Universal free-fermion multiply-excited eigenstates and their experimental signatures in 1D arrays of two-level atoms

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One-dimensional subwavelength atom arrays display multiply-excited subradiant eigenstates which are reminiscent of free fermions. In this Letter, we show that such free-fermion eigenstates appear in case of a quadratic dispersion relation of the band of singly-excited states, by demonstrating that near the band-edge, Hamiltonians of the long-range resonant dipole-dipole interactions can be approximated by a nearest-neighbour-tunneling model diagonalized by Jordan-Wigner fermions. The universal mechanism for this phenomenon implies that the free-fermion ansatz extends to states with finite decay rates and we propose schemes for their observation, exploiting a physical transfer process between sub- and super-radiant free-fermion eigenstates, and by angular coincidences in the emission from a laser driven atomic array.

The resonant dipole-dipole interaction (RDDI) mediated between atoms by the quantized radiation field can be described by an effective non-Hermitian Hamiltonian and displays strong all-to-all interactions \cite{1}. This makes analytical theories challenging, especially for the multi-excitation regime. Recently, significant efforts have been devoted to the multiply-excited eigenstates of the RDDI Hamiltonians of 1D atom arrays \cite{2–28}. While many results have been derived for the case of arrays coupled to ideal 1D waveguides \cite{29} where RDDI has a simple form \cite{30}, some of them are regarded as universal and expected to apply for RDDI mediated by other quantum fields, e.g., the 3D free space field \cite{31}, or photonic crystal waveguides \cite{32}, etc. One such feature is the appearance of free-fermion eigenstates \cite{3–5} represented as Slater determinants of spatially distributed singly-excited eigenstates. Within the ideal 1D waveguide model \cite{5}, we have mapped the RDDI Hamiltonian to the Lieb-Liniger model \cite{34} and interpreted the free-fermion subradiant states as a Tonks-Girardeau gas \cite{35, 36}. However, universal features must be rooted in principles at a more fundamental level. To verify or substantiate if the free-fermion eigenstates are universal for the RDDI, a more generic, system-independent theory is necessary.

In this Letter, we show that if the band of singly-excited states induced by RDDI has a quadratic extremum point \(k_{\text{ex}}\), i.e., its dispersion relation can be expanded as \(\omega_{\text{eff}}(k) \approx \omega_{\text{eff}}(k_{\text{ex}}) + \alpha_2(k - k_{\text{ex}})^2\) for \(k \approx k_{\text{ex}}\) with \(\alpha_2\) an expansion coefficient, there is a family of free-fermion multiply-excited eigenstates defined in the vicinity of \(k_{\text{ex}}\). This result provides a criterion for the free-fermion states that is easy to verify. Moreover, it implies the existence of free-fermion states with finite decay rates and properties that may hence be observed in the emitted field, which is not an attractive option for the previously discovered subradiant free-fermion states \cite{3–5}. Dispersion relations with a higher power law leads to even more subradiant states \cite{37}, but they correspond to interacting fermions and do not follow the free-fermion ansatz.

Preliminaries. We consider atoms with two levels, the ground state \(|g\rangle\) and an excited state \(|e\rangle\), between which the energy gap is \(\omega_0 (\hbar = 1)\). In a regular 1D array, the atoms are equally spaced with coordinates \(z_m = m d\). The light field can be specified by its dyadic Green’s tensor \(G\). Assuming the Born-Markov approximation and translation symmetry of the light field in the direction along the array, the effective RDDI Hamiltonian is expressed as \cite{38–40}

\[
H_{\text{eff}} = -\mu_0 \omega_0^2 \sum_{m,n=1}^N \mathbf{d}_m^\dagger \cdot G(z_m - z_n, \omega_0) \cdot \mathbf{d}_n \sigma^+_m \sigma_n, \tag{1}
\]

where \(\mu_0\) denotes the vacuum permeability, \(\mathbf{d}\) is the transition dipole moment, and \(\sigma^+_m = |e\rangle \langle g|\). The Hamiltonian (1) can be rewritten in Fourier space as

\[
H_{\text{eff}} = N d \int_{-\pi/d}^{\pi/d} \frac{dk}{2\pi} \omega_{\text{eff}}(k) \sigma^+_k \sigma_k, \tag{2}
\]

where the spin-wave operator reads

\[
\sigma^+_k = \frac{1}{\sqrt{N}} \sum_{m=1}^N e^{ikz_m} \sigma^+_m, \tag{3}
\]

and \(\omega_{\text{eff}}(k)\) is the complex dispersion relation of the band of singly-excited eigenstates. For an infinite array, the state \(|k\rangle \equiv \sigma^+_k |G\rangle\), with \(|G\rangle\) the atomic ground state, has the energy \(\Re \omega_{\text{eff}}(k)\) and decay rate \(\gamma(k) = -2\Im \omega_{\text{eff}}(k)\), where \(\Re\) and \(\Im\) denote the real and imaginary parts, respectively.
According to Eq. (2) the full information of the $2^N$-dimensional Hamiltonian $H_{\text{eff}}$ is contained in the dispersion relation $\omega_{\text{eff}}(k)$, and thus, any universal features of the multiply-excited system must reflect a common property of the single excitation dispersion relation, $\omega_{\text{eff}}(k)$. The dispersion relation near a band edge is such a characteristic property of periodic systems, and we shall now show that it accounts for the universal existence of excitations that can be described as free fermions.

**Free-fermion states.** In our analysis we shall approximate $H_{\text{eff}}$ by a simpler Hamiltonian

$$H_1 = c_1 \hat{N}_e - \frac{2}{d^2} \sum_{j=1}^{N-1} \left( t_{\text{ex}} \sigma_j^+ \sigma_{j+1} + t_{\text{ex}}^* \sigma_{j+1}^+ \sigma_j \right),$$  

(4)

where the choice of parameters, $c_1 = \omega_{\text{eff}}(k_{\text{ex}}) + 2\alpha_2/d^2$ and $t_{\text{ex}} = e^{-ik_{\text{ex}}d}$ leads to the same $\omega_{\text{eff}}(k)$ as $H_{\text{eff}}$ in the vicinity of $k_{\text{ex}}$ ($\hat{N}_e = \sum_{j=1}^{N} \sigma_j^+ \sigma_j$ is the total number of excitations). $H_1$ has the exact dispersion relation, $\omega_1(k) = c_1 - 2\alpha_2/d^2 \cos[(k - k_{\text{ex}})d]$, and it can be diagonalized by the Jordan-Wigner transformation [41] $\sigma_j^+ \rightarrow e^{i\xi_j/2} \sigma_j$ and its Hermitian conjugate, where $f_m$ and $f_m^*$ are fermionic operators satisfying the anti-commutation relations $\{f_i, f_j^\dagger\} = \delta_{i,j}$ and $\{f_i, f_j\} = 0$. The transformation leads to a free-fermion Hamiltonian

$$H_1 = \sum_{\xi=1}^{N} \omega_1(k_{\text{ex}} + q_\xi) f_\xi^\dagger f_\xi,$$  

(5)

where $f_\xi = \sum_{j=1}^{N} \langle \psi_\xi | \sigma_j^\dagger | G \rangle f_j$ is the annihilation operator for the single-excitation eigenmode

$$|\psi_\xi\rangle = \frac{1}{\sqrt{2}} \left( \sigma_{k_{\text{ex}} + q_\xi} - \sigma_{k_{\text{ex}} - q_\xi} \right) |G\rangle,$$  

