Research Article

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Dressed emitters as impurities

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Abstract: Dressed states forming when quantum emitters or atoms couple to a photonic bath underpin a number of phenomena and applications, in particular nonradiating effective interactions occurring within photonic bandgaps. Here, we present a compact formulation of the resolvent-based theory for calculating atom-photon dressed states built on the idea that the atom behaves as an effective impurity. This establishes an explicit connection with the standard impurity problem in condensed matter. Moreover, it allows us to formulate and settle – independently of the bath Hamiltonian – a number of properties previously known only for specific models or not entirely formalized. The framework is next extended to the case of more than one emitter, which is used to derive a general expression of dissipationless effective Hamiltonians explicitly featuring the overlap of single-emitter dressed bound states.

Keywords: photonic band-gap materials; quantum optics; waveguide-QED.

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1 Introduction

Quantum emitters ("atoms") coupled to structured and/or low-dimensional photonic environments are an important paradigm of quantum optics and nanophotonics. Important setups are photonic waveguides [1], a major focus of waveguide QED [2–4], and engineered photonic lattices implemented in various ways such as coupled cavities/resonators, photonic crystals or optical lattices [5–9]. Among others, a major appeal of such systems is the possibility of harnessing photon-mediated interactions between the emitters for implementing effective many-body Hamiltonians. Remarkably, for emitters energetically lying within photonic bandgaps, such effective second-order interactions can be dissipationless. These are usually explained in terms of mediating *dressed* bound states (BSs) [10–15]. In one such BSs, the atom is dressed by a photon exponentially localized in its vicinity. Overlapping single-emitter dressed BSs then result in an effective interatomic potential, somewhat similarly to the formation of molecules.

A quantum emitter coupled to a homogeneous photonic reservoir has interesting analogies with the textbook *impurity* problem in condensed matter [16]. For instance, the reflection and transmission coefficients of a photon scattering off an atom in a waveguide are formally the same as those for an impurity described by an effective, energy-dependent, scattering potential [17, 18]. Moreover, as first suggested in Ref. [10], the aforementioned in-gap atom-photon BSs are quite reminiscent of bound states induced by an impurity inside lattice bandgaps [16]. Recently, some of us identified a class of dressed states (dubbed "vacancy-like dressed states") whose photonic wavefunction is just the same that would arise if the atom were replaced by a vacancy (i.e. an impurity described by a point-like potential of infinite strength) [15]. These states play a central role

in topological quantum optics [19–21] and, additionally, encompass a type of dressed bound states in the continuum (BIC) that are currently investigated in waveguide QED [22–29].

A natural question is to what extent the emitter-impurity analogy holds, in particular whether it can be formalized in a framework independent of the bath Hamiltonian and applied to the calculation of both bound and unbound dressed states (the latter ones rule photon scattering processes). Mostly motivated by this question, this work introduces a novel formulation of the non-perturbative resolvent-based framework for studying atom-photon dressed states [30–32]. We show that the resolvent operator (or Green function) can be expressed in a compact form structurally analogous to that arising in the standard impurity problem. This condenses the effect of atom-photon coupling in a single rank-one projector, thus allowing for a unified treatment of several kinds of dressed states (either bound and unbound). The framework is then extended to the case that more than one emitter is present and used to derive a general expression of dissipationless effective Hamiltonians (mentioned above), which explicitly connects the interatomic potential to overlapping single-atom dressed states independently of the specific photonic bath.

2 Model and Hamiltonian

We consider a two-level quantum emitter ("atom") coupled under the usual rotating-wave approximation to an unspecified photonic bath which is effectively modelled as a discrete set of N coupled cavities (see sketch in Figure 1). The Hamiltonian reads (we set $\hbar = 1$ throughout the paper)

$$H = H_0 + V \tag{1}$$

with $H_0 = H_e + H_B$ (unperturbed Hamiltonian), where

$$H_e = \omega_0 \sigma_+ \sigma_-, \tag{2}$$

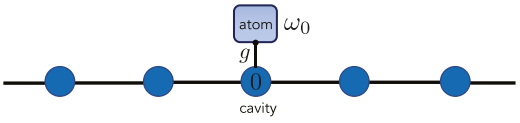

Figure 1: Schematic sketch of the considered model: a two-level quantum emitter (atom) coupled with strength g to a photonic bath B (field) modelled as a set of coupled cavities. The coupling is local in that the atom is directly coupled to only one cavity (labelled with 0). Here, B is represented as a simple one-dimensional lattice (although our framework applies to a generic bath).

$$H_B = \sum_{x=1}^{N} \omega_x b_x^\dagger b_x + \sum_{x \neq x'} J_{xx'} b_x^\dagger b_{x'}, \tag{3}$$

$$V = g\,(b_0^\dagger \sigma_- + b_0 \sigma_+) \tag{4}$$

with $\sigma_- = \sigma_+^\dagger = |g\rangle\langle e|$ and b_x the annihilation operators of the cavities fulfilling usual bosonic commutation rules ($|g\rangle$ and $|e\rangle$ are the atom's ground and excited states, respectively, and ω_0 their energy separation). Here, $x = 0$ (in the following sometimes referred to as the "position" of the atom) labels the cavity directly coupled to the atom. Finally, ω_x is the bare frequency of cavity x, while $J_{x'x} = J_{xx'}^*$ denote the cavity–cavity hopping rates.

In all the remainder, we will be concerned solely with the single-excitation subspace spanned by $\{|e\rangle|\mathrm{vac}\rangle, \{|g\rangle|x\rangle\}\}$ with $|\mathrm{vac}\rangle$ the field's vacuum state and $|x\rangle = b_x^\dagger|\mathrm{vac}\rangle$ single-photon states. We conveniently introduce a light notation such that $|e\rangle|\mathrm{vac}\rangle \to |e\rangle$, $|g\rangle|x\rangle \to |x\rangle$, that is $|e\rangle$ ($|x\rangle$) is the state with one excitation on the atom (xth cavity). Accordingly, in the single-excitation sector the Hamiltonian terms (2)–(4) take the effective forms

$$H_e = \omega_0\,|e\rangle\langle e|\,, \tag{5}$$

$$H_B = \sum_{x=1}^{N} \omega_x\,|x\rangle\langle x| + \sum_{x \neq x'} J_{xx'}\,|x\rangle\langle x'|\,, \tag{6}$$

$$V = g\,(|0\rangle\langle e| + |e\rangle\langle 0|)\,. \tag{7}$$

The essential problem we are interested in is working out all the stationary states of the total Hamiltonian, i.e. all single-photon dressed states.

Before concluding this section, we mention that the model defined by Eqs. (5)–(7) is a special case of the so called Friedrichs–Lee model investigated in the Mathematical Physics literature (see e.g. Refs. [33, 34]). In particular, the local coupling we assume [cf. Eq. (7)] constraints the shape of the function that measures the coupling strength between the emitter and each normal mode of H_B.

3 Resolvent

The resolvent method [16] is a powerful non-perturbative approach to compute eigenstates and eigenvalues of a Hamiltonian H, which is routinely used in many fields including quantum optics (see e.g. Refs. [30–32, 35]). A few basics of the approach are briefly recalled next.

