective interaction in 1d diverges not at the 3d Feshbach resonance but when the 3d scattering length is positive and finite (see also fig. 10.8).

10.5.5   Experimental studies of geometric resonances

Experimentally geometrical resonance in 1d has been studied in Ref. [13]. Results are shown in fig. 10.9.

Bound states in 2d pancakes have been studied by Frohlich et al. in [10]. Results are shown in fig. 10.10. While they see clear differences from the three dimensional case, many-body effects have been argued to be important for interpreting results. In particular, it was argued that they observed polarons rather than molecules[17].
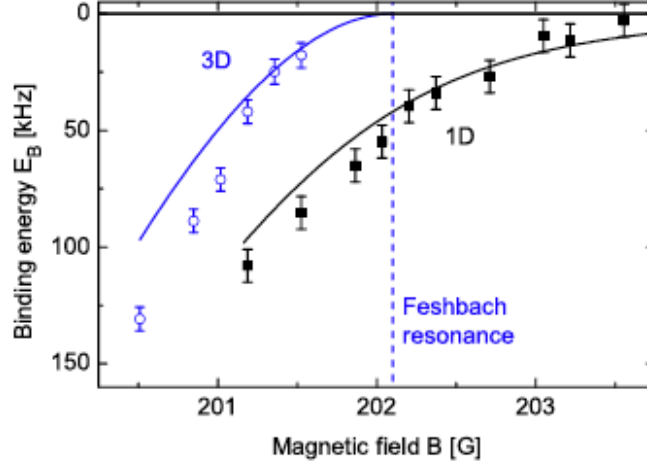
Figure 10.9: Experimental measurements of the biding energy of molecules in 1d systems. Figure taken from [13].

10.6   Appendix.   Alternative derivation of the geometrical resonance in 1d

Let us now consider the full three dimensional problem. The full Hamiltonian is given by

$$\mathcal{H} = -\frac{\nabla_1^2}{2m} - \frac{\nabla_2^2}{2m} + \frac{m\omega^2}{2}\left(r_{1\perp}^2 + r_{2\perp}^2\right) + V_0\delta(r_1 - r_2) \qquad (10.88)$$

Here $r_\perp$ correspond to the x and y components. And we assume that delta function in the interaction term has a cutoff at energy $E_R = 1/mR^2$.

The center of mass and relative coordinates parts of the Hamiltonian separate. We discuss the relative motion of two particles. We use oscillator eigenstates for the transverse direction and plane waves along the z axis. We assume that the incoming particles come in the lowest band in the transverse direction

$$\Psi_{n'}(z) = \delta_{n'=0}e^{ikz} + \Psi_{sc\,n'}e^{ik'z'} \qquad (10.89)$$

Harmonic oscillator states in transverse direction should have two quantum numbers. However angular momentum L_z is a conserved quantity in the Hamiltonian (10.63). Incoming particles have $m = 0$, so we only need to take $m = 0$ states. This means that we only need to keep track of the radial quantum number. Another important factor is the symmetry of the wavefunction. Wavefunction of incoming particles is symmetric in $\vec{r}_\perp$, hence we only need to include states with even radial quantum numbers, because the odd ones are odd in $\vec{r}_\perp$ (this is most easily seen by considering harmonic eigenstates in the x,y basis).
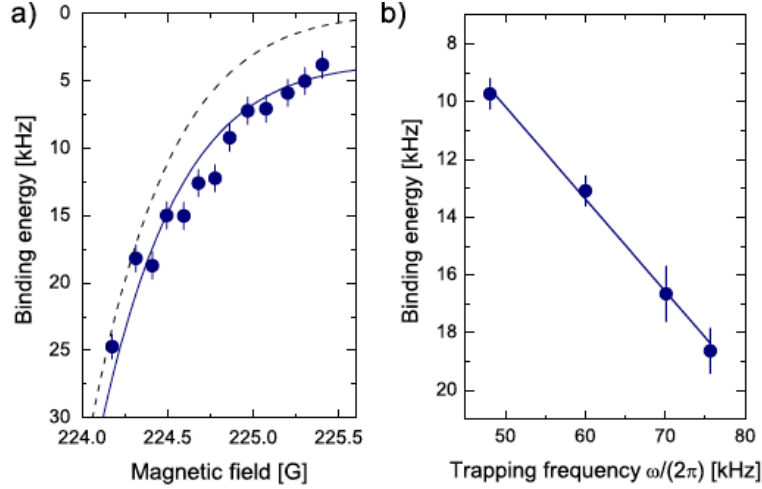
Figure 10.10: Experimental measurements of the biding energy of molecules in 2d systems. Figure taken from [10]. a) Shows bindingenergy as a function of three diemensional scattering length tuned by the magnetic field. Dashed line shows theoretical prediction. b) shows binding energy at the magnetic field corresponding to 3d resonance.