(6a)

with

$$q_\xi = \frac{\pi/d}{N+1}, \quad 1 \leq \xi \leq N.$$  

(6b)

We have $\langle \psi_\xi | \psi_{\xi'} \rangle = \delta_{\xi,\xi'}$ and $\{f_\xi, f_{\xi'}^\dagger\} = \delta_{\xi,\xi'}$, and states $|\psi_\xi\rangle$ with $\xi \ll N$ have wavenumbers in the vicinity of $k_{\text{ex}}$, where the quadratic expansion of $\omega_{\text{eff}}(k)$ is valid. Then an eigenstate of $H_1$ with $n_e$ excitations has the form

$$|F_\xi\rangle = f_{\xi_1}^\dagger f_{\xi_2}^\dagger \cdots f_{\xi_{n_e}}^\dagger |G\rangle,$$  

(7)

where $\xi$ denotes the string $\xi_1 \leq \xi_2 \leq \cdots \leq \xi_{n_e}$.

A similar idea of studying a (different) simpler Hamiltonian was recently used to prove a universal power-law scaling of the decay rates of the singly-excited subradiant states [37]. As in [37] we shall validate our solution by treating the difference between the exact $H_{\text{eff}}$ and the approximate $H_1$ as a perturbation, $\Delta H = H_{\text{eff}} - H_1$, which can also be written in the form of Eq. (2) with a dispersion relation $\delta \omega(k) = \omega_{\text{eff}}(k) - \omega_1(k)$. To proceed, we consider the perturbative expression

$$\langle F_\xi | \Delta H | F_{\xi'} \rangle = N \delta \omega(k) \langle \xi | \sigma_k^\dagger \sigma_k | \xi \rangle.$$  

(8)

By definition, $\delta \omega(k)$ scales as $N^{-3}$ for $|k - k_{\text{ex}}| \sim N^{-1}$, but generally as $O(1)$ outside the neighborhood of $k_{\text{ex}}$, while the occupation $\langle F_\xi | \sigma_k^\dagger \sigma_k | F_{\xi'} \rangle$ scales as $O(1)$ for $|k - k_{\text{ex}}| \sim N^{-1}$ and as $N^{-4}$ elsewhere. We assume that $\omega_{\text{eff}}(k_{\text{ex}})$ is not degenerate with $\omega_{\text{eff}}(k)$ at other wave numbers, as hybridization of these states may requires further treatment. The reported scalings are inferred from an inequality derived in the Supplemental Material [42]:

$$\left\| \sigma_k | \xi \rangle \right\| \leq \frac{1}{N} \sum_{\alpha=1}^{n_e} \left| h_k(-q_{\xi_\alpha}, q_{\xi_\alpha}) \right| + \frac{2\sqrt{N_n}}{N} \sum_{1 \leq \alpha < \beta \leq n_e} \left| h_k(\epsilon_1 q_{\xi_\alpha}, \epsilon_2 q_{\xi_\beta}) \right|,$$  

(9)

where $h_k(q_1, q_2) = \cot[(k - k_{\text{ex}} - q_1)/d] - \cot[(k - k_{\text{ex}} - q_2)/d]$. Eq. (8) thus yields the scaling $\langle F_\xi | \Delta H | F_{\xi'} \rangle \propto N^{-3}$, which is a factor $N$ smaller than the separation of the eigenvalues of $H_1$. The same scaling also holds for off-diagonal terms $\langle F_\xi | \Delta H | F_{\xi'} \rangle$ where $\xi \neq \xi'$. Therefore, $\Delta H$ can be consistently viewed as a perturbation to $H_1$, and the free-fermion states $|F_\xi\rangle$ are the leading order eigenstates of $H_{\text{eff}}$.

The above derivation solidifies the following more physical argument for the free-fermion states: A quadratic $\omega_{\text{eff}}(k)$ corresponds to a kinetic energy that can be represented by $\propto (\partial_k)^2$. Discrete versions of this operator, defined on a lattice, reduce to nearest-neighbor tunneling. Therefore, although displaying long-range hopping terms, $H_{\text{eff}}$ can be approximated by $H_1$, and give rise to Jordan-Wigner fermions due to the nature of two-level atoms.

**Experimental signatures of free-fermion eigenstates.** The above derivation did not apply any assumption about the vanishing or smallness of $\Im \omega_{\text{eff}}(k)$ and $\Im \alpha_2$, and the free-fermion states are not necessarily subradiant [3–5]. This makes it possible to observe their properties in experiments by their optical emission. Within the Markov approximation, the electric field (positive frequency part) of the emission from the atomic ensemble reads

$$\hat{E}^{(+)}(r) = \mu_0 \omega_0^2 \sum_{j=1}^{N} G(r - r_j, \omega_0) \cdot \partial_j \sigma_j(t).$$  

(10)

In the far field, $G(r, \omega_0) \propto r^{-1} e^{i k_0 f(\theta, \phi)}$, where $k_0$ is the resonant wavenumber and $f(\theta, \phi)$ the radiation pattern at polar angle $\theta$ and azimuthal angle $\phi$ [43].
Thus, $\hat{E}^+ (\theta) \propto \sqrt{N} \sigma_k \cos \theta$. This implies that distributions and correlation functions in the form of $\langle \sigma_k^+ \sigma_k \rangle$ and $\langle \sigma_k^+ \sigma_q \sigma_q \sigma_k \rangle$, etc., can be efficiently measured if $k, q \in [-k_0, k_0]$. In the following, we propose two experimental schemes for the study of signatures of the free-fermion states.

Detection scheme-1. First, we exploit the experimental ability to rapidly evolve the atomic system between the extremely subradiant and the superradiant free-fermion states: Systems with parity symmetry $\omega_{eff}(k) = \omega_{eff}(-k)$ have at least two extremum points, $k_{ex,0} = 0$ and $k_{ex,\pi} = \pi/d$. If the dispersion relations is quadratic around both extrema, they both support families of free-fermion states, that we can denote by $|F_0^\pm \rangle$ and $|F_3^\pm \rangle$, respectively. (Without parity symmetry, e.g., in chiral systems, the two extremum points may occur at other wavenumbers.) States $|F_3^\pm \rangle$ are extremely subradiant if the atom-atom separation $d$ is smaller than half of the resonant wavelength of the light field, while states $|F_0^\pm \rangle$ are usually radiant and even superradiant. The super- and sub-radiant states are connected by a single unitary $U_\pi = \sigma_z \otimes \mathbb{1} \otimes \sigma_z \otimes \mathbb{1} \otimes \sigma_z \otimes \cdots$, so that $U_\pi |F_0^\xi \rangle = |F_3^\xi \rangle$ and $U_\pi |F_3^\xi \rangle = |F_0^\xi \rangle$ for any $\xi$. $U_\pi$ factorizes and its $\pi$ phase shifts between the excited states of any two neighboring atoms can be realized, e.g., exploiting Raman energy shifts induced by a gradient magnetic field or the AC Stark shift induced by an off-resonant standing wave laser field [44].

