

# Bose–Fermi mixtures near an interspecies Feshbach resonance: testing a non-equilibrium approach

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## Abstract

We test a non-equilibrium approach to study the behaviour of a Bose–Fermi mixture of alkali atoms in the presence of a Feshbach resonance between bosons and fermions. To this end we derive the Hartree–Fock–Bogoliubov (HFB) equations of motion for the interacting system. This approach has proven very successful in the study of resonant systems composed of Bose particles and Fermi particles. However, when applied to a Bose–Fermi mixture, the HFB theory fails to identify even the correct binding energy of molecules in the appropriate limit. Through a more rigorous analysis we are able to ascribe this difference to the peculiar role that noncondensed bosons play in the Bose–Fermi pair correlation, which is the mechanism through which molecules are formed. We therefore conclude that molecular formation in Bose–Fermi mixtures is driven by three-point and higher-order correlations in the gas.

## 1. Introduction

Feshbach resonances have been recently discovered in ultracold mixtures of bosonic fermionic alkali atoms [1, 2]. Together with the achievement of degenerate states of such systems [3–5], this experimental feat has opened investigative opportunities for the study of new ultracold regimes. From the theoretical point of view, on the other hand, studies of Bose–Fermi mixtures to date have been mostly limited to nonresonant physics, focusing mainly on mean-field effects in trapped systems [6–13], phases in optical lattices [14–17], or equilibrium studies of homogeneous gases, focusing mainly on phonon-induced superfluidity or beyond-mean-field effects [18–23].

This paper introduces a time-dependent theory of the Bose–Fermi mixture that accounts for the resonant interaction. In systems where the resonant interaction is between two bosons [24–26] or between two fermions [27–33], the theory of ‘resonant superfluidity’ has already

been articulated. This theory is, so far, a big success. In the Bose case, it quantitatively describes the coherent conversion of bosonic atoms into bosonic pairs and back. Indeed, Ramsey interferometry on this system, coupled with this theoretical analysis, has produced the most accurate interaction potentials yet between ultracold rubidium atoms [9]. In the Fermi case, the theory has produced important qualitative insights into the crossover regime between weakly-interacting Cooper pairs on one hand and Bose-condensed molecules on the other [27–34].

It seems worthwhile, therefore, adapting the same level of theory to the resonant Bose–Fermi mixture. In this paper we formulate the problem by writing down the relevant equations of motion at the level of Hartree–Fock–Bogoliubov (HFB) approximation. The equations of motion are suitably number and energy conserving, as are their counterparts in boson or fermion systems. However, in sharp contrast to these systems, the HFB theory applied to the Bose–Fermi resonance does not provide quantitatively reasonable results. Specifically we show, by direct numerical solution, that the theory cannot reproduce the binding energy of a Bose–Fermi molecule, even in the limit of low density.

The source of this difficulty lies in the approximate treatment of three-body correlations in the theory. The molecules, after all, are composed of two atoms, so the atom–atom–molecule correlation function is of central importance in determining properties of the resulting molecules. In the HFB theory, this three-body correlation function is approximated in terms of two-body correlation functions, which is adequate for Bose–Bose and Fermi–Fermi resonances, but not for the Bose–Fermi mixture. Ultimately, the critical missing piece will turn out to involve the noncondensed bosonic atoms.

This paper is organized as follows: we begin our discussion in section 2 by introducing the Hamiltonian of the system, and justifying such choice. We then proceed to outline the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) formalism used to derive the HFB equations of motion, and show the form they take in free space. In section 3 we present our results, by first analysing the equations by physical and analytical insight, and then presenting numerical results in support of our conclusions.

Section 4 approaches the problem from an alternative, perturbative point of view, relevant to low fermionic densities. From this analysis it is clear that molecular binding energies will not be recovered without adequately accounting for the noncondensed bosons, thus pointing to their need for a higher-order theory.

## 2. Theoretical formalism

### 2.1. The Hamiltonian

We are interested primarily in the effects of resonant behaviour on the otherwise reasonably understood properties of the system. To this end we use a model which, in the last few years, has become one of the standards in the literature, and which was used to study the effect of resonant scattering in systems composed of bosons [24–26] and fermions [27–32]. Because there is already a significant literature explaining the details involved in the choice of the appropriate model Hamiltonian, we only outline the extent of the approximation involved in such a choice.

An accurate approach to the problem would have to incorporate several scattering channels, since the resonance in question is a consequence of the intertwined behaviour of the complex internal structures of the atoms. In a field theoretical sense that would imply having to consider vector fields for the bosons and fermions with as many components as there are spin states involved in the interaction, and a nonlocal interaction tensor of adequate

size, to account for all coupling between such components. Fortunately, if we assume that the resonances in the system are sufficiently far from each other, such that it is possible to define a ‘background,’ or away from resonance behaviour, we can focus on only one resonance at a time, which in turn makes it possible for an effective two-channel model to describe the resonance. Furthermore, since the closed channel threshold is energetically inaccessible at the temperatures of interest, we can ‘integrate out’ the closed channel components of the fermion and boson field, in favour of fermion fields which we identify as representative of the motion of one boson and one fermion, and which we dub into the ‘molecular field.’ In the appropriate limit the molecular field identifies bound states between fermions and bosons. We emphasize that the molecular field is a theoretical artifice that alleviates the need to treat relative motion of two atoms on the natural scale of the interaction (tens of Bohr radii). However, this model is appropriate for the study of the systems in hand, typically composed of  $10^{12-40}$ K atoms per cubic centimetre, whereby the characteristic length scale associated with the many-body system is of the order of the inverse Fermi wavenumber, (thousands of Bohr radii), implying an average interparticle distance, which is given by  $(\frac{9}{4\pi})^{1/3} \frac{1}{k_F}$ , of the same order. Last, since the coupling terms in the Hamiltonian represent an effective interaction, we can choose its functional form, and we do so by choosing to deal with contact interactions, which simplify the calculations immensely.

