Jaynes–Cummings dynamics of fermionic heteronuclear dimers in the Mott regime

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We formulate and exactly solve a model for coherent association and dissociation of fermionic heteronuclear dimers in the deep-lattice Mott regime. Starting from the onsite three-component atom–molecule Hamiltonian, we show how the single-site model maps to the paradigmatic Jaynes–Cummings Hamiltonian from quantum optics. In this mapping, the fermionic molecular/free-atom sector forms an effective two-level system, while the bosonic atomic mode plays the role of the oscillator degree of freedom. We fix the conserved number of fermionic constituent atoms to one but allow an arbitrary conserved number N of bosonic constituent atoms. The accessible doublet is then $|e, N-1\rangle \leftrightarrow |g, N\rangle$, and the coherent conversion coupling is bosonically enhanced to $\chi\sqrt{N}$. Exact analytic expressions are derived for molecular dissociation, atom-pair association, mode populations, and boson–fermion correlation dynamics. The model provides a transparent matter-wave realization of Jaynes–Cummings physics in a heteronuclear Bose–Fermi system and an exactly solvable setting for understanding coherent atom–molecule conversion and bosonic enhancement in lattice systems.

I. INTRODUCTION

Coherent atom–molecule conversion in ultracold gases provides a powerful setting for exploring nonequilibrium quantum dynamics, controlled chemical association, and strongly correlated many-body physics [1]. Since the late 1990s, coherently coupled atomic–molecular degenerate gases have developed through several major theoretical and experimental advances. Early theoretical work established the basic concepts of coherent atom–molecule condensate dynamics via coherent photoassociation or magnetic Feshbach-resonance coupling [2–7]. The proposal of quantum "superchemistry" [8] then identified many-body chemical conversion as a collective, Bose-enhanced process, with subsequent work clarifying related dynamical, interferometric, and microscopic aspects of atom–molecule coherence [9–14]. Experimentally, coherent atom–molecule oscillations were observed in a Bose–Einstein condensate [15], while the creation of molecular condensates from fermionic atoms opened the way to the BEC–BCS crossover programme [16–18]. More recently, many-body chemical dynamics in a quantum-degenerate gas has provided a modern experimental realization of the superchemistry paradigm [19].

In this paper, we are concerned with heteronuclear Bose–Fermi mixtures near interspecies Feshbach resonances, which support coherent interconversion processes of the form

$$b + f \leftrightarrow m, \tag{1}$$

where a bosonic atom b and a fermionic atom f associate into a fermionic heteronuclear diatomic molecule m, or dissociate back into their constituent atoms.

Such systems have been realized experimentally using quantum gas mixtures such as ^{87}Rb–^{40}K. Early experiments demonstrated the production of ultracold heteronuclear molecules in optical lattices and their controlled association from ultracold atomic mixtures [20–22]. Coherent atom–molecule oscillations in a Bose–Fermi mixture have also been observed near an interspecies Feshbach resonance [23]. Subsequent work achieved several important milestones, including the creation of ultracold polar molecules in their rovibrational ground state [24], the coherent transfer of weakly bound Feshbach molecules to deeply bound molecular states [24, 25], and the production of long-lived dipolar molecular gases [26]. Closely related experiments have also realized coherent atom-pair–molecule Rabi oscillations in optical lattices [27]. More broadly, ultracold polar molecules provide a versatile platform for the study of dipolar quantum matter, precision measurements, and quantum simulation [28–30].

Previous theoretical work on heteronuclear atom–molecule systems has addressed many-body lattice physics, photoassociation dynamics, Anderson-lattice-type models, and coherent conversion near Feshbach resonances [31, 32]. Optical lattices provide a particularly natural setting for these systems because strong confinement and interaction blockade can suppress tunnelling and reduce the dynamics to local conversion processes, building on the standard lattice route to Mott physics in ultracold gases [33, 34]. In the deep-Mott regime, the onsite dynamics becomes especially transparent and admits an exact treatment.

In this work, we isolate and exactly solve the coherent atom–molecule conversion problem for heteronuclear fermionic dimers in a deep optical lattice. We consider one bosonic atomic mode, one fermionic atomic mode, and one fermionic molecular mode on each lattice site, with tunnelling neglected and the fermionic constituent number fixed to one. Unlike the minimal single-boson sector, we allow an arbitrary conserved number N of bosonic constituent atoms on each site. Starting from the full onsite Hamiltonian, we show that the local dynamics reduces exactly to a Jaynes–Cummings Hamiltonian [35]. The fermionic molecular/free-atom sector forms an

effective two-level system, while the bosonic atomic mode plays the role of the quantized oscillator degree of freedom. For fixed N, the relevant Jaynes–Cummings doublet is $|e, N-1\rangle \leftrightarrow |g, N\rangle$, with a bosonically enhanced matrix element $\chi\sqrt{N}$. The collection of fixed-N sectors reproduces the occupation-dependent doublet structure of the Jaynes–Cummings ladder. The resulting system therefore provides a matter-wave realization of Jaynes–Cummings physics in which the oscillator quanta correspond to physical constituent atoms rather than photons.