The resolvent operator or Green function is defined as

$$G(z) = \frac{1}{z - H} = \sum_n \frac{1}{z - \omega_n}\,|n\rangle\langle n| + \int dk\, \mathcal{D}(k)\, \frac{1}{z - \omega(k)}\,|k\rangle\langle k|\,, \tag{8}$$

where $z = \omega + i\omega'$ (with ω, ω' real) runs over the entire complex plane. Here, $\{|n\rangle\}$ are the bound eigenstates of H with corresponding discrete energies $\{\omega_n\}$, while $\{|k\rangle\}$ is the continuum of all unbound eigenstates with energy $\omega(k)$ [index k is in general a multi-dimensional variable and $\mathcal{D}(k)$ the associated density of states[1]]. Energies and eigenstates of H can be inferred from the non-analyticity points of $G(z)$ on the real axis. Specifically, the stationary *bound* states (BSs) $\{|n\rangle\}$ are the residues of $G(z)$ around real poles $z = \omega_n$. Instead, unbound eigenstates $\{|k\rangle\}$ are associated with branch cuts of $G(z)$ on the real axis, each cut generally corresponding to an energy band of H [at each point $z = \omega(k)$ on a branch cut, $G(E(k) + i\omega')$ jumps at $\omega' = 0$].

Usually, the Hamiltonian is the sum of an unperturbed Hamiltonian H_0 and a perturbation V, $H = H_0 + V$. In this case, if $\{|\varphi_k\rangle\}$ are the unbound eigenstates of H_0 each with energy ω_k and provided that the perturbation is compact [36], the unbound eigenstates of H have the same spectrum and are worked out from these through the Lippmann–Schwinger equation as

$$|\Phi_k\rangle = |\varphi_k\rangle + G(\omega_k^+)V|\varphi_k\rangle, \tag{9}$$

where we introduced the compact notation $h(\omega^+) = \lim_{\delta\to 0^+} h(\omega + i\delta)$. These thus fulfil $H|\Phi_k\rangle = \omega_k|\Phi_k\rangle$.

For our model in Eq. (1), the bare atomic and field resolvents (in the thermodynamic limit $N \gg 1$) are respectively given by

$$G_e(z) = \frac{1}{z - H_e} = \frac{|e\rangle\langle e|}{z - \omega_0}, \tag{10}$$

$$G_B(z) = \frac{1}{z - H_B} = \int dk\, \mathcal{D}(k)\, \frac{|k\rangle\langle k|}{z - \omega_k}. \tag{11}$$

Here, we assumed that $G_B(z)$ *has no poles*, i.e. H_B has no bound eigenstates (as it is typically the case when H_B describes a photonic lattice or waveguide). Accordingly, the only eigenstates of H_B are the continuum of single-photon states $\{|k\rangle\}$, associated with the field normal modes, such that $H_B|k\rangle = \omega_k|k\rangle$ with ω_k the corresponding normal frequency.

In order to simplify the notation, in the remainder we will follow a frequent convention (see e.g. Ref. [37]) and formally write $G_B(z)$ as a discrete sum

$$G_B(z) = \sum_k \frac{|k\rangle\langle k|}{z - \omega_k}. \tag{12}$$

with the understanding that the thermodynamic limit $N \gg 1$ must be eventually carried out.

3.1 Resolvent in the impurity problem: review

A longstanding topic in condensed matter and beyond is studying the effect of introducing an impurity into a lattice (although what follows does not require B to be a lattice). The impurity is usually modelled as a contact potential of the form [16].

$$V_{\text{imp}} = \epsilon\, |0\rangle\langle 0|, \tag{13}$$

where ϵ is the potential strength and $x = 0$ the impurity position. When contextualized to our coupled-cavity lattice [cf. Eq. (3)], the impurity corresponds to an effective detuning of cavity $x = 0$ [see Figure 2], which changes the field Hamiltonian as $H_B \to H_B + V_{\text{imp}}$. Correspondingly, the field's resolvent $G_B(z)$ [cf. Eq. (12)] turns into $G(z) = (z - H_B - V_{\text{imp}})^{-1}$. This can be worked out as [16]

$$G(z) = G_B(z) + \frac{1}{f(z)}\, |\psi(z)\rangle\rangle\langle\langle\psi(z)|, \tag{14}$$

with

$$|\psi(z)\rangle\rangle = G_B(z)\,|0\rangle, \tag{15}$$

$$f(z) = \frac{1}{\epsilon} - \langle 0|G_B(z)|0\rangle. \tag{16}$$

Eq. (14) states that the entire effect of the impurity is condensed in the rank-one projector featuring the z-dependent (unnormalized) state $|\psi(z)\rangle\rangle$.

3.2 Resolvent of the atom-field system

Let us come back to our atom-field system and address now the total resolvent $G(z)$ corresponding to the total Hamiltonian H [see Eq. (1)], i.e. when the atom-field coupling V is included. As the atom can be seen as a sort of impurity although with internal degrees of freedom ("quantum impurity" [38]), it is tempting to ask whether the total resolvent $G(z) = 1/(z - H)$ with H given by Eq. (1) can be expressed in a form structurally analogous to Eq. (14). This

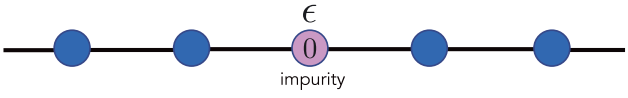

Figure 2: Impurity problem. A local static potential is added to the photonic bath, which is equivalent to a detuning ϵ changing the frequency of cavity 0 as $\omega_{x=0} \to \omega_{x=0} + \epsilon$.

1 In the case of many bands, a discrete band index is also needed. In these cases, the integral over k should be intended as implicitly including a sum over the band index.

is indeed possible, which can be shown through a transfer matrix method (see Supp. Mater.). The result is[2]

$$G(z) = G_B(z) + \frac{1}{F(z)} \left|\Psi(z)\right\rangle \left\langle\Psi(z)\right|, \tag{17}$$

where in place of Eq. (15) and (16), we now have

$$\left|\Psi(z)\right\rangle = \frac{1}{g} \left|e\right\rangle + \left|\psi(z)\right\rangle, \tag{18}$$

$$F(z) = \frac{1}{\epsilon(z)} - \langle 0|G_B(z)|0\rangle, \tag{19}$$

with

$$\epsilon(z) = \frac{g^2}{z - \omega_0}. \tag{20}$$

Thus the fictitious impurity potential (20) is z-dependent and scales as $(z-\omega_0)^{-1}$. Interestingly, Eq. (18) shows that $\left|\Psi(z)\right\rangle$ can be seen as resulting from the hybridization of $\left|\psi(z)\right\rangle$, which is just the same as Eq. (15), with the atom. It is also worth observing that for $g = 0$ the projector term in Eq. (17) correctly reduces to the bare atomic resolvent $G_e(z)$ [cf. Eq. (10)].

Projecting the resolvent (see Eq. (17)) on the excitonic subspace, i.e. on the state $|e\rangle$ (atom excited and field in vacuum), results in

$$\mathcal{P}_e G(z) \mathcal{P}_e = \frac{|e\rangle\langle e|}{z - \omega_0 - \Sigma(z)} \tag{21}$$

with the projector $\mathcal{P}_e$ defined as $\mathcal{P}_e = |e\rangle\langle e|$. Here,

$$\Sigma(z) = g^2 \langle 0|G_B(z)|0\rangle \tag{22}$$

is the so called "self-energy" [30]. By comparing Eq. (21) with Eq. (10), we retrieve the familiar picture [31, 32] according to which – from the atom's viewpoint – the effect of the interaction is to correct the atom's frequency ω_0 with a z-dependent, generally complex, energy shift $\Sigma(z)$.

