

Chapter 7

Path integral approach to the crossover problem

7.1 Resonant action

To begin our discussion of the resonant crossover problem we consider a Feshbach resonance for s -wave scattering of atoms in the lowest two hyperfine states $\sigma \in \{\uparrow, \downarrow\}$ of a fermionic alkali atom [84]. For a homogeneous system we have the following generalized Hamiltonian:

$$\begin{aligned}
 \hat{H}(t) = & \sum_{\sigma} \int \psi_{\sigma}^{\dagger}(x)(\hat{H}_{\sigma} - \mu)\psi_{\sigma}(x)d^3x + \int \psi_m^{\dagger}(x)(\hat{H}_m - 2\mu + \nu)\psi_m(x)d^3x \\
 & + \int \psi_{\uparrow}^{\dagger}(x)\psi_{\downarrow}^{\dagger}(x')U(\mathbf{x} - \mathbf{x}')\psi_{\downarrow}(x')\psi_{\uparrow}(x)d^3xd^3x' \\
 & + \int \left(\psi_m^{\dagger}\left(\frac{x+x'}{2}\right)g(\mathbf{x} - \mathbf{x}')\psi_{\downarrow}(x)\psi_{\uparrow}(x') + \text{h.c.} \right) d^3xd^3x', \tag{7.1}
 \end{aligned}$$

where the operators ψ_{σ}^{\dagger} (ψ_{σ}) create (annihilate) fermions at $x = (\mathbf{x}, t)$, and ψ_m^{\dagger} (ψ_m) create (annihilate) composite bosons. The free dispersion Hamiltonian for fermions (bosons) is \hat{H}_{σ} (\hat{H}_m) and ν is the detuning of the resonant molecular state from the collision continuum. The collisional interactions are described by both background fermion-fermion scattering, U , and an interconversion between composite bosons and fermions, g .

Functional methods prove to be especially convenient in describing the thermodynamics of the resonant system. For a finite-temperature field theory, the connection with statistical mechanics is made by Wick rotating the time coordinate $t \rightarrow -i\tau$ so that one works in terms of the spatial coordinate x and temperature τ [85]. The action

is defined in the usual way:

$$S = \sum_l \int_0^\beta d\tau \int d^3x \psi_l^\dagger(\mathbf{x}, \tau) \partial_\tau \psi_l(\mathbf{x}, \tau) - \int_0^\beta \hat{H}(\tau) d\tau, \quad (7.2)$$

where the sum in l runs over both the Fermi and the Bose degrees of freedom. In this functional formulation we treat the fermion fields ψ_σ as Grassmann variables and the composite Bose fields ψ_m as classical fields [86].

Let us consider a system comprised of fermions at some finite temperature τ inside a box of volume V (for convenience, let us work in the set of units where $\hbar = k_b = 1$). By imposing periodic boundary conditions upon the fields ψ_σ and ψ_m , we form the following Fourier series expansions:

$$\begin{aligned} \psi_\sigma(\mathbf{x}, \tau) &= (\beta V)^{-1/2} \sum_{\mathbf{k}, \omega} e^{i(\omega\tau + \mathbf{p} \cdot \mathbf{x})} a_\sigma(\mathbf{p}), \\ \psi_m(\mathbf{x}, \tau) &= (\beta V)^{-1/2} \sum_{\mathbf{q}, v} e^{i(v\tau + \mathbf{q} \cdot \mathbf{x})} b(\mathbf{q}), \end{aligned} \quad (7.3)$$

with even thermal (Matsubara) frequencies for the bosons ($v = 2\pi n/\beta$, where n is an integer) and odd frequencies for the fermions ($\omega = 2\pi(n + 1)/\beta$) [87]. Here $a_\sigma(\mathbf{p})$ annihilates a fermion at $\mathbf{p} = (\mathbf{k}, \omega)$ and $b(\mathbf{q})$ annihilates a molecule at $\mathbf{q} = (\mathbf{q}, \omega)$.

