Mean-field stationary state of a Bose gas at a Feshbach resonance

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We study the steady state of a zero-temperature Bose gas near a Feshbach or photoassociation resonance using a two-channel mean-field model that incorporates atomic and molecular condensates, as well as correlated atom pairs originating from dissociation of molecules into pairs of atoms. We start from a many-body Hamiltonian for atom-molecule conversion, and derive the time-dependent version of the mean-field theory. The stationary solution of the time-dependent model is rendered unique with an approximation that entails that all noncondensate atoms are correlated, as if emerging from dissociation of molecules. The steady state is solved numerically, but limiting cases are also found analytically. The system has a phase transition in which the atomic condensate emerges in a nonanalytic fashion. We quantify the scaling of the observable quantities, such as fractions of atomic and molecular condensates, with the detuning and the atom-molecule conversion strength. Qualitatively, the dependence on detuning rounds out with increasing coupling strength. A study of the thermodynamics shows that the pressure of the atom-molecule system is negative, even on the molecule side of the resonance. This indicates the possibility of mechanical instability.

I. INTRODUCTION

Photoassociation [1,2] and especially the mathematically equivalent Feshbach resonance [3,4] have been main themes in the physics of quantum degenerate Bose and Fermi gases for a while. The earliest experimental work was carried out on bosons. The widest-known examples are probably Feshbach resonance in a Bose-Einstein condensate (BEC) [5], two-photon photoassociation [6] in a BEC, purported [7] mechanical collapse of a BEC when the atom-atom interaction is made attractive by using a Feshbach resonance [8], and Ramsey fringes in the conversion between atomic and molecular condensates [9].

In an aspect that is often concealed by phrases to the effect that the Feshbach resonance is used to tune atom-atom interactions, at least in principle photoassociation and Feshbach resonance always involve conversion of atom pairs to the corresponding diatomic molecules. These molecules are in a highly excited vibrational state and are prone to collisional quenching. In a Bose gas the molecules tend to be short-lived (~ 10 ms). However, it turns out [10,11] that the diatomic molecules created at the 834 G Feshbach resonance from fermionic ^{6}Li atoms may persist for seconds. Thermal-equilibrium experiments are feasible, which has spurred enormous experimental and theoretical interest. Molecular condensates are now prepared routinely [12,13]. Of particular interest to our theme of atom-molecule conversion is a measurement of the equilibrium fraction of molecules as a function of the magnetic field [14], while a comparison of the thermodynamical properties between experiments [15] and quantum Monte Carlo simulations [16] serves as an illustration of the present state of the art in the modeling of fermion systems.

Given that the initial Feshbach resonance experiments were time dependent in an essential way, the corresponding theories were time dependent as well. Our approach is based on field-theoretical modeling of atom-molecule systems [17–19], but there are methods springing, e.g., from theory

of molecular structure, as reviewed recently in Ref. [20]. For instance, a good agreement with the atom-molecule Ramsey fringe experiments in a BEC [9] has been reported by several groups [21–25]. Our time-dependent method has produced [26] a passable theoretical description of atom-molecule conversion in an experiment [27] and yielded valid [28] predictions about the temperature dependence and the maximum value of the conversion efficiency also for fermionic atoms.

With the emergence of thermal-equilibrium experiments in Fermi systems, the equilibrium-oriented theoretical machinery of condensed matter physics has been brought to bear [16,29,30]. On the other hand, we have noticed [31] that the stationary solution of our time-dependent formalism for fermions [26] may also serve as a zero-temperature thermal equilibrium theory. The stationary solution is not unique, but it may be made so by assuming that all fermions appear in correlated pairs, as if from the dissociation of molecules. The result turns out to be a variant of the atom-molecule version of the BCS theory [32–35] for Fermi gases. We [31] and others [30,36] have reported favorable theoretical comparisons with the equilibrium fraction of molecules in the experiments [14] in which the magnetic field was varied in the neighborhood of the broad ^{6}Li Feshbach resonance.

The immediate purpose of the present paper is to introduce a similar "BCS" theory for bosonic atoms at zero-temperature thermal equilibrium. Basically, we take our time-dependent theory [22,25,37] and find the time-independent solution. As with fermions, the stationary solution may be rendered unique with a pairing approximation, which, however, turns out to be more subtle for bosons than for fermions. As the secondary goal, we discuss the technicalities of our work on both bosons [22,25,37] *and* fermions [26,31] that were not detailed in the original publications.

The main qualitative finding is that the atom-molecule system exhibits a phase transition in which the atomic BEC emerges in a nonanalytic fashion when the detuning, the atom-molecule energy difference, is varied. What we now call a two-mode model including only atomic and molecular

condensates, no atom pairs at all, exhibits this same feature [38], and it survives, even at finite temperature, if atom pairs are taken into account more or less like in the standard BCS theory [39–41]. In the limit of weak atom-molecule conversion, for instance, in the limit of a very dilute gas, the phase transition is at the position of the two-body Feshbach resonance, but for increasing atom-molecule conversion strength it moves to the molecule side of the Feshbach resonance or photoassociation. We characterize the phase transition and the variation of quantities such as the molecule fraction with both the detuning and the atom-molecule conversion strength. Broadly speaking, the dependence on detuning rounds out with increasing interaction strength. Finally, we investigate the thermodynamics of the atom-molecule system. The two-mode model is known to be dynamically unstable if there is an atomic condensate present [42], but the present model produces another puzzling surprise: The calculated pressure of the gas is negative for all parameter values, which indicates mechanical instability.

II. FORMULATION OF THE PROBLEM

A. Hamiltonian

We model conversion of bosonic atoms into bosonic diatomic molecules using the momentum (wave-vector) representation Hamiltonian [19,38]

$$\frac{H}{\hbar} = \sum_{\mathbf{k}} \left[\epsilon_{\mathbf{k}} a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + \left(\delta + \frac{1}{2} \epsilon_{\mathbf{k}} \right) b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}} \right]$$
$$- \frac{1}{2} \sum_{\mathbf{p},\mathbf{q}} (\kappa_{\mathbf{p},\mathbf{q}} b_{\mathbf{p}+\mathbf{q}}^{\dagger} a_{\mathbf{p}} a_{\mathbf{q}} + \kappa_{\mathbf{p},\mathbf{q}}^{*} a_{\mathbf{q}}^{\dagger} a_{\mathbf{p}}^{\dagger} b_{\mathbf{p}+\mathbf{q}}), \quad (1)$$

as appropriate for a free (nontrapped) gas. Here $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are boson annihilation operators for atoms and molecules with momentum $\hbar\mathbf{k}$, and $\hbar\epsilon_{\mathbf{k}} \equiv \hbar^2\mathbf{k}^2/2m$ is the kinetic energy for an atom with wave vector $\mathbf{k}$. For a molecule with twice the mass of an atom, the kinetic energy for a given momentum is half of the energy of an atom. The detuning δ gives the energy difference between a stationary molecule ($\mathbf{k}=0$) and two stationary atoms in the form $\hbar\delta$. This parameter is varied in a Feshbach resonance by varying the magnetic field, and in photoassociation by tuning the frequency (frequencies) of the laser(s).

Atom-molecule conversion entails that a pair of atoms is either converted to a molecule or a molecule is dissociated to a pair of atoms, all the while conserving the momentum. The governing matrix elements are denoted by $\kappa_{\mathbf{p},\mathbf{q}}$. Ordinarily we deal with s-wave processes that dominate at low temperature. By virtue of translational and rotational invariance, the corresponding coupling matrix element is then of the form $\kappa_{\mathbf{p},\mathbf{q}}=\kappa(|\mathbf{p}-\mathbf{q}|)$. Furthermore, we mostly write the coupling matrix element as a once-and-for-all constant $\kappa_{\mathbf{p},\mathbf{q}}=\kappa$. This means that atom-molecule conversion is a zero-range contact interaction; in the position representation for the atomic and molecular fields $\hat{\phi}$ and $\hat{\psi}$, the corresponding term in the Hamiltonian density would be $\propto \kappa[\hat{\psi}^{\dagger}(\mathbf{r})\hat{\phi}(\mathbf{r})\hat{\phi}(\mathbf{r})+\hat{\phi}^{\dagger}(\mathbf{r})\hat{\phi}^{\dagger}(\mathbf{r})\hat{\psi}(\mathbf{r})]$. The contact interaction model is convenient for our aims for two reasons: it reduces

the number of parameters to consider, and endowing the coupling coefficients with a realistic momentum dependence would much complicate the solution of the model. The downside is an ultraviolet divergence [37], which will require a renormalization.

Consider two atoms that may combine into a molecule in the center-of-mass frame. Then a molecular bound state is coupled to the continuum of the relative motion of the two atoms. By redefining the global phases of the continuum wave functions, one may always arrange things so that the coupling coefficients $\kappa_{\mathbf{p},\mathbf{q}}$ and κ are real, and κ is also nonnegative. This is assumed to be the case below. We write *sums* over the wave vectors in Eq. (1), which presumes box normalization of the dissociated states. The quantization volume V therefore enters the matrix element, $\kappa_{\mathbf{p},\mathbf{q}} \propto V^{-1/2}$ [19,38].

Conspicuously missing from the model is a background scattering length that would prevail, say, far away from the Feshbach resonance. It could, and given the nature of our results, maybe should be included; but again, since our focus is on the nature of the system in the vicinity of the resonance $\delta=0$, we keep the model and the attendant technical complications to the bare minimum.

A breakup of a molecule produces two atoms, and it takes precisely two atoms to make a molecule. The Hamiltonian (1) correspondingly has the conserved quantity

$$\hat{N} = \sum_{\mathbf{k}} (a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + 2b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}), \quad (2)$$

number of atoms plus twice the number of molecules. We use the value N of the invariant $\hat{N}$ to characterize the number of particles in the system, and occasionally, slightly inaccurately, call it the atom number. The total momentum

$$\hat{\mathbf{P}} = \hbar \sum_{\mathbf{k}} \mathbf{k}(a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + b_{\mathbf{k}}^{\dagger} b_{\mathbf{k}}) \quad (3)$$

is likewise a constant of the motion.