We derive exact analytic solutions for both molecular dissociation and atom-pair association dynamics and calculate the resulting population transfer and atom–atom correlation functions for arbitrary N. The conversion frequency increases as $\sqrt{N}$, displaying the expected bosonic enhancement. The normalized pair correlations depend qualitatively on the initial bosonic occupation: for $N = 1$, dissociation creates atoms into an initially empty bosonic mode and produces a divergent short-time normalized correlation, whereas for $N > 1$ the pre-existing bosons provide a finite background and regularize this divergence.

The model considered here should be viewed as the exactly solvable coherent-conversion limit of more general atom–molecule lattice systems. Although the exact idealized limit has not, to our knowledge, been realized as a site-resolved Jaynes–Cummings experiment for fermionic heteronuclear dimers, the essential ingredients — heteronuclear Bose–Fermi molecules in optical lattices, coherent atom–molecule oscillations, and lattice-confined atom-pair conversion — have already been demonstrated experimentally. The model therefore provides a transparent and experimentally motivated setting for understanding how coherent atom–molecule conversion, bosonic enhancement, and occupancy constraints combine to produce characteristic atom–molecule and atom–atom correlation dynamics across the Jaynes–Cummings ladder.

II. ONSITE ATOM–MOLECULE HAMILTONIAN

We consider one lattice site containing a bosonic atomic mode ($\hat{b}$), a fermionic atomic mode ($\hat{f}$), and a fermionic molecular mode ($\hat{m}$), as appropriate for the local conversion channel in heteronuclear Bose–Fermi atom–molecule systems [20, 23, 31, 36]. The minimal onsite Hamiltonian is

$$\begin{aligned}\hat{H} =& \hbar\omega_b \hat{b}^\dagger \hat{b} + \hbar\omega_f \hat{f}^\dagger \hat{f} + \hbar\omega_m \hat{m}^\dagger \hat{m} \\ &+ \hbar\chi \left(\hat{b}^\dagger \hat{f}^\dagger \hat{m} + \hat{m}^\dagger \hat{f} \hat{b}\right), \end{aligned} \tag{2}$$

where the creation (annihilation) operators $\hat{b}^\dagger$, $\hat{f}^\dagger$, and $\hat{m}^\dagger$ ($\hat{b}$, $\hat{f}$, and $\hat{m}$) satisfy the standard bosonic commutation and fermionic anticommutation relations, $[\hat{b}, \hat{b}^\dagger] = \{\hat{f}, \hat{f}^\dagger\} = \{\hat{m}, \hat{m}^\dagger\} = 1$. Here, ω_b, ω_f, and ω_m are the onsite energies of the bosonic atom, fermionic atom, and fermionic molecule, respectively, while χ is the coherent atom–molecule conversion coupling. The term $\hat{b}^\dagger \hat{f}^\dagger \hat{m}$ describes molecular dissociation into one bosonic atom and one fermionic atom, whereas $\hat{m}^\dagger \hat{f} \hat{b}$ describes the reverse association process.

In the present work, we consider the minimal atom–molecule conversion Hamiltonian, retaining only the single-particle energies and the coherent conversion term. While strong onsite interactions are responsible for preparing and stabilizing the initial Mott state, their contribution to the atom–molecule energy difference during the coherent atom–molecule conversion dynamics is neglected in the minimal model presented here. In a more complete description of the Mott-regime lattice system, such interactions would generally produce occupation-dependent energy shifts. Within the restricted two-state subspace considered here, however, they contribute only diagonal matrix elements and therefore renormalize the effective atom–molecule detuning without altering the conversion matrix element or the exact solvability of the fixed-occupation subspace. Their effect is discussed in Appendix B, where we show that each fixed-occupation sector remains an exactly solvable two-state problem with the same coupling $\chi\sqrt{N}$ as the corresponding Jaynes–Cummings doublet, but with an interaction-shifted detuning.