By making use of the above transformation, Eq. (7.3), we may write out the action for the resonant system in terms of the Fourier coefficients $a_\sigma(\mathbf{p})$ and $b(\mathbf{q})$. To help clarify the following calculation, we split the resulting resonant action into two parts, the first being the usual BCS action

$$S_{BCS} = \sum_{\mathbf{p}, \sigma} \left(i\omega - \frac{p^2}{2m} + \mu \right) a_\sigma^*(\mathbf{p}) a_\sigma(\mathbf{p}) - \frac{1}{\beta V} \sum_{\mathbf{p}_1 + \mathbf{p}_2 = \mathbf{p}_3 + \mathbf{p}_4} U a_\uparrow^*(\mathbf{p}_1) a_\downarrow^*(\mathbf{p}_2) a_\downarrow(\mathbf{p}_3) a_\uparrow(\mathbf{p}_4), \quad (7.4)$$

and the second we will label the molecular action

$$\begin{aligned} S_M &= \sum_{\mathbf{q}} \left(iv - \frac{q^2}{4m} - \nu + 2\mu \right) b^*(\mathbf{q}) b(\mathbf{q}) \\ &\quad - \frac{1}{\sqrt{\beta V}} \sum_{\mathbf{q} = \mathbf{p}_1 + \mathbf{p}_2} g \left(b^*(\mathbf{q}) a_\downarrow(\mathbf{p}_1) a_\uparrow(\mathbf{p}_2) + a_\uparrow^*(\mathbf{p}_2) a_\downarrow^*(\mathbf{p}_1) b(\mathbf{q}) \right). \end{aligned} \quad (7.5)$$

In deriving Eqs. (7.4) and (7.5) we have inserted contact potentials for the couplings $U(\mathbf{x} - \mathbf{x}') \rightarrow U\delta(\mathbf{x} - \mathbf{x}')$ and $g(\mathbf{x} - \mathbf{x}') \rightarrow g\delta(\mathbf{x} - \mathbf{x}')$. The full partition function for our

resonant system, under the model Hamiltonian of Eq. (7.1), can now be written as

$$Z = \int \left(\prod_{\sigma} Da_{\sigma}^* Da_{\sigma} \right) \left(\prod Db^* Db \right) e^{S_{BCS} + S_M}, \quad (7.6)$$

with the functional integral, $Dc \equiv \prod_i dc^i$, ranging over all Fermi and Bose fields.

7.2 Saddle-point approximation

From the form of the action in Eq. (7.6), it should be apparent that all of the resonant contributions are contained within the molecular action. In practice this gives rise to the integral of a displaced Gaussian that can be easily evaluated (see Appendix C). After integrating out the molecular degrees of freedom, we are left with the following partition function:

$$Z = Z_B(q^2/4m + \nu - 2\mu) \int Da_{\sigma}^* Da_{\sigma} e^{S_{BCS'}}. \quad (7.7)$$

Here $Z_B(q^2/4m + \nu - 2\mu)$ is a Bose partition function describing the formation of bound molecules and $S_{BCS'}$ is the BCS action with a potential that is now dependent on both thermal frequencies and momentum. The interaction potential in the BCS action, therefore, is modified in the presence of a Feshbach resonance in the following way:

$$U \rightarrow U - \frac{g^2}{q^2/4m + \nu - 2\mu - iv}. \quad (7.8)$$

With the above partition function, Eq. (7.7), we may go on to calculate all thermodynamic properties of interest. Here we are primarily interested in calculating the critical temperature of the superfluid phase transition. This can be done by solving for a gap and number equation and then self-consistently solving these two equations for both the chemical potential μ and the critical temperature τ . The procedure is straightforward since the full resonant calculation has been reduced to the usual BCS calculation (however, we must now deal with the interaction given by Eq. (7.8)). Following Popov's derivation [86], we perform a Hubbard-Stratonovich transformation about an auxiliary