The resulting Hamiltonian has the following form:

$$H = H_0 + H_I, \quad (1)$$

where

$$H_0 = \sum_p \epsilon_p^F \hat{a}_p^\dagger \hat{a}_p + \sum_p \epsilon_p^B \hat{b}_p^\dagger \hat{b}_p + \sum_p (\epsilon_p^M + \nu) \hat{c}_p^\dagger \hat{c}_p + \frac{\gamma}{2V} \sum_{p,p',q} \hat{b}_{p-q}^\dagger \hat{b}_{p'+q}^\dagger \hat{b}_p \hat{b}_{p'} \quad (2)$$

$$H_I = \frac{V_{bg}}{V} \sum_{p,p',q} \hat{a}_{p-q}^\dagger \hat{b}_{p'+q}^\dagger \hat{a}_p \hat{b}_{p'} + \frac{g}{\sqrt{V}} \sum_{q,p} (\hat{c}_q^\dagger \hat{a}_{-p+q/2} \hat{b}_{p+q/2} + \text{h.c.}).$$

Here  $\hat{a}_p, \hat{b}_p$  are the annihilator operators for, respectively, fermions and bosons,  $\hat{c}_p$  is the annihilator operator for the molecular field [27, 31, 32];  $\gamma = 4\pi a_b/m_b$  is the interaction term for bosons, where  $a_b$  is the boson–boson scattering length; and  $V_{bg}, \nu$ , and  $g$  are parameters related to the Bose–Fermi interaction, yet to be determined. Also we define single particle energies  $\epsilon^\alpha = p^2/2m_\alpha$ , where  $m_\alpha$  indicates the mass of bosons, fermions, or pairs, and  $V$  as the volume of a quantization box with periodic boundary conditions.

## 2.2. Two-body scattering parameters

The first step is to find the values for  $V_{bg}, \nu, g$  in terms of measurable parameters. We will, for this purpose, calculate the two-body  $T$ -matrix resulting from the Hamiltonian in equation (2). Integrating the molecular field out of the real time path integral [41], leads to the following Bose–Fermi interaction Hamiltonian

$$H_I^{2\text{body}} = \frac{1}{V} \left( V_{bg} + \frac{g^2}{E - \nu} \right) \sum_p \hat{a}_p^\dagger \hat{b}_{-p}^\dagger \hat{a}_p \hat{b}_{-p}. \quad (3)$$

This expression is represented in centre-of-mass coordinates, and  $E$  is the collision energy of the system. From the above equation we read trivially the zero energy  $T$ -matrix in the saddle point approximation

$$T = \left( V_{bg} - \frac{g^2}{\nu} \right), \quad (4)$$

which corresponds to the Born approximation. We emphasize that this approximation is only valid at exactly zero energy, and it does not, therefore, describe the correct binding energy as a function of detuning, and will be improved in the many-body treatment in section 4. However, with this approach we obtain an adequate description of the behaviour of scattering length as a function of detuning, which allows us to relate the parameters of our theory to experimental observables via the conventional parameterization [25, 27]

$$T(B) = \frac{2\pi}{m_{\text{bf}}} a_{\text{bg}} \left( 1 - \frac{\Delta_B}{(B - B_0)} \right), \quad (5)$$

where  $a_{\text{bg}}$  is the value of the scattering length far from resonance,  $\Delta_B$  is the width, in magnetic field, of the resonance,  $m_{\text{bf}}$  is the reduced mass and  $B_0$  is the field at which the resonance is centred.

The identification of parameters between equations (4) and (5) proceeds as follows: far from resonance,  $|B - B_0| \gg \Delta_B$ , the interaction is defined by a background scattering length, via  $V_{\text{bg}} = \frac{2\pi a_{\text{bg}}}{m_{\text{bf}}}$ . Relating magnetic field dependent quantity  $B - B_0$  to its energy-dependent analogue  $\nu$  requires defining a parameter  $\delta_B = \partial \nu / \partial B$ , which may be thought of as a kind of magnetic moment for the molecules. It is worth noting that  $\nu$  does not represent the position of the resonance nor the binding energy of the molecules, and that, in general  $\delta_B$  is a field-dependent quantity, since the thresholds move quadratically with field, because of nonlinear corrections to the Zeeman effect. For current purposes we identify  $\delta_B$  by its behaviour far from resonance, where it is approximately constant. Careful calculations of scattering properties using the model in equation (2), however, leads to the correct Breit–Wigner behaviour of the two-body  $T$ -matrix, as we show in section 4.

Finally we get the following identifications:

$$V_{\text{bg}} = \frac{2\pi a_{\text{bg}}}{m_{\text{bf}}} \quad g = \sqrt{V_{\text{bg}} \delta_B \Delta_B} \quad \nu = \delta_B (B - B_0). \quad (6)$$

For our calculations we use the 511G resonance in the  $^{40}\text{K}$ – $^{87}\text{Rb}$  system, the parameters we use in the calculations to follow are  $a_{\text{bg}} = -202a_0$ ,  $\delta_B = 5.1 \times 10^{-5}$  K/G, and  $\Delta_B = 1$  G.

### 2.3. The formalism

We now move on to the many-body analysis, and derive the Heisenberg equations of motion for the many-body system. The way this is done is to find equation of motion for correlation functions,  $f_s(x_1, \dots, x_s)$ , which represent the probability of finding  $s$  particles at positions  $x_1, \dots, x_s$ . As it turns out, the equation of motion for the correlation function  $f_1$  will depend on the function  $f_2$ , which in turn will depend on  $f_3$ , and so on all the way to  $f_N$ , where  $N$  is the total number of particles in the system. This is known as a Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchy [35]. In practice we will be concerned with momentum space correlation functions, but the idea is the same.

Given the large number of particles in the system, it is impossible to calculate equation of motions for all correlation functions, and we need to invoke an approximation. In practice, correlation functions are often calculated only up to two-body correlations,  $s = 2$ . This is justified under the assumption that interactions are suitably ‘weak.’ Higher-order correlations are included in an approximate way by considering not the actual atomic constituents, but rather combinations called quasiparticles. The quasiparticles are defined to be noninteracting, so that their higher-order correlation functions can be written in terms of second order correlation functions [41].

Using this qualitative idea we proceed to develop a more formal understanding. In statistical field theory, given an operator  $\mathcal{O}$ , and Hamiltonian  $H$ , we define the thermal average

of  $\mathcal{O}$  with respect to  $H$  as  $\langle \mathcal{O} \rangle_H = 1/Z \text{Tr}\{\mathcal{O} e^{-\beta H}\}$ , where  $\beta = (k_B T)^{-1}$  is the inverse temperature, and  $Z = \text{Tr}\{e^{-\beta H}\}$  is the partition function. In this framework, the one-particle correlation function is defined as the thermal average of the number operator with respect to the Hamiltonian of the system.

In the quasiparticle representation, we define the annihilation operator for quasiparticles as  $\alpha$ , reminding ourselves that it is a complicated function of  $a, a^\dagger, b, b^\dagger, c, c^\dagger$ . In momentum space, the one-particle correlation function in this representation will then be  $\langle \alpha_{p1} \alpha_{p2} \rangle_{H_{\text{qp}}}$ , where  $H_{\text{qp}}$  is the (noninteracting) quasiparticle Hamiltonian.

