Bound mode of an atom laser

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We use a Fano diagonalization technique to find the eigenmodes of an atom laser consisting of a single-mode atomic cavity that is coherently coupled to the continuum of free space modes. Under very general conditions the system exhibits a single, stationary bound mode. We discuss the properties of this bound mode depending on the system parameters and investigate its effect on the output beam of the atom laser.

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I. INTRODUCTION

Following the first experimental demonstrations of Bose-Einstein condensation in dilute atomic gases, the study of quantum degenerate bosonic systems has become a major subject in atomic physics. For recent experimental and theoretical overviews of the field of Bose-Einstein condensation see, for example, [1–3].

Attention has now shifted toward the investigation of possible applications. One of the most promising of these is the possibility of using a condensate as the source for an atom laser, a device producing a well collimated beam of coherent atoms with a large spectral density analogous to an optical laser. Both pulsed [4–6] and continuous [7,8] atom lasers have recently been demonstrated experimentally.

A large number of theoretical models for atom lasers have been proposed using various different mathematical frameworks such as Lindblad master equations [9–12] or nonlinear Gross-Pitaevskii equations [13–17]. In either case, the models hold only under certain operating conditions. As an example, it has been pointed out recently that for experimentally achievable parameters atom lasers exhibit non-Markovian dynamics [18–21], which limits the validity of most master equation models to the case of weak output coupling strength. The aim of this paper is to provide a better understanding of the effects that lead to this non-Markovian behavior by calculating the exact eigenmodes of the atom laser.

Our calculations are based on the simple model discussed by Savage and co-workers [22–24] which consists of a single mode of an atom cavity coherently coupled to the continuum of free space modes. The Hamiltonian of this system is given by

$$\hat{H}=k_0^2\hat{a}^\dagger\hat{a}+\int_{-\infty}^{\infty}k^2\hat{b}^\dagger(k)\hat{b}(k)dk+\int_{-\infty}^{\infty}V(k)[\hat{a}^\dagger\hat{b}(k)+\hat{b}^\dagger(k)\hat{a}]dk, \tag{1}$$

where $\hat{a}$ is the boson annihilation operator for the cavity mode, $\hat{b}(k)$ is the annihilation operator for the free mode with wave vector k, k_0 is the cavity wave vector, and $V(k)$ is the wave-vector-dependent coupling.

We diagonalize this Hamiltonian by using a Fano technique [25] and obtain a complete set of orthogonal atom laser eigenmodes characterized by creation and annihilation operators that satisfy the usual boson commutation relations. Our main finding is that under very general conditions this set of eigenmodes comprises a continuum of (positive energy) modes as well as a single bound mode (of negative energy) [21].

The paper is organized as follows. In Sec. II we outline the Fano diagonalization and give the main results and mathematical properties of the system eigenmodes, while the technical details are deferred to Appendix A. In Sec. III we discuss the dependence of the energy and occupation of the bound mode on the various system parameters such as cavity mode energy, coupling strength, and coupling width. The following sections deal with the effect that the existence of the bound mode has on the output spectrum of the atom laser, Sec. IV, and on the dynamics of the cavity state, Sec. V. Finally, we summarize the analytical formulas for some specific types of the coupling $V(k)$ in Appendix B.

II. FANO DIAGONALIZATION OF THE ATOM OUTPUT COUPLER

The first step of our discussion is to diagonalize the Hamiltonian (1) using a Fano technique [25]. For simplicity we will restrict the calculations here to a one-dimensional model and will only briefly outline the generalization to three dimensions afterward.

The first step in our diagonalization process is done solely for convenience of calculation. We begin by writing the Hamiltonian in terms of operators defined solely for positive k. It then takes the form

$$\hat{H}=k_0^2\hat{a}^\dagger\hat{a}+\int_0^{\infty}k^2[\hat{c}^\dagger(k)\hat{c}(k)+\hat{d}^\dagger(k)\hat{d}(k)]dk+\int_0^{\infty}\lambda(k)[\hat{a}^\dagger\hat{c}(k)+\hat{c}^\dagger(k)\hat{a}]dk, \tag{2}$$

where

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$$\hat{c}(k)=\frac{1}{\lambda(k)}[V(k)\hat{b}(k)+V(-k)\hat{b}(-k)], \tag{3}$$

$$\hat{d}(k)=\frac{1}{\lambda(k)}[-V(-k)\hat{b}(k)+V(k)\hat{b}(-k)], \tag{4}$$

and $\lambda^2(k)=V^2(k)+V^2(-k)$. The operators $\hat{d}(k)$ do not couple to the cavity, so any bosons in the cavity will not excite these modes. We therefore drop them from consideration in the rest of this paper, but it should be noted that the fact that these superpositions are unexcited will have an effect in interference experiments performed with the atom laser output.