Bose field $c(q)$ (see Appendix C) to derive the gap equation at the critical point

$$1 = \left(-U + \sum_j \frac{g_j^2}{\nu_j - 2\mu} \right) \sum_k \frac{\tanh(\beta(k^2/2m - \mu)/2)}{2(k^2/2m - \mu)}. \quad (7.9)$$

A self-consistent equation for the total particle number can be found by expanding the action to lowest order about the auxiliary field $c(q) = c^*(q) = 0$. This is commonly referred to as the saddle-point approximation. The thermodynamic identity $N = -\partial \ln Z / \partial \mu$ yields:

$$N = N_b + N_f = 2 \sum_k \frac{1}{e^{\beta(k^2/4m + \nu - 2\mu)} - 1} + 2 \sum_k \frac{1}{e^{\beta(k^2/2m - \mu)} + 1}. \quad (7.10)$$

Thus, our number equation counts all free fermions, N_f , plus an additional boson population N_b . Equations (7.9) and (7.10) provide a set of equations for determining the critical temperature T_c and chemical potential μ . In conventional BCS theory, this level of approximation proves reasonable for calculating T_c for weak, attractive interactions, but diverges as the interaction strength grows. The reason for this is that the mechanism which signals the phase transition within the weak coupling BCS limit is the formation and disassociation of Cooper pairs. As the coupling increases, the particles tend to pair at higher and higher temperatures which means that the critical transition is no longer signaled by the formation of Cooper pairs, but rather by a coherence across the sample caused by condensation of pre-formed Cooper pairs. Since we are interested in describing the resonant system at all detunings, the equations that we have derived so far are insufficient because they do not account for this process. We should, therefore, next focus on how to more accurately incorporate atom pairing into our model.

7.3 Beyond the saddle-point approximation

To account for fluctuations in the fermion field, we follow the method of Nozières and Schmitt-Rink [82] in its functional form as put forth by Randeria et al. [83, 88]. This procedure will introduce a next order (Gaussian) correction to the saddle-point

calculation of the previous section. By expanding the action to second order in $c(\mathbf{q})$, and then calculating the number equation in the same way as was done when deriving Eq. (7.10), we introduce an additional population into the equation. The action becomes

$$S(c(\mathbf{q}), c^*(\mathbf{q}))_{BCS'} \approx S_{BCS'}(0, 0) + \sum_{\mathbf{q}} |c(\mathbf{q})|^2 \chi(\mathbf{q}), \quad (7.11)$$

where we have defined the auxiliary function $\chi(\mathbf{q})$ as

$$\chi(\mathbf{q}) = \left(U - \frac{g^2}{\frac{q^2}{4m} + \nu - 2\mu - i\omega} \right) \sum_k \frac{1 - f(\epsilon_{\frac{q}{2}+k}) - f(\epsilon_{\frac{q}{2}-k})}{\epsilon_{\frac{q}{2}+k} + \epsilon_{\frac{q}{2}-k} - i\omega}. \quad (7.12)$$

Here $f(\epsilon_k)$ is the Fermi distribution function and $\epsilon_k = k^2/2m - \mu$. $\chi(\mathbf{q})$ is often referred to as the susceptibility (or the pair propagator) and results from the Matsubara summation of the single particle, free Green's functions G_0 (see Appendix D):

$$\frac{1}{\beta} \sum_{\omega} G_0(\mathbf{p}, \nu) G_0(\mathbf{k}, \omega - \nu). \quad (7.13)$$

Once again we make use of the thermodynamic identity $N = -\partial \ln Z / \partial \mu$ resulting in a modified number equation

$$\begin{aligned} N &= N_b + N_f + N_p \\ &= 2 \sum_k \frac{1}{e^{\beta(k^2/4m + \nu - 2\mu)} - 1} + 2 \sum_k \frac{1}{e^{\beta(k^2/2m - \mu)} + 1} - \frac{1}{\beta} \sum_{\mathbf{q}, \omega} \frac{\partial}{\partial \mu} \log[1 - \chi(\mathbf{q}, i\omega)]. \end{aligned} \quad (7.14)$$

This inclusion of the first order fluctuations introduces a new population which we will refer to as atom pairs N_p to distinguish them from the other bosonic population N_b already accounted for at the saddle-point level. We are now able to solve for the fluctuation corrected critical temperature from a self-consistent solution of Eqs. (7.9) and (7.14).