States with the fermionic anti-symmetry are difficult to excite directly, and we propose instead to initially prepare the array in the symmetrically excited state, e.g., $|\Psi_0 \rangle = |B_{0,0,0} \rangle \propto (\sigma_{k=0}^+)^3 |G \rangle$ (see methods in Ref. [4]), and subsequently apply $U_\pi$ to transfer the excitations to the vicinity of $k_{ex,\pi}$. The resulting state does not exclusively populate an anti-symmetric free-fermion state, but it may be realized through a subsequent “evaporative cooling” process: Given no light emission is observed, the atomic state follows the “no-jump” trajectory $|\Psi_t \rangle \propto e^{-i H_{eff} t} U_\pi |\Psi_0 \rangle$ and gradually converges to the most long-lived component in the eigenstate expansion of $U_\pi |B_{0,0,0} \rangle$. This state, in turn, is dominated by the desired free-fermion state, $|F_{1,2,3}^\pi \rangle$ (in some systems a class of bound states appear with even longer lifetime [6, 7]).

Note that we can arrest the “cooling” at any time $t$, and apply $U_\pi$ to convert the system to a radiant or superradiant state around $k_{ex,0}$. Then the time evolution is governed by the radiative master equation

$$i \frac{d}{dt} \rho = H_{eff} \rho - \rho H_{eff}^\dagger + i \sum_{\xi=1}^N \gamma_\xi \sigma_{\phi_\xi} \rho \sigma_{\phi_\xi}^\dagger$$  \hspace{1cm} (11)

where $\sigma_{\phi_\xi} = \sum_{j=1}^N \langle \phi_\xi | \sigma_j^+ | G \rangle \sigma_j$. $\gamma_\xi$ and $|\phi_\xi \rangle$ are eigenvalues and eigenstates of $2H_{eff}^\dagger$, the dissipative part of $H_{eff}$ defined through $H_{eff} = H_{eff}^{Re} - iH_{eff}^{Im}$ [45]. Since $k_{ex,0}$ is also a quadratic extremum point of $3\omega_{eff}(k)$, we have $|\phi_\xi \rangle \approx |\psi_\xi \rangle$ for $\xi \ll N$.

As an example, we consider an atom array with $k_{0d} = \pi/2$ and $N = 20$ in 3D free space, where the atomic transition dipoles $d$ are aligned parallel to the array (further details are given in the Supplemental Material [42]). In Fig. 1(a), we simulate the “evaporative cooling” process and plot the fidelities $F_0 = |\langle \Psi_t | U_\pi | B_{0,0,0} \rangle |^2$ (blue line) and $F_3 = |\langle \Psi_t | F_{1,2,3}^\pi \rangle |^2$ (red line), respectively. The free-boson and free-fermion states are not orthogonal, and fully populating one implies a 0.53 population of the other. Along the no-jump trajectory, the atomic coincides with the symmetrically excited and then phase flipped free-boson state $U_\pi |\Psi_0 \rangle$, an intermediate state $|\Psi_{inter} \rangle$ with equal overlap with the phase flipped free-boson and free-fermion state, and, finally, the free-fermion state $|F_{1,2,3}^\pi \rangle$. In the simulations of the optical emission, these three states are acted upon by $U_\pi$ and then used as the initial state for the simulation of radiative emission governed by the master equation (11).

In Fig. 1(b), we plot the renormalized axial photon momentum distribution $P_k = \int_{0}^{\infty} d\tau \langle \sigma_k^\dagger (\tau) \sigma_k (\tau) \rangle$, integrated over time. The distribution is defined according to Eq. (10), and it is evaluated by averaging over 200 quantum trajectories [45].

The quantum states $|F_{1,2,3}^\pi \rangle$ and $|B_{0,0,0} \rangle$ are not orthogonal, but, as shown in Fig. 1(b), the free-fermion state $|F_{1,2,3}^\pi \rangle$ has a distinct emission profile, $P_k$ with a
lower peak value and wider shoulders than the free-boson state \(|B_{0,0,0}\rangle\). The insert in Fig. 1(b) emphasizes the destructive interference in \(P_k\) for \(|B_{0,0,0}\rangle\) at \(k \approx \pm 0.1\pi/d\). The intermediate state \(U_\pi |\Psi_{\text{inter}}\rangle\) overlaps equally with \(|B_{0,0,0}\rangle\) and \(|F^0_{1,2}\rangle\), and shares emission features of both states.

Detection scheme-2. An alternative detection of the free-fermion state characteristics may employ continuous laser excitation with a constant spatial phase, driving excitations with \(k \approx k_{\text{ex},0}\) of the atoms. Such driving is also studied in Refs. [26, 46, 47]. The collective driving is modeled by

\[
H_L = \Omega (e^{-i\delta_L t} \sigma_{k=0}^\dagger + e^{i\delta_L t} \sigma_{k=0})
\]  

and we assume the detuning \(\delta_L = \omega_0 + \Re \omega_{\text{eff}}(k_{\text{ex},0})\) so that \(|F_{1,2}\rangle\) is the doubly-excited state closest to resonance. The amplitude \(\Omega\) is assumed to be weak so that excited state components with \(n_e \geq 3\) are neglected. The emitted radiation signal may be dominated by the most populated singly-excited components of the steady state, but we can extract the properties of the doubly-excited components by observation of photon coincidences, described by the 2nd-order equal-time correlation function \(G(k_1, k_2) = N^2 (\sigma_{k_1}^\dagger \sigma_{k_2}^\dagger \sigma_{k_1} \sigma_{k_2})\) of the scattered field.