For the T-matrix we need to introduce a band label

$$T_{n'}(k',k,E) = U_{n'0}(k',k) + \sum_{n''} \int \frac{dk"}{2\pi} \frac{U_{n'n''}(k',k)\,T_{n''}(k'',k,E)}{\left(\frac{k^2}{m} - \left(\frac{k''^2}{m} + 2n\omega\right) + i\delta\right)} \quad (10.90)$$

Summation over n'' and integration over k'' now has a high energy cutoff at E_R. For the delta function interaction matrix element $U_{n'n''}(k',k)$ are given by $U_{n'n''}(k',k) = \Psi^*_{n'}(0)\Psi_n(0)$, where $\Psi_n(r_\perp)$ are eigenstates of the 2D harmonic oscillator with angular momentum $m = 0$ and radial number n. Remarkably they are all the same $U_{n'n''} = V_0/2\pi l^2$. We set $E = k^2/m$ again and note that the right hand side of (10.90) does not depend on n' or k'. Hence the T matrix should depend on k only by $T_{n'}(k',k,E)(k)$

$$\tilde{T}(k) = \frac{V_0}{2\pi l^2} + \frac{V_0\,\tilde{T}(k)}{2\pi l^2} \sum_{n'=0}^{n_c} \int \frac{dk"}{2\pi} \frac{1}{\frac{k^2}{m} - \left(\frac{k''^2}{m} + 2n\omega\right) + i\delta} \quad (10.91)$$

Here $2n_c\omega = \left(\frac{2}{\pi}\right)^2 E_R$. When $n > 0$ we can neglect k^2/m compared to ω, so

$$\sum_{n'=0}^{n_c} \int \frac{dk"}{2\pi} \frac{1}{\frac{k^2}{m} - \left(\frac{k''^2}{m} + 2n\omega\right) + i\delta} \simeq \int \frac{dk"}{2\pi} \frac{1}{\left(\frac{k^2}{m} - \frac{k''^2}{m} + i\delta\right)} - \sum_{n'=1}^{n_c} \int \frac{dk"}{2\pi} \frac{1}{\left(\frac{k''^2}{m} + 2n\omega\right)}$$

$$= -\frac{m}{2ik} - \frac{m}{2\sqrt{2m\omega}} \sum_{n=1}^{n_c} \frac{1}{\sqrt{n}} \quad (10.92)$$

We can write

$$\sum_{n=1}^{n_c} \frac{1}{\sqrt{n}} = \int_0^{n_c} \frac{dn}{\sqrt{n}} + (\sum_{n=1}^{n_c} \frac{1}{\sqrt{n}} - \int_0^{n_c} \frac{dn}{\sqrt{n}}) \tag{10.93}$$

Expression in brackets converges as $n_c \to \infty$, so we take its value for $n_c = \infty$. Then

$$\sum_{n=1}^{n_c} \frac{1}{\sqrt{n}} \simeq 2\sqrt{n_c} - \alpha = 2 \left[\frac{1}{2\omega} (\frac{2}{\pi})^2 E_R \right]^{1/2} - \alpha = \frac{2\sqrt{2}}{\pi} \frac{l}{R} - \alpha \tag{10.94}$$

where $\alpha \simeq 1.46$. Thus we find for the T-matrix

$$\tilde{T}(k) = \frac{V_0}{2\pi l^2} + \frac{V_0 \tilde{T}(k)}{2\pi l^2} \left(-\frac{m}{2} \frac{i}{k} - \frac{lm}{2\sqrt{2}} (\frac{2\sqrt{2}\, l}{\pi R} - \alpha) \right) \tag{10.95}$$

This can be written as

$$\frac{2}{m} \frac{1}{T} = \frac{4\pi l^2}{mV_0} + \frac{2l^2}{\pi R} - \frac{\alpha l}{2\sqrt{2}} + \frac{i}{k} \tag{10.96}$$

From formula (10.22) we know that

$$\frac{4\pi}{mV_0} + \frac{2}{\pi R} = \frac{1}{a_{3D}} \tag{10.97}$$

Thus

$$\frac{2}{m} \frac{1}{\tilde{T}} = \frac{l^2}{a_{3D}} - \frac{\alpha\, l}{2\sqrt{2}} + \frac{i}{k} \tag{10.98}$$

10.7   Problems to Chapter 10

Problem 1.

The Lippmann-Schwinger equation on the T-matrix is

$$T(k', k, E) = U(k', k) + \frac{1}{V} \sum_{k''} U(k', k'')(E - \frac{k''^2}{m} + i\delta)^{-1} T(k'', k, E) \tag{10.99}$$

When solving this equation it is often convenient to introduce an intermedite energy scale ϵ_c and define

$$\tilde{U}(k', k, E) = U(k', k) + \frac{1}{V} \sum_{|k''|>k_c} U(k', k'')(E - \frac{k''^2}{m} + i\delta)^{-1} \tilde{U}(k'', k, E) \tag{10.100}$$

Show that equations (10.101) and (10.100) lead to the following equation for the T-matrix

$$T(k', k, E) = \tilde{U}(k', k, E) + \frac{1}{V} \sum_{|k''|<k_c} \tilde{U}(k', k'', E)(E - \frac{k''^2}{m} + i\delta)^{-1} T(k'', k, E)$$

$$\tag{10.101}$$

Problem 2.

Consider two identical bosonic particles in a one dimensional system with parabolic confinement (transverse confinement is assumed to be infinitely strong in this problem). Assume contact interaction between particles. The Hamiltonian is given by

$$\mathcal{H} = -\frac{1}{2m}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2m}\frac{\partial^2}{\partial x_2^2} + \frac{m\omega^2 x_1^2}{2} + \frac{m\omega^2 x_2^2}{2} + V_0\delta(x_1 - x_2) \quad (10.102)$$

Calculate the full spectrum of the system as a function of V_0.

Problem 3.

Analyze bound states in a pancake geometry, $d_\perp = 1$, (see equation (10.82)).

Problem 4.

Consider equation (10.78). Show that when a is small and positive the bound state is at $E = -1/ma^2$ for any $d_\perp$.

Problem 5.

Derive equation (10.74).

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