In a more complete description of the Mott-regime lattice system

The total number of atoms of the bosonic species, whether free or bound into molecules, is

$$\hat{N}_b^{\mathrm{tot}} = \hat{b}^\dagger \hat{b} + \hat{m}^\dagger \hat{m}. \tag{3}$$

Similarly, the total number of atoms of the fermionic species, whether free or bound into molecules, is

$$\hat{N}_f^{\mathrm{tot}} = \hat{f}^\dagger \hat{f} + \hat{m}^\dagger \hat{m}. \tag{4}$$

Both commute with the Hamiltonian,

$$[\hat{H}, \hat{N}_b^{\mathrm{tot}}] = [\hat{H}, \hat{N}_f^{\mathrm{tot}}] = 0, \tag{5}$$

and hence are conserved.

We restrict the fermionic constituent number to

$$N_f^{\mathrm{tot}} = 1, \tag{6}$$

but allow the conserved bosonic constituent number to take an arbitrary positive integer value,

$$N_b^{\mathrm{tot}} = N, \qquad N = 1, 2, \ldots. \tag{7}$$

For each fixed N, the local Hilbert space relevant to coherent conversion is two-dimensional and is spanned by

$$|N - 1_b, 0_f, 1_m\rangle, \qquad |N_b, 1_f, 0_m\rangle. \tag{8}$$

The first state contains one fermionic molecule, zero free fermionic atoms, and $N-1$ free bosonic atoms, whereas

the second contains zero molecules, one free fermionic atom, and N free bosonic atoms. Both states contain the same total number N of atoms of the bosonic species (either all free, or $N-1$ free and one in the bound molecular state) and one atom of the fermionic species (again either free or in the bound molecular state). The case $N = 1$ reproduces the minimal doublet, while arbitrary N exposes the occupation-dependent coupling characteristic of the full Jaynes–Cummings ladder (see below).

Although each fixed-N problem can be solved directly by exact diagonalisation (see Appendix A), we proceed by mapping the model to the paradigmatic Jaynes–Cummings Hamiltonian [35], whose well-known structure makes the bosonic enhancement and the relation between different number sectors transparent.

III. REDUCTION TO A JAYNES–CUMMINGS HAMILTONIAN

Within the sector $N_f^{\mathrm{tot}} = 1$, the molecular and free-fermion configurations form an effective two-level system. We define

$$|e\rangle \equiv |0_f, 1_m\rangle, \qquad |g\rangle \equiv |1_f, 0_m\rangle. \tag{9}$$

The corresponding pseudo-spin operators are

$$\hat{\sigma}_z = \hat{m}^\dagger \hat{m} - \hat{f}^\dagger \hat{f}, \tag{10}$$
$$\hat{\sigma}_- = \hat{f}^\dagger \hat{m}, \tag{11}$$
$$\hat{\sigma}_+ = \hat{m}^\dagger \hat{f}. \tag{12}$$

Using

$$\hat{m}^\dagger \hat{m} = \frac{1}{2}\left(\hat{N}_f^{\mathrm{tot}} + \hat{\sigma}_z\right), \tag{13}$$
$$\hat{f}^\dagger \hat{f} = \frac{1}{2}\left(\hat{N}_f^{\mathrm{tot}} - \hat{\sigma}_z\right), \tag{14}$$

the Hamiltonian becomes

$$\begin{aligned}\hat{H} =& \hbar\omega_b \hat{b}^\dagger \hat{b} + \frac{\hbar}{2}(\omega_m - \omega_f)\hat{\sigma}_z \\ &+ \hbar\chi\left(\hat{b}^\dagger \hat{\sigma}_- + \hat{b}\hat{\sigma}_+\right) + \frac{\hbar}{2}(\omega_f + \omega_m)\hat{N}_f^{\mathrm{tot}}.\end{aligned} \tag{15}$$

Since the dynamics is restricted to the sector $N_f^{\mathrm{tot}} = 1$, the term $\frac{\hbar}{2}(\omega_f + \omega_m)\hat{N}_f^{\mathrm{tot}}$ is a constant energy offset, $\frac{\hbar}{2}(\omega_f + \omega_m)$, and hence can be omitted.

We next define

$$\omega_0 = \omega_m - \omega_f, \tag{16}$$

which gives

$$\hat{H} = \hbar\omega_b \hat{b}^\dagger \hat{b} + \frac{\hbar\omega_0}{2}\hat{\sigma}_z + \hbar\chi\left(\hat{b}^\dagger \hat{\sigma}_- \hat{b}\hat{\sigma}_+\right). \tag{17}$$

Equation (17) is precisely the Jaynes–Cummings Hamiltonian [35]. The effective two-level transition corresponds to coherent conversion between a fermionic molecular state and a fermionic free-atom state, while the bosonic oscillator mode is provided by the atomic matter-wave field.