Diagonalization in this case amounts to reexpressing the Hamiltonian in the form

$$\hat{H}=\int_0^\infty k^2\hat{A}^\dagger(k)\hat{A}(k)dk, \tag{5}$$

where $\hat{A}(k)$ is a diagonal operator which, when written in terms of the initial operators, is

$$\hat{A}(k)=\alpha(k)\hat{a}+\int_0^\infty \gamma(k,k')\hat{c}(k')dk'. \tag{6}$$

The functions $\alpha(k)$ and $\gamma(k,k')$ are determined by imposing the commutators

$$[\hat{A}(k),\hat{H}]=k^2\hat{A}(k), \tag{7}$$

$$[\hat{A}(k),\hat{A}^\dagger(k')]=\delta(k-k'). \tag{8}$$

The mathematical details of the process are confined to Appendix A, where the forms of $\alpha(k)$ and $\gamma(k,k')$ are given and where it is shown that such a diagonalization is complete only if the coupling satisfies

$$k_0^2\geqslant\int_0^\infty\frac{\lambda^2(k)}{k^2}dk. \tag{9}$$

This criterion is not satisfied by any coupling that has $\lambda^2(0)\neq 0$. This means that there exists a negative energy bound mode of the coupled system. The Hamiltonian therefore requires an extra term, and can be written

$$\hat{H}=\int_0^\infty k^2\hat{A}^\dagger(k)\hat{A}(k)dk-\mu^2\hat{A}_\mu^\dagger\hat{A}_\mu, \tag{10}$$

where $-\mu^2$ is the energy of the bound mode and $\hat{A}_\mu$ is its annihilation operator,

$$\hat{A}_\mu=\alpha_\mu\hat{a}+\int_0^\infty\gamma_\mu(k)\hat{c}(k)dk. \tag{11}$$

Again the coefficients α_μ and $\gamma_\mu(k)$ are given in Appendix A. We shall see in the next sections that it is the existence of this bound mode that gives rise to the non-Markovian coupling between the cavity and the external modes for the condensate output coupler. It also explains the unusual evolution of the cavity boson number previously found by others [20].

The existence of bound modes in coupled systems is not an unusual occurrence in physics. In quantum optics a single mode of a field coupled to a continuum with a lower energy bound gives rise to a dressed state with an energy below that of the continuum [26]. Also, in superconductivity a continuum of phonon states coupled to electron states leads to a bound mode of electron pairs at negative energy, the so-called Cooper pairs [27].

We should also note here that the existence of the bound mode may be affected by other factors such as geometry, gravity, and the atom-atom interaction within the condensate. In particular, the theory presented here is one dimensional. In three dimensions the density of atomic states will be proportional to k^2. This factor will appear in the numerator of Eq. (9), and so the existence or otherwise of the bound mode will depend upon the solid angle of the output coupling. For the ideal case of a unidirectional output beam, however, the mode exists and full account must be taken of it.

The inverse transformations between the original operators and the new diagonal and bound mode operators are

$$\hat{a}=\int_0^\infty\alpha(k)\hat{A}(k)dk+\alpha_\mu\hat{A}_\mu, \tag{12}$$

$$\hat{c}(k)=\int_0^\infty\gamma(k',k)\hat{A}(k')dk'+\gamma_\mu(k)\hat{A}_\mu. \tag{13}$$

Evaluation of the commutators of these operators amounts to a consistency check on the diagonalization process. We find that, as required,

$$[\hat{a},\hat{a}^\dagger]=\int_0^\infty\alpha^2(k)dk+\alpha_\mu^2=1, \tag{14}$$

$$[\hat{c}(k),\hat{c}^\dagger(k')]=\int_0^\infty\gamma(k'',k)\gamma^*(k'',k')dk''+\gamma_\mu(k)\gamma_\mu^*(k') =\delta(k-k'). \tag{15}$$

We will verify the first of these in Appendix A.

III. DISCUSSION OF THE BOUND MODE

In this section we will discuss some properties of the bound mode found as a consequence of the coupling of the cavity mode of the atom cavity with the free space modes, as discussed in the previous section. For the sake of simplicity, and also in order to allow graphical presentations, we will mainly focus on the specific example of a Gaussian coupling

$$\lambda^2(k)=\lambda_0^2e^{-\Gamma k^2}. \tag{16}$$

A physical motivation for this choice of coupling has been given by Moy, Hope, and Savage [20,24] for an atom laser based on a harmonic trap. In Appendix B we summarize the analytical results for the relevant quantities (bound mode energy, population) for this model. Note, however, that most of

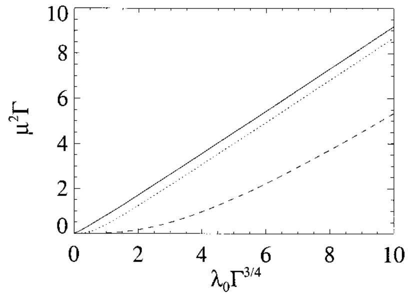

FIG. 1. Energy μ^2 of the bound mode versus coupling strength λ_0 for Gaussian coupling for $k_0^2\Gamma=0$ (solid line), $k_0^2\Gamma=1$ (dotted), $k_0^2\Gamma=10$ (dashed).