Now we introduce the real approximation, namely that the quasiparticles can be written as linear combinations of all possible products of two operators (except for averages involving one fermionic and one bosonic operator, which are easily shown to vanish). The procedure is then to find the Heisenberg equations of motion for these pairs of operators, and then averaging over the quasiparticle Hamiltonian

$$i\hbar \frac{\partial}{\partial t} \langle \mathcal{O} \rangle_{H_{\text{qp}}} = \langle [\mathcal{O}, H] \rangle_{H_{\text{qp}}}, \quad (7)$$

which being Gaussian allows us to invoke Wick's theorem to decompose all higher-order correlations in one-particle correlations, thus truncating the BBGKY hierarchy.

#### 2.4. The equations of motion

Before generating Heisenberg equations, we need to take a little care in the treatment of the Bose field, to properly treat the condensed part. To this end we perform the usual separation of mean field and fluctuations of the Bose field, substituting  $b_0$  (the zero-momentum component of the Bose gas) with a c-number  $\phi = \langle b_0 \rangle_{H_{\text{qp}}}$ , and identifying it with the condensate amplitude, while  $\langle b_{p \neq 0} \rangle_{H_{\text{qp}}} = 0$  are the fluctuations. We insert these definitions in the Hamiltonian in equation (2), then proceed to calculate commutators.

Since we wish to limit our analysis to a homogeneous gas, we note that the correlation functions  $f_1(x, x')$  can be written in terms of a relative coordinate  $y = x - x'$ . Thus in momentum space  $f_1(p)$  is the probability of finding a particle with momentum  $p$  in the gas, or in other words it is the momentum distribution of the system.

Having taken all appropriate commutators, and applied Wick's theorem, (for more details on the procedure see [36], or appendix A for the derivation of a sample equation.), we obtain the following self-consistent set of equations of motion for the system:

$$i\hbar \frac{\partial}{\partial t} \phi = V_{\text{bg}} \rho_F \phi + \gamma (2\phi \tilde{\rho}_B + \Delta_B \phi^*) + g \rho_{MF}^* + \gamma |\phi|^2 \phi \quad (8a)$$

$$\hbar \frac{\partial}{\partial t} \tilde{\eta}_B(p) = 2\gamma \Im m[\kappa_B(p)(\phi^{*2} + \Delta_B^*)] \quad (8b)$$

$$i\hbar \frac{\partial}{\partial t} \kappa_B(p) = [\epsilon_p^B + 2V_{\text{bg}} \rho_F + 4\gamma(|\phi|^2 + \tilde{\rho}_B)] \kappa_B(p) + \gamma (2\tilde{\eta}_B(p) + 1)(\phi^2 + \Delta_B) \quad (8c)$$

$$\hbar \frac{\partial}{\partial t} \eta_F(p) = -2g \Im m(\phi \eta_{MF}(p)) \quad (8d)$$

$$i\hbar \frac{\partial}{\partial t} \kappa_F(p) = [\epsilon_p^F + 2V_{\text{bg}}(\tilde{\rho}_B + |\phi|^2)] \kappa_F(p) \quad (8e)$$

$$\hbar \frac{\partial}{\partial t} \eta_M(p) = 2g \Im m(\phi \eta_{MF}(p)) \quad (8f)$$

$$i\hbar \frac{\partial}{\partial t} \kappa_M(p) = [\epsilon_p^M + v] \kappa_M(p) \quad (8g)$$

$$i\hbar \frac{\partial}{\partial t} \eta_{MF}(p) = [\epsilon_p^F - \epsilon_p^M - \nu + V_{\text{bg}}(\tilde{\rho}_B + |\phi|^2)]\eta_{MF}(p) - g\phi^*(\eta_F(p) - \eta_M(p)) \quad (8h)$$

$$i\hbar \frac{\partial}{\partial t} \kappa_{MF}(p) = [\epsilon_p^F + \epsilon_p^M + \nu + V_{\text{bg}}(\tilde{\rho}_B + |\phi|^2)]\kappa_{MF}(p) - g[\phi\kappa_F(p) + \phi^*\kappa_M(p)], \quad (8i)$$

where  $\tilde{\eta}_B(p) = \langle b_{p \neq 0}^\dagger b_{p \neq 0} \rangle_{H_{\text{qp}}}$  is the momentum distribution of non-condensed bosons, and  $\tilde{\rho}_B = \int \frac{dp}{2\pi^2} p^2 \tilde{\eta}_B(p)$  is the density of noncondensed bosons;  $\kappa_B(p) = \langle b_{p \neq 0} b_{p \neq 0} \rangle_{H_{\text{qp}}}$  is the anomalous distribution of bosonic fluctuations and  $\Delta_B = \int \frac{dp}{2\pi^2} p^2 \kappa_B(p)$  is the anomalous density. Similarly  $\eta_{F,M}(p)$  are the fermionic and molecular distributions,  $\rho_{M,F}$  are the densities and  $\kappa_{F,M}(p)$  and  $\Delta_{F,M}$  are the anomalous molecular and fermionic distributions and densities. Finally  $\eta_{MF}(p) = \langle c_p^\dagger a_p \rangle_{H_{\text{qp}}}$  and  $\kappa_{MF}(p) = \langle c_p a_p \rangle_{H_{\text{qp}}}$  are the normal and anomalous distribution for molecule–fermion correlation, with the associated densities  $\rho_{MF}$  and  $\Delta_{MF}$ .

### 3. Analysis and results

Equations (8a)–(8i) describe the complete self-consistent set of HFB equations for the resonant BF mixture. Inspection of these equations, however, allows us to simplify the set quite dramatically, without sacrificing almost any of the physics thereby contained. First, we note that the evolution of the anomalous fermionic densities  $\kappa_{MF}(p)$ ,  $\kappa_F(p)$  and  $\kappa_M(p)$  is entirely decoupled from the evolution of all other quantities, and can therefore be considered separately. This implies that, since we are mainly interested in the evolution of the normal densities, we can eliminate without approximation all the anomalous ones.

The next thing we note is that the evolution of the normal and anomalous bosonic averages is completely independent of the resonant interaction, and is controlled only by the background interactions between bosons and with fermions. For typical background interaction strengths, and cold enough temperatures, it is well established that the role of noncondensed bosons is minor, and the system is well described at the Gross–Pitaevskii level of approximation.