Taking advantage of Eq. (17), we can also straightforwardly project $G(z)$ on the field via the projector $\mathcal{P}_B = \sum_x |x\rangle\langle x|$. Based on Eq. (18), we see that this is equivalent to replacing $\left|\Psi(z)\right\rangle$ with $\left|\psi(z)\right\rangle$ in Eq. (17)

$$\mathcal{P}_B G(z) \mathcal{P}_B = G_B(z) + \frac{1}{F(z)} \left|\psi(z)\right\rangle \left\langle\psi(z)\right|. \tag{23}$$

Comparing with (14), this shows that the field effectively behaves as if the atom were replaced by a fictitious impurity but with a z-dependent potential $\epsilon(z)$ [cf. Eqs. (13), (15) and (19)]. This fact was already noted in Ref. [17] but for a specific dynamics and model. In contrast, Eq. (23) shows that it is a general property, irrespective of the field Hamiltonian and interaction strength (so long as the rotating wave approximation holds). In a semantic analogy with the atom's self-energy, we will refer to $\epsilon(z)$ as the "self-potential".

Thus, to sum up, while the atom acquires an effective self-energy $\Sigma(z)$, the field is subject to an impurity self-potential with strength $\epsilon(z)$.

4 Dressed states

In line with the previous section, we will first quickly review the scheme for calculating bound and unbound eigenstates in the standard impurity problem and next consider dressed states in our atom-field system.

4.1 Stationary states in the impurity problem

Applying the resolvent method (see first part of Section 2) to the impurity problem, the energy $\omega_{\rm BS}$ of a stationary BS (if any) is a real pole of the resolvent (see Eq. (14)). Hence, it is a real solution of the pole equation [16]

$$f(\omega) = 0, \tag{24}$$

i.e. $\frac{1}{\epsilon} = \langle 0|G_B(\omega)|0\rangle$ (recall that we assume throughout that $G_B(z)$ has no poles). The associated stationary BS (density matrix form) is then just the residue of the resolvent Eq. (14) at $z = \omega_{\rm BS}$. The corresponding (unnormalized) BS ket is given by $\left|\psi(z=\omega_{\rm BS})\right\rangle$. Upon normalization, we get $\mathcal{N}\left|\psi(\omega_{\rm BS})\right\rangle$ with the normalization factor given by $\mathcal{N} = (\langle 0|\, G_B^2(\omega_{\rm BS})\, |0\rangle)^{-1/2}$.

The unbound eigenstates $\{\left|\psi_k\right\rangle\}$ are instead obtained in terms of the unbound eigenstates $\{|k\rangle\}$ of H_B [cf. Eq. (12)] through the Lippmann–Schwinger Eq. (9). This generally yields (see Supp. Mater. for details)

$$\left|\psi_k\right\rangle = \begin{cases} |k\rangle + \dfrac{\langle 0|k\rangle}{f(\omega_k^+)} \left|\psi(z=\omega_k^+)\right\rangle & \text{if } f(\omega_k) \neq 0 \\ |k\rangle & \text{if } f(\omega_k) = 0 \end{cases} \tag{25}$$

with $(H_0 + V_{\rm imp})\left|\psi_k\right\rangle = \omega_k \left|\psi_k\right\rangle$.

We note that the latter case, namely ω_k such that $f(\omega_k) = 0$, occurs when there exists a solution of Eq. (24) *within* a continuous band of H_B (that is when, using the previous notation, $\omega_{\rm BS} \equiv \omega_k$ for some ω_k). The corresponding eigenstate is then a BIC. Eq. (25) shows that all the unbound eigenstates of H_B at this specific energy remain stationary states also in the presence of the impurity (thus in such a case $\omega_{\rm BS}$ will be at least twofold degenerate).

2 In Ref. [39] an expression of $G(z)$ equivalent to (14) was presented, which is yet relatively involved and as such its physical interpretation not straightforward.

This highlights the role of states $|\psi(z)\rangle$ featured in the rank-one-projector term in the resolvent [cf. Eq. (14)], showing their close connection with stationary states. Indeed, the above can be summarized as follows: if there exists a real solution $\omega_{\rm BS}$ of Eq. (24) then $|\psi(z=\omega_{\rm BS})\rangle$ (once normalized) is already a stationary state. This yields all the BSs. To obtain an unbound eigenstate state at energy ω_k, we distinguish two cases: (i) ω_k does not fulfil Eq. (24), (ii) $\omega_k = \omega_{\rm BS}$ with $\omega_{\rm BS}$ a solution of Eq. (24). In case (i), the stationary state results from the superposition of $|\psi(z=\omega_k^+)\rangle$, once weighted by $\langle 0|k\rangle/f(\omega_k^+)$, with the unperturbed unbound state $|k\rangle$. In case (ii), the eigenstate simply coincides with the unperturbed state $|k\rangle$.

4.2 Stationary states of the atom-field system

Much like in the standard impurity problem, where the BSs correspond to the real solutions of $f(\omega)=0$, the BSs of the atom-field total Hamiltonian Eq. (1) are obtained from the real solutions of $F(\omega)=0$ [recall Eqs. (14) and (17)]. This is equivalent [cf. Eq. (19)] to the usual pole equation used in quantum optics in structured reservoirs [31, 32]

$$\omega = \omega_0 + g^2\langle 0|G_B(\omega)|0\rangle. \tag{26}$$

Note that this equation (hence its solutions) differs from the impurity-problem analogue (see Eq. (24)) ultimately due to the z-dependence of the impurity self-potential (see Eq. (20)).

In formal analogy with the impurity problem, if $\omega_{\rm BS}$ is now a real solution of Eq. (26), then the corresponding dressed BS is just $\propto |\Psi(z=\omega_{\rm BS})\rangle$ [cf. Eq. (18)]. Upon normalization, the dressed BS can be arranged as

$$|\Psi_{\rm BS}\rangle = \mathcal{N}\left(|e\rangle + g\,|\psi\left(\omega_{\rm BS}\right)\rangle\right) \tag{27}$$

where we recall that $|\psi(z)\rangle = G_B(z)\,|0\rangle$ [cf. Eq. (15)] and with the normalization factor given by

$$\mathcal{N} = \left(1 + g^2\,\langle 0|\,G_B^2(\omega_{\rm BS})\,|0\rangle\right)^{-\frac{1}{2}}. \tag{28}$$

Again in formal analogy with the impurity problem [see Eqs. (25)], unbound dressed states are found from the unperturbed unbound states $\{|k\rangle\}$ as (see Supp. Mater.)

$$|\Psi_k\rangle = \begin{cases} |k\rangle + \dfrac{\langle 0|k\rangle}{F(\omega_k^+)}\,|\Psi(z=\omega_k^+)\rangle & \text{if } F(\omega_k)\neq 0 \\ |k\rangle & \text{if } F(\omega_k)=0 \end{cases}. \tag{29}$$

To conclude this section, note that, like its impurity analogue (see end of Section 3.1), the state $|\Psi(z)\rangle$ in Eq. (17) is strictly connected with stationary states. A dressed BS (if any) is given by $|\Psi(z=\omega_{\rm BS})\rangle$ (to be normalized) with $\omega_{\rm BS}$ being a real solution of $F(\omega)=0$ [i.e. of Eq. (26)]. An unbound dressed state at energy ω_k not fulfilling Eq. (26) instead results from the superposition of $|\Psi(z=\omega_k^+)\rangle$, once weighted by $\langle 0|k\rangle/F(\omega_k^+)$, with the unperturbed unbound state $|k\rangle$. If instead $\omega_k=\omega_{\rm BS}$, i.e. ω_k is a solution of Eq. (26), the corresponding unperturbed $|k\rangle$ is a stationary state even in the presence of the atom which adds to the dressed BS $\propto |\Psi(z=\omega_{\rm BS})\rangle$.[3] Note that the last property immediately entails the known impossibility to populate dressed BICs via single-photon scattering [27]: a photon at frequency ω_0 sent from far away will just not see the atom.