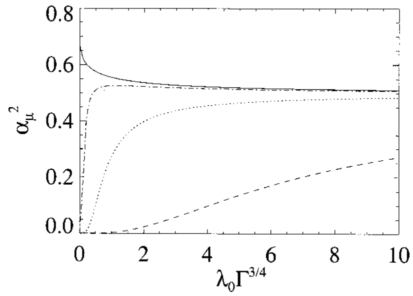

FIG. 2. Overlap α_μ^2 of the cavity mode with the bound mode for Gaussian coupling for $k_0^2\Gamma=0$ (solid line), $k_0^2\Gamma=0.1$ (dash-dotted), $k_0^2\Gamma=1$ (dotted), $k_0^2\Gamma=10$ (dashed).

our findings also hold for other forms of coupling or can be proven generally for arbitrary forms.

Let us first discuss the binding energy μ^2 of the bound mode as a function of the other system parameters, as depicted in Fig. 1. We found in the previous section that the bound mode always exists in the one-dimensional model even for arbitrarily small coupling strengths λ_0. However, in this limit ($\lambda_0 \to 0$) the energy of the bound mode tends to zero and the bound mode thus approaches the continuum of free modes. A small thermal excitation can then couple any atoms out of this mode. Additionally, as we will show later, the overlap between the bound and cavity modes tends to zero with λ_0. Thus the bound mode population also vanishes. From the defining equation (B2), in the limit $\lambda_0 \to 0$, we see that

$$\mu^2 \approx \left(\frac{\lambda_0^2 \pi}{2k_0^2}\right)^2 \tag{17}$$

for $\mu^2 \ll k_0^2, \Gamma^{-1}$, while

$$\mu^2 \approx \left(\frac{\lambda_0^2 \pi}{2}\right)^{2/3} \tag{18}$$

for $k_0=0$ and $\mu^2 \ll \Gamma^{-1}$.

With increasing coupling strength λ_0, the binding energy increases monotonically and in the limit where $\mu^2 \gg k_0^2, \Gamma^{-1}$ we find

$$\mu^2 \approx \lambda_0 \sqrt[4]{\pi/(4\Gamma)}. \tag{19}$$

This linear dependence on the coupling strength is in close analogy with cavity quantum electrodynamics, where the coupling of a two-level atom to a (single) mode of an optical cavity shifts the eigenstate energies by the coupling strength (Rabi frequency) Ω.

Finally, we note from Fig. 1 that the binding energy decreases with increasing cavity mode energy k_0^2. This can be understood from the fact that the Gaussian coupling chosen here connects the cavity mode more strongly to the low energy modes with $k \approx 0$, whereas energy conservation requires that an atom leaving a high energy cavity mode has a high kinetic energy outside the cavity. Increasing k_0^2 shifts the cavity out of resonance, thus decreasing the effective coupling strength and thereby the binding energy.

Next we turn to the overlap α_μ^2 of the cavity mode with the bound mode, the fraction of atoms found in the bound mode if initially only the cavity mode is populated. Figure 2 shows the dependence of this quantity on the coupling strength λ_0 for different values of the cavity mode energy k_0^2.

For very weak coupling where $\mu^2 \ll k_0^2, \Gamma^{-1}$ we find that

$$\alpha_\mu^2 \approx 2\left(\frac{\lambda_0^2 \pi}{2k_0^3}\right)^2, \tag{20}$$

and hence the bound mode population tends to zero with the coupling strength. This again is related to the difference in energy of the two modes for $k_0^2>0$. If, on the other hand, $k_0=0$, then the cavity mode and the bound mode energies approach each other as $\lambda_0 \to 0$ and the overlap is given by

$$\alpha_\mu^2 \approx \tfrac{2}{3}(1-\lambda_0^{2/3}\tfrac{2}{3}\sqrt{\Gamma/\pi}\sqrt[3]{\pi/2}. \tag{21}$$

Clearly in this case the limit of α_μ^2 as $\lambda_0 \to 0$ is 2/3.