B. Dressed molecule

Before proceeding to many-body systems, we investigate the solvable model with the invariant atom number equal to two [31,37,43]. Without restricting the generality, we also assume that the conserved center-of-mass momentum equals zero. The state space is then spanned by vectors of the form [31]

$$|\psi\rangle = \left(\sum_{\mathbf{k}} A(\mathbf{k}) a_{\mathbf{k}}^{\dagger} a_{-\mathbf{k}}^{\dagger} + \beta b_0^{\dagger} \right) |0\rangle, \quad (4)$$

where $A(\mathbf{k})$ [with $A(\mathbf{k})=A(-\mathbf{k})$] and β are complex numbers, and $|0\rangle$ is the particle vacuum. The time-dependent Schrödinger equation follows from Hamiltonian (1) in the form

$$i\dot{\beta} = \delta\beta - \frac{\kappa}{2} \sum_{\mathbf{k}} A(\mathbf{k}), \quad (5)$$

$$i\dot{A}(\mathbf{k}) = 2\epsilon_{\mathbf{k}}A(\mathbf{k}) - \kappa\beta. \tag{6}$$

If rotational invariance prevails at the initial time so that $A(\mathbf{k})$ is only a function of $|\mathbf{k}|$, or equivalently, a function of $\epsilon_{\mathbf{k}} \equiv \epsilon$, the same symmetry holds at all later times. Moreover, in a two-atom system we may replace the sum over $\mathbf{k}$ by a continuum approximation without running into problems with the atomic BEC. We write the continuum approximation as

$$\sum_{\mathbf{k}} f(\epsilon(\mathbf{k})) \rightarrow \frac{V}{(2\pi)^3} \int d^3k f(\epsilon(\mathbf{k})) \rightarrow \frac{3N}{2\epsilon_F^{3/2}} \int_0^\infty d\epsilon \sqrt{\epsilon} f(\epsilon). \tag{7}$$

We prefer quantities with the dimension of frequency over $\hbar$ times the same quantities with the dimension of energy, so that the integral runs over frequencies. Although it is silly if not misleading in the present case of only two atoms ($N=2$), for future use we have defined the energy $\hbar\epsilon_F$ by

$$\epsilon_F = \frac{\hbar}{2m}\left(\frac{6\pi N}{V}\right)^{2/3}. \tag{8}$$

It equals the Fermi energy for a single-component gas with the density N/V, but obviously has nothing to do with any physical Fermi energy. Instead, ϵ_F is a measure of the density of the gas; the essentially unique frequency that can be constructed out of density (N/V) for a quantum mechanical ($\hbar$) gas of atoms (m). Below we often refer to ϵ_F *without* the $\hbar$ as Fermi energy, and similarly with other quantities with the dimension of frequency.

To cap our introduction of the notations, we define the frequency parameter characterizing the atom-molecule coupling

$$\Omega = \sqrt{N}\kappa. \tag{9}$$

It is essential to keep in mind that in this bound-continuum problem the analogy of the Rabi frequency Ω is proportional to the square root of density, $\Omega \propto (N/V)^{1/2}$. In line with what was said before of the coefficient κ, we also take $\Omega \geq 0$. The time dependent Schrödinger equation for the coefficients β and $A(\epsilon(\mathbf{k}))$ finally reads

$$i\dot{\beta}(t) = \delta\beta(t) - \frac{3\Omega}{2\sqrt{2}\epsilon_F^{3/2}} \int_0^\infty d\epsilon \sqrt{\epsilon} A(\epsilon,t), \tag{10}$$

$$i\dot{A}(\epsilon,t) = 2\epsilon A(\epsilon,t) - \frac{\Omega}{\sqrt{2}}\beta(t). \tag{11}$$

The essence of the two-channel theory is to regard atoms and molecules as distinct though coupled degrees of freedom. The boson operators in Hamiltonian (1) create and annihilate bare atoms and molecules that would be observed if there were no atom-molecule coupling. As such, they would represent the observable atoms and molecules immediately after the atom-molecule coupling was switched off. In the case of photoassociation this could be achieved literally by switching off the lasers. For the Feshbach resonance an equivalent decomposition could be effected (in principle) by suddenly switching the magnetic field so far off the reso-

nance that the atoms and the molecules effectively decouple. There are also experimental probes that directly see the bare molecules, for instance, by making use of optical transitions in the bare molecules [14].

However, standard radio frequency spectroscopy at a Feshbach resonance [27,44] probes transitions between energy eigenstates of the system in the presence of the atom-molecule coupling, i.e., stationary states of Eqs. (10) and (11). These are superpositions of a bare molecule and pairs of bare atoms, and so we refer to the coupled system as the dressed molecule [18].

Renormalization

The energy eigenstates are obtained by inserting an ansatz of the form $\beta(t) = e^{-i\omega t}\beta$, $A(\epsilon,t) = e^{-i\omega t}A(\epsilon)$ into Eqs. (10) and (11), which gives

$$(\omega - \delta)\beta = -\frac{3\Omega}{2\sqrt{2}\epsilon_F^{3/2}} \int_0^\infty d\epsilon \sqrt{\epsilon} A(\epsilon), \tag{12}$$

$$(\omega - 2\epsilon)A(\epsilon) = -\frac{\Omega}{\sqrt{2}}\beta. \tag{13}$$

Simple elimination of $A(\epsilon)$ from Eq. (12) using Eq. (13) gives a relation to determine the eigenfrequency ω,

$$\omega - \delta = \frac{3\Omega^2}{4\epsilon_F^{3/2}} \int_0^\infty d\epsilon \frac{\sqrt{\epsilon}}{\omega - i\eta - 2\epsilon}. \tag{14}$$

Here $-\eta$, with $\eta = 0+$, is the usual imaginary part in the energy that needs to be added to handle the divergence of the integrand at $2\epsilon = \omega$. This practice is the same as if we took Fourier transformations of the time-dependent equations and used them to study the evolution of the system forward in time. Such an asymmetry in the direction of time is not desirable if we are looking for true stationary states of the atom-molecule system. We outline in the Appendix a method, following Ref. [45], to find the proper stationary states, but here the main issue is the ultraviolet divergence of the integral in Eq. (14).

Physically, Eqs. (10) and (11) describe the coupling of the bare-molecule state to many (actually, a continuum of) atom-pair states. One obvious consequence is that, if there still is a bound state in the system, it is shifted in energy from the original bare molecular state. In the contact-interaction model the shift simply is infinite.

We renormalize as follows [31,37]. We adopt an upper limit of the integral M, write Eq. (14) as

$$\omega - \left(\delta - \frac{3\Omega^2}{4\epsilon_F^{3/2}} \int_0^M \frac{\sqrt{\epsilon}}{2\epsilon}\right) = \frac{3\Omega^2}{4\epsilon_F^{3/2}} \int_0^M d\epsilon \left(\frac{\sqrt{\epsilon}}{\omega - i\eta - 2\epsilon} + \frac{\sqrt{\epsilon}}{2\epsilon}\right), \tag{15}$$

and let $M \rightarrow \infty$ at the end of the calculation. The right-hand side then converges nicely, but ostensibly not so the left-hand side; the detuning δ gets modified by the infinite level shift. The idea of the renormalization is to incorporate the level shift into the definition of the energies, and take the renormalized detuning

$$\lim_{M \to \infty} \delta - \frac{3\Omega^2}{8\epsilon_F^{3/2}} \int_0^M \frac{1}{\sqrt{\epsilon}} = \bar{\delta} \quad (16)$$

to have a finite value.

In this way Eq. (14) turns into a well-behaved equation,

$$\omega - \bar{\delta} = \frac{3\Omega^2}{4\epsilon_F^{3/2}} \int_0^\infty d\epsilon \frac{1}{\sqrt{\epsilon}} \frac{\omega}{\omega + i\eta - 2\epsilon}. \quad (17)$$

The salient point is that for $\bar{\delta} < 0$ Eq. (17) has precisely one real solution (with $\omega < 0$), and no real solution if $\bar{\delta} > 0$. The system has a true stationary state that does not evolve in time only for $\bar{\delta} < 0$. In the Appendix we replace this statement with the more precise observation that the dressed molecule has a *normalizable* stationary state if and only if $\bar{\delta} < 0$. A bound state is found for the dressed molecule for $\bar{\delta} < 0$, otherwise the dressed molecule only exists in a dissociated form as a pair of bare atoms with a component of the bare molecule mixed in. We take this to mean that the renormalized detuning $\bar{\delta} = 0$ denotes the position of the Feshbach resonance in the two-atom system.

C. Mean-field approximation

We make the many-particle system solvable by a mean-field approximation, the idea of which is to treat possible atomic and molecular condensates as classical fields not quantum fields anymore [17,19,26]. Although it is not essential for the structure of the mean-field theory but rather a technical assumption to facilitate the analysis, we also assume that all molecules present in the system belong to a condensate of zero-momentum molecules. Hence only the molecule operator $b_0 \equiv b$ is kept in the Hamiltonian. Moreover, to accommodate the corresponding atomic BEC, we already at this point track separately the zero-momentum atoms with $a_0 \equiv a$. Using Hamiltonian (1) we then find the Heisenberg picture equations of motion for the atomic and molecular operators

$$i\dot{a} = -\kappa b a^\dagger, \quad (18)$$

$$i\dot{b} = \delta b - \frac{1}{2}\kappa aa - \frac{1}{2}\kappa \sum_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}}, \quad (19)$$

$$i\dot{a}_{\mathbf{k}} = \epsilon_{\mathbf{k}} a_{\mathbf{k}} - \kappa b a_{-\mathbf{k}}^\dagger. \quad (20)$$

Out of these primary equations one may form equations of motion for quadratic operator products, e.g.,

$$i\frac{d}{dt}(a_{\mathbf{k}}^\dagger a_{\mathbf{k}}) = \kappa(b^\dagger a_{\mathbf{k}} a_{-\mathbf{k}} - a_{-\mathbf{k}}^\dagger a_{\mathbf{k}}^\dagger b), \quad (21)$$

$$i\frac{d}{dt}(a_{\mathbf{k}} a_{-\mathbf{k}}) = 2\epsilon_{\mathbf{k}} a_{\mathbf{k}} a_{-\mathbf{k}} - \kappa(1 + a_{\mathbf{k}}^\dagger a_{\mathbf{k}} + a_{-\mathbf{k}}^\dagger a_{-\mathbf{k}})b. \quad (22)$$

We implement the mean-field approximation at this juncture by stating that in the equations of motion a and b are c numbers not operators anymore [26,37]. The quantum me-

chanical expectation values for the products then factorize as in this example,

$$\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} b \rangle = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle b \equiv \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle \langle b \rangle. \quad (23)$$

Applying the factorization to Eqs. (18)–(22) gives a closed set of equations of motion involving the expectation values of the form $\langle a \rangle$, $\langle b \rangle$, $\langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle$, and $\langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle$.