If the RDDI is negligible, the two-excitation component of the steady state will be \(|B_{0,0}\rangle \propto (\sigma_{k=0}^\dagger)^2 |G\rangle\), and only for sufficiently strong interactions will the atomic steady state, and hence the optical emission show features of \(|F_{1,2}\rangle\). To focus on the essential physical mechanisms rather than system-dependent details, we propose a minimal model

\[
i \frac{d}{dt} \rho = \mathbb{H}_1 \rho - \rho \mathbb{H}^\dagger_1 - [\rho, H_L] + i\beta \gamma_{\text{ex}} \sum_{\xi=1}^N \sigma_{\psi_\xi} \rho \sigma_{\psi_\xi}^\dagger - \frac{\Re a_2}{d^2} \sum_{j=1}^{N-1} (\sigma_j^\dagger \sigma_{j+1} + \sigma_{j+1} \sigma_j^\dagger).
\]  

(13)

where \(\mathbb{H}_1\) is derived from \(H_1\),

\[
\mathbb{H}_1 = \beta \gamma_{\text{ex}} \frac{N}{2t} \mathbb{N}_{\text{ex}} - \frac{\Re a_2}{d^2} \sum_{j=1}^{N-1} (\sigma_j^\dagger \sigma_{j+1} + \sigma_{j+1} \sigma_j^\dagger).
\]  

(14)

In this model \(\Delta \omega = \Re a_2/(Nd)^2\) characterizes the energy gaps between the free-fermion states and \(\beta \gamma_{\text{ex}}\) characterizes their linewidths, where \(\beta\) is introduced to explicitly control the value of the dimension-less ratio \(r_\beta = \Delta \omega / (\beta \gamma_{\text{ex}})\). When \(r_\beta\) is large, eigenstates other than \(|F_{1,2}\rangle\) are far from resonance and the doubly-excited states predominantly occupy \(|F_{1,2}\rangle\). Moreover, the quantum jump operators in Eq. (13) appear with the same magnitude. Thus they are equivalent to individual atomic decay described by \(\sum_j \sigma_j \rho \sigma_j^\dagger\). Eq. (13) hence describes atoms decaying independently with decay rate \(\beta \gamma_{\text{ex}}\) while being coherently coupled to the nearest neighbors with “renormalized” tunneling strength \(\Re a_2/d^2\).

We have both solved Eq. (13) and Eq. (11), including \(H_L\), for the same parameters as used in Scheme-1 but allowing variation of the dissipative part through the factor \(\beta\), i.e., \(H_{\text{eff}} \rightarrow H_{\text{eff}}^{(a)} - i\beta H_{\text{eff}}^{(b)}\). This choice of \(H_{\text{eff}}\) yields \(\Re a_{\text{eff}}(k_{\text{ex}}) \approx -1.03 \gamma_0, \gamma_{\text{ex}} \approx 3 \gamma_0\) and \(\Re a_2/d^2 \approx 0.17 \gamma_0\), that we apply in Eq. (13). In Fig. 2 we show the results of the simulation for \(N = 20\) atoms with paired parameters (\(\beta = 1/25, \Omega = 0.01 \gamma_0\)) and (\(\beta = 1/150, \Omega = 0.008 \gamma_0\)). In the Supplemental Material [42], we show results for a larger value of \(N = 30\) which blurs some of the features of \(|F_{1,2}\rangle\). The results are obtained by averaging over 200 quantum trajectories following the Monte-Carlo wavefunction formalism [45].

In Fig. 2(a), we extract the two-excitation component of each quantum state trajectory, renormalize it, and we plot its fidelity with \(|F_{1,2}\rangle\) \(|B_{0,0}\rangle\) (blue lines) [The solid lines are for Eq. (13) and the dotted lines are for Eq. (11)]. We see that for the simulation of Eq. (11), the choice of \(\beta = 1/25\) (left panel, dotted lines, \(r_\beta \approx 0.004\)) leads to a dominant steady state overlap with \(|F_{1,2}\rangle\) while for Eq. (13) (solid line) the dominant overlap is with \(|B_{0,0}\rangle\). For \(\beta = 150\) (right panel, \(r_\beta \approx 0.02\)), both models yield dominant overlap with the free-fermion state \(|F_{1,2}\rangle\).

In Fig. 2(b), we plot the two-photon coincidences, \(\log_{10} G(k_1, k_2)\) with \(0 \leq k_1, k_2 \leq 2\pi/d\) for the steady states of Eq. (13) (the first row, labelled by “toy“) and Eq. (11) (the second row). In the plots, the patterns colored by dark blue represent suppression of two-photon coincidences. In each row, plots for \(\beta = 1/25\) and \(\beta = 1/150\) are shown in the left and right column, respectively. In the third row we show results evaluated as expectation values in the states \(|B_{0,0}\rangle\) (left) and \(|F_{1,2}\rangle\) (right).

The almost identical patterns obtained for the same \(\beta\) in Fig. 2(b) show that Eq. (13) approximates Eq. (11) well. For \(\beta = 1/25\) and \(\beta = 1/150\), the patterns display an upright cross as a signature of the state \(|B_{0,0}\rangle\) and two sloping lines, characteristic of the state \(|F_{1,2}\rangle\), respectively. To distinguish them more quantitatively, in Fig. 2(c) we plot the diagonal terms, i.e., \(\log_{10} G(k, k)\), of the four subplots labeled “1-4“ in Fig. 2(b), and plot those of \(|B_{0,0}\rangle\) and \(|F_{1,2}\rangle\) in the insert. The insert shows that the upright cross of \(|B_{0,0}\rangle\) results in anti-bunching at \(k \approx 0.1 \pi/d\), while the avoided crossing of \(|F_{1,2}\rangle\) leads to a more smooth curve. The anti-bunching is clearly seen in the blue solid and dashed lines (\(\beta = 1/25\)), but are smoothed in the red lines (\(\beta = 1/150\)). The qualitative agreement between the dashed lines and solid lines in Fig. 2(c) further validates the approximate treatment by Eq. (13).

Candidate systems supporting large values of \(r_\beta\) are atom arrays coupled to photonic crystals where the atomic transition frequency \(\omega_0\) is in the vicinity of the photonic band edge [33, 48]; and atom arrays coupled to 1D waveguide modes, where at \(k_{\text{ex}} = 0\) \(H_{\text{eff}}^{(b)}\) is enhanced while \(H_{\text{eff}}^{(a)}\) is reduced due to coupling via residual non-guided modes [3].

With a more sophisticated state preparation, one may
extremum point of $\omega_{\text{eff}}(k)$ is not quadratic. Quartic extremum points exist in atom arrays in 3D free space [37]. In this case, $H_1$ (4) should be replaced by one with beyond nearest neighbor tunneling processes. After the Jordan-Wigner transformation, this corresponds to a strongly-interacting fermionic model.

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Supplemental Material to “Universal free-fermion multiply-excited eigenstates and their experimental signatures in 1D arrays of two-level atoms”

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In this Supplemental Material, we present the detailed proof of our main result that a quadratic single excitation dispersion relation implies free-fermion multiply-excited states of arrays of atomic dipoles in Sec. S-I; we present elements of the theory of atomic arrays in 3D free-space and evidence of free-fermion superradiant states that are used in our detection scheme-1 in Sec. S-II, and we show simulations of our detection scheme-2 with \( N = 30 \) atoms in Sec. S-III.