In the limit of very strong coupling where $\mu^2 \gg k_0^2, \Gamma^{-1}$, or equivalently, by using Eq. (19), $\lambda_0\Gamma^{-1/4} \gg k_0^2, \Gamma^{-1}$, the overlap tends to 1/2. This is the same result as is found in near-threshold ionization [26].

Some of the above features occur for more general couplings. In particular, we always find the largest fraction of atoms in the bound mode for $k_0=0$, with the value 2/3 in the limit $\lambda_0 \to 0$.

IV. OUTPUT SPECTRUM

The spectrum of the cavity output is essentially given by the form of the function $\alpha^2(k)$, which is the contribution of the continuous eigenmodes of the Hamiltonian to the cavity mode *a*. In this section we investigate the behavior and physical consequences of the form of this function. In particular, we are interested in the way in which the existence of the bound mode effects the properties of the output beam. In Fig. 3 we plot the output spectrum $\alpha^2(k)$ for the model with Gaussian coupling for fixed cavity mode energy and Gaussian width with various different coupling strengths λ_0.

Let us first concentrate on the case of small coupling strength $\lambda_0\Gamma^{3/4} \ll 1$ (solid curve in the figure). Here we see

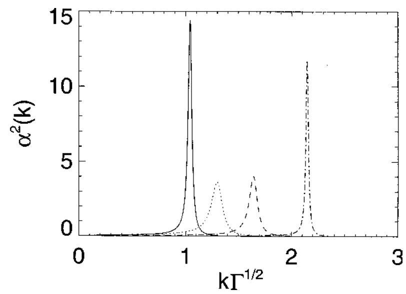

FIG. 3. Spectrum $\alpha^2(k)$ (units of $\Gamma^1/2$) against dimensionless wave number for $k_0^2\Gamma=1$ and $\lambda_0\Gamma^{3/4}=0.3$ (solid line), 1 (dotted), 2 (dashed), 4 (dash-dotted).

that the spectrum is centered around k_0 and symmetric. In fact, the analytic solution can be approximated by

$$\alpha^2(k)\approx\frac{\lambda^2(k_0)}{(k^2-k_0^2)^2+[\pi\lambda^2(k_0)/(2k_0)]^2}, \tag{22}$$

that is, the energy spectrum is a Lorentzian around k_0^2 with a width of $\pi\lambda^2(k_0)/(2k_0)$. This coincides with the limit in which the Born and Markov approximations are valid [20], and hence this width also determines the time scale of the exponential decay of the cavity mode.

For increasing coupling strength λ_0 we see that the center of the spectrum is shifted to higher momenta (and therefore higher energies). This is due to the increasing role of the function $F(k)$ in the general expression (A11) for $\alpha(k)$. Physically, this shift of the mean output energy can be understood in terms of energy conservation. Consider a system that initially has N atoms in the cavity mode a. The energy expectation value is then

$$\langle\hat{H}\rangle=Nk_0^2. \tag{23}$$

On the other hand, we have seen in the previous section that for increasing coupling strength both the bound mode energy and population increase simultaneously. This part of the Hamiltonian thus contains a *negative* amount of energy

$$-N\mu^2\alpha_\mu^2. \tag{24}$$

Hence the mean energy of the continuous (free) eigenmodes must be increased by this value. If the energy spectrum is approximately symmetric, we can then estimate the position of the spectral maximum to be

$$k_{max}^2=\langle k^2\rangle\approx\frac{k_0^2+\mu^2\alpha_\mu^2}{1-\alpha_\mu^2}, \tag{25}$$

which agrees well with the curves of Fig. 3.

The width of the spectrum is altered in accordance with this change in its central energy since we can now write

$$\alpha^2(k)\approx\frac{\lambda^2(k_{max})}{(k^2-k_{max}^2)^2+[\pi\lambda^2(k_{max})/(2k_{max})]^2}. \tag{26}$$

This explains why the width of the Lorentzian decreases (and the maximum increases) for larger values of λ_0, after the initial increase discussed above. Note, however, that an approximation of the spectrum by a Lorentzian is not always accurate. It depends upon the form of the coupling and hence the actual behavior of the function $F(k)$. As a final remark on Fig. 3 we should mention that the areas below the spectra are not the same for the different curves, since for the normalization we also have to take into account the contribution of the bound mode.