For the convenience of the formulation we assume that the problem is effectively rotationally symmetric, so that, e.g., the expectation value $\langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle$ only depends on the energy $\epsilon \equiv \epsilon_{\mathbf{k}}$. We write

$$P(\epsilon) = \langle a_{\mathbf{k}}^\dagger a_{\mathbf{k}} \rangle,$$

$$A(\epsilon) = \langle a_{\mathbf{k}} a_{-\mathbf{k}} \rangle. \quad (24)$$

It should be noted that $P(\epsilon)$ stands for the expectation value of the number of atoms in a one-particle state with the energy $\hbar\epsilon$, not for a quantity such as the number of atoms per unit energy interval. We also define the amplitudes for atomic and molecular condensates

$$\alpha = \sqrt{\frac{1}{N}} a, \quad \beta = \sqrt{\frac{2}{N}} b \quad (25)$$

so that $|\alpha|^2$ and $|\beta|^2$ stand for the fractions of the atoms that are in the system as part of either the atomic or the molecular condensate. Finally, as the atomic BEC has already been taken into account separately, the continuum approximation (7) should work as before.

We finally have the equations of motion of our mean-field theory for atom-molecule conversion in a boson system,

$$i\dot{\alpha}(t) = -\frac{\Omega}{\sqrt{2}}\beta(t)\alpha^*(t), \quad (26)$$

$$i\dot{\beta}(t) = \delta\beta(t) - \frac{\Omega}{\sqrt{2}}\alpha^2(t) - \frac{3\Omega}{2\sqrt{2}\epsilon_F^{3/2}}\int d\epsilon \sqrt{\epsilon} A(\epsilon,t), \quad (27)$$

$$i\dot{A}(\epsilon,t) = 2\epsilon A(\epsilon,t) - \frac{\Omega}{\sqrt{2}}[1 + 2P(\epsilon,t)]\beta(t), \quad (28)$$

$$i\dot{P}(\epsilon,t) = \frac{\Omega}{\sqrt{2}}[\beta^*(t)A(\epsilon,t) - \beta(t)A^*(\epsilon,t)]. \quad (29)$$

The similarity to the notation we employed in the discussion of the two-atom problem in Sec. II B is no accident. In fact, in the absence of a BEC of atoms, and assuming that the occupation numbers of the atomic states $P(\epsilon,t)$ are negligible compared to unity, Eqs. (26) and (27) coincide with the two-atom theory Eqs. (10) and (11). We view the mean-field theory as the two-atom theory amended with the possibility of a BEC and Bose enhancement for the atoms. An analogous interpretation applies to the corresponding mean-field theory for fermions [31].

Writing the expectation value of the invariant atom number (2) in terms of the mean-field variables gives the equation

$$|\alpha|^2 + |\beta|^2 + \frac{3}{2\epsilon_F^{3/2}} \int d\epsilon \sqrt{\epsilon} P(\epsilon) = 1. \tag{30}$$

The left-hand side is indeed a constant of the motion under Eqs. (26)–(29), so that the present mean-field approximation successfully reflects a basic property of the Hamiltonian. Finally, one may write the expectation value of the Hamiltonian in the mean-field approximation as

$$e = \frac{\langle H \rangle}{\hbar N} = \frac{1}{2} \delta |\beta|^2 + \frac{3}{2\epsilon_F^{3/2}} \int d\epsilon \epsilon^{3/2} P(\epsilon)$$
$$- \frac{\Omega}{2\sqrt{2}} \left(\alpha^2 \beta + \frac{3\beta}{2\epsilon_F^{3/2}} \int d\epsilon \sqrt{\epsilon} A(\epsilon) + \text{c.c.} \right). \tag{31}$$

Using Eqs. (26)–(29) it may be shown straightforwardly that, provided one is willing to subtract certain formally equal divergent integrals to obtain zero, the energy per particle $\hbar e$ from Eq. (31) is also a constant of the motion. The divergent integrals are part of the issue of renormalization, which was already discussed above and will be revisited again shortly.

We have made use of Eqs. (26)–(30) in different variations, notations, and approximations many a time in the past in our boson theories [19,22,25,37]. Similarly, we have repeatedly resorted to basically the same approach in the theory of the conversion between a two-species Fermi gas and the corresponding diatomic molecules [26,31]. Besides the obvious absence of the fermionic condensate, the difference is that where the boson problem shows the factor $1 + 2P(\epsilon)$ for Bose enhancement in Eq. (28), the corresponding fermion equation has the factor $1 - 2P(\epsilon)$ reflecting the exclusion principle.

D. Pairing approximation for steady state

Barring circumstances such as interference of the atomic BEC component of the atom-molecule system with another reference BEC, a multiplicative complex phase factor in the quantities α, β, and $A(\epsilon)$ is not observable. Besides, it is obvious from the equations of motion (26)–(29) that a certain combination of exponentially evolving phases is self-sustained. Specifically, we search for a stationary solution in the form [31]

$$\alpha(t) \equiv e^{-i\mu t}\alpha, \quad \beta(t) \equiv e^{-2i\mu t}\beta,$$
$$A(\epsilon,t) \equiv A(\epsilon)e^{-2i\mu t}, \quad P(\epsilon,t) \equiv P(\epsilon), \tag{32}$$

where μ is a real frequency. It will turn out that $\hbar\mu$ is the chemical potential for the atoms in this system (and half of the chemical potential for the molecules), but such an interpretation is not a given at this stage. In the rest of the paper we will again ignore the $\hbar$, and call μ the chemical potential.

Now, by a suitable choice of the zero of time we may always make the coefficient β in Eqs. (32) real and nonnegative, $\beta \geq 0$; let us assume so from now on. To keep Eq. (29) valid with an ansatz of the form (32) at all times is then only possible if ($\beta = 0$ or if) $A(\epsilon)$ is real. Likewise, by Eq. (26), the amplitude α must be real. With these restrictions, the time independent coefficients must satisfy

$$\alpha\left(\mu + \frac{\beta\Omega}{\sqrt{2}}\right) = 0, \tag{33}$$

$$(2\mu - \delta)\beta = -\frac{\Omega}{\sqrt{2}}\left[\alpha^2 + \frac{3}{2\epsilon_F^{3/2}} \int d\epsilon \sqrt{\epsilon} A(\epsilon)\right], \tag{34}$$

$$(\mu - \epsilon)A(\epsilon) = -\frac{\Omega}{2\sqrt{2}}[1 + 2P(\epsilon)]\beta, \tag{35}$$

and, of course, the norm condition (30).

The unknowns in the steady state are μ, α, β, $A(\epsilon)$, and $P(\epsilon)$. Thinking about a numerical solution with a discrete set of values for ϵ, it is clear that there are many more unknowns than equations. The problem is the original Eq. (29), which will not lead to any useful relation between $A(\epsilon)$ and $P(\epsilon)$ in the steady state. Additional conditions are needed to constrain the solution.

The same dilemma came up in a system of two fermion species combining into bosonic molecules. We resolved it [31] by the assumption that the fermions only come in pairs with opposite momenta and spins, as from dissociation of molecules. This leads immediately to the relation between pairing amplitudes and occupation numbers

$$|\langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}\rangle|^2 = \langle c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow}\rangle - \langle c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\uparrow}\rangle^2, \tag{36}$$

or, in the notation of the mean-field theory in Ref. [31],

$$|C(\epsilon)|^2 - [P(\epsilon) - P^2(\epsilon)] = 0. \tag{37}$$

$C(\epsilon)$ is the fermion pairing amplitude analogous to $A(\epsilon)$ of the present paper. With Eq. (37), the number of equations was sufficient for a (presumably) unique solution. Moreover, while we have not mentioned this before, the left-hand side of Eq. (37) is a constant of the motion in our BCS style mean-field theory for fermions [31].