4.3 Vacancy-like dressed states

An important special case occurs when there exists a dressed BS having the same energy as the atom, i.e. $\omega=\omega_0$. If this is a BS then (as previously discussed) $F(\omega_0)=0$, entailing

$$\langle 0|G_B(\omega_0)|0\rangle = 0 \tag{30}$$

[cf. Eqs. (19) or (26)]. This means that the photonic component $|\psi(\omega_0)\rangle$ is just the all-photonic BS that would occur (at the same energy ω_0) if the atom-photon interaction V were replaced by $V_{\rm imp}$ with $\epsilon\to\infty$, i.e. a vacancy on the cavity $x=0$ [recall Eqs. (13), (15) and (16)]. Also, Eq. (30) states that $|\psi(\omega_0)\rangle = G_B(\omega_0)\,|0\rangle$ has a node at $x=0$ (as it must be due to the infinite potential strength). If instead the dressed state at energy ω_0 is unbound, then ω_0 lies within some band and $F(\omega_0)\neq 0$. Using Eq. (29), it can be expressed as

$$|\Psi_{k_0}\rangle = |k_0\rangle - \frac{\langle 0|k_0\rangle}{\langle 0|G_B(\omega_0)|0\rangle}\,|\Psi(\omega_0)\rangle, \tag{31}$$

where k_0 is defined such that $\omega_{k_0}=\omega_0$. Projecting both sides on $|0\rangle$ and using again $|\psi(\omega_0)\rangle = G_B(\omega_0)\,|0\rangle$ [cf. Eq. (18)] yield $\langle 0\,|\Psi_{k_0}\rangle = 0$. Thus the dressed state also in this case has a node on $|0\rangle$.

This class of stationary states occurring at energy ω_0, named "vacancy-like dressed states" (VDSs), were introduced and studied in Ref. [15] without using the resolvent method. The above discussion shows that their properties are straightforwardly retrieved in our resolvent-based framework. More importantly, it clarifies the peculiarity of VDSs against all the other dressed states as follows. A

3 To our knowledge, this is the first general formulation of this property, which was discussed in Ref. [22] but for a specific model.

dressed state can always be associated with an effective impurity seen by the field: VDSs are the subset of dressed states whose corresponding impurity has an infinite potential strength (namely it reduces to a vacancy).

5 More than one emitter

It is natural to ask how the one-emitter framework developed so far generalizes when another emitter is present. We thus consider next two atoms, labelled 1 and 2, each coupled to the photonic bath at site x_i (for $i = 1, 2$) with strength g, see sketch in Figure 3. Accordingly, Eq. (5) is now replaced by $H_e = \omega_0 \sum_{i=1}^{2} |e_i\rangle\langle e_i|$ (with ω_0 the frequency of each atom), while Eq. (7) now turns into $V = g\,|x_1\rangle\langle e_1| + g\,|x_2\rangle\langle e_2| + \text{H.c.}$ (we consider equal couplings for the sake of simplicity).

The total resolvent in this case can be arranged as (see Supp. Mater.)

$$G(z) = G_B(z) + \sum_{ij=1}^{2} (\mathbf{F}^{-1})_{ij}\, |\Psi_i\rangle\langle\Psi_j|, \tag{32}$$

where we defined the z-dependent states $|\Psi_i(z)\rangle$ and the z-dependent matrix $\mathbf{F}(z)$ as [their z-dependence is implicit in Eq. (32)]

$$|\Psi_i(z)\rangle = \frac{1}{g}\,|e_i\rangle + G_B(z)\,|x_i\rangle\,, \tag{33}$$

$$F_{ij}(z) = \frac{z-\omega_0}{g^2}\delta_{ij} - \langle x_i|G_B(z)|x_j\rangle, \tag{34}$$

with $\langle x_j|\Psi_i\rangle = \langle\Psi_j|x_i\rangle = \langle x_j|G_B(z)|x_i\rangle$. Notice that, for $z \notin \mathbb{R}$, generally $F_{12} \neq F_{21}^*$, and that $|\Psi_i(z)\rangle$ and $F_{ii}(z)$ coincide with Eqs. (18) and (19), respectively, when $|0\rangle$ is replaced by $|x_i\rangle$.

This exact expression already points towards an effective interaction mediated by one-emitter dressed states. Indeed, the resolvent $G(z)$ reduces to $G_1(z) + G_2(z)$ (isolated emitters) when $\mathbf{F}(z)$ is diagonal, i.e. $F_{12} = F_{21} = 0$: this can only occur when $|\Psi_i(z)\rangle$ has a node on $x_{j\neq i}$ [cf. Eq. (34)]. This shows that the crosstalk between the emitters is mediated by $|\Psi_i(z)\rangle$ (via its photonic component $|\psi_i(z)\rangle$).

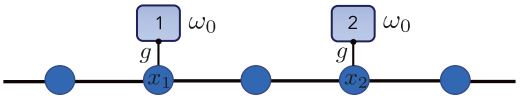

Figure 3: Schematics of two atoms, 1 and 2, coupled to a photonic bath (in this case sketched as a simple lattice). Each emitter has frequency ω_0 and is coupled to the cavity x_i with strength g.

Each BS energy ω_{BS} fulfils the pole equation $\det \mathbf{F}(\omega_{\text{BS}}) = 0$, whose solutions are implicitly given by

$$\omega_{\text{BS}}^{\pm} = \tilde{\omega}_0(\omega_{\text{BS}}^{\pm}) \pm \delta(\omega_{\text{BS}}^{\pm}) \tag{35}$$

where the function $\tilde{\omega}_0(z)$ and $\delta(z)$ (here calculated at $z = \omega_{\text{BS}}^{\pm}$) are defined as

$$\tilde{\omega}_0(z) = \omega_0 + \frac{g^2}{2}\sum_{i=1,2}\langle x_i|G_B(z)|x_i\rangle, \tag{36}$$

$$\delta(z) = \sqrt{g^4 F_{12}F_{21} + \mathcal{A}^2}, \tag{37}$$

with $\mathcal{A}(z) = \frac{g^2}{2}(F_{22} - F_{11})$ [the dependence on z of F_{ij} and $\mathcal{A}$ is implicit in Eq. (37)].