Due to the contact form of the couplings that we have chosen, however, we are immediately plagued with problems of divergences in our equations. These may be remedied by a proper renormalization as outlined in Chapter 2.6. We may also account for mean-field shifts due to all 2-body scattering processes by adjusting the chemical

potential $\mu = \bar{\mu} - \langle Un_k \rangle$ where n_k is the Fermi distribution and $\langle \rangle$ denotes an averaging. This shift, however, is sufficiently small to neglect; inclusion has demonstrated corrections of the order of 1% or less.

7.4 Bound states and asymptotes

The renormalization of the resonance theory forces us to take a closer look at the bound state physics of the system. In Fig. 7.1 we show the bound state energies for a single resonance system with a positive background scattering length. The figure results from a coupled square well calculation of the bound state energies, as in Chapter 2.4, and shows an avoided crossing between two molecular states. The upper state behaves to a fairly good approximation as $E_b = (ma_{\text{eff}}^2)^{-1}$, which is the molecular binding energy regularly associated with a contact interaction [89]. The lower state, however, is offset from the detuning by an energy $\sim \kappa$ and goes linear with the detuning. We find this similar behavior in the first term of Eq. (7.14). Taking the cutoff to infinity, which is justified since this term does not diverge, the renormalized detuning approaches $\nu \rightarrow \bar{\nu} - \bar{g}^2/\bar{U}$. This produces a constant shift of $\bar{g}^2/\bar{U} = \kappa$ between the detuning and the molecular binding energy. Keeping this term in the number equation would incorrectly cause a transfer of the entire population into the wrong molecular state. In order to avoid this unwanted behavior, we set this term to zero, i.e., $N_b = 0$. In the case of a negative background scattering length, we would not have encountered this problem and only one molecular state would have appeared (see Fig. 7.2). We will show in the next section that the pairing term fully accounts for the correct population of molecules in this system with $a_{\text{bg}} > 0$.

However, before we present the full crossover solution for the case of ^{40}K , let us look at the analytical solutions to Eqs. (7.9) and (7.14) in the strong (BEC) and weak (BCS) coupling regimes. We will first turn our attention to the weak coupling (BCS) limit. In this limit we would expect only free fermions to contribute to the

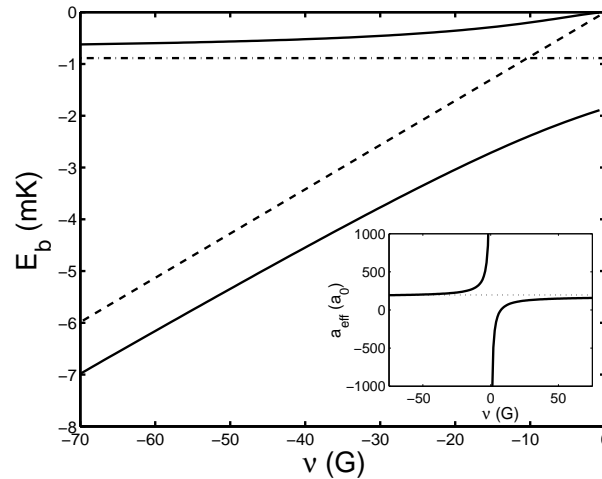


Figure 7.1: Binding energies for ^{40}K resonance at positive background scattering length $a_{\text{bg}} = 176a_0$. A single resonance with a positive background scattering length produces an effective scattering length $a_{\text{eff}} = a_{\text{bg}}(1 - \kappa/\nu)$, as seen in the figure inset where we plot the effective scattering length vs. detuning (the dotted line is at $176a_0$). A positive a_{bg} , which is larger than the range of the potential, implies that another bound state is not far below threshold (dash-dotted line). In combination with the Feshbach state (dashed detuning line) this results in an avoided crossing and the molecular state of interest asymptotes quickly to the dash-dotted line.