V. DYNAMICS OF THE CAVITY MODE

In this section we will discuss the time evolution of the atom number in the cavity if initially only the cavity mode is populated. This time evolution is easily obtained from our decomposition of the cavity mode into the eigenstates of the Hamiltonian,

$$\hat{a}(t)=\int_0^\infty\alpha(k)\hat{A}(k)e^{-ik^2t}dk+\alpha_\mu e^{i\mu^2t}\hat{A}_\mu. \tag{27}$$

If at time $t=0$ only the cavity mode is populated, we find that the fraction of atoms left in the cavity at any time t is given by

$$\frac{\langle\hat{a}^\dagger(t)\hat{a}(t)\rangle}{\langle\hat{a}^\dagger(0)\hat{a}(0)\rangle}=\left|\int_0^\infty\alpha^2(k)e^{-ik^2t}dk+\alpha_\mu^2e^{i\mu^2t}\right|^2. \tag{28}$$

It can be shown that for $t\to\infty$ the integral vanishes, and thus the fraction of atoms left in the cavity in the long time limit is given by α_μ^4. Note that α_μ^2 is the fraction of atoms in the bound mode $\hat{A}_\mu$, which itself comprises a fraction α_μ^2 of the cavity mode $\hat{a}$. The difference is accounted for by the nonzero overlap between the bound mode and the free modes. The fact that atoms remain inside the cavity forever is thus a consequence of the existence of the bound mode due to the coupling of the cavity mode to the continuum of free modes. Theoretical descriptions of the atom output coupler that neglect coherences between the cavity mode and the free modes artificially remove this bound mode and hence must fail whenever this mode is significantly populated.

In Fig. 4 we show the time evolution of the cavity population for different values of the coupling strength. For very weak coupling the time evolution becomes Markovian and hence we find an exponential decay. The decay rate of this is given by the width of the Lorentzian as discussed in the previous section. The steady-state population in the cavity is essentially zero in accordance with our results of Sec. III in the weak coupling limit.

For slightly larger coupling small oscillations are superimposed on this exponential decay. These oscillations arise from the beating of the two terms corresponding to the bound mode and the free modes in Eq. (28) and therefore are of the order of α_μ^2. For even stronger coupling the bound mode population increases and hence the amplitude of the oscillations grows. Simultaneously the oscillations become faster since the binding energy μ^2 and the mean energy k_{max}^2

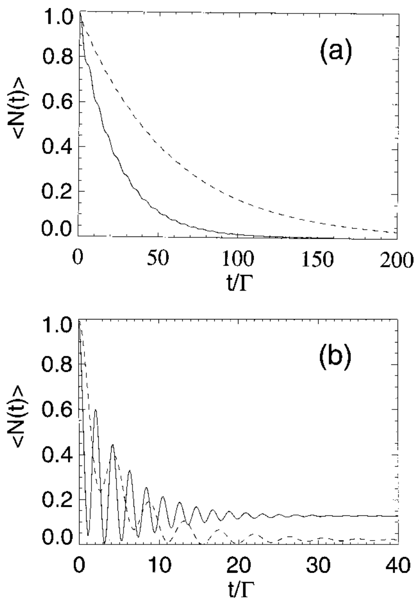

FIG. 4. Time evolution of the cavity mode population $\langle \hat{a}^{\dagger}(t)\hat{a}(t)\rangle$ (normalized to the initial number of atoms) for $k_0^2\Gamma = 1$. (a) Weak coupling $\lambda_0\Gamma^{3/4} = 0.125$ (dashed line) and 0.2 (solid). (b) Stronger coupling $\lambda_0\Gamma^{3/4} = 0.6$ (dashed) and 1.5 (solid).

of the output beam increase as discussed before. Energy conservation allows us to estimate the frequency of these oscillations,

$$\omega_{osc} \approx k_{max}^2 + \mu^2 \approx \frac{k_0^2 + \mu^2}{1 - \alpha_\mu^2}. \tag{29}$$

Finally, we see that the steady-state cavity population α_μ^4 increases with increasing coupling. In the limit of very large coupling the steady-state bound mode population tends to 1/4 of the initial population of the cavity mode.

Although we have dealt only with the time evolution of the atom number operator $\hat{a}^{\dagger}\hat{a}$ in this section, it is straightforward to generalize our results to any product of the cavity mode annihilation and creation operators. By using the normal-ordered characteristic function we have been able to show that at any time the state of the cavity mode is the attenuated version of the initial state with amplitude attenuated by the factor

$$L(t) = \int_0^\infty \alpha^2(k) e^{-ik^2 t} dk + \alpha_\mu^2 e^{i\mu^2 t}. \tag{30}$$

For example, if the cavity mode is initially in a coherent state with $\langle \hat{a}(0)\rangle = \beta$, then the state at time t satisfies $\langle \hat{a}(t)\rangle = L(t)\beta$. More generally, for any initial state,

$$\langle \hat{a}^{\dagger n}(t)\hat{a}^m(t)\rangle = L^{*n}(t)L^m(t)\langle \hat{a}^{\dagger n}(0)\hat{a}^m(0)\rangle. \tag{31}$$