The residues of $G(z)$, $|\Psi_{\text{BS}}^{\pm}\rangle\langle\Psi_{\text{BS}}^{\pm}|$, on the two poles $\omega_{\text{BS}}^{\pm}$ can be calculated directly although their expression is too lengthy to be reported here (see Supp. Mater.). The states $|\Psi_{\text{BS}}^{\pm}\rangle$ are especially relevant when the emitters are far-detuned from all unbound photonic modes. Under weak-coupling condition, this guarantees that $\omega_{\text{BS}}^{\pm}$ will also be far-detuned from the unbound photonic modes and close to ω_0. Correspondingly, the emitters bare states $|e_i\rangle$ will have vanishing overlap with the unbound dressed states and lie (up to second order in g) in the eigenspace spanned by $|\Psi_{\text{BS}}^{\pm}\rangle$. Thus, the atomic dynamics is described by the effective Hamiltonian $H_{\text{eff}} \simeq \sum_{i=\pm}\omega_{\text{BS}}^{i}\,|\Psi_{\text{BS}}^{i}\rangle\langle\Psi_{\text{BS}}^{i}|$. In this regime, we can derive the approximate explicit expressions for $\omega_{\text{BS}}^{\pm}$ and $|\Psi_{\text{BS}}^{\pm}\rangle$, which provides the following effective Hamiltonian (see Supp. Mater.)

$$H_{\text{eff}} = H_{\text{s}} + H_{\text{a}} \tag{38}$$

with

$$H_{\text{s}} = \lambda_{\text{s}}\Bigg(\sum_{i=1,2}\omega_{\text{BS}}^{(i)}\,|\Psi_i\rangle\langle\Psi_i| - (g^2F_{12}\,|\Psi_1\rangle\langle\Psi_2| + \text{H.c.})\Bigg), \tag{39}$$

$$H_{\text{a}} = \lambda_{\text{a}}\Bigg(\sum_{i=1,2}\Omega_i\,|\Psi_i\rangle\langle\Psi_i| - (g^2F_{12}\,|\Psi_1\rangle\langle\Psi_2| + \text{H.c.})\Bigg), \tag{40}$$

where

$$\omega_{\text{BS}}^{(i)} = \omega_0 + g^2\langle x_i|G_B(\omega_0)|x_i\rangle \qquad (i = 1, 2) \tag{41}$$

$$\lambda_{\text{s}} = -\frac{2\delta^2\,(\langle\Psi_1|\Psi_1\rangle + \langle\Psi_2|\Psi_2\rangle)}{\beta^+\beta^-}, \tag{42}$$

$$\lambda_{\text{a}} = \frac{2\omega_0\mathcal{A}\,(\langle\Psi_1|\Psi_1\rangle - \langle\Psi_2|\Psi_2\rangle)}{\beta^+\beta^-}, \tag{43}$$

$$\Omega_1 = \frac{\delta^2}{\omega_0} + \mathcal{A}, \quad \Omega_2 = \frac{\delta^2}{\omega_0} - \mathcal{A}, \tag{44}$$

$$\beta^{\pm} = \mathcal{A}\left(\langle\Psi_1|\Psi_1\rangle - \langle\Psi_2|\Psi_2\rangle\right) \pm \delta(\langle\Psi_2|\Psi_2\rangle + \langle\Psi_1|\Psi_1\rangle). \tag{45}$$

Here, all z-dependent quantities such as $|\Psi_i\rangle$, F_{ij}, $\omega_{\mathrm{BS}}^{(i)}$, $\mathcal{A}$ and δ [cf. Eqs. (33)–(37)] are calculated at $z = \omega_0$. In particular, $|\Psi_i\rangle$ and $\omega_{\mathrm{BS}}^{(i)}$ are the (unnormalized) dressed BS of atom i and the corresponding energy in the absence of the other emitter, respectively.

Eq. (38) expresses the effective Hamiltonian explicitly in terms of overlapping one-atom dressed BSs. A similar task was carried out in Ref. [12] yet for the specific model of a simple homogeneous photonic lattice.

Notably, terms H_{s} and H_{a} are interpreted as follows. When the two atoms are located in equivalent positions then $\langle\Psi_1|\Psi_1\rangle = \langle\Psi_2|\Psi_2\rangle$ and thus $H_{\mathrm{a}} = 0$. Otherwise, in general $\langle\Psi_1|\Psi_1\rangle \neq \langle\Psi_2|\Psi_2\rangle$ so that both H_{s} and H_{a} contribute to H_{eff}. Thus the term H_{a} describes the effect of inequivalent emitters' positions. A noteworthy example is a translationally-invariant bath featuring a unit cell with more than one site. In this case it is known that changing from equivalent to inequivalent positions (or vice versa) can dramatically affect the effective coupling strength (which may even vanish) [15, 19].

We conclude by noting that for equivalent positions we get the particularly compact form

$$\begin{aligned} H_{\mathrm{eff}} &= H_s \\ &= \sum_{i=1,2} \omega_{\mathrm{BS}}^{(i)} \left|\tilde{\Psi}_i\right\rangle\!\left\langle\tilde{\Psi}_i\right| - (g^2 F_{12} \left|\tilde{\Psi}_1\right\rangle\!\left\langle\tilde{\Psi}_2\right| + \mathrm{H.c.}) \end{aligned} \tag{46}$$

where $\left|\tilde{\Psi}_i\right\rangle = \langle\Psi_i|\Psi_i\rangle^{-1/2}|\Psi_i\rangle$ is a normalized dressed BS (due to the hypothesis of equivalent positions, $\langle\Psi_1|\Psi_1\rangle = \langle\Psi_2|\Psi_2\rangle$).

The above arguments can be generalised (see Supp. Mater.) to the case of M emitters. Indeed, Eqs. (32)–(34) are naturally generalized, yielding in the weak coupling regime the effective Hamiltonian

$$H_{\mathrm{eff}} = \sum_{i=1}^{M} \omega_{\mathrm{BS}}^{(i)} \left|\tilde{\Psi}_i\right\rangle\!\left\langle\tilde{\Psi}_i\right| - g^2 \sum_{i\neq j} F_{ij} \left|\tilde{\Psi}_i\right\rangle\!\left\langle\tilde{\Psi}_j\right| \tag{47}$$

with x_i the location of the ith atom and where $\left|\tilde{\Psi}_i\right\rangle$ and $\omega_{\mathrm{BS}}^{(i)}$ are defined exactly as in the $M = 2$ case.

6 Conclusions

To sum up, we considered a general model of quantum emitter coupled to an *unspecified photonic bath* under the rotating wave approximation. Inspired by analogies between an atom and a standard impurity, we have shown that the resolvent operator used in the non-perturbative description of atom-photon interactions can be re-arranged in a compact form so as to make it structurally analogous to that occurring in the textbook impurity problem. This complements the usual picture according to which the atom acquires a self-energy, showing that the field sees the atom as a fictitious impurity with an associated self-potential. As a hallmark, the presence of the atom in the resolvent is fully captured by a rank-one projector term appearing in the resolvent. This in turn features a dressed-state function $|\Psi(z)\rangle$ (defined on the complex plane) which in a sense encompasses already the stationary states (especially BSs). An extension of the framework to the case of more than one emitter was carried out, which allows for a natural derivation of dispersive Hamiltonians explicitly in terms of overlapping one-atom dressed states.

This work settles the atom-photon resolvent formalism in a form arguably easier to handle. This can be beneficial for instance in view of generalizations to the topical paradigm of giant atoms [40], i.e. emitters non-locally coupled to the bath and as such more complicated to describe [21, 41, 42]. Moreover, the connection with the familiar impurity problem makes the atom-photon resolvent apparatus physically more intuitive. We took advantage from the last circumstance in order to highlight some general properties having an impurity-problem counterpart (e.g. the coexistence of dressed BICs with unperturbed photonic states).