To address the corresponding boson case, let us take two momentum states $\pm$, short for $\pm\mathbf{k}$, with the occupation number states $|n_+n_-\rangle$. The most general completely paired state is of the form

$$|\psi\rangle = \sum_n c_n |n,n\rangle, \tag{38}$$

with $\sum_n |c_n|^2 = 1$. Given the propensity of bosons to Poissonian statistics, we take

$$c_n = e^{|\alpha|^2/2} \frac{\alpha^n}{\sqrt{n!}}, \tag{39}$$

where α is a complex number. In the limit $|\alpha| \ll 1$ this is a generic description for a situation when only the states $|00\rangle$ and $|11\rangle$ are occupied, and the latter with a much smaller probability. Similarly, in the limit of a real $\alpha \equiv x \gg 1$ we have a generic description of the state in which $|c_n|$ peaks around $n \simeq x^2$, and c_n vary slowly as a function of n around this maximum. In fact, we cover the case $|\alpha| \ll 1$, too, if we just use a real and positive x in our argument, so that is how we proceed. Given the model, we have the expectation values
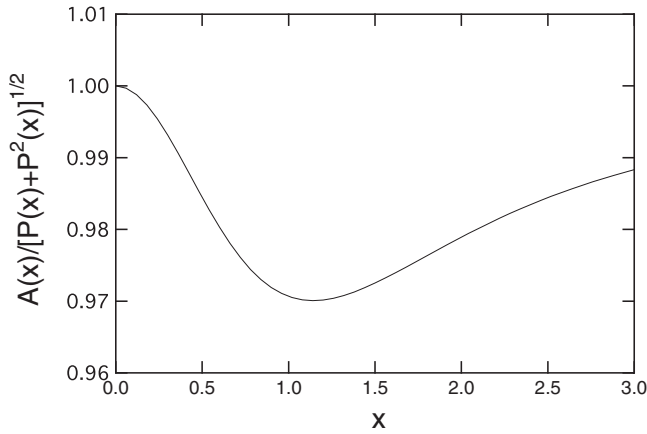
FIG. 1. The ratio of the actual pairing amplitude $A(x)$ and the quantity $[P(x)+P^2(x)]^{1/2}$ derived from the occupation number of the boson state $P(x)$ for the Poissonian paired state, (38) and (39), as a function of the real parameter of the state $x=\alpha$. If the pairing approximation (42) were exact, this ratio would identically equal unity.

$$P \equiv \langle a_+^\dagger a_+ \rangle = x^2, \tag{40}$$

$$A \equiv \langle a_+ a_- \rangle = e^{-x^2} x \sum_n \frac{x^{2n}\sqrt{n+1}}{n!}. \tag{41}$$

Mindful of the sign differences between bosons and fermions, on the basis of Eq. (37) we expect a relation for bosons of the form

$$|A(\epsilon)|^2 - [P(\epsilon) + P^2(\epsilon)] = 0. \tag{42}$$

To find out if it works, we plot in Fig. 1 the ratio $A/\sqrt{P+P^2}$ from Eqs. (40) and (41) as a function of the variable x. The maximum deviation of this ratio from unity is about 3%. We surmise that Eq. (42) is a reasonable approximation between pairing amplitudes and occupation numbers for boson states of the form (38).

The pairing approximation for bosons is further cemented by the observation that, fully analogously to the fermion theory, in our mean-field theory for bosons the left-hand side of Eq. (42) is a constant of the motion. This also gives an interesting piece of insight into the problem of finding the steady state: There is a large (infinite) number of constants of the motion, so that time evolution cannot lead to a unique steady state without an explicit specification of the values of the constants. Physically, on the other hand, it is generally up to the interactions with the environment to force specific values, such as the zero on the right-hand side of Eq. (42). In the corresponding fermion problem the zero would follow even without the interactions with the environment if the system started out as a condensate of molecules, and the same holds for the boson system. As advertised, our stationary solution corresponds to the assumption that all noncondensate atoms are correlated as if they came from dissociation of molecules.

Given that $A(\epsilon)$ is real and that it must be positive in the limit $\epsilon \to \infty$ by virtue of Eq. (35), Eqs. (35) and (42) may be solved for the pairing amplitudes and occupation numbers,

$$A(\epsilon) = \frac{\beta\Omega}{2\sqrt{2(\epsilon-\mu)^2 - \beta^2\Omega^2}}, \tag{43}$$

$$P(\epsilon) = \frac{1}{2}\left(\sqrt{\frac{\beta^2\Omega^2}{2(\epsilon-\mu)^2 - \beta^2\Omega^2} + 1} - 1\right). \tag{44}$$

Hence given the chemical potential μ and the amplitude of the molecular condensate β, both the occupation numbers $P(\epsilon)$ and the pairing amplitudes $A(\epsilon)$ are uniquely determined. The inequality

$$\mu \le -\frac{\beta\Omega}{\sqrt{2}} \tag{45}$$

must hold, else complex occupation numbers would result. The equality in Eq. (45) presents no problem, since the ensuing singularities in the occupation numbers and pairing amplitudes are sufficiently mild not to hamper the analysis.

E. Renormalization

Equations (33), (34), and (30) suffice to determine the remaining unknowns α, β, and μ, although a few issues remain. Next we discuss renormalization.

Consideration of the form of $A(\epsilon)$ in Eq. (43) shows right away that the integral $\int d\epsilon \sqrt{\epsilon} A(\epsilon)$ in Eq. (34) diverges. However, it turns out that the same renormalization that we devised for the two-atom case also resolves this divergence. We replace $A(\epsilon)$ with

$$\bar{A}(\epsilon) = \frac{\beta\Omega}{2\sqrt{2(\epsilon-\mu)^2 - \beta^2\Omega^2}} - \frac{\beta\Omega}{2\sqrt{2\epsilon}}, \tag{46}$$

which makes the integral convergent; but, to keep Eq. (34) valid, we need to add the the divergent integral $\int_0^\infty d\epsilon \, \epsilon^{-1/2}$ with an appropriate factor to the left-hand side as well. It turns out that the net effect is precisely to replace the detuning δ on the left-hand side with the renormalized detuning $\bar{\delta}$. Here we have played fast and loose with mathematical rigor, but this could be remedied by introducing the upper limit M to the integration just as in Eq. (15) and then letting $M \to \infty$.

Given the occupation numbers (44), the integral in the normalization equation (30) converges as written, but not so the integral involving $P(\epsilon)$ in the expression for the energy per particle (31). However, if one analogously to Eq. (46) replaces $P(\epsilon)$ with

$$\bar{P}(\epsilon) = P(\epsilon) - \frac{(\beta\Omega)^2}{8\epsilon^2}, \tag{47}$$

in the integral involving $A(\epsilon)$, does the subtraction (46), *and* replaces the detuning with the renormalized value $\bar{\delta}$, all divergences in Eq. (31) cancel. We regard this as an impressive demonstration of the consistency of the mean-field theory.

F. Statement of numerical problem

We now have to deal with the equations

$$\alpha\left(\mu + \frac{\beta\Omega}{\sqrt{2}}\right) = 0,$$

$$(2\mu - \bar{\delta})\beta + \frac{\Omega}{\sqrt{2}}\left[\alpha^2 + \frac{3(\beta\Omega)^{3/2}}{2^{11/4}\epsilon_F^{3/2}}A_{1/2}\left(-\frac{\sqrt{2}\mu}{\beta\Omega}\right)\right] = 0,$$

$$\alpha^2 + \beta^2 + \frac{3(\beta\Omega)^{3/2}}{2^{11/4}\epsilon_F^{3/2}}P_{1/2}\left(-\frac{\sqrt{2}\mu}{\beta\Omega}\right) = 1; \qquad (48)$$

$$e = \frac{\beta^2\bar{\delta}}{2} - \frac{\beta\Omega}{\sqrt{2}}\left\{\alpha^2 + \frac{3(\beta\Omega)^{3/2}}{2^{11/4}\epsilon_F^{3/2}}\left[A_{1/2}\left(-\frac{\sqrt{2}\mu}{\beta\Omega}\right)\right.\right.$$
$$\left.\left. - P_{3/2}\left(-\frac{\sqrt{2}\mu}{\beta\Omega}\right)\right]\right\}; \qquad (49)$$

$$A_{1/2}(m) = \int_0^\infty dx \frac{-m^2 - 2xm + 1}{\sqrt{x}\sqrt{[(m+x)^2 - 1][x + \sqrt{(m+x)^2 - 1}]}}; \qquad (50)$$

$$P_{1/2}(m) = \int_0^\infty dx \frac{\sqrt{x}}{\sqrt{(m+x)^2 - 1}[m + x + \sqrt{(m+x)^2 - 1}]}; \qquad (51)$$

$$P_{3/2}(m) = \int_0^\infty dx \frac{-8mx^3 - 4m^2x^2 + 3x^2 - 2mx - m^2 + 1}{2\sqrt{x}\sqrt{(m+x)^2 - 1}[2(x+m)x^2 + (2x^2 + 1)\sqrt{(m+x)^2 - 1}]}. \qquad (52)$$

Equations (48) are the ones to solve for the unknown quantities α, β, and μ, and Eq. (49) gives the resulting mean-field energy per particle. The integral $A_{1/2}(m)$ is a representation of the integral $\int d\epsilon\,\epsilon^{1/2}\bar{A}(\epsilon)$ as a function of the chemical potential μ, and similarly for $P_{1/2}$, $P_{3/2}$. These integrals are properly renormalized and dimensionless, and we have gone so far as to write them in forms that do not involve near-canceling subtractions of large numbers. They are suitable for use in numerical computations as written.

III. SOLVING THE THEORY

We have solved Eqs. (48)–(52) using MATHEMATICA [46] in a combination of analytical and numerical calculations. We double-checked many of the results by independent programming on MAPLE [47]. Unlike in the fermion case [31] where the production of accurate numerical results for arbitrary parameter values was a major project in numerical analysis, with bosons we never had to resort to a general-purpose programming language such as C++.

In detailed studies we first investigated numerically how the results behave, and used this knowledge to formulate ansatz solutions to find analytical results. The discussion preceding Eqs. (60) below serves as an example. An enormous amount of detail could be extracted in this way, but our aim is to demonstrate a few major qualitative features only.