The resonance condition for coherent atom–molecule conversion is $\omega_m = \omega_f + \omega_b$, or equivalently $\omega_0 = \omega_b$. We define the atom–molecule detuning

$$\Delta = \omega_0 - \omega_b = \omega_m - \omega_f - \omega_b. \tag{18}$$

and transform to the interaction picture with respect to

$$\hat{H}_0 = \hbar\omega_b\left(\hat{b}^\dagger \hat{b} + \frac{1}{2}\hat{\sigma}_z\right), \tag{19}$$

using the unitary operator

$$\hat{U}(t) = \exp\left(-\frac{i}{\hbar}\hat{H}_0 t\right). \tag{20}$$

The transformed interaction-picture Hamiltonian is

$$\hat{H}_I = \hat{U}^\dagger \hat{H} \hat{U} - \hat{H}_0, \tag{21}$$

and one obtains

$$\hat{H}_I = \frac{\hbar\Delta}{2}\hat{\sigma}_z + \hbar\chi\left(\hat{b}^\dagger \hat{\sigma}_- + \hat{b}\hat{\sigma}_+\right). \tag{22}$$

Equation (22) is the standard Jaynes–Cummings Hamiltonian in the interaction picture [35].

IV. EXACT DYNAMICS FOR ARBITRARY BOSONIC CONSTITUENT NUMBER

For fixed $N_b^{\mathrm{tot}} = N$ and $N_f^{\mathrm{tot}} = 1$, the two states in Eq. (8), forming the Jaynes–Cummings doublet associated with $N_b^{\mathrm{tot}} = N$, can be written as

$$|e, N-1\rangle \equiv |N-1_b, 0_f, 1_m\rangle, \qquad |g, N\rangle \equiv |N_b, 1_f, 0_m\rangle, \tag{23}$$

using Eq. (9). The conversion matrix element contains the familiar bosonic enhancement factor $\sqrt{N}$,

$$\langle g, N|\hat{b}^\dagger \hat{\sigma}_-|e, N-1\rangle = \sqrt{N}, \tag{24}$$

which is the microscopic origin of bosonic stimulation in the atom–molecule conversion process. Consequently, in the ordered basis $\{|e, N-1\rangle, |g, N\rangle\}$, the interaction-picture Hamiltonian is

$$\hat{H}_I^{(N)} = \hbar\begin{pmatrix} \Delta/2 & \chi\sqrt{N} \\ \chi\sqrt{N} & -\Delta/2 \end{pmatrix}. \tag{25}$$

The eigenvalues of $H_I^{(N)}$ are $E_{N,\pm} = \pm\hbar\Omega_N$, where

$$\Omega_N = \sqrt{\left(\frac{\Delta}{2}\right)^2 + N\chi^2} \tag{26}$$

is the generalized Rabi frequency in the $N_b^{\rm tot} = N$ doublet, associated with the detuned atom–molecule conversion dynamics. The corresponding dressed eigenstates may be written as

$$|N,+\rangle = \cos\frac{\theta_N}{2}\,|e,N-1\rangle + \sin\frac{\theta_N}{2}\,|g,N\rangle\,, \tag{27}$$

$$|N,-\rangle = -\sin\frac{\theta_N}{2}\,|e,N-1\rangle + \cos\frac{\theta_N}{2}\,|g,N\rangle\,, \tag{28}$$

with $\cos\theta_N = \Delta/2\Omega_N$, $\sin\theta_N = \chi\sqrt{N}/\Omega_N$, $0 \le \theta_N \le \pi$. The scaling $\Omega_N \propto \sqrt{N}$ on resonance ($\Delta = 0$) is the standard bosonic enhancement of the Jaynes–Cummings coupling.

In Appendix B we show that when we include onsite collisional interactions between bosonic atoms, fermionic atoms, and molecules, the conserved occupation numbers decompose the dynamics into independent two-dimensional sectors, each having the structure of a Jaynes–Cummings doublet with an interaction-shifted detuning.

A. Dissociation dynamics

We first consider the initial molecular state $|\psi(0)\rangle = |e,N-1\rangle$. The exact time evolution is

$$|\psi(t)\rangle = A_{\mathrm{dissoc},N}(t)|e,N-1\rangle + B_{\mathrm{dissoc},N}(t)|g,N\rangle, \tag{29}$$

where

$$A_{\mathrm{dissoc},N}(t) = \cos(\Omega_N t) - i\frac{\Delta}{2\Omega_N}\sin(\Omega_N t), \tag{30}$$

$$B_{\mathrm{dissoc},N}(t) = -i\frac{\chi\sqrt{N}}{\Omega_N}\sin(\Omega_N t). \tag{31}$$

The dissociation probability, i.e. the probability that the system is found in the atom-pair state after starting from a molecule, is

$$P_N(t) = \left|\langle g,N|\psi(t)\rangle\right|^2 = \frac{N\chi^2}{\Omega_N^2}\sin^2(\Omega_N t). \tag{32}$$

It is identical to the probability that the system has converted from one of its initial basis states to the other basis state. On resonance, $\Delta = 0$, one has $\Omega_N = \chi\sqrt{N}$ and $P_N(t) = \sin^2(\chi\sqrt{N}\,t)$, so complete conversion remains possible, but the oscillation frequency is enhanced by $\sqrt{N}$.