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Supplementary Material for "Dressed emitters as impurities"'

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CONTENTS

This Supplemental Material presents technical proofs of some properties and theorems discussed in the main text. We note that Section SM2 is essentially a review of known material.

SM1. PROOF OF EQS. (16) AND (31)

We will derive Eqs. (16) and (31) as a special case of a general formula for M emitters coupled to the field. For M emitters the Hamiltonian terms of section IV generalise to

$$H_e = \omega_0 \sum_{i=1}^{M} |e_i\rangle\langle e_i| \,, \qquad V = g \sum_{i=1}^{M} (|x_i\rangle\langle e_i| + |e_i\rangle\langle x_i|) \,, \tag{S1}$$

with obvious meaning of the symbols, and H_B remains as in Eq. (6). In standard Green function theory [**?**], for a given a Hamiltonian $H = H_0 + V$ and associated resolvent $G(z) = (z - H)^{-1}$, the T-matrix is defined as

$$T(z) = V + T(z)G_0(z)V \,, \tag{S2}$$

where $G_0(z) = (z - H_0)^{-1}$ is the resolvent of the unperturbed Hamiltonian $H_0 = H_e + H_B$. The resolvent can be expressed in terms of $T(z)$ as

$$G(z) = G_0(z) + G_0(z)T(z)G_0(z) \,. \tag{S3}$$

Using the expression (S2) recursively yields a formal expression for $T(z)$ in series

$$T(z) = \sum_{k=1}^{+\infty} T^k(z) \;\text{ with }\; T_k(z) = V\left(G_0(z)V\right)^{k-1} = T_k(z) = V\left(\mathcal{P}G_0(z)\mathcal{P}V\right)^{k-1} \,, \tag{S4}$$

where $\mathcal{P}$ is the projector on the support of V. Since V has only support on $\{\{|x_i\rangle\}_{i=1}^{M}, |e_i\rangle_{i=1}^{M}\}$, $\mathcal{P}$ is the projector operator onto this subspace. Notice that in the single particle sector $G_0(z) = G_e(z) + G_B(z)$, with $G_e(z) = (z - H_e)^{-1}$

and $G_B(z) = (z - H_B)^{-1}$. Thus, in the ordered basis $\{|x_1\rangle, \ldots, |x_M\rangle, |e_1\rangle, \ldots, |e_M\rangle\}$, the relevant operators assume the following block-matrix structures

$$\mathcal{P}G_0(z)\mathcal{P} \sim \begin{pmatrix} \boldsymbol{\gamma}^B(z) & 0 \\ 0 & \boldsymbol{\gamma}^e(z) \end{pmatrix} \qquad \text{and} \qquad V \sim g \begin{pmatrix} 0 & \mathbb{1}_M \\ \mathbb{1}_M & 0 \end{pmatrix}, \tag{S5}$$

where $\sim$ is a shorthand notation for matrix representation in the mentioned basis, $\mathbb{1}_M$ is the $M \times M$ identity matrix while $\boldsymbol{\gamma}^B(z)$ and $\boldsymbol{\gamma}^e(z)$ are $M \times M$ matrices with elements $\gamma^B_{ij}(z) = \langle x_i|G_B(z)|x_j\rangle$ and $\gamma^e_{ij}(z) = \langle x_i|G_e(z)|x_j\rangle = \gamma_e(z)\delta_{ij}$, respectively where $\gamma_e(z) = (z - \omega_0)^{-1}$. Thanks to the simplicity of V, one can get explicit expressions for odd and even terms of $T(z)$ as

$$\begin{aligned} T_{2k-1}(z) \sim\ & g\left[g^2 \begin{pmatrix} \gamma_e(z)\boldsymbol{\gamma}^B(z) & 0 \\ 0 & \gamma_e(z)\boldsymbol{\gamma}^B(z) \end{pmatrix}\right]^{k-1} \cdot \begin{pmatrix} 0 & \mathbb{1}_M \\ \mathbb{1}_M & 0 \end{pmatrix}, \\ T_{2k}(z) \sim\ & g^2\left[g^2 \begin{pmatrix} \gamma_e(z)\boldsymbol{\gamma}^B(z) & 0 \\ 0 & \gamma_e(z)\boldsymbol{\gamma}^B(z) \end{pmatrix}\right]^{k-1} \cdot \begin{pmatrix} \boldsymbol{\gamma}^e(z) & 0 \\ 0 & \boldsymbol{\gamma}^B(z) \end{pmatrix}. \end{aligned}$$

We thus end up with

$$T(z) \sim g \begin{pmatrix} \boldsymbol{h}(z) & 0 \\ 0 & \boldsymbol{h}(z) \end{pmatrix} \cdot \begin{pmatrix} g\boldsymbol{\gamma}^e(z) & \mathbb{1}_M \\ \mathbb{1}_M & g\,\boldsymbol{\gamma}^B(z) \end{pmatrix},$$

where $\boldsymbol{h}(z)$ is a geometric serie of $M \times M$ matrices, which for sufficiently weak coupling (i.e. $||g^2\boldsymbol{\gamma}^e(z) \cdot \boldsymbol{\gamma}^B(z)||<1$) converges, yielding

$$\boldsymbol{h}(z) = \sum_{k=0} \left[g^2\gamma_e(z)\boldsymbol{\gamma}^B(z)\right]^k = \frac{1}{\mathbb{1}_M - g^2\gamma_e(z)\boldsymbol{\gamma}^B(z)}. \tag{S6}$$

Plugging this in Eq. (S3) we get the full Green function in the following form (where the repeated index summation convention is used and the z dependences are omitted),

$$\begin{aligned} G(z) &= G_B + G_e + g^2\gamma_e G_0 \,|x_i\rangle\, h_{ij}\, \langle x_j|\, G_0 + gG_0\,|x_i\rangle\, h_{ij}\, \langle e_j|\, G_0 + gG_0\,|e_i\rangle\, h_{ij}\, \langle x_j|\, G_0 + g^2 G_0\,|e_i\rangle\, h_{ij}\gamma^B_{jk}\, \langle e_k|\, G_0 \\ &= G_B + \gamma_e\,|e_i\rangle\,\langle e_i| + \gamma_e h_{ij}\left\{g^2 G_B\,|x_i\rangle\,\langle x_j|\, G_B + gG_B\,|x_i\rangle\,\langle e_j| + g\,|e_i\rangle\,\langle x_j|\, G_0 + g^2\gamma_e\,|e_i\rangle\,\gamma^B_{jk}\,\langle e_k|\right\} \\ &= G_B + g^2\gamma_e\, h_{ij}\,|\Psi_i\rangle\,\langle\Psi_j|\,, \end{aligned} \tag{S7}$$

with h_{ij} denoting the elements of the matrix $\boldsymbol{h}(z)$. We recall that $|\Psi_i(z)\rangle = \frac{1}{g}\,|e_i\rangle + G_B(z)\,|x_i\rangle$. Finally, we obtain the expression

$$G(z) = G_B(z) + \sum_{ij}\{\boldsymbol{F}^{-1}(z)\}^M_{ij=1}\,|\Psi_i(z)\rangle\,\langle\Psi_j(z)|\,, \tag{S8}$$

where $\boldsymbol{F}(z) = \frac{\mathbf{1}_M}{g^2\gamma_e(z)} - \boldsymbol{\gamma}^B(z)$, whose elements are $F_{ij}(z) = \frac{z-\omega_0}{g^2}\delta_{ij} - \langle x_i|G_B(z)|x_j\rangle$. For M=1, Eq. (S8) reduces to Eq. (16) upon identifying the matrix $\boldsymbol{F}(z)$ with the scalar $F(z)$. For $M = 2$, we recover Eq. (31).