1. Atomic condensate present

One way of satisfying Eq. (33), or the same equation as the first member of Eqs. (48), is to require that the expression inside the parentheses vanishes. This leads to

$$\mu = -\frac{\beta\Omega}{\sqrt{2}}, \qquad (53)$$

the integrals become $A_{1/2}(1) = -2\sqrt{2}$, $P_{1/2}(1) = 2\sqrt{2}/3$, and $P_{3/2}(1) = -8\sqrt{2}/5$, and the equations to solve for α and β are

$$(\bar{\delta} - 2\mu)\beta = \frac{\alpha^2\Omega}{\sqrt{2}} - \frac{3\beta^{3/2}\Omega^{5/2}}{2^{7/4}\epsilon_F^{3/2}}, \qquad (54)$$

$$\alpha^2 + \beta^2 + \frac{(\beta\Omega)^{3/2}}{2^{5/4}\epsilon_F^{3/2}} = 1. \qquad (55)$$

In principle these have an explicit closed-form solution, but in practice we have found it useless and proceed numerically. Given the solution, the energy per particle may be found from

$$e = \frac{3(-\mu)^{5/2}}{5\sqrt{2}\epsilon_F^{3/2}} + \alpha^2\mu. \qquad (56)$$

Now, by eliminating α from Eqs. (54) and (55) we have a necessary condition for the solution,

$$\beta^2 + \frac{\sqrt{2}(\sqrt{2}\beta\Omega + \bar{\delta})\beta}{\Omega} + \frac{2^{3/4}(\beta\Omega)^{3/2}}{\epsilon_F^{3/2}} = 1. \qquad (57)$$

It is easy to see numerically that for any real $\bar{\delta}$ and $\Omega > 0$ this has at most one solution with $0 \leq \beta \leq 1$. Moreover, numerically one may demonstrate that such a solution $\beta(\Omega, \bar{\delta})$ is a decreasing function of $\bar{\delta}$. Therefore a lower limit on the existence of a solution as a function of $\bar{\delta}$ is a possibility: Once β has reached a certain value <1, Eq. (55) dictates that $\alpha^2 = 0$. Suppose one decreases $\bar{\delta}$ further, then β would increase further and Eq. (55) would require $\alpha^2 < 0$, which is not allowed for a real α.

The limiting case is found setting $\alpha = 0$ in Eqs. (53)–(55), which gives a relation between $\bar{\delta}$ and Ω. We plot in Fig. 2 the detuning $\bar{\delta}$ obtained numerically in this way as a function of the Rabi frequency Ω, effectively using the Fermi frequency
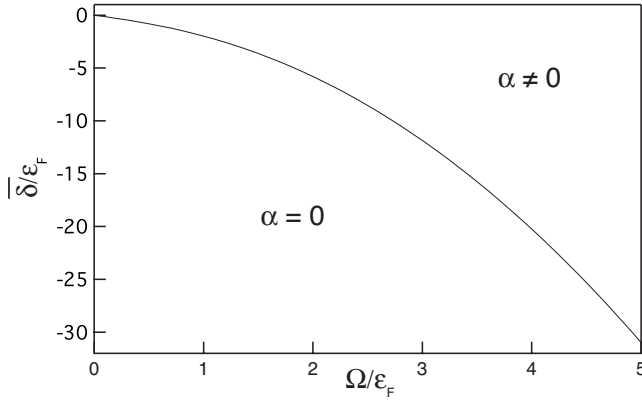
FIG. 2. The line in the $(\Omega, \bar{\delta})$ plane separating the phases of the system with a BEC of atoms present ($\alpha \neq 0$) and absent ($\alpha = 0$).

as a scale of frequencies. Given the equations to solve, we may also attempt power series solutions. For instance, we may insert the series

$$-\bar{\delta} = K_1 \Omega^1 + K_{3/2} \Omega^{3/2} + K_2 \Omega^2 + \cdots, \tag{58}$$

$$-\mu = M_1 \Omega^1 + M_{3/2} \Omega^{3/2} + M_2 \Omega^2 + \cdots, \tag{59}$$

into Eqs. (53)–(55) and attempt to satisfy the equations power by power in Ω. This ansatz works and gives solvable equations for the coefficients K and L. Following such principles, we find the expressions of the curve in Fig. 2 for the limits of both small and large Ω,

$$\bar{\delta}(\Omega) = \begin{cases} -\sqrt{2}\Omega + O(\Omega^{5/2}), & \Omega \ll \epsilon_F, \\ -\dfrac{3}{2^{4/3}} \dfrac{\Omega^2}{\epsilon_F} + O(\Omega^0), & \Omega \gg \epsilon_F. \end{cases} \tag{60}$$

2. Atomic condensate absent

The other way to satisfy Eq. (33) is to set

$$\alpha = 0, \tag{61}$$

which corresponds to the up-front statement that there is no atomic condensate. Equations (48) then turn into

$$\mu \equiv -\frac{\beta\Omega}{\sqrt{2}} m, \tag{62}$$

$$(\bar{\delta} - 2\mu)\beta = \frac{3\Omega(\beta\Omega)^{3/2} A_{1/2}(m)}{2^{13/4} \epsilon_F^{3/2}}, \tag{63}$$

$$1 = \beta^2 + \frac{3(\beta\Omega)^{3/2} P_{1/2}(m)}{2^{11/4} \epsilon_F^{3/2}}, \tag{64}$$

which are to be solved for β and μ; we have expressed the chemical potential μ using the dimensionless variable $m \in [1, \infty)$. The integrals (50)–(52) may be written in terms of elliptic integrals, but this fact appears to be useless and the practical solutions again proceed numerically. Once the solution is found, the energy per particle is given by Eq. (49) as written.

Now, consider Eqs. (62)–(64) for a fixed value of the parameter Ω, regarding β and $\bar{\delta}$ as functions of the variable m. By plotting the respective functions, it may be seen that, for $m > 1$, $P_{1/2}(m) > 0$, $P'_{1/2}(m) < 0$, $A_{1/2}(m) < 0$, and $A'_{1/2}(m) < 0$, with the prime denoting the derivative. Equation (64) then implies that $\beta'(m) > 0$, and Eq. (63) consequently gives $\bar{\delta}'(m) < 0$. In other words, when the parameter $\bar{\delta}$ is increased while keeping Ω fixed, m and β resulting from Eqs. (62)–(64) decrease; but, by the time the detuning $\bar{\delta}$ has reached the line in Fig. 2 the parameter m has attained the minimum permissible value $m = 1$, and there cannot be a solution for any larger $\bar{\delta}$.

3. Role of atomic condensate

The two classes of solutions we have found, $\alpha > 0$ and $\alpha \equiv 0$ corresponding to the presence and absence of an atomic condensate, join continuously. On the line drawn in Fig. 2 $\alpha = 0$ and $\mu = -\beta\Omega/\sqrt{2}$ both hold true, so that all of the Eqs. (53)–(55) as well as Eqs. (62)–(64) are satisfied simultaneously.

Summarizing, we have the following observations about the structure of the theory. There are two different kinds of solutions for μ, α, and β when the parameters Ω and $\bar{\delta}$ are varied, characterized by the conditions $\mu = -\beta\Omega/\sqrt{2}$ and $\alpha = 0$. Only the former (latter) exists in the region of parameters Ω and $\bar{\delta}$ labeled $\alpha \neq 0$ ($\alpha = 0$) in Fig. 2. On the borderline between the regions both solutions exist and agree, so that they go continuously from one to the other as the variable $\bar{\delta}$ and/or Ω crosses the line. The solution is unique for all $\bar{\delta}$ and Ω under the assumptions $\Omega > 0$, $\alpha \geq 0$, and $\beta > 0$, which are a matter of convenience and can always be made. Finally, our numerical computations demonstrate that the unique solution always exists.

IV. FEATURES OF THE THEORY

The present boson theory has three parameters with the dimension of frequency, Ω, $\bar{\delta}$, and ϵ_F. In our discussions we regard Fermi energy, ϵ_F, as the scale of frequencies, although we always write it down explicitly. In present-day dilute quantum degenerate gases the representative value is $\epsilon_F \sim 2\pi \times 10$ kHz. In the classic Feshbach resonance experiments with bosons orders of magnitude of the coupling Rabi frequencies $\Omega \sim 10\epsilon_F$ are typical [37], but a narrower Feshbach resonance could change this comparison significantly. In photoassociation the ratio Ω/ϵ_F may be varied by varying the intensity (intensities) of the laser(s). In a Feshbach resonance the detuning $\bar{\delta}$ depends on the product of magnetic field and the difference of the magnetic dipole moments of the bound molecular state and of the free-atom state. Roughly, $\bar{\delta} \sim \epsilon_F$ corresponds to a 10 mG change in the magnetic field. In photoassociation the parameter $\bar{\delta}$ is directly a matter of tuning of the laser(s).

For comparison it is useful to recall a few basic facts about the usual one-channel theory for a BEC [20,48]. In such modeling there are no explicit molecules at all, but it is
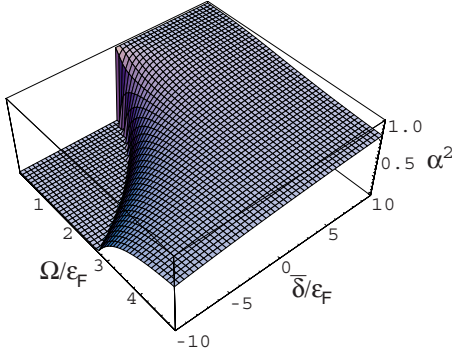
FIG. 3. (Color online) Fraction of atoms in the atomic BEC, α^2, as a function of the coupling strength, Ω, and detuning, $\bar{\delta}$.

assumed that the atoms interact among themselves as characterized by a scattering length a that may be tuned by varying the magnetic field around the Feshbach resonance, i.e., by varying the detuning. At positive detunings the scattering length is negative, which indicates an attractive interaction between the atoms and collapse of the (untrapped) condensate. At negative detunings, at least close to the resonance, the scattering length is positive and large. According to the theory of molecular structure, this means that there must be a weakly bound molecular state, which, however, is not included explicitly in the one-channel theory. By elementary thermodynamics, at low temperatures these molecules should make the thermal-equilibrium state. Positive (negative) detunings thus indicate the atom (molecule) side of the resonance.