S-I. QUADRATIC DISPERSION IMPLIES FREE-FERMION STATES

Here we present our main result in details. Without loss of generality, we assume \( k_{\infty} = 0 \) throughout this section. Cases of \( k_{\infty} \neq 0 \) can be obtained by a formal translation in the Brillouin zone.

S-I.A. Write \(|F_{\xi} \rangle\) in the spin basis

In the main text, the free-fermion state \(|F_{\xi} \rangle\) is expressed with the Jordan-Wigner fermions. Here we write them in the spin basis for later convenience.

To start, we introduce a state of \( n_e \) excitations, which are ordered in the 1D array and specified by a wavenumber

\[
|k_{\xi} \rangle = |k_{\xi_1}, k_{\xi_2}, \ldots, k_{\xi_{n_e}} \rangle
\]

\[= \frac{1}{(\sqrt{N})^{n_e}} \sum_{x_{\uparrow}} \epsilon^{\sum_{j=1}^{n_e} k_{\xi_j} x_j} |x_1, x_2, \ldots x_{n_e} \rangle. \tag{S1}\]

Above we have used the basis in real space

\[
|x_1, x_2, \ldots x_{n_e} \rangle = \bigotimes_{j=1}^{n_e} \sigma^x_j |G\rangle, \tag{S2}\]

with the short-hand notation

\[
\sum_{x_{\uparrow}} \cdots \equiv \sum_{z_1 \leq x_1 < x_2 \ldots < x_{n_e} \leq z_N} \cdots, \tag{S3}\]

where \( z_1 = d \) and \( z_N = N d \) are coordinates of the first and last atom. Similarly, we will use the notation

\[
|\psi_1, \psi_2, \ldots \psi_{n_e} \rangle = \sum_{x_{\uparrow}} \prod_{j=1}^{n_e} \psi_j(x_j) |x_1, x_2, \ldots, x_{n_e} \rangle. \tag{S4}\]

Then the free-fermion state \(|F_{\xi} \rangle\) is expressed as

\[
|F_{\xi} \rangle = \sum_{p} (-1)^{P} |\psi_{p(\xi_1)}, \psi_{p(\xi_2)}, \ldots, \psi_{p(\xi_{n_e})}\rangle
\]

\[= \sum_{p} (-1)^{P} \sum_{x_{\uparrow}} \prod_{j=1}^{n_e} \psi_{p(\xi_j)}(x_j) |x_1, x_2, \ldots x_{n_e} \rangle
\]

\[= \frac{1}{\sqrt{2^{n_e}}} \sum_{p} (-1)^{P} \prod_{j=1}^{n_e} \epsilon_j |\epsilon_1 k_{p(\xi_1)}, \ldots, \epsilon_{n_e} k_{p(\xi_{n_e})}\rangle \tag{S5}\]

where \((-1)^{P}\) denotes the parity of the permutation of \( \xi \), \( \psi_{p(\xi_j)}(x_j) = \langle G | \sigma_j | \psi_{p(\xi)} \rangle \) with \( |\psi_{p(\xi)}\rangle \) defined in Eq. (6) of the main text, which can be rephrased as

\[
|\psi_{\xi} \rangle = \frac{1}{\sqrt{2}} (|q_{\xi} \rangle - |q_{\xi}^\prime \rangle). \tag{S6}\]

In the 3rd equality of Eq. (S5), \( \epsilon_j = \pm 1 \) for \( j = 1, 2, \ldots, n_e \).

1. Normalization of \(|F_{\xi} \rangle\)

We use the above notation to verify the normalization of \(|F_{\xi} \rangle\). Consider the inner product

\[
\langle F_{\xi} | F_{\xi} \rangle = \sum_{P, P'} (-1)^{P+P'} \sum_{x_{\uparrow}} \prod_{j=1}^{n} \psi_{P(\xi_j)}^* (x_j) \psi_{P(\xi)} (x_j). \tag{S7}\]

We can replace the summation of permutation \( P \) and \( P' \) by first choosing a \( P_0 \) and sum over \( P \) and \( P' = P P_0 \):

\[
\langle F_{\xi} | F_{\xi} \rangle = \sum_{P_0, P} (-1)^{P_0} \sum_{x_{\uparrow}} \prod_{j=1}^{n} \psi_{P_0(\xi_j)}^* (x_j) \psi_{P(\xi)} (x_j)
\]

\[= \sum_{P_0, P} (-1)^{P_0} \sum_{x_{\uparrow}} \prod_{j=1}^{n} \psi_{\xi_j}^* (P^{-1}(x_j)) \psi_{P_0(\xi)} (P^{-1}(x_j)). \tag{S8}\]

\[= \sum_{P_0} (-1)^{P_0} \sum_{P x_{\uparrow}} \prod_{j=1}^{n} \psi_{\xi_j}^* (x_j) \psi_{P_0(\xi)} (x_j),\]

\[\text{where}\]

\[\sum_{P x_{\uparrow}} \equiv \sum_{\{j \in P_{\text{x}\uparrow}\}} \prod_{j=1}^{n} \psi_{\xi_j}^* (x_j) \psi_{P_0(\xi)} (x_j) \]

...
where in the 2nd equality, the permutation is moved from subindex of $\psi$ to its coordinate argument; and in the 3rd equality, the replacement $x_i \to \mathcal{P}(x_i)$ is used.

Next, we notice that now the following substitution is allowed:

$$\sum_{\mathcal{P}} \sum_{x \uparrow} \to \sum_{x_1=1}^{z_N} \sum_{x_2=1}^{z_N} \cdots \sum_{x_n=1}^{z_N}.$$  \hspace{1cm} (S9)

Note that nonphysical contributions with $x_i = x_j$ cancel each other due to the anti-symmetry of the free-fermion states implied in our calculation. Using the equality $\langle \psi_{\xi} | \psi_{\xi_m} \rangle = \delta_{i,m}$, we immediately obtain

$$\langle \mathcal{F}_k | \mathcal{F}_q \rangle = \sum_{\mathcal{P}_0} (-1)^{\mathcal{P}_0} \delta_{k,q}.$$  \hspace{1cm} (S10)

This shows that the free-fermion states are orthonormal.

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**S-1.B. An equality for $\sigma_k | F_\mathcal{F} \rangle$**

Here we derive an expansion of $\sigma_k | F_\mathcal{F} \rangle$, which will be used to estimate its magnitude. The derivation is separated into a few steps.