The expectation values of atom and molecule number operators, $\langle\hat{n}_f\rangle = \langle\hat{f}^\dagger\hat{f}\rangle$, $\langle\hat{n}_b\rangle = \langle\hat{b}^\dagger\hat{b}\rangle$, and $\langle\hat{n}_m\rangle = \langle\hat{m}^\dagger\hat{m}\rangle$, follow directly from the probabilities of occupying the two basis states. Since the state $|e,N-1\rangle$ contains $N-1$ free bosons and one molecule, whereas $|g,N\rangle$ contains N free bosons and one fermionic atom, the number-operator expectation values are simply the probability-weighted averages over these two configurations. More specifically, the fermionic-atom and molecular populations are

$$\langle\hat{n}_f\rangle = P_N(t), \qquad \langle\hat{n}_m\rangle = 1 - P_N(t), \tag{33}$$

whereas the number of free bosonic atoms is

$$\begin{aligned}\langle\hat{n}_b\rangle &= (N-1)[1-P_N(t)] + NP_N(t)\\ &= N - 1 + P_N(t).\end{aligned} \tag{34}$$

Thus each dissociation event increases the free-boson occupation by one while creating one free fermionic atom. At short times,

$$P_N(t) = N\chi^2 t^2 + O(t^4), \tag{35}$$

which displays the bosonic enhancement directly.

Figure 1(a) illustrates the $N = 1$ conversion probability $P_1(t)$ for several detunings. The arbitrary-N dynamics has the same functional form after the replacements $\chi \to \chi\sqrt{N}$ and $\Omega \to \Omega_N$. Increasing either N or $|\Delta|$ increases the oscillation frequency, while detuning also reduces the maximum conversion probability to $N\chi^2/\Omega_N^2$.

B. Association dynamics

For coherent association, the initial condition is

$$|\psi(0)\rangle = |g,N\rangle. \tag{36}$$

The exact evolution is

$$|\psi(t)\rangle = A_{\mathrm{assoc},N}(t)|g,N\rangle + B_{\mathrm{assoc},N}(t)|e,N-1\rangle, \tag{37}$$

where

$$A_{\mathrm{assoc},N}(t) = \cos(\Omega_N t) + i\frac{\Delta}{2\Omega_N}\sin(\Omega_N t), \tag{38}$$

$$B_{\mathrm{assoc},N}(t) = -i\frac{\chi\sqrt{N}}{\Omega_N}\sin(\Omega_N t). \tag{39}$$

The molecular conversion probability is the same function as in Eq. (32),

$$P_N(t) = \left|\langle e,N-1|\psi(t)\rangle\right|^2 = \frac{N\chi^2}{\Omega_N^2}\sin^2(\Omega_N t). \tag{40}$$

The populations are now

$$\langle\hat{n}_m\rangle = P_N(t), \qquad \langle\hat{n}_f\rangle = 1 - P_N(t), \tag{41}$$

and

$$\begin{aligned}\langle\hat{n}_b\rangle &= N[1-P_N(t)] + (N-1)P_N(t)\\ &= N - P_N(t).\end{aligned} \tag{42}$$

Thus association removes one bosonic atom and one fermionic atom whenever a molecule is created. The same conversion probability governs both directions, but the free-boson populations differ by the bosonic background present in the two initial conditions.