VI. CONCLUSIONS

In this paper we have applied a Fano technique to diagonalize the Hamiltonian for the atomic output coupler proposed by Moy *et al.* [20]. This consists of a cavity mode of a particular wave vector (and hence energy), a set of external modes with a continuum of energies, and a coupling between the two. We have found a complete set of eigenmodes for the Hamiltonian. There are a set of positive energy free modes and a single negative energy bound mode. This bound mode, the binding energy of which increases with the coupling strength, gives rise to the dynamics described in this paper, none of which can be explained if the Born-Markov approximation is made. An illustration of this is given by the fact that the number of atoms in the cavity does not decay to zero. The overlap of the cavity mode and the bound mode is nonzero, so some fraction of atoms in the cavity must also be bound. There are also oscillations in the cavity atom number due to interference between the free modes and the bound mode.

In addition to the cavity dynamics we have also calculated the output spectrum. For low coupling strength it was found to be symmetric and centered on the cavity wave vector. For higher coupling strength the spectral maximum is shifted to higher energies to offset the increased binding energy of the bound mode. The oscillation frequency of the decaying cavity atom number is found to be approximately the sum of the spectral energy maximum and the binding energy of the bound mode.

There are two sources of influence to which atom lasers are subjected which do not exist for their optical counterparts: interparticle interactions and gravity. Both of these alter the atomic states. In particular, for some geometries, gravity may cause atoms to drop out of the bound mode after a short time [21]. Also, in more realistic three-dimensional analyses of the atom laser, the bound mode may not exist at all if the coupling strength is low compared with the cavity energy. For an ideal one-dimensional laser, however, the bound mode will always occur. In practice, the bound mode will have a finite lifetime. Its existence, however, will affect the output characteristics of the atom laser.

ACKNOWLEDGMENT

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APPENDIX A: DERIVATION OF THE DIAGONALIZED HAMILTONIAN

The Hamiltonian that we will diagonalize is written

$$\hat{H} = k_0^2 \hat{a}^{\dagger}\hat{a} + \int_0^\infty k^2 \hat{c}^{\dagger}(k)\hat{c}(k) dk + \int_0^\infty \lambda(k)[\hat{a}^{\dagger}\hat{c}(k) + \hat{c}^{\dagger}(k)\hat{a}] dk, \tag{A1}$$

with $\hat{c}$ and $\hat{d}$ given by Eqs. (3) and (4). Let

$$\hat{A}(k) = \alpha(k)\hat{a} + \int_0^\infty \gamma(k,k')\hat{c}(k') dk'. \tag{A2}$$

We impose the commutator

$$[\hat{A}(k),\hat{H}]=E(k)\hat{A}(k)=k_0^2\alpha(k)\hat{a}+\alpha(k)\int_0^\infty \lambda(k')\hat{c}(k')dk' + \int_0^\infty \gamma(k,k')k'^2\hat{c}(k')dk' + \int_0^\infty \gamma(k,k')\lambda(k')\hat{a}dk' = E(k)\alpha(k)\hat{a} + E(k)\int_0^\infty \gamma(k,k')\hat{c}(k')dk', \tag{A3}$$

where $E(k)$ is a function of k. If we take the commutator of this equation with $\hat{a}^\dagger$ and $\hat{c}^\dagger$ we obtain the following two equations:

$$k_0^2\alpha(k)+\int_0^\infty \gamma(k,k')\lambda(k')dk' = E(k)\alpha(k), \tag{A4}$$

$$\alpha(k)\lambda(k')+k'^2\gamma(k,k')=E(k)\gamma(k,k'). \tag{A5}$$

Equation (A5) gives γ in terms of α,

$$\gamma(k,k')=\alpha(k)\lambda(k')\mathrm{P}\left[\frac{1}{E(k)-k'^2}+z(k')\delta(E(k)-k'^2)\right], \tag{A6}$$

where P denotes the principal value and z is some function to be determined. Next substitute this into Eq. (A4) and cancel α,

$$k_0^2+\int_0^\infty \lambda^2(k')P\left[\frac{1}{E(k)-k'^2}+z(k')\delta(E(k)-k'^2)\right]dk' = E(k). \tag{A7}$$

If $E(k)>0$ (positive energy) this equation gives us the function $z(k)$. For negative energy the δ function contribution does not exist. These cases are treated separately below.