1. **the evaluation of $\sigma_k | \bar{q} \rangle$**

Consider a state $| \bar{q} \rangle$ defined in the form of Eq. (S1), which is a component of $| F_\mathcal{F} \rangle$ given in Eq. (S5). We have the following expansion

$$\sqrt{N} \sigma_k | \bar{q} \rangle = \sum_{j=1}^{N} \frac{1}{N_n^{n/2}} \sum_{x \uparrow} e^{i \sum_{i=1}^{n} q_i (x_{i-1} - x_i)} \sigma_j | x_1, x_2, \cdots, x_n \rangle$$

$$= \sum_{m=1}^{n} \frac{1}{N_n^{n/2}} \sum_{x \uparrow} e^{i \sum_{i=1}^{n} q_i x_{i-m}} | \cdots, x_{m-1}, x_{m+1}, \cdots, x_n \rangle.$$  \hspace{1cm} (S11)

In the 2nd equality, the summation over $x_m$ can be evaluated using the fact that $x_m < x_{m+1}$:

$$\sum_{x_m=x_{m-1}+d}^{x_{m+1}-d} e^{i(q_m-k)x_m} = \frac{e^{i(q_m-k)(x_{m+1}-d)} - e^{i(q_m-k)x_{m-1}}}{1 - e^{i(q_m-k)d}}.$$  \hspace{1cm} (S12)

The above formula assumes $q_m \neq k$, while the case of $q_m = k$ can be recovered by taking the limit of the further derived expressions as $q \to k_m$. Finally, we have

$$N \sigma_k | \bar{q} \rangle = \frac{e^{i(q_1-k)z_1}}{1 - e^{i(q_n-k)d}} | q_2, q_3, \cdots, q_n \rangle - \frac{e^{i(q_n-k)(z_N+d)}}{1 - e^{i(q_n-k)d}} | q_1, q_2, \cdots, q_{n-1} \rangle$$

$$+ \sum_{m=1}^{n-1} f_k(q_m, q_{m+1}) | q_1, \cdots, q_{m-1}, q_m, q_{m+1} - k, q_{m+2}, \cdots, q_n \rangle$$

where

$$f_k(q_m, q_{m+1}) = -1 + \frac{i}{2} \cot\left(\frac{q_{m+1} - k}{2} \right) - \frac{i}{2} \cot\left(\frac{q_m - k}{2} \right).$$  \hspace{1cm} (S13)

2. **the calculation of $\sigma_k | F_\mathcal{F} \rangle$**

We start from one particular sequence of arguments $\vec{\xi}$,

$$N \sigma_k | \psi_{\xi_1}, \psi_{\xi_2}, \cdots, \psi_{\xi_{n-1}} \rangle = f_{k,L}(q_1) | \psi_{\xi_2}, \psi_{\xi_3}, \cdots, \psi_{\xi_{n-1}} \rangle - f_{k,R}(q_n) | \psi_{\xi_1}, \psi_{\xi_2}, \cdots, \psi_{\xi_{n-1}} \rangle$$

$$+ \sum_{m=1}^{n-1} \epsilon_{1,2} \epsilon_m f_k(\epsilon_1 q_m, \epsilon_2 q_{m+1}) | \psi_{\xi_1}, \cdots, \psi_{\xi_{m-1}}, \epsilon_1 q_m + \epsilon_2 q_{m+1} - k, \psi_{\xi_{m+2}}, \cdots, \psi_{\xi_{n-1}} \rangle$$

where the chain-end coefficients are

$$f_{k,L}(q_1) = \frac{e^{i(q_1-k)z_1}}{1 - e^{i(q_1-k)d}} - \frac{e^{i(-q_1-k)z_1}}{1 - e^{i(-q_1-k)d}}$$  \hspace{1cm} (S16a)

$$f_{k,R}(q_n) = \frac{e^{i(q_n-k)(z_N+d)}}{1 - e^{i(q_n-k)d}} - \frac{e^{i(-q_n-k)(z_N+d)}}{1 - e^{i(-q_n-k)d}}.$$  \hspace{1cm} (S16b)
Following Eq. (S5), now we consider the permutations and evaluate
\[ N\sigma_k \sum_p (-1)^p |\psi_{P(\xi_1)}\cdots\psi_{P(\xi_{n_c})}|. \]  
(S17)

Substituting Eq. (S15) into the permutations, we see that terms corresponding to the right hand side of the first lines of Eq. (S15) are straightforward \((n_c - 1)\)-excitation states, but those in the second line are more involved with \((n_c - 2)\) arguments in the form of \(\epsilon_1q_\alpha + \epsilon_2q_\beta - k\). We start by collecting all terms that have the same group of arguments but in different orders. We assume that \(\alpha = m = m + 1\), and we fix a particular order of \((n_c - 2)\) indices,
\[ (\xi_1, \cdots, \xi_{m-1}, \xi_{m+2}, \cdots, \xi_{n_c}). \]  
(S18)

Next, we insert \((\xi_m, \xi_{m+1})\), as a pair in one of the \((n_c - 1)\) possible locations in the above string of \((n - 2)\) indices. This yields \((n_c - 1)\) different permutations of the string \(\vec{\xi}\), which all have the same parity.

For every one of these \((n_c - 1)\) permutations, one can apply Eq. (S15) and obtain one term resembling the second line of Eq. (S15), i.e., a state denoted with \(\epsilon_1q_m + \epsilon_2q_{m+1} - k\) inserted in a string of \(\psi\). The sum of all these \((n-1)\) terms is hence

\[ \epsilon_1\epsilon_2f_k(\epsilon_1q_m, \epsilon_2q_{m+1})\sigma^\dagger_{\epsilon_1q_m + \epsilon_2q_{m+1} - k} |\psi_{\xi_1}\cdots|\psi_{\xi_{n_c}}\rangle_{m+1} \]  
(S19)

where we have used a short-hand notation
\[ |\psi_{\xi_1}\cdots|\psi_{\xi_{n_c}}\rangle_{m+1} = |\psi_{\xi_1}\cdots, \psi_{\xi_{m-1}}, \psi_{\xi_{m+2}}, \cdots, \psi_{\xi_{n_c}}\rangle, \]  
(S20)

and used the fact that
\[ \sigma^\dagger_k |q\rangle = |k,q_1,q_2,\cdots\rangle + |q_1,k,q_2,\cdots\rangle + |q_1,q_2,k,\cdots\rangle + \cdots + |q_1,q_2,\cdots,q_{n_c}\rangle. \]  
(S21)

Next, these states can also be generated in the same way by inserting the ordered pair \((q_{m+1}, q_m)\) into Eq. (S18). The parity of these permutations are just opposite to those obtained above. By adding them together, we replace the factor \(f_k(\cdots)\) in Eq. (S19) by
\[ \lambda_k(\epsilon_1q_m, \epsilon_2q_{m+1}) \equiv f_k(\epsilon_1q_m, \epsilon_2q_{m+1}) - f_k(\epsilon_2q_{m+1}, \epsilon_1q_m) = i\cot\left(\frac{k - \epsilon_1q_m}{2}\right) - i\cot\left(\frac{k - \epsilon_2q_{m+1}}{2}\right) \]  
(S22)