We can therefore write the following reduced set of equations:

$$i\hbar \frac{\partial}{\partial t} \phi = (V_{\text{bg}}\rho_F + \gamma|\phi|^2)\phi + g\rho_{MF}^* \quad (9a)$$

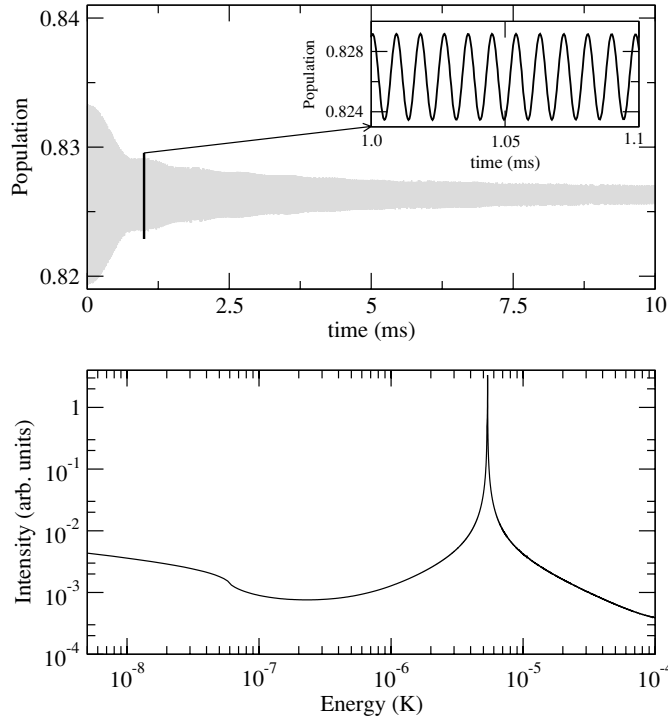
$$\hbar \frac{\partial}{\partial t} \eta_F(p) = -2g \text{Im}(\phi\eta_{MF}(p)) \quad (9b)$$

$$\hbar \frac{\partial}{\partial t} \eta_M(p) = 2g \text{Im}(\phi\eta_{MF}(p)) \quad (9c)$$

$$i\hbar \frac{\partial}{\partial t} \eta_{MF}(p) = [\epsilon_p^F - \epsilon_p^M - \nu + V_{\text{bg}}|\phi|^2]\eta_{MF}(p) - g\phi^*(\eta_F(p) - \eta_M(p)). \quad (9d)$$

Together with the prospect of simulating time-dependent experiments, such a set of equations allow us to calculate many characteristics of the system, which we could use to understand further physics or, more importantly at this stage, to test the theory against our knowledge of the system in various limits.

A relevant quantity we can calculate to this end is the binding energy of the molecules. This can be done by an instantaneous jump of the detuning from large and positive values, where we know the equilibrium distributions very well, to some other arbitrary value. The system thus perturbed oscillates at a specific characteristic frequency, which identifies as the (unique) pole of the HFB many-body  $T$ -matrix of the system. For negative detunings, as



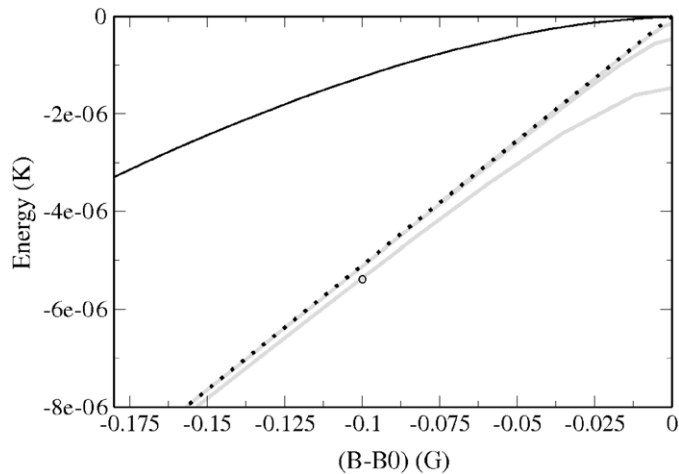
**Figure 1.** The top panel represents the time evolution of the population of condensed atoms after detuning is suddenly shifted from infinitely positive to  $-5.1$  K ( $-0.1$  G magnetic detuning). The bottom panel shows the absolute value of Fourier transform of said time evolution. The main peak in this graph represents the computed value of the binding energy, which we see is about  $5.4 \times 10^{-6}$  K. The system under consideration is composed of fermionic densities of  $10^{12}$   $\text{cm}^{-3}$  for a constant density ratio of five bosons per fermion.

shown below, this pole corresponds to the binding energy of the molecules, dressed by the interactions in the system.

Figure 1 shows a representative example of time evolution of the condensate population (number conservation guarantees that all three populations oscillate with the same frequency) under the conditions described above. In this particular example, at time  $t = 0$  the detuning is suddenly shifted to  $-5.1 \times 10^{-6}$  K, corresponding to a magnetic field detuning of approximately 0.1 G. The response of the population shows an envelope function, indicated by the grey shaped area that arises from nonlinearities in the equations of motion. The inset shows that under this envelope is a well-defined sinusoidal oscillation.

The nearly monochromatic character of the response is made clear by Fourier transforming the time-dependent population. The Fourier Transform shown in the second panel of figure 1 is strongly peaked at  $5.4 \times 10^{-6}$  K. Similarly, the position of the peak in the frequency spectrum, for different final detunings, should map the molecular binding energy as a function of magnetic field.

Figure 2 shows the results obtained by this method. This plot represents the binding energy of the molecules, dressed by the interactions in the system. This dressing is expected to be weaker for smaller densities of atoms and molecules. In this limit, we should thus recover the two-body molecular binding energy, which can be calculated quite accurately from two-body close coupling calculations (solid line in figure 2). Instead we see that the pole behaviour



**Figure 2.** Plot representing the poles of the scattering  $T$ -matrix for the 511G  $^{87}\text{Rb}$ - $^{40}\text{K}$  Feshbach resonance. The dotted line represents the ‘bare’ molecular detuning as a function of field, as defined in the text. The solid black line is the correct binding energy of the molecular state, obtained by means of full close coupling calculations, while the grey solid lines are the eigenenergies obtained from equations (9a)–(9d), for different atomic densities. From top to bottom on the right the grey lines refer to fermionic densities of  $10^{10}\text{ cm}^{-3}$ ,  $10^{11}\text{ cm}^{-3}$  and  $10^{12}\text{ cm}^{-3}$ , for a constant density ratio of five bosons per fermion. We note that for lower and lower densities the calculated binding energy incorrectly approaches the bare detuning instead of the correct two-body binding energy.

approaches the bare detuning (dashed line in figure 2), indicating that the renormalization of the binding energy obtained at the present level of approximation is inadequate to correctly include the two-body physics. This behaviour is in sharp contrast to the Bose–Bose resonant interaction, where the correct binding energy is preserved at the HFB level [24]. This is also true for the Fermi–Fermi case [37].