1. Positive energy

If $E(k)>0$ we put $E(k)=k^2$ and solve to find

$$z(k)=\frac{2k[k^2-k_0^2-F(k)]}{\lambda^2(k)}, \tag{A8}$$

where

$$F(k)=\mathrm{P}\int_0^\infty \frac{\lambda^2(k')dk'}{k^2-k'^2}. \tag{A9}$$

We now know γ in terms of α, so in order to find α we impose the commutator

$$[\hat{A}(k),\hat{A}^\dagger(k')]=\delta(k-k'). \tag{A10}$$

We use Eqs. (A2), (A6), (A8), and (A9) to find after some algebra that the commutator is satisfied if

$$\alpha(k)=\frac{2k\lambda(k)}{\sqrt{4k^2[k^2-k_0^2-F(k)]^2+\pi^2\lambda^4(k)}} = \frac{2k}{\lambda(k)\sqrt{z^2(k)+\pi^2}}. \tag{A11}$$

2. Negative energy

For $E(k)<0$ the δ function contribution to Eq. (A7) vanishes and the equation becomes

$$k_0^2-E(k)=\int_0^\infty \frac{\lambda^2(k')}{k'^2-E(k)}dk'. \tag{A12}$$

We put $E(k)=-\mu^2$, so the equation for μ is

$$k_0^2+\mu^2=\int_0^\infty \frac{\lambda^2(k)dk}{k^2+\mu^2}. \tag{A13}$$

If $\lambda^2(0)\neq 0$ the right hand side tends to infinity for $\mu\to 0$, and decreases monotonically as $\mu\to\infty$. Since the left-hand side is a monotonically increasing function of μ, this equation has exactly one solution for μ. We can now use Eq. (A6) to write γ_μ in terms of α_μ as

$$\gamma_\mu(k)=\frac{-\alpha_\mu\lambda(k)}{k^2+\mu^2}, \tag{A14}$$

and so from Eq. (A2)

$$\hat{A}_\mu=\alpha_\mu\left(\hat{a}-\int_0^\infty \frac{\lambda(k)\hat{c}(k)dk}{k^2+\mu^2}\right). \tag{A15}$$

As was the case for the positive energy solutions, we can find α_μ from this equation by imposing the unit commutator on $\hat{A}_\mu$, to obtain

$$\alpha_\mu=\left(1+\int_0^\infty \frac{\lambda^2(k)dk}{(k^2+\mu^2)^2}\right)^{-1/2}. \tag{A16}$$

If we now write our original operators in terms of the new operators,

$$\hat{a}=\int_0^\infty \alpha(k)\hat{A}(k)dk+\alpha_\mu\hat{A}_\mu, \tag{A17}$$

$$\hat{c}(k)=\int_0^\infty \gamma(k',k)\hat{A}(k')dk'+\gamma_\mu(k)\hat{A}_\mu, \tag{A18}$$

and substitute these into the original Hamiltonian it is relatively easy to verify that the expression obtained is that of Eq. (10).

3. Consistency check

The full diagonalization scheme including the negative energy mode is consistent only if it preserves the commutators. As a check on this we verify that the unit commutator for $\hat{a}$, the original annihilation operator of the cavity, is preserved,

$$[\hat{a},\hat{a}^{\dagger}]=\int_0^{\infty}\alpha^2(k)dk+\alpha_\mu^2=I+\alpha_\mu^2=1. \tag{A19}$$

Consider the integral I, extend the range of integration to $-\infty$, and decompose into partial fractions,

$$I=\frac{1}{2}\int_{-\infty}^{\infty}\frac{4k^2\lambda^2(k)dk}{4k^2[k^2-k_0^2-F(k)]^2+\pi^2\lambda^4(k)}$$
$$=\frac{1}{\pi i}\int_{-\infty}^{\infty}\left(\frac{k^2}{2k[k^2-k_0^2-F(k)]-i\pi\lambda^2(k)}-\frac{k^2}{2k[k^2-k_0^2-F(k)]+i\pi\lambda^2(k)}\right)dk. \tag{A20}$$

Since $\lambda^2(k)$ is an even function, $F(k)$ can be written

$$F(k)=\frac{1}{2}\mathrm{P}\int_{-\infty}^{\infty}\frac{\lambda^2(k')dk'}{k^2-k'^2}. \tag{A21}$$

Now consider the function $G(k)$ defined for *complex* k in the upper half plane (UHP) by

$$G(k)=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\lambda^2(k')dk'}{k^2-k'^2}=F(k)+\pi i\frac{\lambda^2(k)}{-2k}, \tag{A22}$$

so that $F(k)=G(k)+\pi i\lambda^2(k)/(2k)$. The integrand of I analytically continued into the UHP can then be written

$$\frac{1}{\pi i}\left(\frac{k^2}{2k[k^2-k_0^2-G(k)]-2\pi i\lambda^2(k)}-\frac{k}{2[k^2-k_0^2-G(k)]}\right). \tag{A23}$$