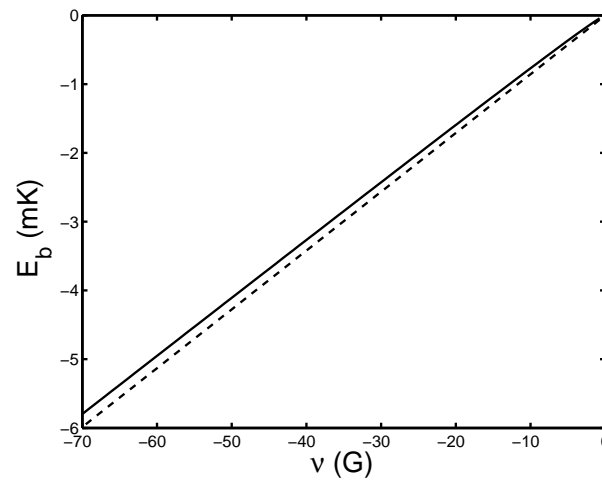


Figure 7.2: Same as Fig. 7.1, but now for an artificial situation with $a_{\text{bg}} < 0$. A resonance system with a negative background scattering length has only one bound state relatively close to threshold, which is shifted positive of the detuning. The next bound state in the potential is too far away to be of any significant influence. The line styles are the same as for Fig. 7.1.

population, so from equation (7.14) we find that the chemical potential is at the Fermi surface ($\mu = E_F$). With this information, we solve the gap equation for the critical temperature. The result is the usual exponential dependence on the effective scattering length

$$T_c/T_F \approx \frac{8}{\pi} e^{\gamma-2} \exp\left(\frac{-\pi}{2k_F|a_{\text{eff}}|}\right), \quad (7.15)$$

where $\gamma \sim 0.5772$ is the Euler-Mascheroni constant, k_F is the Fermi wave number, and $a_{\text{eff}} < 0$ is the effective scattering length produced by the Feshbach resonance $a_{\text{eff}} = a_{\text{bg}}(1 - \kappa/\bar{\nu})$.

The other limit we may consider is the strong coupling (BEC) limit. When the argument of the tanh function in the gap equation, Eq. (7.9), becomes sufficiently negative, it is a good approximation to use its asymptotic value of unity. What this implies, physically, is that the fermion statistics are unimportant in determining the value of the gap. This allows us to solve the gap equation for the chemical potential as a function of detuning. In the limit of large negative detuning we find that $\mu \rightarrow -E_b/2$, where $E_b \approx 1/ma_{\text{eff}}^2$. Within this limit the entire population has been converted to molecules and we can solve the number equation to get the noninteracting BEC condensation temperature of $T_c/T_F \sim 0.218$.

7.5 Numerical results

To study the transition between the BEC and BCS regimes, we numerically solve Eqs. (7.9) and (7.14) for ^{40}K . The single resonance curve is produced using a background scattering length of $176a_0$ and $\kappa = 7.68\text{G}$ at a density of 10^{14}cm^{-3} .

Figure 7.3 shows the critical temperature as a function of magnetic field detuning. The crossover calculation clearly merges with the BEC result for large-positive detunings and smoothly connects between positive and negative detunings, limiting to the Bose condensation temperature of $T_c/T_F \sim 0.218$ for large negative detuning. This approach

gives a maximum near zero detuning ($T_c/T_F \sim 0.26$).