A. Scaling with detuning and coupling strength

In Fig. 3 we plot the fraction of atoms in the atomic BEC, α^2, as a function of the coupling strength Ω and detuning $\bar{\delta}$. At $\Omega \ll \epsilon_F$, the system switches abruptly (compared to ϵ_F) from having all atoms to no atoms in the condensate when the detuning crosses the two-body resonance position $\bar{\delta}=0$. As the coupling Ω increases, the transition from $\alpha^2 \simeq 1$ to $\alpha^2 \ll 1$ rounds out. However, $\alpha^2=0$ is always reached on the line shown in Fig. 2. Given that on this line the solution of the system is not analytic, we predict a phase transition.

The analogous plot for the chemical potential μ as a function of coupling strength and detuning is given in Fig. 4. The function $\mu(\Omega, \bar{\delta})$ is also nonanalytic on the line shown in Fig. 2, but the kink is not visible in Fig. 4. The rounding-out with increasing coupling strength is again obvious.

We quantify the rounding-out starting with the numerical observation that in the regime $\alpha \neq 0$ the following limits hold true:

$$\alpha^2(\Omega, \bar{\delta}) = \begin{cases} f_\alpha^< \left[\dfrac{\bar{\delta}}{\Omega} \right], & \Omega \ll \epsilon_F; \\[4mm] f_\alpha^> \left[\left(\dfrac{\bar{\delta}}{\Omega} \right)^2 \right], & \Omega \gg \epsilon_F; \end{cases} \tag{65}$$
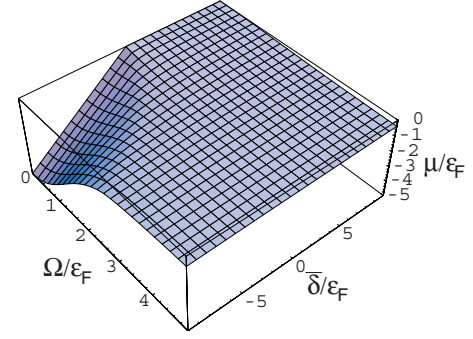

FIG. 4. (Color online) Chemical potential μ as a function of the coupling strength Ω and detuning $\bar{\delta}$.

$$\beta^2(\Omega, \bar{\delta}) = \begin{cases} f_\beta^< \left[\dfrac{\bar{\delta}}{\Omega} \right], & \Omega \ll \epsilon_F; \\[4mm] \left(\dfrac{\epsilon_F}{\Omega} \right)^2 f_\beta^> \left[\left(\dfrac{\bar{\delta}}{\Omega} \right)^2 \right], & \Omega \gg \epsilon_F. \end{cases} \tag{66}$$

Knowing these scalings it is easy to work out analytical expressions for the functions $f_\alpha^<$, etc., from Eqs. (62)–(64); simply put in the scalings and see what becomes of the equations in the corresponding limit of Ω. For instance, we have $f_\beta^>(x)=[y(x)]^2$, where y is a solution to the polynomial equation

$$8y^3 - 4\sqrt{2}x^2y^2 + 8xy - 2\sqrt{2} = 0 \tag{67}$$

for the fixed value of x. We have plotted the scaling functions in Fig. 5. They tend to the proper limits in both ends of the range of the variable x, and, as is appropriate for useful dimensionless scaling functions, their magnitudes and scales of variation with the argument x are both on the order of unity.

We next turn to the behavior of the chemical potential and the energy per particle, particularly in the region $\alpha=0$ in Fig. 2 with both $\bar{\delta}<0$ and $\mu<0$. To this end we first note the asymptotic expansions of the functions (50)–(52) for $m \to \infty$:
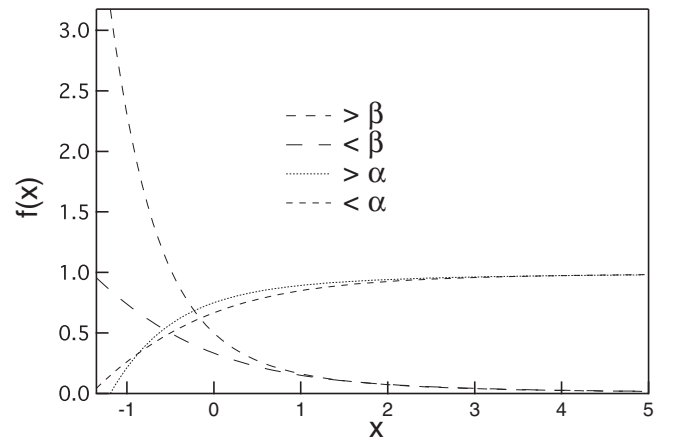

FIG. 5. Scaling functions $f_\beta^>(x)$, etc., in Eqs. (65) and (66). The legend identifies the combination of $<$ or $>$ and α or β for each curve.

$$A_{1/2}(m) \sim -\pi\sqrt{m} + \frac{\pi}{16}m^{-3/2} + O(m^{-7/2}), \qquad (68)$$

$$P_{1/2}(m) \sim \frac{\pi}{4\sqrt{m}} + \frac{3\pi}{128}m^{-5/2} + O(m^{-9/2}), \qquad (69)$$

$$P_{3/2}(m) \sim -\frac{3\pi}{4}\sqrt{m} + \frac{3\pi}{128}m^{-3/2} + O(m^{-7/2}). \qquad (70)$$

The coefficients were inferred from numerical results as given by MATHEMATICA's NIntegrate function. They are probably exact; the coefficients of the leading terms appear to be precise to at least 10^{-8}, and the coefficients of the next-to-leading terms to about 10^{-3}.

Now, inserting power series expansions of the form

$$-\mu = \frac{|\bar{\delta}|}{2} + M_{1/2}|\bar{\delta}|^{1/2} + M_0|\bar{\delta}|^0 + \cdots, \qquad (71)$$

$$\beta = 1 + B_{-1/2}|\bar{\delta}|^{-1/2} + B_{-1}|\bar{\delta}|^{-1} + \cdots \qquad (72)$$

into Eqs. (62)–(64) and expanding the result to a power series in $1/|\bar{\delta}|$ using Eqs. (68)–(70), we discover that we may determine the coefficients M and B in Eqs. (71) and (72) down to and including M_{-3} and B_{-4} in terms of the explicit coefficients in Eqs. (68)–(70). These, in turn, will give an expression for the energy per particle (49) in the form

$$e = -\frac{\bar{\delta}}{2} + E_{1/2}|\bar{\delta}|^{1/2} + E_0|\bar{\delta}|^0 + \cdots, \qquad (73)$$

also down to and including the order $|\bar{\delta}|^{-3}$.

We will not write down the expansions (71)–(73) in detail, but a few notes are relevant. The expansions of chemical potential and energy go with powers of the dimensionless number $z = \Omega^4/\epsilon_F^3|\bar{\delta}|$ down to and including the order $|\bar{\delta}|^{-1}$, and the expansion of condensate amplitude down to and including the order $|\bar{\delta}|^{-2}$, although in the expansions of μ and e the coefficients of $|\bar{\delta}|^{-1}$ happen to be zero, $M_{-1} = E_{-1} = 0$. However, since we have $\Omega \propto \rho^{1/2} = (N/V)^{1/2}$ and $\epsilon_F \propto \rho^{2/3} = (N/V)^{2/3}$, the parameter z does not depend on density, or particle number, or volume, at all. It is a single-molecule quantity. In fact, with the identification (A9), down to the order $|\bar{\delta}|^{-1}$ the expansions of μ and e coincide with the expansion of $\omega_b/2$, where ω_b is the bound-state energy of a single molecule as given in Eq. (A15) in the Appendix.

Many-body phenomena start at the order $|\bar{\delta}|^{-3/2}$, from which onwards other combinations of Ω and ϵ_F than z also emerge. For instance, asymptotically, $|\bar{\delta}| \to \infty$, the dependence of chemical potential and energy on detuning and density goes as $\propto \rho/|\bar{\delta}|^{3/2}$. The analogous mean-field theory for fermions [31] behaves in this respect in the same way.

The conventional scattering length for atoms behaves as $a \propto -\bar{\delta}^{-1}$ near the Feshbach resonance, and for fermions the scattering length of the molecules near the resonance should be 0.6 times the scattering length for the atoms [11]. This means that the density dependence of energy should emerge in the order $\bar{\delta}^{-1}$. The present mean-field theory does not conform with the standard expectations. Whether this is a contradiction or not, we cannot say. First, by their very nature the asymptotic expansions are valid far away from the resonance, not close where one expects the 0.6a for molecules made of fermions. Second, as a practical matter, the frequency Ω^4/ϵ_F^3 is typically quite large for a Feshbach resonance; we estimate $\sim 2\pi \times 10$ GHz for the usual Feshbach resonance in ^{85}Rb [51], and indeed THz scale values for the 834 G Feshbach resonance in fermionic ^{6}Li [31]. Our asymptotic expansions only become useful at extremely large detunings, when in practice some physics assumption of our theory such as the contact interaction or the neglect of the background scattering length has already become invalid. We do not expect the expansions (71)–(73) to be of much practical value, which is one reason why we have not listed the coefficients. We will return to their theoretically interesting properties below, though.

We next turn to the limit of strong coupling, $\Omega \to \infty$. Let us first fix $\bar{\delta} = 0$, so that the argument is within the regime $\alpha \neq 0$. We set $\bar{\delta} = 0$ in Eqs. (53)–(55), attempt a solution of the form

$$\alpha = A_0 + A_{-2}\Omega^{-2} + A_{-4}\Omega^{-4} + \cdots, \qquad (74)$$

$$-\mu = M_0 + M_{-2}\Omega^{-2} + M_{-4}\Omega^{-4} + \cdots, \qquad (75)$$

and find that it works; asymptotically, with $\Omega \to \infty$, we have $\mu = -\frac{1}{2}\epsilon_F$ and $\alpha^2 = 3/4$. From Eq. (56), the corresponding expression for energy per particle is $e = -\frac{1}{3}\epsilon_F$. As expected on the basis of unitarity [49,50], in the limit of very strong interactions the interaction strength vanishes from the result and the only energy scale that remains, ϵ_F, is set by the density of the gas.