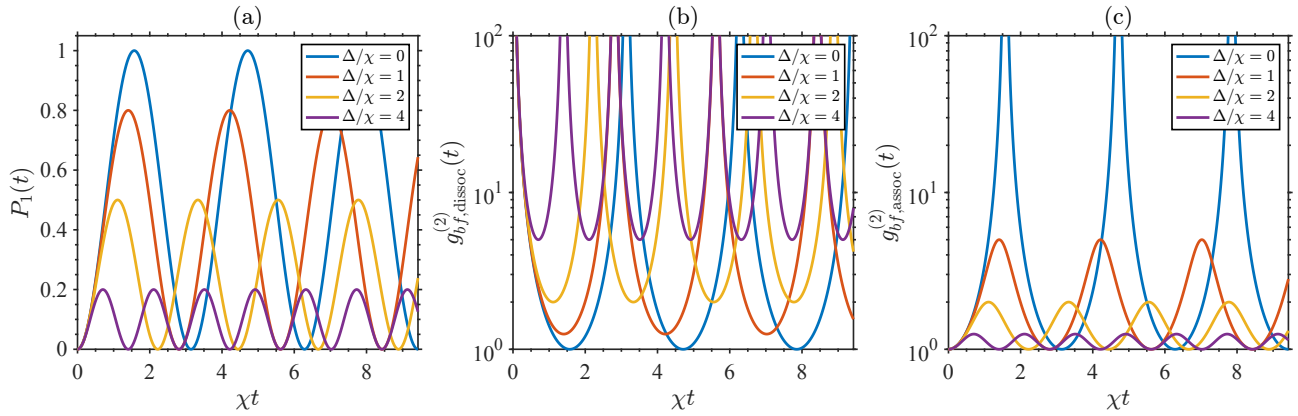

FIG. 1. Coherent conversion and correlation dynamics in the $N = 1$ Jaynes–Cummings doublet. (a) Conversion probability $P_1(t)$ for several detunings Δ/χ. Detuning reduces the maximum conversion probability while increasing the generalized Rabi frequency. (b) Normalized boson–fermion atom correlation $g^{(2)}_{bf,\mathrm{dissoc}}(t) = 1/P_1(t)$ in dissociation, showing the strong enhancement associated with conditional onsite pair production. (c) Normalized boson–fermion atom correlation $g^{(2)}_{bf,\mathrm{assoc}}(t) = 1/[1-P_1(t)]$ in association, showing the corresponding enhancement near times of strong atom-pair depletion; a true divergence occurs only for complete resonant conversion. For $N > 1$, the conversion frequency is enhanced according to Ω_N in Eq. (26), while the pre-existing bosonic population regularizes the limiting divergence of the normalized correlations, as discussed in the text.

C. Boson–fermion correlation functions

The onsite boson–fermion atom correlation function is

$$G^{(2)}_{bf}(t) = \left\langle \hat{b}^\dagger \hat{f}^\dagger \hat{f} \hat{b} \right\rangle = \langle \hat{n}_b \hat{n}_f \rangle. \tag{43}$$

For dissociation, only the state $|g, N\rangle$ contains a free fermionic atom, and it contains N free bosons. Hence

$$G^{(2)}_{bf,\mathrm{dissoc}}(t) = N P_N(t). \tag{44}$$

Using Eqs. (33) and (34), the normalized correlation is

$$g^{(2)}_{bf,\mathrm{dissoc}}(t) = \frac{G^{(2)}_{bf,\mathrm{dissoc}}(t)}{\langle \hat{n}_b \rangle \langle \hat{n}_f \rangle} = \frac{N}{N - 1 + P_N(t)}. \tag{45}$$

At the isolated times for which $P_N(t) = 0$, the normalized correlator is formally undefined because the free-fermion population vanishes. For $N = 1$, this reduces to $g^{(2)}_{bf,\mathrm{dissoc}} = 1/P_1(t)$ and diverges whenever $P_1(t) \to 0^+$. For $N > 1$, however,

$$\lim_{P_N \to 0^+} g^{(2)}_{bf,\mathrm{dissoc}}(t) = \frac{N}{N-1}, \tag{46}$$

so the pre-existing population of $N-1$ bosons regularizes the limiting divergence of the normalized correlation and reduces it to unity for large N. The atoms created by dissociation remain perfectly paired at the event level, but the normalized correlator includes the unconverted bosonic background and therefore no longer exhibits the vacuum-pair divergence.

For association, the atom-pair component $|g, N\rangle$ occurs with probability $1 - P_N(t)$, giving

$$G^{(2)}_{bf,\mathrm{assoc}}(t) = N[1 - P_N(t)]. \tag{47}$$

Using Eqs. (41) and (42), one finds

$$g^{(2)}_{bf,\mathrm{assoc}}(t) = \frac{G^{(2)}_{bf,\mathrm{assoc}}(t)}{\langle \hat{n}_b \rangle \langle \hat{n}_f \rangle} = \frac{N}{N - P_N(t)}. \tag{48}$$

This correlation begins at unity. For $N = 1$, it reduces to $1/[1 - P_1(t)]$ and diverges as complete association removes the last atom pair. For $N > 1$, the limiting value near complete resonant conversion is $N/(N-1)$; exactly at a time when $\langle \hat{n}_f \rangle = 0$, the normalized correlator is again formally undefined, but this finite value describes the continuous limit.

The $N = 1$ correlations are shown in Figs. 1(b) and 1(c). Equations (45) and (48) show that the singular normalized correlations are a special property of conversion into or out of an initially empty atomic mode. At larger bosonic occupation, the dominant new effect is instead the $\sqrt{N}$ enhancement of the coherent conversion frequency.