This discrepancy is due to the fact that the creation of molecules requires the formation of correlations between bosons and fermions, which, as shown in the following, cannot exist if the density matrix is assumed to be Gaussian. Specifically what is required is a more careful consideration of the noncondensed bosons

#### 4. The importance of noncondensed bosons

The reason for the failure of the HFB theory is not immediately clear from the theory itself. To bring out the inadequacy of this theory in the dilute limit, we now recast the problem in an alternative perturbative form that can reproduce the correct behaviour in the two-body limit. This path integral approach will also lay bare the role of noncondensed bosons.

What we will see in the upcoming analysis may be qualitatively understood in the following simple terms. A molecule in the gas can decay into a pair of ‘virtual’ (i.e. non-energy conserving) atoms, which can then meet again and reform the molecule. The incidence of these events modifies the behaviour of the molecule, and an appropriate treatment of these virtual excitations is therefore necessary to correctly include the two-body properties of the molecules in the many-body theory. In particular, the molecules can decay forming a virtual noncondensed boson, and the contribution of this set of events to the physics of the molecules turns out to be very important. An appropriate theory would therefore consider the coupling of the molecules to noncondensed bosons explicitly, which implies that one has to include



in the equations of motion three point averages, such as  $\langle c_q^\dagger a_{-p+q/2} b_{(p+q/2)} \rangle$ . Since the HFB theory disregards three point averages, it only contains molecule–atom–atom couplings of the form  $\langle c_q^\dagger a_q \rangle \phi_0$ , where molecules can only decay forming a condensed boson.

It is straightforward to see that the HFB theory treats three-body correlation functions differently depending on the quantum statistics of the constituents. For a Bose–Bose mixture, the correlation function is approximated (schematically) by

$$\langle b b m \rangle \approx \langle m \rangle \langle b(-q) b(q) \rangle + 2 \langle b \rangle \langle b m \rangle. \quad (10)$$

The first term of the right of this expression allows explicitly for virtual bosonic pairs of arbitrary momentum, provided that the molecular field  $\langle m \rangle$  accounts for most of the molecules, which is assumed to be the case. Similarly, in a mixture of distinct fermions, the correlation function reads

$$\langle f_1 f_2 m \rangle \approx \langle m \rangle \langle f_1(q) f_2(-q) \rangle, \quad (11)$$

and the same argument applies, since the molecules are bosons.

For the Bose–Fermi mixture, on the other hand, the correlation function would be approximated by

$$\langle b f m \rangle \approx \langle b \rangle \langle f m \rangle + \langle f \rangle \langle b m \rangle + \langle m \rangle \langle b f \rangle. \quad (12)$$

The required virtual atom–atom pairs would arise from the third term on the right-hand side of this expression. However, these molecules are fermions, which have no mean field,  $\langle m \rangle = 0$ . The only surviving term is then the first one, which accounts only for condensed bosons, and somehow correlates the fermionic atoms to the fermionic molecules. This is only an indirect way to get the bosons and fermions correlated.

#### 4.1. Two-body scattering

The perturbative analysis begins by recasting the Hamiltonian in equation (2) in terms of a two-body action, in centre-of-mass coordinates:

$$S[\psi, \psi^\dagger, \phi, \phi^\dagger, \xi, \xi^\dagger] = S_B[\phi, \phi^\dagger] + S_F[\psi, \psi^\dagger] + S_M[\xi, \xi^\dagger] + S_C[\psi, \psi^\dagger, \phi, \phi^\dagger, \xi, \xi^\dagger], \quad (13)$$

where the field  $\phi$  represents the bosons,  $\psi$  the fermions and  $\xi$  the fermionic molecules, and where

$$\begin{aligned} S_B[\phi, \phi^\dagger] &= \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}} (-\hbar\omega + \epsilon_p^B) \phi_{\omega, \mathbf{p}}^\dagger \phi_{\omega, \mathbf{p}} + \frac{1}{2V} \gamma \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}, \mathbf{p}' \mathbf{q}} \phi_{\omega, \mathbf{p}-\mathbf{q}}^\dagger \phi_{\omega, \mathbf{p}'+\mathbf{q}}^\dagger \phi_{\omega, \mathbf{p}'} \phi_{\omega, \mathbf{p}} \\ S_F[\psi, \psi^\dagger] &= \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}} (-\hbar\omega + \epsilon_p^F) \psi_{\omega, \mathbf{p}}^\dagger \psi_{\omega, \mathbf{p}} \\ S_M[\xi, \xi^\dagger] &= \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}} (-\hbar\omega + \epsilon_p^M + \nu) \xi_{\omega, \mathbf{p}}^\dagger \xi_{\omega, \mathbf{p}} \\ S_C[\psi, \psi^\dagger, \phi, \phi^\dagger, \xi, \xi^\dagger] &= \frac{V_{\text{bg}}}{V} \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}, \mathbf{p}' \mathbf{q}} \psi_{\omega, \mathbf{p}-\mathbf{q}}^\dagger \phi_{\omega, \mathbf{p}'+\mathbf{q}}^\dagger \psi_{\omega, \mathbf{p}'} \phi_{\omega, \mathbf{p}} + g \\ &\quad \times \int \frac{d\omega}{2\pi} \sum_{\mathbf{p} \mathbf{q}} (\xi_{\omega, \mathbf{p}}^\dagger \psi_{\omega, \mathbf{q}-\mathbf{p}} \phi_{\omega, \mathbf{p}} + \text{c.c.}), \end{aligned} \quad (14)$$

where  $\hbar\omega$  is the frequency associated with the motion of the various fields.