For any pair \((q_\alpha, q_\beta)\), we introduce the notation
\[ \sigma^\dagger_{q_\alpha,q_\beta;k} = (-1)^{\alpha + \beta - 1} \sum_{\epsilon_\alpha, \epsilon_\beta = \pm 1} \epsilon_\alpha\epsilon_\beta\lambda_k(\epsilon_\alpha q_\alpha, \epsilon_\beta q_\beta)\sigma^\dagger_{\epsilon_\alpha q_\alpha + \epsilon_\beta q_\beta - k} \]  
(S23)

and obtain the concise formula that
\[ N\sigma_k |\vec{F}_\vec{\xi}\rangle = \sum_{\alpha = 1}^{n_c} f_{k,LR}(q_\alpha) |\vec{F}_\alpha\rangle + \sum_{\alpha < \beta} \sigma^\dagger_{q_\alpha,q_\beta;k} |\vec{F}_\alpha\beta\rangle. \]  
(S24)

Here, \(|\vec{F}_\alpha\rangle\) and \(|\vec{F}_\alpha\beta\rangle\) are defined in the manner of Eq. (S20), i.e., fermionic states defined upon the ordered sequence \(\vec{\xi}\) with \(\xi_\alpha\) or both \(\xi_\alpha\) and \(\xi_\beta\), removed, respectively; and \(f_{k,LR}\) reads
\[ f_{k,LR}(q_\alpha) \equiv (-1)^{n+1}[f_{k,L}(q_\alpha) + (-1)^{n}\epsilon f_{k,R}(q_\alpha)] = (-1)^{n+1}[1 + (-1)^ne^{-i(q_\alpha-k)(N+1)d}]\frac{i}{2}\left[\cot\left(\frac{k + q_\alpha}{2}\right) - \cot\left(\frac{k - q_\alpha}{2}\right)\right]. \]

In the second equality we have employed the conditions that \(e^{2iq_\alpha(N+1)d} = 1\) and \(z_1 = d\).

---

**S-I.C. Eigenvalues of \(\sigma_k^\dagger\sigma_k\) and \(\sigma_k\sigma_k^\dagger\)**

Here we study the eigenvalues of \(\sigma_k^\dagger\sigma_k\), which will be used in the next subsection. First of all, we use a local unitary transformation
\[ U_k = \bigotimes_{i = -\infty}^{+\infty} \left( e^{iE_i\tau_i} |e_i\rangle \langle e_i| + |g_i\rangle \langle g_i| \right). \]  
(S26)
to transform \( \sigma_k \) into the standard collective spin operator

\[
S_\dagger S = U_k \sigma_k U_k \tag{S27}
\]

where \( S_\dagger = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \sigma_i \). Then the problem is reduced to the spectrum of \( S_\dagger S \), which can be expressed by angular momentum operators:

\[
S_\dagger S = \frac{4}{N} (L^2 - L_z^2 + L_z) \tag{S28}
\]

where \( L^2 \) is the squared magnitude of the total angular momentum and \( L_z = \frac{1}{2} \sum_i \sigma_i^z \) is the z-component.

In the space of \( n_e \)-excitation states, the eigenvalue of \( L_z \) is \( l = -N/2 + n_e \). The eigenvalue of \( L^2 \) is \( l(l+1) \), where the values of \( l \) should satisfy the relation that \( |l| \leq l \leq N/2 \). Let us introduce \( x = l - |l| \). Then the eigenvalues of \( S_\dagger S \) are expressed as

\[
\frac{4}{N} x(N - 2n_e + x + 1), \quad 0 \leq x \leq n_e. \tag{S29}
\]

Given that \( n_e \ll N \), the magnitude of the eigenvalues of \( S_\dagger S \) do not scale with \( N \), i.e., \( \| S_\dagger S \| \approx O(1) \). Similarly, the eigenvalues of \( SS_\dagger = \frac{4}{N}(L^2 - L_z^2 - L_z) \) are

\[
\frac{4}{N} (x + 1)(N - 2n_e + x), \quad 0 \leq x \leq n_e, \tag{S30}
\]

hence \( \| SS_\dagger \| \approx O(1) \) as well.

**S-I.D. Derivation of Eq. (9) of the main text**

Here we estimate the magnitude of \( \| \sigma_k | F_{\tilde{q}}^\gamma \| \) by using the triangle inequality on Eq. (S24)

\[
\| \sigma_k | F_{\tilde{q}}^\gamma \| \leq \frac{1}{N} \sum_{\alpha=1}^{n_e} | f_{k,LR}(q_\alpha) \| + \frac{1}{N} \sum_{\alpha < \beta} \| \sigma_{q_{\alpha}q_{\beta}}^\dagger | F_{\tilde{q}}^\gamma \| \tag{S31}
\]

where we have used the normalization \( \| F_{\tilde{q}}^\gamma \| = 1 \). There are totally \( n_e(n_e + 1)/2 \) terms in the right hand side of the inequality (S31), but \( n_e^2 \) does not scale with \( N \), given that we restrict ourselves to \( n_e \ll N \).

From Eq. (S25), it can be seen that the first term on the right hand side of the inequality (S31) is bounded from above by

\[
| f_{k,LR}(q_\alpha) \| \leq | h_k(-q_\alpha, q_\alpha) \|
= \left| \cot \left( \frac{k + q_\alpha}{2}d \right) - \cot \left( \frac{k - q_\alpha}{2}d \right) \right|, \tag{S32}
\]

where \( h_k(q_1, q_2) \) is defined in the main text.

For the second term on the right hand side of the inequality (S31), we notice that

\[
\| \sigma_{q_{\alpha}q_{\beta}}^\dagger | F_{\tilde{q}}^\gamma \| \leq \sum_{\epsilon_\alpha, \epsilon_\beta = \pm 1} \lambda_k(\epsilon_\alpha q_\alpha, \epsilon_\beta q_\beta) \| \sigma_{q_{\alpha}q_{\beta}}^\dagger \| \tag{S33}
\]

where by \( \max_{n_e - 2} \| \cdots \| \) we mean the largest eigenvalue in the subspace of \( (n_e - 2) \) excitations. We have

\[
\max_{n_e - 2} \| \sigma_{q_{\alpha}q_{\beta}}^\dagger \sigma_{q_{\alpha}q_{\beta} + q_{\alpha}q_{\beta} - k} \| = \frac{4}{N} (N - n_e - 2)(n_e - 1) < 4n_e. \tag{S34}
\]

Substituting the above inequality and Eq. (S22) into Eq. (S33), we obtain that

\[
\| \sigma_{q_{\alpha}q_{\beta}}^\dagger | F_{\tilde{q}}^\gamma \| < 2 \sqrt{n_e} \sum_{\epsilon_\alpha, \epsilon_\beta = \pm 1} | h_k(\epsilon_\alpha q_\alpha, \epsilon_\beta q_\beta) \|. \tag{S35}
\]

Assembling the above results we obtain Eq. (9) in the main text.
S-I.E. Consistency of our perturbation theory approach

The assumption $\xi_n \ll N$ implies that for $|k| \sim N^{-1}$, the magnitude of $\sigma |F_\xi^\dagger\rangle$ scales as $O(1)$. This is because $|k|$ overlaps with states in the form of $|\psi_{\xi,i}\rangle$ that constitute $|F_\xi^\dagger\rangle$.