SM2. IMPURITY PROBLEM

The total Hamiltonian reads (see main text) $H = H_B + V_{\text{imp}}$ with $V_{\text{imp}} = \epsilon\,|0\rangle\langle 0|$. One can show [**?**] that the transfer matrix in this case is

$$T(z) = |0\rangle\,\frac{\epsilon}{1 - \epsilon\,\langle 0|G_B(z)|0\rangle}\,\langle 0|\,, \tag{S9}$$

if $|\,\epsilon\,\langle 0|G_B(z)|0\rangle\,| < 1$. The total Green function for this model is then

$$G(z) = G_B(z) + G_B(z)T(z)G_B(z), \tag{S10}$$

which coincides with Eq. (13) in the main text.

The only possible BS (if any) is the solution of the pole equation $\gamma_0(\omega_{\rm BS}) = \frac{1}{\epsilon}$ with the corresponding residue being [**?**]

$$\text{Res}\ [G(z), z = \omega_{\rm BS}] = \frac{1}{\langle 0|G_B^2(\omega_{\rm BS})|0\rangle}\ |\psi(\omega_{\rm BS})\rangle\langle\psi(\omega_{\rm BS})|\,, \tag{S11}$$

The BS is non-degenerate since the degeneracy is calculated as $\text{Tr}\{\text{Res}\ [G(z), z = \omega_{\rm BS}]\} = 1$ [**?**]. The normalized BS wavefunction is given by $\mathcal{N}|\psi(\omega_{\rm BS})\rangle$ with $\mathcal{N} = \langle 0|G_B^2(\omega_{\rm BS})|0\rangle^{-1/2}$.

Applying the Lippmann-Schwinger equation, an unbounded eigenstate of energy ω is given by

$$|\psi_k^{\pm}\rangle = |k(\omega)\rangle + G^{\pm}(\omega)V_{\rm imp}\,|k(\omega)\rangle\,. \tag{S12}$$

This gives

$$|\psi_k^{\pm}\rangle = |k(\omega)\rangle + \lim_{\delta\to 0}\frac{1}{f(\omega \pm i\delta)}\,\langle 0|k(\omega\pm i\delta)\rangle\,|\psi(\omega\pm i\delta)\rangle\,, \tag{S13}$$

for each ω such that $\gamma_0(\omega) \neq \frac{1}{\epsilon}$ [namely $f(\omega) \neq 0$]. If instead $\gamma_0(\omega) = \frac{1}{\epsilon}$, then $|\psi_k^{\pm}\rangle = |k(\omega)\rangle$.

SM3. UNBOUND DRESSED STATES

Similarly to the previous section, based on the Lippmann–Schwinger equation, an unbound dressed state of energy ω fulfils

$$|\psi_k\rangle = |k(\omega)\rangle + G^{+}(\omega)V_{\rm imp}\,|k(\omega)\rangle\ . \tag{S14}$$

Using Eqs. (12), (17) and (18) (see main text) then yields Eq. (28) in the main text.

In our case, the modes that belong to the bands are the modes of the bare bath, and this equation simply becomes

$$|\psi_k\rangle = |k(\omega)\rangle + \frac{\langle 0|k(\omega)\rangle}{F^{+}(\omega)}\,|\Psi(\omega)\rangle\,. \tag{S15}$$

To work out a more explicit expression for the unbound dressed states, we recall the identities

$$\lim_{y\to 0}\frac{1}{x\pm iy} = \mathcal{P}\frac{1}{x} \mp i\pi\delta(x)\,,\ \ \delta(g(x)) = \sum_i \frac{\delta(x-x_i)}{|g'(x_i)|}\ \text{ with } g(x_i) = 0 \tag{S16}$$

and expand Eq. (S15) as

$$|\psi_k\rangle = |k(\omega)\rangle + \langle 0|k(\omega)\rangle\,\mathcal{P}\tfrac{1}{F(\omega)}\,|\Psi(\omega)\rangle - i\pi\sum_i \frac{\langle 0|k(\omega_i)\rangle\,\delta(\omega-\omega_i)}{\frac{1}{g^2} + \langle 0|G_B^2(\omega_i)|0\rangle}\ |\Psi(\omega_i)\rangle\,, \tag{S17}$$

with $F(\omega_i) = 0$. If $F(\omega) \neq 0$, only the second term (featuring the principal part) adds to $|k(\omega)\rangle$. If instead $F(\omega) = 0$ (namely ω coincides with some ω_i) then the only possible corrrection to $|k(\omega)\rangle$ can come from the third term. This is yet zero since

$$\langle 0|k(\omega_i)\rangle = 0\,. \tag{S18}$$

To show this, we note that the bath resolvent on the real axis can be expanded as

$$G_B(\omega^{\pm}) = \int \mathrm{d}\omega'\,\mathcal{P}\,\frac{\rho_B(\omega')\,|k(\omega')\rangle\langle k(\omega')|}{\omega-\omega'} \mp i\pi\rho_B(\omega)\,|k(\omega)\rangle\langle k(\omega)|\,, \tag{S19}$$

where the density of state $\rho_B(\omega)$ is $\frac{\partial k}{\partial\omega}$. Taking the expectation value of both sides on state $|0\rangle$, we see that $\text{Im}\,\langle 0|G_B(\omega^{\pm})|0\rangle = 0$ if and only if (S18) holds. Then if there exists a solution of $F(\omega) = 0$ in the continuum then the associated eigenstate of the same energy of the bare bath is unaffected by the atom, entailing $|\psi_k\rangle = |k(\omega_i)\rangle$.

Thus Eqs. (28) in the main text are proven.

SM4. TWO ATOMS

Based on Eqs. (31) and (33) in the main text, the two-atom BS energy $\omega_{\rm BS}$ fulfils the two-atom pole equation $\det \mathbf{F}(\omega_{\rm BS}) = 0$. The solution is given implicitly by

$$\omega_{\rm BS}^{\pm} = \tilde{\omega}_0(\omega_{\rm BS}^{\pm}) \pm \delta(\omega_{\rm BS}^{\pm}) \tag{S20}$$

with $\tilde{\omega}_0(z)$ and $\delta(z)$ depending on z according to

$$\tilde{\omega}_0^{\pm} = \omega_0 + \tfrac{g^2}{2}\left(\langle G_B(z)\rangle_{x_1} + \langle G_B(z)\rangle_{x_2}\right)\,,\ \delta(z) = \sqrt{g^4 F_{12}F_{21} + \mathcal{A}^2}\,, \tag{S21}$$

with the asymmetry coefficient $\mathcal{A}$ defined as

$$\mathcal{A}(z) = \tfrac{g^2}{2}\left(F_{22}(z) - F_{11}(z)\right)\,. \tag{S22}$$

The residues of $G(z)$ on the two poles $\omega_{\rm BS}^{\pm}$ can be calculated directly, yielding (we use a vector-matrix formalism)

$$|\Psi_{\rm BS}^{\pm}\rangle\langle\Psi_{\rm BS}^{\pm}| = \operatorname*{Res}_{\omega_{\rm BS}}\left[G(z)\right] = \frac{g^2}{\beta}\left[\begin{pmatrix}|\Psi_1\rangle & |\Psi_2\rangle\end{pmatrix}\begin{pmatrix}F_{11} & -F_{12}\\ -F_{21} & F_{22}\end{pmatrix}\begin{pmatrix}\langle\Psi_1|\\ \langle\Psi_2|\end{pmatrix}\right]\Bigg|_{z=\omega_{\rm BS}^{\pm}} \tag{S23}$$

with

$$\beta(z) = g^2\left[F_{11}\langle\Psi_2|\Psi_2\rangle + F_{22}\langle\Psi_1|\Psi_1\rangle - F_{12}\langle x_2|G_B^2|x_1\rangle - F_{21}\langle x_1|G_B^2|x_2\rangle\right] \tag{S24}$$

[the dependence on z is left implicit in the expressions for $G_B(z)$, $F_{ij}(z)$ and $\Psi_i(z)$].