Figure 7.4 shows the chemical potential as a function of detuning, beginning at the Fermi energy for positive detuning and approaching half the bound state energy at large negative detuning $\mu \rightarrow -E_b/2$. Figure 7.5 shows the change in population as a function of detuning. For large positive detuning, the system is composed solely of free fermions. As the detuning is decreased (i.e., from positive to negative) the contribution of the fermions begins to decrease until all the population is transferred into the atom pair component at $\nu \sim -0.5G$. The chemical potential is then equal to $-E_b/2$ and we may identify the atom pairs from that point on as the molecules. The superfluid behavior then comes from the condensation of these molecules.

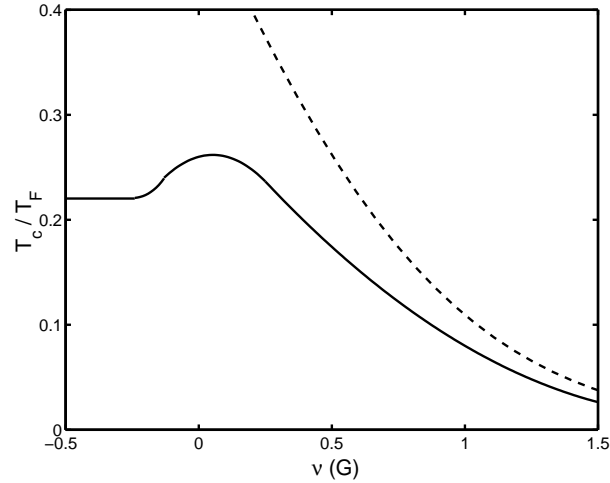


Figure 7.3: Critical temperature T/T_F as a function of detuning ν in Gauss. The dashed line corresponds to the usual BCS solution, which limits to the full crossover theory at large positive detuning. At negative detuning, T_c drops to the BEC condensation temperature of $T_c/T_F \sim 0.218$.

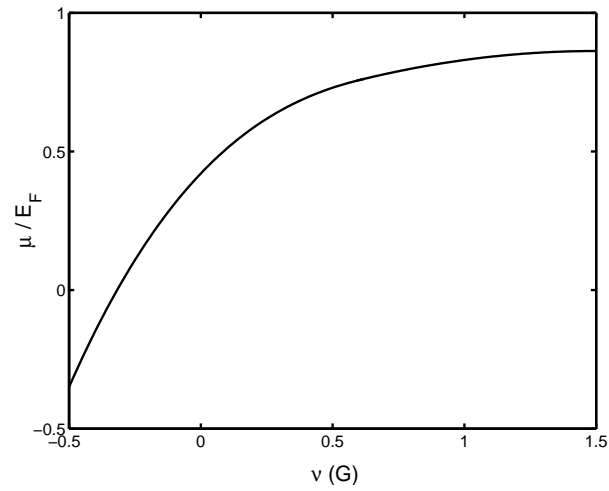


Figure 7.4: Chemical potential as a function of detuning ν in Gauss. For large negative detuning 2μ approaches the bound state energy of the molecular state. At increasing positive detuning, the chemical potential slowly approaches the Fermi energy.

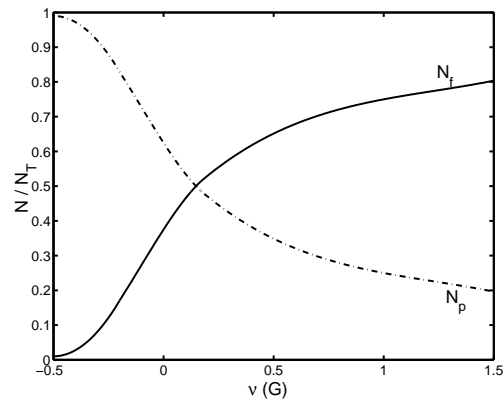


Figure 7.5: The fraction of the total population as a function of detuning ν in Gauss. The dot-dashed line corresponds to the pairing fraction N_p and the solid to the free fermion fraction N_f .