V. MANY-SITE MOTT STATES

We now consider a translationally invariant lattice in which every occupied site has the same conserved constituent numbers $N_b^{\mathrm{tot}} = N$ and $N_f^{\mathrm{tot}} = 1$. An initial molecular Mott state with one molecule and $N - 1$ free bosons per site is

$$|\Psi(0)\rangle = \prod_j |e, N-1\rangle_j, \tag{49}$$

motivated by optical-lattice Mott physics and by the production of heteronuclear molecules in lattice sites [20, 25, 34, 36].

Since tunnelling is neglected, the dynamics factorizes into independent single-site evolutions. The conversion probability on every site is $P_N^{(j)}(t) = P_N(t)$, and the populations per site are

$$N_m^{(j)}(t) = 1 - P_N(t), \tag{50}$$
$$N_f^{(j)}(t) = P_N(t), \tag{51}$$
$$N_b^{(j)}(t) = N - 1 + P_N(t). \tag{52}$$

Similarly, an initial atom-pair Mott state with N bosons and one fermion per site is

$$|\Psi(0)\rangle = \prod_j |g, N\rangle_j. \tag{53}$$

The corresponding association dynamics gives

$$N_m^{(j)}(t) = P_N(t), \tag{54}$$
$$N_f^{(j)}(t) = 1 - P_N(t), \tag{55}$$
$$N_b^{(j)}(t) = N - P_N(t). \tag{56}$$

Because different lattice sites evolve independently, the many-body dynamics factorizes into an array of identical onsite Jaynes–Cummings doublets. For uniform N, all sites oscillate at the same frequency Ω_N. If instead the initial lattice contains a distribution of local bosonic occupations, different sites evolve with different frequencies Ω_N, producing dephasing of the spatially averaged conversion signal even in the absence of tunnelling or dissipation. This independent-site limit is the opposite limit to the cooperative dynamics discussed in resonantly coupled Bose–Fermi lattice models with finite tunnelling [37].

VI. CONCLUSION

The exactly solvable model developed here provides a simple testbed for coherent heteronuclear atom–molecule conversion in deep optical lattices. Experimentally, fermionic heteronuclear Feshbach and ground-state molecules have been realized in several platforms, including KRb, NaK, and NaLi systems [22, 24, 38–43]. Beginning with the full onsite Hamiltonian containing the free energies of the three components, we have shown explicitly how the sector with one fermionic constituent atom and an arbitrary number N of bosonic constituent atoms maps to the Jaynes–Cummings doublet corresponding to $N_b^{\rm tot} = N$ [35].

The coherent coupling in this doublet is $\chi\sqrt{N}$, giving the generalized Rabi frequency $\Omega_N = [(\Delta/2)^2 + N\chi^2]^{1/2}$. We derived exact population dynamics for both dissociation and association. In dissociation, the free-boson population evolves as $N - 1 + P_N(t)$, whereas in association it evolves as $N - P_N(t)$. The normalized boson–fermion correlations also acquire a nontrivial dependence on the initial bosonic occupation: the divergent conditional correlations of the $N = 1$ sector are regularized for $N > 1$ by the background bosonic population, while the $\sqrt{N}$ enhancement of coherent conversion becomes the dominant occupation-dependent effect.

The model provides a transparent matter-wave realization of Jaynes–Cummings physics and a useful conceptual starting point for more general atom–molecule lattice systems [31, 37]. Several extensions are natural. Finite tunnelling would couple the onsite doublets and generate competition between coherent conversion and transport. Spatially varying bosonic occupations would produce dephasing through the occupation-dependent frequencies Ω_N. Dissipation and molecular loss could be incorporated through Lindblad dynamics, while coherent superpositions of bosonic number states would permit the collapse-and-revival phenomena associated with the full Jaynes–Cummings ladder.

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Appendix A: Direct solution in the fixed-constituent-number subspace

Although the mapping to the Jaynes–Cummings model provides a useful physical interpretation, each fixed-N sector can also be solved directly without introducing effective spin operators.

The conserved quantities

$$N_f^{\rm tot} = n_f + n_m = 1, \qquad N_b^{\rm tot} = n_b + n_m = N, \tag{A1}$$

restrict the dynamics to the two states $|N-1_b, 0_f, 1_m\rangle$ and $|N_b, 1_f, 0_m\rangle$. In this basis, the Hamiltonian (2) takes the matrix form

$$\hat{H}^{(N)} = \hbar \begin{pmatrix} (N-1)\omega_b + \omega_m & \chi\sqrt{N} \\ \chi\sqrt{N} & N\omega_b + \omega_f \end{pmatrix}. \tag{A2}$$

The factor $\sqrt{N}$ follows from $\hat{b}^\dagger|N-1\rangle = \sqrt{N}|N\rangle$.