Given that the line separating the $\alpha = 0$ and $\alpha \neq 0$ regions in Fig. 2 may, perhaps, be thought of as the position of the Feshbach resonance shifted by many-body effects, it is also instructive to find the asymptotic limits of chemical potential and energy as one moves along this line. To find them, we set $\alpha = 0$ in Eqs. (53)–(55) and put in the ansatz

$$-\bar{\delta} = D_2\Omega^2 + D_0\Omega^0 + D_{-2}\Omega^{-2} + \cdots, \qquad (76)$$

$$-\mu = M_0 + M_{-2}\Omega^{-2} + M_{-4}\Omega^{-4} + \cdots. \qquad (77)$$

Aside from reproducing the second of Eqs. (60), this analysis shows that in the limit of large interaction strength we have $\mu = -\sqrt[3]{2}\epsilon_F$. This, in turn, gives $e = -3\sqrt[3]{2}/5\epsilon_F$.

B. Thermodynamics

The atom-molecule BEC has some interesting thermodynamical properties, in particular a propensity for negative pressure. We now discuss these aspects.

It seems natural to identify the mean-field value of the energy $E = \hbar N e$ as the thermodynamic internal energy U of the system. Moreover, the system is at zero temperature, which indicates an entropy identically equal to zero. In the

sense of thermodynamics, the chemical potential should then equal

$$\mu_T = \left(\frac{\partial U}{\partial N}\right)_V. \tag{78}$$

There is a subtlety to this definition, in that N is the invariant atom number that combines both atoms and molecules, yet we have used it to find the chemical potential for atoms only. On the other hand, the condition for chemical equilibrium for atoms and molecules dictates that the thermodynamic chemical potentials for atoms and molecules satisfy $2\mu_{T,a} = \mu_{T,m}$. From this observation it is easy to deduce that the procedure (78) gives the correct chemical potential for the atoms. There are related issues elsewhere in our thermodynamics discussions that could be resolved similarly, but henceforth we will not bring them up.

We have talked of the quantity μ as the chemical potential, which is consistent with our thermodynamics identification $E \leftrightarrow U$ if

$$\mu = \left(\frac{\partial [Ne]}{\partial N}\right)_V. \tag{79}$$

As already noted repeatedly, both atom number and volume are ingredients in our theory because the parameters Ω and ϵ_F depend on the density; for instance,

$$\left(\frac{\partial \Omega}{\partial N}\right)_V = \frac{\Omega}{2N}, \quad \left(\frac{\partial \epsilon_F}{\partial N}\right)_V = \frac{2\epsilon_F}{3N}. \tag{80}$$

However, verifying Eq. (79) by simply taking the analytical N derivative of Eq. (49) appears cumbersome, since we should then take into account the implicit dependence on N of the quantities α and β, and even of μ itself. Instead, we have carried out the verification numerically, by calculating the derivative of e numerically using Eqs. (80), and found that Eq. (79) is indeed satisfied.

We have also found that the analytical asymptotic expansions (73) and (71) satisfy Eq. (79) to all orders, down to and including $|\bar{\delta}|^{-3}$, for which the expansion coefficients are explicitly known. This is a rather impressive confirmation of our originally numerical identification of the expansion coefficients in Eqs. (68)–(70).

Finally, there is the question of pressure. The thermodynamical expression for pressure in the present case with identically zero entropy is

$$p = -\left(\frac{\partial U}{\partial V}\right)_N = -\hbar N\left(\frac{\partial e}{\partial V}\right)_N; \tag{81}$$

but, given the identifications we have already made, the Gibbs-Duhem relation of thermodynamics reads

$$\hbar Ne = -pV + \hbar N\mu \tag{82}$$

or

$$\frac{p}{\hbar \rho} = \mu - e. \tag{83}$$

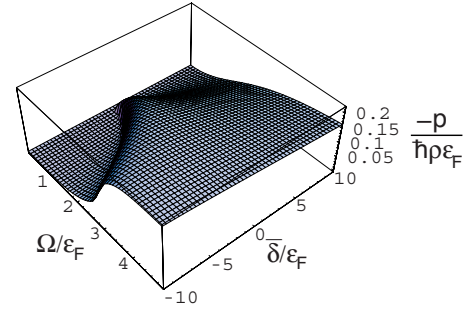We have calculated the pressure both ways numerically, too, and found that Eqs. (81) and (83) are consistent.

FIG. 6. (Color online) Pressure p of the atom-molecule BEC plotted as a function of the interaction strength Ω and detuning $\bar{\delta}$.

We have already noted that in the case $\bar{\delta}=0$ and $\Omega \to \infty$, the limits $\mu \to -\frac{1}{2}\epsilon_F$ and $e \to -\frac{1}{3}\epsilon_F$ hold true, which gives $p/(\hbar\rho) \to -\frac{1}{6}\epsilon_F$. The pressure becomes negative. In a way, this is as expected. Assuming that the transition line between the regions with $\alpha=0$ and $\alpha \neq 0$ denotes the true Feshbach resonance as shifted by the interactions in the system, this limiting case is on the atom side of the Feshbach resonance where, according to the standard one-channel model, the scattering length is negative and the BEC of the atoms is liable to collapse. This is also what one would expect for negative pressure.

The situation becomes more peculiar after a look at Fig. 6, which plots the negative of the pressure for a range of the parameters Ω and $\bar{\delta}$. Although the absolute value of the pressure drops sharply toward of the borderline between the regions with $\alpha=0$ and $\alpha \neq 0$ when entering from the $\alpha \neq 0$ side, as far as we can tell, the pressure remains negative for all values of Ω and $\bar{\delta}$. For instance, the expansions (73) and (71) give

$$\frac{p}{\hbar\rho} = -\frac{3\pi\Omega^4}{256\sqrt{2}\epsilon_F^{3/2}|\bar{\delta}|^{3/2}} + O(|\bar{\delta}|^{-2}). \tag{84}$$

For comparison, we have plotted in Fig. 7 the pressure of a two-component Fermi gas from Eq. (83) in complete analogy with Fig. 6. No negative pressure develops for a Fermi gas in the corresponding mean-field theory [31]. Moreover, there is no question about the experimental stability of the Fermi gas in the vicinity of the Feshbach resonance.

As it comes to the Bose gas, the negative pressure is a mixed blessing. It is an interesting prediction in its own right but complicates the observation of the other features we have discussed. We hope that additional atom-atom, atom-molecule, and molecule-molecule interactions not included in our model might stabilize the Bose gas sufficiently, especially on the $\alpha=0$ side, that the phase transition-like feature and the many-body shift of the Feshbach resonance could be seen under favorable circumstances.

V. CONCLUDING REMARKS

So far the molecular lifetimes have not allowed atom-molecule equilibration in a Bose gas near a Feshbach resonance, so that the kind of systems we have studied are pres-
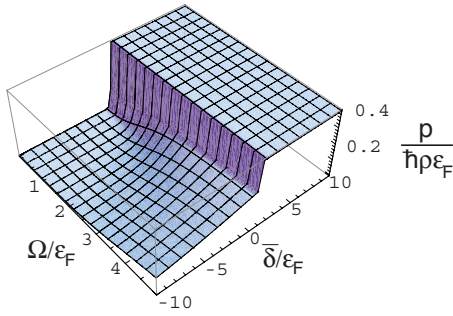
FIG. 7. (Color online) Pressure p of two-component Fermi gas plotted as a function of the interaction strength Ω and detuning $\bar{\delta}$. The definition of the interaction strength Ω is as in Ref. [31], but, for compatibility with the present paper, the detuning here is the detuning of Ref. [31] divided by two. For comparison, for an ideal Fermi gas at zero temperature, $p = \frac{2}{5}\hbar\rho\epsilon_F$.

ently not feasible experimentally. However, progress is continually made [52] in two-photon (two-color) photoassociation in a Raman scheme [6], and in heteronuclear systems direct one-photon photoassociation [53] from the dissociation continuum to a low-lying vibrational level is possible in principle. We are of the opinion that photoassociation to a stable molecular state will eventually be achieved in a BEC.

There is a semantic issue with the mean-field theory, in that, for instance, the review [20] regards our approach as going beyond the mean-field theory. Now, in a usual atomic BEC "mean-field theory" means Gross-Pitaevskii equation for the condensate [48]. The analogy in atom-molecule systems would, indeed, be an analysis in terms of atomic and molecular condensates only, with no noncondensate atoms or molecules. This was the case in the early two-mode models [17,19].

However, such an analysis ignores an inherent asymmetry in atom-molecule conversion. According to momentum conservation, in a Feshbach resonance in free space two zero-momentum condensate atoms may only combine into a zero-momentum condensate molecule, but in the reverse process the two atoms dissociated from a zero-momentum molecule may have arbitrary opposite momenta. Taking into account such "rogue"dissociation [37] was the original aim of our present modeling that accounts for correlated pairs of atoms. Initially we regarded this as an extension of mean-field theory, but after we discovered that the time independent version for fermions is a variation of the BCS theory, one of the quintessential mean-field theories, we refer to our approach simply as mean-field theory.

Mean-field theories, of course, are an interesting case in their own right. They are typically the first, and occasionally the last, tool in the analysis of a new phase transition, even though it is well-known that they cannot be expected to be quantitatively accurate. In fact, we cannot think of any instance in the area of quantum degenerate dilute gases in which a properly formulated mean-field theory has given a qualitatively wrong prediction, and only very recently has it become possible to distinguish between mean-field theory and a strongly correlated approach quantitatively in an experiment; cf. Refs. [15,16].

These observations cast an interesting light on our prediction of negative pressure even on the molecule side of the

Feshbach resonance, where the standard picture is that the scattering length should be large and positive. Granted, our calculations are missing the usual background scattering length and are cursory about the structure and collisions of the molecules. One may also argue that, as we have no time scale to offer for the associated instability, it may be unobservable even if it really existed. After all, at sub-Kelvin temperatures, at any pressure, the thermodynamic ground state of alkali metals is a solid not a gas, which has not precluded innumerable successful BEC experiments.