As before we will then proceed to integrate out the molecular degree of freedom [41] to get

$$S'_C[\psi, \psi^\dagger, \phi, \phi^\dagger] = \int \frac{d\omega}{2\pi} \frac{d\omega'}{2\pi} \sum_{\mathbf{p} \mathbf{p}'} \left( V_{\text{bg}} + \frac{g^2}{E - \nu} \right) \phi_{\omega, \mathbf{p}}^\dagger \psi_{E-\omega, -\mathbf{p}}^\dagger \phi_{\omega', \mathbf{p}'} \psi_{E-\omega', -\mathbf{p}'} \quad (15)$$

where  $E$  is the collision energy between the fermions and the bosons. We then undergo the inverse transformation to obtain

$$\begin{aligned} S_M''[\xi, \xi^\dagger] &= - \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}} \left( V_{\text{bg}} + \frac{g^2}{\omega - \frac{p^2}{2(m_b+m_f)} - \nu} \right)^{-1} \xi_{\omega, \mathbf{p}}^{\dagger} \xi'_{\omega, \mathbf{p}} \\ S_C''[\psi, \psi^\dagger, \phi, \phi^\dagger, \xi, \xi^\dagger] &= \int \frac{d\omega}{2\pi} \sum_{\mathbf{p}} (\xi'_{E, \mathbf{0}}^\dagger \psi_{E-\omega, -\mathbf{p}} \phi_{\omega, \mathbf{p}} + \text{c.c.}). \end{aligned} \quad (16)$$

Here  $\xi'$  represents the new effective (i.e. primed) molecules. The first line of figure 3 shows the diagrams describing the resonant collisions between bosons and fermions. Here the continuous lines refer to fermions, the squiggles to bosons and the broken lines to effective molecules. Since we are looking for poles of the S-matrix, we can disregard the trivial fermion and boson propagators, and proceed, as outlined in figure 3, to calculate the renormalized propagator for  $\xi'$ , denoted as  $\mathbf{M}$ , represented there as a heavy broken line. This object coincides with the  $T$ -matrix of the system, and shares its poles. Using the definition of the retarded molecular self-energy  $\Sigma^M$  given in figure 3, and calling the molecular propagator  $M_0$  (again for  $\xi'$ ), we get the following Dyson series:

$$\begin{aligned} T = \mathbf{M} &= M_0 - M_0 \Sigma^M M_0 + M_0 \Sigma^M M_0 \Sigma^M M_0 - \dots \\ &= M_0 - M_0 \Sigma^M \mathbf{M}, \end{aligned} \quad (17)$$

where  $T$  is the  $T$ -matrix for the collision, and which has formal solution

$$T = \mathbf{M} = \frac{1}{M_0^{-1} + \Sigma^M}. \quad (18)$$

These quantities take the explicit form

$$\begin{aligned} M_0(E) &= \left( V_{\text{bg}} + \frac{g^2}{E - \nu} \right) \\ \Sigma^M(E) &= i \int \frac{d\omega}{2\pi} \frac{d\mathbf{p}}{(2\pi)^3} \frac{1}{(\hbar\omega - \frac{p^2}{2m_b} + i0^+)(E - \hbar\omega - \frac{p^2}{2m_f} + i0^+)} \\ &\approx -i \frac{m_{\text{bf}}^{3/2}}{\sqrt{2\pi}} \sqrt{E} - \frac{m_{\text{bf}} \Lambda}{\pi^2}, \end{aligned} \quad (19)$$

where  $m_{\text{bf}}$  is the boson–fermion reduced mass, and  $\Lambda$  is an ultraviolet momentum cutoff needed to hide the unphysical nature of the contact interactions; we will dwell more on that shortly. Finally inserting equation (19) into equation (18), we obtain the following expression for the  $T$ -matrix:

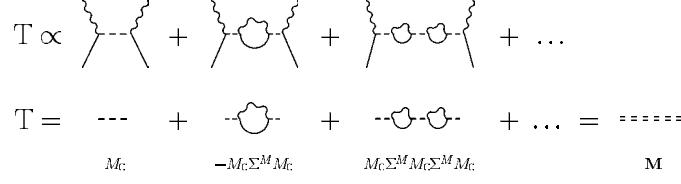
$$T(E) = \left[ \frac{1}{V_{\text{bg}} + \frac{g^2}{E - \nu}} + i \frac{m_{\text{bf}}^{3/2}}{\sqrt{2\pi}} \sqrt{E} + \frac{m_{\text{bf}} \Lambda}{\pi^2} \right]^{-1}. \quad (20)$$

To show that this expression correctly represents the two-body  $T$ -matrix for two-channel resonant scattering, we will compare it to the results we know from standard theoretical treatments [38], which teach us that

$$T(E) = \frac{\pi i}{m_{\text{bf}} \sqrt{2m_{\text{bf}} E}} 0(S(E) - 1), \quad (21)$$

where  $S(E)$  is the S matrix given by

$$S(E) = e^{-2i\sqrt{2m_{\text{bf}} E} a_{\text{bf}}} \left( 1 - \frac{2i\Gamma\sqrt{E}}{E - \epsilon_0 + i\Gamma\sqrt{E}} \right). \quad (22)$$



**Figure 3.** Feynman diagrams representing the resonant collision of a fermion and a boson. Straight lines represent fermions, squiggles bosons, and dashed lines represent the effective composite fermions.

Here  $\Gamma\sqrt{E}$  is the width of the resonance,  $\epsilon_0$  is a shift associated with the detuning with respect to threshold of the resonance and  $a_{\text{bf}}$  is the  $s$ -wave scattering length for the boson–fermion collision; all of these quantities can be extracted from experimental observables, through accurate two-body scattering calculations.

From the parameterization of the zero energy  $T$ -matrix in equation (5), and the  $E \rightarrow 0$  limit of (21), we easily derive  $\Gamma = \sqrt{2m_{\text{bf}}a_{\text{bf}}\delta_{\mu}\Delta B}$ . With these definitions we can relate equations (21) and (20), to find a regularization scheme for the theory, by substituting the nonobservable parameters  $g$ ,  $\nu$  and  $V_{\text{bg}}$  by the  $\Lambda$ -dependent (renormalized) quantities  $\bar{g}$ ,  $\bar{\nu}$  and  $\bar{V}_{\text{bg}}$ , such that the observable  $T$ -matrix will not be itself  $\Lambda$  dependent

Following [27] we compare equations (20) and (21), in the limit  $E \rightarrow 0$ , where we have (once we include the definitions of the bare quantities)

$$V_{\text{bg}} - \frac{(g)^2}{\nu} = \left[ \frac{1}{\bar{V}_{\text{bg}} - \frac{\bar{g}^2}{\bar{\nu}}} + \frac{m_{\text{bf}}\Lambda}{\pi^2} \right]^{-1}. \quad (23)$$