In the weak-coupling regime, we can make the following approximations

$$\tilde{\omega}_0(\omega_{\rm BS}^{\pm}) \simeq \tilde{\omega}_0(\omega_0) = \omega_0 + \tfrac{g^2}{2}\left[\langle G_B(\omega_0)\rangle_{x_1} + \langle G_B(\omega_0)\rangle_{x_2}\right]\,, \tag{S25}$$

$$F_{ij}(\omega_{\rm BS}^{\pm}) \simeq F_{ij}(\omega_0) \pm \tfrac{\delta(\omega_0)}{g^2}\delta_{ij}\,,\ \ \mathcal{A}(\omega_{\rm BS}^{\pm}) \simeq \mathcal{A}(\omega_0) = \mathcal{A}_0\,,\ \ |\Psi_i(\omega_{\rm BS}^{\pm})\rangle \simeq |\Psi_i(\omega_0)\rangle = |\Psi_i\rangle\,, \tag{S26}$$

$$\delta(\omega_{\rm BS}^{\pm}) \simeq \delta(\omega_0) = \delta_0\,,\ \ \beta(\omega_{\rm BS}^{\pm}) \simeq \beta^{\pm} = \mathcal{A}_0\left(\langle\Psi_1|\Psi_1\rangle - \langle\Psi_2|\Psi_2\rangle\right) \pm \delta_0(\langle\Psi_2|\Psi_2\rangle + \langle\Psi_1|\Psi_1\rangle)\,, \tag{S27}$$

hence (S23) reduces to

$$|\Psi_{\rm BS}^{\pm}\rangle\langle\Psi_{\rm BS}^{\pm}| = \frac{1}{\beta^{\pm}}\left[(\mathcal{A}_0 \pm \delta_0)\,|\Psi_1\rangle\langle\Psi_1| + (-\mathcal{A}_0 \pm \delta_0)\,|\Psi_2\rangle\langle\Psi_2| - g^2F_{12}\,|\Psi_1\rangle\langle\Psi_2| - g^2F_{21}\,|\Psi_2\rangle\langle\Psi_1|\right]\,. \tag{S28}$$

The full Hamiltonian can be spectrally decomposed as

$$H = \sum_{i=\pm}\omega_{\rm BS}^{i}\,|\Psi_{\rm BS}^{i}\rangle\langle\Psi_{\rm BS}^{i}| + \text{unbound dressed states}\,. \tag{S29}$$

For ω_0 out of the photonic continuum and g sufficiently small, states $|e_1\rangle$ and $|e_2\rangle$ will negligibly overlap unbound states (as these are far-detuned). Hence, the atomic dynamics is in this case fully captured by the BSs contribution in Eq. (S29). Accordingly, the effective atomic Hamiltonian is thus given by Eq. (37) in the main text, where $\omega_{\rm BS}^{(i)} = \omega_0 + g^2\,\langle G_B(\omega_{\rm BS}^{(i)})\rangle_{x_i}$.

SM5. MANY-ATOM EFFECTIVE HAMILTONIAN

Recall from Eqs. (31) and (33) the many atom BS energy equation

$$\det \boldsymbol{F}(z) = \tfrac{1}{g^2}\det[z - \omega_0 - g^2\boldsymbol{\gamma}^{\boldsymbol{B}}(z)] = 0\,. \tag{S30}$$

This is a non-linear equation which yields M (possibly coinciding) solutions $\{\omega_{\rm BS}^{(i)}\}_{i=1}^{M}$. Correspondingly, the bound states can be calculated as the residues of $G(z)$ on the poles $\omega_{\rm BS}^{(i)}$, which can be expressed

$$|\Psi_{\rm BS}^{(i)}\rangle\langle\Psi_{\rm BS}^{(i)}| = \operatorname*{Res}_{\omega_{\rm BS^{(i)}}}\left[G(z)\right] = \sum_{jk}\left\{\operatorname*{Res}_{\omega_{\rm BS^{(i)}}}\left[\boldsymbol{F}^{-1}(z)\right]\right\}_{jk}|\Psi_j(\omega_{\rm BS}^{(i)})\rangle\,\langle\Psi_k(\omega_{\rm BS}^{(i)})| \tag{S31}$$

In the weak-coupling regime, i.e. for $g \ll \Delta$ where Δ is the detuning of ω_0 from the continuum of frequencies (e.g. energy bands) of the lattice, equation (S30), up to second order in g/Δ, can be approximated by $\det[z - \omega_0 - g^2\boldsymbol{\gamma}^{\boldsymbol{B}}(\omega_0)] = 0$. Thus, decomposing $\boldsymbol{\gamma}^B(\omega_0) = \sum_i \gamma_i|\gamma_i)(\gamma_i|$ in terms of its eigenvalues γ_i and eigenvectors $|\gamma_i)$ ($\gamma^B(z)$ is Hermitian, for $z \in \mathbb{R}$) yields

$$\omega_{\mathrm{BS}}^{(i)} \simeq \omega_0 + g^2\gamma_i \tag{S32}$$

$$\operatorname*{Res}_{\omega_{\mathrm{BS}^{(\mathrm{i})}}} \left[\boldsymbol{F}^{-1}(z)\right] \simeq g^2|\gamma_i)(\gamma_i| \,. \tag{S33}$$

As for the two-atom case, in the weak coupling regime, the atomic dynamics is described by the BSs contribution of the full Hamiltonian analogue of Eq. (S29). Hence, the effective Hamiltonian is given by

$$\begin{aligned} H_{\mathrm{eff}} &\simeq \sum_i \omega_{\mathrm{BS}}^{(i)} |\Psi_{\mathrm{BS}}^{(i)}\rangle\langle\Psi_{\mathrm{BS}}^{(i)}| \simeq g^2 \sum_{jk} \left\{ \sum_i (\omega_0 + g^2\gamma_i)|\gamma_i)(\gamma_i| \right\}_{jk} |\Psi_j\rangle \langle\Psi_k| \\ &= g^2 \sum_{jk} \{\omega_0 \mathbb{1}_M + g^2\boldsymbol{\gamma}^B(\omega_0)\}_{jk} |\Psi_j\rangle \langle\Psi_k| = g^2 \sum_{jk} \left[\omega_0\delta_{jk} + g^2 \langle x_j|G_B(\omega_0)|x_k\rangle\right] |\Psi_j\rangle \langle\Psi_k| \,, \end{aligned} \tag{S34}$$

which, upon renormalisation of the states $|\Psi_i\rangle$, coincides with Eq. (46) in the main text.