Nonetheless, the negative pressure may be viewed as an opportunity rather than a nuisance. It either exists, or is a qualitatively wrong prediction from a mean-field theory. Speculating further, since we do not have any time scale for the collapse associated with the negative pressure, we do not know that it is short either. It is a well-known empirical fact that in the neighborhood of a Feshbach resonance, on both sides of the resonance, atoms are lost from a BEC. Perhaps the negative pressure contributes to, or even dominates, the loss.

We close with a remark about a rather esoteric original motivation for this particular piece of work on bosons. Some time ago we noticed [54] in a simple model for two trapped ions that the statistics has no effect on the thermodynamic properties. Our interpretation was that the Coulomb interaction between the ions keeps them sufficiently far apart, so that they are effectively distinguishable and quantum statistics is moot. Calculations in which strongly interacting bosons crystallize [55] in a trap just like ions do then led us to the idea of "superuniversality": If strong interactions between the particles keep them apart, the state could not only not depend on the strength of the interactions, but could also be independent of atom statistics. Now, within the confines of mean-field theory, our results for bosons and fermions are quite different. Technically, superuniversality in mean-field theories is neither a necessary nor a sufficient condition for superuniversality in nature, but nonetheless, the notion of superuniversality did not pass this particular test.

APPENDIX: STEADY STATE

In this appendix we study the steady state of the two-atom model as a bound-continuum problem along the lines of the classic paper by Fano [45], with due consideration to renormalization of the ultraviolet divergence.

We imagine that there is initially a bound molecular state $|b\rangle$ and a continuum of states $|\epsilon\rangle$ labeled by frequency and normalized in such a way that $\langle\epsilon|\epsilon'\rangle = \delta(\epsilon - \epsilon')$, coupled by a photoassociative or Feshbach resonance coupling. We write the Hamiltonian as

$$\frac{H}{\hbar} = |b\rangle\delta\langle b| + \int d\epsilon |\epsilon\rangle\epsilon\langle\epsilon| + \int d\epsilon K(\epsilon)[|b\rangle\langle\epsilon| + |\epsilon\rangle\langle b|],$$

(A1)

with

$$K(\epsilon) = \sqrt[4]{\frac{4\kappa\epsilon}{\pi^2}}. \qquad (A2)$$

The relevant features in Eq. (A2) are the fourth root of frequency (energy) and the constant κ with the dimension of frequency; the rest of the constants are an attempt to simplify the appearance of a few results below. Similarly, the state vector is

$$|\psi\rangle = b(t)|b\rangle + \int d\epsilon a(\epsilon;t)|\epsilon\rangle. \qquad (A3)$$

The time dependent Schrödinger equation becomes

$$i\frac{\partial}{\partial t}b = \delta b + \int d\epsilon K(\epsilon)a(\epsilon), \qquad (A4)$$

$$i\frac{\partial}{\partial t}a(\epsilon) = \epsilon a(\epsilon) + K(\epsilon)b, \qquad (A5)$$

and the time independent Schrödinger equation for an eigenstate of the Hamiltonian with the eigenfrequency ω is

$$(\omega - \delta)b = \int d\epsilon K(\epsilon)a(\epsilon), \qquad (A6)$$

$$(\omega - \epsilon)a(\epsilon) = K(\epsilon)b. \qquad (A7)$$

The substitution

$$a(\epsilon) = -\frac{3\sqrt{\pi}\sqrt[4]{\epsilon}\Omega}{\sqrt{2}\sqrt[4]{\kappa}\epsilon_F^{3/2}}A\left(\frac{\epsilon}{2}\right) \qquad (A8)$$

converts Eqs. (A6) and (A7) to Eqs. (12) and (13). Moreover, let us solve Eqs. (A4) and (A5) in the pole approximation for a positive detuning δ, and likewise solve Eqs. (10) and (11) in the pole (Wigner-Weisskopf) approximation, then the ensuing decay rates for the molecules are equal if the parameters are related by

$$\kappa = \frac{9\pi^2\Omega^4}{512\epsilon_F^3}. \qquad (A9)$$

The present continuum problem (A1) simply solves the dilute-gas (single-molecule) limit of our mean-field theory, but with the advantage that the amplitudes b and $a(\epsilon)$ also have the normalization conditions that follow from the orthonormality conditions of the states $|b\rangle$ and $|\epsilon\rangle$ and the manifest Hermiticity of Eqs. (A4) and (A5). In the steady state the amplitudes b and $a(\epsilon)$, of course, depend on the eigenvalue ω, a dependence that we will write down below.

Now, the formal solution for $a(\epsilon)$ of Eq. (A7),

$$a(\epsilon, \omega) = \frac{K(\epsilon)b(\omega)}{\omega - \epsilon}, \qquad (A10)$$

contains a singularity at $\epsilon = \omega$ that renders the meaning of the right-hand side of Eq. (A6) ambiguous. The substitution $\omega \to \omega - i\eta$, with $\eta = 0+$, removes the ambiguity, but gives at most one stationary state. Following Fano [45], we therefore attempt a solution in the form

$$a(\epsilon, \omega) = \left[\mathcal{P}\frac{1}{\omega - \epsilon} + f(\omega)\delta(\epsilon - \omega)\right]K(\epsilon)b(\omega), \qquad (A11)$$

where $\mathcal{P}$ denotes the principal value integral and $\mathcal{P}f(\omega)$ is yet to be determined; $f(\omega) = i\pi$ would give the forward-in-time solutions we have discussed earlier. Inserting Eq. (A11) into Eq. (A6) gives

$$\omega - \delta = \theta(\omega)f(\omega)K^2(\omega) + \mathcal{P}\int d\epsilon\frac{K^2(\epsilon)}{\omega - \epsilon}, \qquad (A12)$$

with θ being the usual unit step function. The integral on the right-hand side has the same ultraviolet divergence as before, and the cure is exactly the same; we add the infinity $\int d\epsilon K^2(\epsilon)/\epsilon$ to both sides of the equation, which renormalizes the detuning and makes the principal value integral convergent,

$$\omega - \bar\delta = \theta(\omega)f(\omega)K^2(\omega) + \mathcal{P}\int d\epsilon\frac{K^2(\epsilon)\omega}{\epsilon(\omega - \epsilon)}. \qquad (A13)$$

1. Bound state

Suppose first that $\omega < 0$. Then the principal value integral is a usual integral, and we have the equation

$$\omega - \bar\delta = 2\sqrt{-\kappa\omega}. \qquad (A14)$$

It turns out that this equation has a real solution if and only if $\bar\delta < 0$, and the unique solution is then

$$\omega_b = \bar\delta - 2\kappa + 2\sqrt{\kappa^2 - \kappa\bar\delta}. \qquad (A15)$$

There is one, and only one, negative-energy solution if and only if the detuning is negative.

One might surmise that the negative-energy solution is bounded, i.e., normalizable to unity. In fact, using Eq. (A10), we find

$$\int d\epsilon|a(\epsilon, \omega_b)|^2 = \sqrt{\frac{\kappa}{-\omega_b}}|b(\omega_b)|^2, \qquad (A16)$$

so that the bound and continuum amplitudes in the wave function normalized to unity are

$$b(\omega_b) = \sqrt{\frac{\sqrt{-\omega_b}}{\sqrt{\kappa} + \sqrt{-\omega_b}}}, \qquad (A17)$$

$$a(\epsilon, \omega_b) = \frac{\sqrt[4]{\kappa\epsilon/\pi^2}}{\omega_b - \epsilon}b(\omega_b). \qquad (A18)$$

2. Continuum states

The system also has a bounty of positive-energy eigenstates. It turns out that for $\omega > 0$

$$\mathcal{P}\int d\epsilon\frac{K^2(\epsilon)\omega}{\epsilon(\omega - \epsilon)} = 0, \qquad (A19)$$

so that Eq. (A13) gives

$$f(\omega) = \frac{\omega - \bar{\delta}}{K^2(\omega)}. \tag{A20}$$

For positive energies we are obviously dealing with continuum states, so that we aim at the normalization

$$b^*(\omega)b(\omega') + \int d\epsilon\, a^*(\epsilon,\omega)a(\epsilon,\omega') = \delta(\omega - \omega'). \tag{A21}$$

Note that while for a unit-normalized bound state the coefficient $b(\omega_g)$ is dimensionless, here the dimension of $b(\omega)$ will be the inverse of the square root of frequency. The calculation based on Eq. (A11) is straightforward except for the ensuing product of principal value integrals, which may be handled as in [45];

$$\mathcal{P}\frac{1}{\omega - \epsilon}\mathcal{P}\frac{1}{\omega' - \epsilon} = \frac{1}{\omega' - \omega}\left(\mathcal{P}\frac{1}{\omega - \epsilon} - \mathcal{P}\frac{1}{\omega' - \epsilon}\right) + \pi^2\delta(\omega - \omega')\delta(\epsilon - \omega). \tag{A22}$$

The principal value integrals arising in this way give zero just as in Eq. (A19), so we have

$$|b(\omega)|^2\left[\pi^2 K^2(\omega) + \frac{(\omega - \bar{\delta})^2}{K^2(\omega)}\right] = 1. \tag{A23}$$

The continuum state vectors for $\omega > 0$ are therefore fully specified by

$$b(\omega) = \sqrt{\frac{2}{\pi}}\frac{\sqrt[4]{\kappa\omega}}{\sqrt{(\omega - \bar{\delta})^2 + 4\kappa\omega}};$$

$$a(\epsilon,\omega) = \left[\sqrt[4]{\frac{4\kappa\omega}{\pi^2}}\mathcal{P}\frac{1}{\omega - \epsilon} + (\omega - \bar{\delta})^2\sqrt[4]{\frac{\pi^2}{4\kappa\omega}}\delta(\epsilon - \omega)\right]b(\omega). \tag{A24}$$

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