Since we have one equation and three unknowns, we will have to insert some physics in the system, analysing it one limit at a time. The first limit is far from resonance, where  $\nu \rightarrow \infty$

$$\bar{V}_{\text{bg}} = V_{\text{bg}} \left( \frac{1}{1 - \frac{m_{\text{bf}}\Lambda V_{\text{bg}}}{\pi^2}} \right). \quad (24)$$

We are now left with the task of defining the resonant quantities, and we have no more leeway to make physically motivated simplifications. The equations which remain are ambiguous, which leaves us with a set of possibilities for the choice of  $\bar{g}$  and  $\bar{\nu}$ . One way is to proceed as follows: insert equation (24) into (23), and solve for  $\bar{\nu}$ , to get

$$\bar{\nu} = \bar{g}^2 \left( 1 - \frac{m_{\text{bf}}\Lambda V_{\text{bg}}}{\pi^2} \right) \left( \frac{m_{\text{bf}}\Lambda}{\pi^2} + \frac{\nu}{g^2} \right). \quad (25)$$

From inspecting the above equation we can choose a definition of  $\bar{g}$ , which will also imply one for  $\bar{\nu}$ , and we get (reporting also equation (24) for completeness)

$$\bar{V}_{\text{bg}} = V_{\text{bg}} \left( \frac{1}{1 - \frac{m_{\text{bf}}\Lambda V_{\text{bg}}}{\pi^2}} \right) \quad \bar{g} = g \left( \frac{1}{1 - \frac{m_{\text{bf}}\Lambda V_{\text{bg}}}{\pi^2}} \right) \quad \bar{\nu} = \nu + \bar{g}g \frac{m_{\text{bf}}\Lambda V_{\text{bg}}}{\pi^2}. \quad (26)$$

Using these definitions of  $\bar{V}_{\text{bg}}$ ,  $\bar{g}$  and  $\bar{\nu}$ , together with the policy of imposing  $\Lambda$  as the upper limit of momentum integrals, will guarantee that observables will not depend on the choice of  $\Lambda$ , as long as it is chosen to be bigger than momentum scales relevant to experiment.

#### 4.2. Many-body generalization

Generalizing the above treatment from two to many particles, we must now account for the fact that, in a many-body system the molecular self-energy is modified by the environment.

Unlike in the scattering problem, the procedure outlined in the previous section is only an approximation to the full many-body problem, but as some evidence seems to suggest, a pretty good one [39, 40].

To perform this generalization, one needs to calculate the many-body self-energy using the many-body free Green functions  $D_{\text{MB}}^0(\omega, p)$  and  $G_{\text{MB}}^0$ , respectively for bosons and fermions, defined as [41]

$$D_{\text{MB}}^0(\omega, p) = |\phi|^2 + \frac{1}{\hbar\omega - \epsilon_p^B + \mu_B + i0^+} \quad (27)$$

$$G_{\text{MB}}^0(\omega, p) = \frac{1}{\hbar\omega - \epsilon_p^F + \mu_B + i0^+ \text{sign}(\epsilon_b^F - \mu_B)}, \quad (28)$$

where  $\mu_{B(F)}$  is the bosonic (fermionic) chemical potential. The molecular self-energy becomes

$$\begin{aligned} \Sigma^M B(\Omega, \mathbf{p}) &= -ig^2 \int \frac{d\omega}{2\pi} \frac{d^3q}{(2\pi)^3} D_0(\mathbf{q}, \omega) G_0(\mathbf{p} - \mathbf{q}, \Omega - \omega) \\ &= \Sigma_0^{\text{MB}}(\Omega, p) + \Sigma_\delta^{\text{MB}}(\Omega, p) = -ig^2 |\phi|^2 G_0(\Omega, \mathbf{p}) \\ &\quad + g^2 \int_{p-kf}^\Lambda \frac{d^3q}{(2\pi)^3} \frac{1}{\Omega - \epsilon_q^B - \epsilon_{\mathbf{p}-\mathbf{q}}^F + \mu_F + \mu_B}, \end{aligned} \quad (29)$$

the two terms in this expression represent contributions from condensed ( $\Sigma_0^{\text{MB}}(\Omega, p)$ ) and noncondensed ( $\Sigma_\delta^{\text{MB}}(\Omega, p)$ ) bosons, respectively.

The (approximate) many-body self-energy in equation (29) can be easily shown to reduce to its correct two-body counterpart defined in equation (19), when the densities and chemical potentials are set to zero. However, if the contribution due to the noncondensed bosons  $\Sigma_\delta^{\text{MB}}$  is omitted, then  $\Sigma^{\text{MB}}$  clearly vanishes in the two-body limit,  $\phi \rightarrow 0$ . There would then be no renormalization of the molecular propagator, and the pole of the  $T$ -matrix would coincide with the bare detuning, as shown in figure 2.

We remind the reader that neglecting the noncondensed component of the bosonic field was a perfectly well-justified approximation of equations (8a)–(8i), which implies that those equations are already inadequate to reproduce the two-body binding energies in the low density limit. Indeed the part of resonant term in the Hamiltonian containing the bosonic fluctuations vanishes according to Wicks theorem, since it is an average of a three operator correlation with respect to a density matrix which is Gaussian, in the HFB approximation. To correct this problem we should extend the HFB approximation and explicitly include three, and possibly higher, particle cumulants, finding some other way to truncate the BBGKY hierarchy. The subtleties involved in such a calculation, however, are many, and nontrivial, and will be the subject of the further work.

## 5. Conclusions

We have performed a study of the non-equilibrium behaviour in Bose–Fermi mixtures subject to an interspecies Feshbach resonance, using the HFB approximation. We have found that this approximation is not adequate to describe the system, which is quite remarkable since it has become one of the standard approaches to resonant cold atom physics due to its successes in Bose gases and two-component Fermi gases.

The reason of this failure is found in the way in which the theory treats noncondensed bosons. This problem could be corrected by the explicit inclusion of three (and possibly higher) point cumulants, which will allow for a mechanism through which bosons and fermions could correlate to form molecules. This task, however is beyo.

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## Appendix

In this appendix we will present a sample derivation of one of the equations of motion, namely that for  $\langle \delta^\dagger \delta \rangle$ .

Starting with the Hamiltonian in coordinate space

$$\begin{aligned}
 H = & \int dx \psi^\dagger(x) T^F(x) \psi(x) + \int dx \phi^\dagger(x) T^B(x) \phi(x) + \int dx \xi^\dagger(x) T^M(x) \xi(x) \\
 & + \frac{1}{2} \gamma \int dx |\phi(x)|^4 + V_{\text{bg}} \int dx |\phi(x)|^2 |\psi(x)|^2 + g \\
 & \times \int dx (\xi^\dagger(x) \phi(x) \phi(x) + \text{c.c.}), \tag{A.1}
 \end{aligned}$$

where  $T^\alpha(x)$  is the kinetic energy of molecules, bosons or fermions.