We will consider the second term. In order to find the poles we take the denominator and set it equal to zero. Put $k=x+iy$ with $y>0$ and take real and imaginary parts,

$$x^2-y^2-k_0^2=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\lambda^2(k)(x^2-y^2-k^2)dk}{(x^2-y^2-k^2)^2+4x^2y^2}, \tag{A24}$$

$$2xy=\frac{1}{2}\int_{-\infty}^{\infty}\frac{-2xy\lambda^2(k)dk}{(x^2-y^2-k^2)^2+4x^2y^2}. \tag{A25}$$

Equation (A25) has no solution for nonzero x and y, and so as $y>0$ the only solution has $x=0$. Then Eq. (A24) becomes

$$y^2+k_0^2=\frac{1}{2}\int_{-\infty}^{\infty}\frac{\lambda^2(k)dk}{y^2+k^2}. \tag{A26}$$

This is the same equation as that for μ [Eq. (A13)] and so $y=\mu$ is its solution. The second term in the integrand therefore has one pole at $k=i\mu$ and its residue is

$$\left(4+\frac{i}{\mu}\int_{-\infty}^{\infty}\frac{-2k\lambda^2(k')dk'}{(k^2-k'^2)^2}\Bigg|_{k=i\mu}\right)^{-1}$$
$$=\frac{1}{4}\left(1+\int_0^{\infty}\frac{\lambda^2(k)dk}{(k^2+\mu^2)^2}\right)^{-1}=\frac{1}{4}\alpha_\mu^2. \tag{A27}$$

Now we add to I the integral of Eq. (A23) around a semicircle of radius R. This term tends to zero as $R\to\infty$ so it does not affect I. Then a simple rearrangement of terms means that we can use Eq. (A27) to write

$$I=\frac{1}{2}(I+1-\alpha_\mu^2), \tag{A28}$$

so $I+\alpha_\mu^2=1$, the commutator (A19) is preserved, and the scheme is consistent.

APPENDIX B: RESULTS FOR SPECIFIC COUPLINGS

In this Appendix we list the analytic results for some specific examples of the coupling $\lambda(k)$.

1. Gaussian coupling

For a Gaussian coupling

$$\lambda^2(k)=\lambda_0^2e^{-\Gamma k^2} \tag{B1}$$

the energy $-\mu^2$ of the bound mode is given by the solution of the equation

$$k_0^2+\mu^2=\frac{\lambda_0^2\pi}{2\mu}\phi(\mu\sqrt{\Gamma}), \tag{B2}$$

where we have defined the function

$$\phi(x)=\exp(x^2)[1-\mathrm{erf}(x)], \tag{B3}$$

with $\mathrm{erf}(x)$ the usual error function. The overlap of the cavity mode with the bound mode is then given by

$$\alpha_\mu^2=\frac{2\mu^2}{2\mu^2+(1-2\mu^2\Gamma)(k_0^2+\mu^2)+\lambda_0^2\sqrt{\pi\Gamma}}. \tag{B4}$$

The function $F(k)$ used in Eqs. (A11) and (A21) can be evaluated in terms of Dawson's integral [28],

$$D(x)=\exp(-x^2)\int_0^x\exp(y^2)dy, \tag{B5}$$

as

$$F(k)=\frac{\lambda_0^2\sqrt{\pi}}{k}D(k\sqrt{\Gamma}). \tag{B6}$$

2. Lorentzian coupling

For Lorentzian coupling

$$\lambda^2(k)=\frac{\lambda_0^2}{k^2+b^2} \tag{B7}$$

the bound mode energy $-\mu^2$ is obtained as the solution of

$$(k_0^2+\mu^2)\mu(\mu+b)=\frac{\lambda_0^2\pi}{2b}. \tag{B8}$$

The population in the bound mode is

$$\alpha_\mu^2=\frac{1}{1+\lambda_0^2 I}, \tag{B9}$$

where

$$I=\frac{\pi(b+2\mu)}{4b\mu^3(b+\mu)^2} \tag{B10}$$

and the function $F(k)$, obtained from Eq. (21) by calculating the residues of $\lambda^2(k')/(k^2-k'^2)$ on and above the real axis, is found to be

$$F(k)=\frac{\lambda_0^2\pi}{2b(k^2+b^2)}. \tag{B11}$$

3. Broadband coupling

The results for broadband coupling

$$\lambda^2(k)=\lambda_0^2 \tag{B12}$$

can be obtained either by taking the limit of a very large width for the Gaussian or Lorentzian coupling or by direct evaluation of the general formulas. The defining equation for μ is

$$\mu(k_0^2+\mu^2)=\frac{\lambda_0^2\pi}{2}. \tag{B13}$$

The bound mode population is

$$\alpha_\mu^2=\frac{1}{1+\lambda_0^2\pi/(4\mu^3)}=\frac{2}{3+k_0^2/\mu^2}. \tag{B14}$$

Finally, we find that

$$F(k)=0. \tag{B15}$$

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