Introducing the detuning Δ as in Eq. (18) and subtracting the average energy

$$\frac{\hbar}{2}\left[(2N-1)\omega_b + \omega_m + \omega_f\right]\hat{I} \tag{A3}$$

gives precisely the interaction-picture matrix in Eq. (25). Its eigenvalues, eigenvectors, and time evolution therefore coincide with those derived in the main text.

Appendix B: Onsite collisional interactions

In the main text we have considered the minimal atom–molecule conversion Hamiltonian, retaining only the

single-particle energies and the coherent atom–molecule conversion term. This allows the onsite Hamiltonian to be mapped exactly onto the standard Jaynes–Cummings Hamiltonian.

In a more complete description of an optical-lattice Mott insulator, however, one should also include onsite collisional interactions between bosonic atoms, fermionic atoms, and molecules. Neglecting molecule–molecule interactions, which are irrelevant in the present restricted Hilbert space containing at most one molecule per lattice site, the interaction Hamiltonian may be written as

$$\hat{H}_{\rm int} = \frac{\hbar U_{bb}}{2}\hat{n}_b(\hat{n}_b - 1) + \hbar U_{bf}\hat{n}_b\hat{n}_f + \hbar U_{bm}\hat{n}_b\hat{n}_m, \quad \text{(B1)}$$

where U_{bb}, U_{bf}, and U_{bm} are the onsite boson–boson, boson–fermion, and boson–molecule interaction strengths, respectively. Terms proportional to $\hat{n}_f\hat{n}_m$ and $\hat{n}_m(\hat{n}_m - 1)$ vanish identically in the sector $N_f^{\rm tot} = 1$, since the free-fermion and molecular modes cannot be occupied simultaneously and the fermionic molecular mode contains at most one particle.

For fixed conserved constituent numbers $N_b^{\rm tot} = N$ and $N_f^{\rm tot} = 1$, the dynamics remains confined to the two basis states

$$|e, N-1\rangle, \qquad |g, N\rangle. \quad \text{(B2)}$$

The interaction energies of these two configurations are

$$E_e^{(\rm int)} = \frac{\hbar U_{bb}}{2}(N-1)(N-2) + \hbar U_{bm}(N-1), \quad \text{(B3)}$$

$$E_g^{(\rm int)} = \frac{\hbar U_{bb}}{2}N(N-1) + \hbar U_{bf}N. \quad \text{(B4)}$$

The projected Hamiltonian therefore becomes

$$\hat{H}^{(N)} = \hbar\begin{pmatrix}(N-1)\omega_b + \omega_m & \chi\sqrt{N} \\ \chi\sqrt{N} & N\omega_b + \omega_f\end{pmatrix} + \begin{pmatrix}E_e^{(\rm int)} & 0 \\ 0 & E_g^{(\rm int)}\end{pmatrix}. \quad \text{(B5)}$$

Subtracting the average diagonal energy merely shifts the overall energy origin and does not affect the dynamics. The remaining Hamiltonian can be written as

$$\hat{H}_I^{(N)} = \hbar\begin{pmatrix}\Delta_N/2 & \chi\sqrt{N} \\ \chi\sqrt{N} & -\Delta_N/2\end{pmatrix}, \quad \text{(B6)}$$

where the effective atom–molecule detuning is

$$\Delta_N = \Delta - (N-1)U_{bb} + (N-1)U_{bm} - NU_{bf}, \quad \text{(B7)}$$

with $\Delta = \omega_m - \omega_f - \omega_b$ being the bare detuning introduced in the main text.

Equation (B6) [*cf.* Eq. (25)] shows that the onsite interactions contribute only diagonal matrix elements within each fixed-occupation sector. Consequently, they preserve the two-dimensional invariant subspaces generated by the conserved occupation numbers and merely renormalize the atom–molecule detuning. The coherent coupling retains the bosonic enhancement factor $\chi\sqrt{N}$, and the generalized Rabi frequency becomes

$$\Omega_N = \sqrt{\left(\frac{\Delta_N}{2}\right)^2 + N\chi^2}. \quad \text{(B8)}$$

Therefore, all analytical results derived in the main text remain valid after the simple replacement

$$\Delta \longrightarrow \Delta_N. \quad \text{(B9)}$$

The main effect of onsite interactions is thus to shift the resonance condition in an occupation-dependent manner, while preserving the exactly solvable two-dimensional structure of each fixed-occupation sector, with the same coupling matrix element $\chi\sqrt{N}$ as the corresponding Jaynes–Cummings doublet.

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