We then write the bosonic field in terms of its average and fluctuations around it  $\phi(x) = \phi_0(x) + \delta(x)$ , where  $\phi_0$  is a complex number. Inserting this expression in the Hamiltonian, we get the following:

$$\begin{aligned}
 H = E_0 + & \int dx \psi^\dagger(x) (T^F(x) + V_{\text{bg}} |\phi_0(x)|^2) \psi(x) + \int dx \delta^\dagger(x) T^B(x) \delta(x) \\
 & + \int dx \xi^\dagger(x) T^M(x) \xi(x) + \gamma \int dx (4 |\phi_0(x)|^2 |\delta(x)|^2 + \phi_0^*(x)^2 \delta(x) \delta(x) \\
 & + \phi_0(x)^2 \delta^\dagger(x) \delta^\dagger(x)) + \int dx (\phi_0^*(x) \delta(x) + \phi_0(x) \delta^\dagger(x)) \\
 & \times \left( \frac{\gamma}{2} |\phi_0(x)|^2 + V_{\text{bg}} |\psi(x)|^2 \right) + \gamma \int dx (\phi_0^*(x) \delta^\dagger(x) \delta(x) \delta(x) + \text{c.c.}) \\
 & + \frac{\gamma}{2} \int dx \delta^\dagger(x) \delta^\dagger(x) \delta(x) \delta(x) + V_{\text{bg}} \int dx |\delta(x)|^2 |\psi(x)|^2 \\
 & + g \int dx [\xi(x)^\dagger (\phi_0(x) + \delta(x)) \phi(x) + \text{c.c.}], \tag{A.2}
 \end{aligned}$$

where  $E_0$  is a constant which depends on  $\phi_0$ , and it is relevant for its motion, but does not contribute to that of  $\delta^\dagger \delta$ .

The next step is to calculate the commutator  $[\delta^\dagger(z) \delta(z'), H]$ , and to take its average, thereby obtaining

$$\begin{aligned}
 \langle [\delta^\dagger(z) \delta(z'), H] \rangle = & T^B(z') - T^B(z) \langle \delta^\dagger(z) \delta(z') \rangle + \gamma [2 |\phi_0(z')|^2 \langle \delta^\dagger(z) \delta(z') \rangle \\
 & + \phi_0^2(z) \langle \delta^\dagger(z) \delta^\dagger(z') \rangle - 2 |\phi_0(z)|^2 \langle \delta^\dagger(z) \delta(z') \rangle - \phi_0^{*2}(z') \langle \delta(z) \delta(z') \rangle] \\
 & + \phi_0(z') \left( \gamma \langle \delta^\dagger(z') \rangle |\phi_0(z')|^2 + V_{\text{bg}} \int dx \langle \delta^\dagger(z') \psi^\dagger(x) \psi(x) \rangle \right) \\
 & - \phi_0^*(z) \left( \gamma \langle \delta(z) \rangle |\phi_0(z)|^2 + V_{\text{bg}} \int dx \langle \delta(z) \psi^\dagger(z) \psi(z) \rangle \right) \\
 & + \gamma \int dx [\phi_0^*(x) (\langle \delta^\dagger(z) \delta(z') \delta^\dagger(x) \delta(x) \delta(x) \rangle - \langle \delta^\dagger(x) \delta(x) \delta(x) \delta^\dagger(z) \delta(z') \rangle)]
 \end{aligned}$$

$$\begin{aligned}
& + \phi_0(x)(\langle \delta^\dagger(z)\delta(z')\delta^\dagger(x)\delta^\dagger(x)\delta(x) \rangle - \langle \delta^\dagger(x)\delta^\dagger(x)\delta(x)\delta^\dagger(z)\delta(z') \rangle) \\
& + \gamma(\langle \delta^\dagger(z)\delta^\dagger(z')\delta(z')\delta(z') \rangle - \langle \delta^\dagger(z)\delta^\dagger(z)\delta(z)\delta(z') \rangle) \\
& + V_{\text{bg}}(\langle \delta^\dagger(z)\delta(z')\psi^\dagger(z')\psi(z') \rangle - \langle \delta^\dagger(z)\delta(z')\psi^\dagger(z)\psi(z) \rangle) \\
& + g(\langle \xi(z')\psi^\dagger(z')\delta^\dagger(z) \rangle - \langle \xi^\dagger(z)\psi(z)\delta(z') \rangle).
\end{aligned} \tag{A.3}$$

The next step is to apply Wick's theorem to correlation functions of three or more operators. This implies that all correlation functions of odd order will vanish. We then get

$$\begin{aligned}
\langle [\delta^\dagger(z)\delta(z'), H] \rangle & = (T^B(z') - T^B(z))\langle \delta^\dagger(z)\delta(z') \rangle + \gamma[2|\phi_0(z')|^2\langle \delta^\dagger(z)\delta(z') \rangle \\
& + \phi_0^2(z)\langle \delta^\dagger(z)\delta^\dagger(z') \rangle - 2|\phi_0(z)|^2\langle \delta^\dagger(z)\delta(z') \rangle - \phi_0^{*2}(z')\langle \delta(z)\delta(z') \rangle] \\
& + \gamma(\langle \delta^\dagger(z)\delta^\dagger(z') \rangle\langle \delta(z)\delta(z') \rangle + 2\langle \delta^\dagger(z')\delta(z') \rangle\langle \delta^\dagger(z)\delta(z') \rangle \\
& - 2\langle \delta(z)\delta^\dagger(z) \rangle\langle \delta^\dagger(z)\delta(z') \rangle - \langle \delta^\dagger(z)\delta^\dagger(z) \rangle\langle \delta(z)\delta(z') \rangle) \\
& \times V_{\text{bg}}(\langle \delta^\dagger(z)\delta(z') \rangle\langle \phi^\dagger(z')\phi(z') \rangle - \langle \delta^\dagger(z)\delta(z') \rangle\langle \phi^\dagger(z)\phi(z) \rangle)
\end{aligned} \tag{A.4}$$

In free space,  $\phi_0$  becomes a constant, and all two-point correlations, which are functions of  $z, z'$ , become functions of  $z - z'$ , so that in momentum space they become functions of a single momentum. We thus obtain equation (8b).

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