On the other hand, for $k$ not in the vicinity of $k_{\text{ex}} = 0$, i.e., $|k| > p_0$ for any constant $p_0$ in the Brillouin zone, there will be a sufficiently large $N_0$ so that for $N > N_0$ we have $\|\sigma_k |F_\xi^\dagger\rangle\| \sim N^{-2}$. To verify this, in the previous section we have introduced

$$h_k(q_1, q_2) = \cot\left(\frac{k - q_1}{2} d\right) - \cot\left(\frac{k - q_2}{2} d\right). \quad (S36)$$

For $|k| > p_0$ and $q_1, q_2 \sim N^{-1}$ hence $q_1, q_2 \ll |k|$ for a sufficiently large $N$. Then the above expression is approximated by

$$h_k(q_1, q_2) \approx \frac{1}{\sin^2(kd/2)} \frac{q_1 - q_2}{2} \sim N^{-1}. \quad (S37)$$

The inequality derived above then leads to $\|\sigma_k |F_\xi^\dagger\rangle\| \sim N^{-2}$, or equivalently, $\langle F_\xi^\dagger | \sigma_k |F_\xi^\dagger\rangle \sim N^{-4}$.

In summary, we have

$$\langle F_\xi^\dagger | \sigma_k |F_\xi^\dagger\rangle \sim \begin{cases} O(1), & \text{if } |k| \sim N^{-1} \\ N^{-4}, & \text{if } |k| > O(N^{-1}) \end{cases} \quad (S38)$$

Recall that we can rewrite $\Delta H$ as

$$\Delta H = N \int_{-\pi/d}^{\pi/d} dk \, \delta\omega(k) |\sigma_k^\dagger\sigma_k| \quad (S39)$$

where $\delta\omega(k) = \omega_{\text{eff}}(k) - \omega_1(k)$ can be given by a Taylor series approximation

$$\delta\omega(k) = a_3 (k - k_{\text{ex}})^3 + O(k^4), \text{ for } k \approx k_{\text{ex}}. \quad (S40)$$

Alternatively, we may use the Lagrange form of the remainder of the 2nd order Taylor polynomial, and write

$$\delta\omega(k) = \frac{\delta\omega^{(3)}(\xi_k)}{6} (k - k_{\text{ex}})^3 \quad (S41)$$

where $\delta\omega^{(3)}$ is given by the 3rd order derivative of $\delta\omega$ and $\xi_k$ is a value in the interval between $k_{\text{ex}}$ and $k$.

To show that $\Delta H$ is a perturbation to $|F_\xi^\dagger\rangle$ with $\xi_n \ll N$, we rewrite Eq. (8) of the main text here:

$$\langle F_\xi^\dagger | \Delta H |F_\xi^\dagger\rangle = N \int_{-\pi/d}^{\pi/d} dk \, \delta\omega(k) \langle F_\xi^\dagger | \sigma_k^\dagger \sigma_k |F_\xi^\dagger\rangle. \quad (S42)$$

We notice that in a short interval of $k \sim N^{-1}$ (the measure of this interval is $O(N^{-1})$) we have $\delta\omega(k) \sim N^{-3}$ and $\langle F_\xi^\dagger | \sigma_k^\dagger \sigma_k |F_\xi^\dagger\rangle \sim O(N^0)$. While for the integral of $k$ not in the vicinity of $k_{\text{ex}} = 0$, for which the measure is $O(1)$, we have $\delta\omega(k) \sim O(1)$ but $\langle F_\xi^\dagger | \sigma_k^\dagger \sigma_k |F_\xi^\dagger\rangle \sim O(N^{-4})$. Therefore, the scaling of the integral must be

$$\langle F_\xi^\dagger | \Delta H |F_\xi^\dagger\rangle \sim N^{-3}. \quad (S43)$$

This shows that $\langle F_\xi^\dagger | \Delta H |F_\xi^\dagger\rangle$ will be much smaller than the energy separation between different $|F_\xi^\dagger\rangle$, which scale as $N^{-2}$, and confirms the consistency of our perturbation approach.

S-II. ATOM ARRAY IN THE 3D FREE SPACE

The RDDI Hamiltonian of an atom array in 3D free space has a closed form expression. It is used in the detection scheme-1 and in detection scheme-2 after supplementing its dissipative part with a scaling factor $\beta$.

The dyadic Green’s tensor is given by

$$G(r, \omega_0) = \frac{e^{ik_0r}}{4\pi k_0^2 r^3} \left[ (k_0^2 r^2 + i k_0 r - 1) I + \right. \left. (k_0^2 r^2 - 3 i k_0 r + 3) r r \right], \quad (S44)$$

where $I$ is the $3 \times 3$ identity tensor, $rr$ is the dyadic vector product, and $r$ is the magnitude of $r$. As in the main text.
we suppose the atomic transition dipoles are aligned parallel to the array direction. Then the dispersion relation is given by

$$\omega_{\text{eff}}(k) = -\frac{3\gamma_0}{2} \sum_{\epsilon=\pm 1}^{\xi=2,3} \xi \text{Li}_\epsilon(e^{i(k_0+\epsilon k)d})$$

where \( \text{Li}_\epsilon(z) = \sum_{n=1}^\infty z^n n^{-\epsilon} \) is the polylogarithm of order \( \xi \). The second order derivative of \( \omega_{\text{eff}}(k) \) is

$$\frac{d^2 \omega_{\text{eff}}(k)}{dk^2} = \frac{3\gamma_0}{2} \sum_{\epsilon=\pm 1}^{\xi=2,3} \xi^2 \text{Li}_\epsilon(e^{i(k_0+\epsilon k)d})$$

where \( \text{Li}_0(z) = \frac{z}{1-z} \) and \( \text{Li}_1(z) = -\ln(1-z) \). We plot \( \Re \omega_{\text{eff}}(k) \) (blue curve) and the decay rate \(-23\omega_{\text{eff}}(k) \) (red curve) in Fig. S1(a), for atom arrays with \( k_{0d} = \pi/2 \). It can be seen that \( k = 0 \) and \( k_{0d} = 2 \) are extremum points. We numerically obtain the two-excitation eigenstates of the effective RDDI Hamiltonian for an array of \( N = 20 \) atoms, and show their fidelities with the free-fermion states (grey bars) in Fig. S1(b), where the states are sorted by increasing decay rates (red curve). Formally, the shown fidelity is defined as

$$\max_{\xi_1,\xi_2} |\langle F_{\xi_1,\xi_2} | \psi_{j} \rangle|^2$$

for all 190 two-excitation eigenstates \( 1 \leq j \leq 190 \). It confirms that there are two families of states around the most subradiant and the most superradiant states that have high fidelities with the free-fermion ansatz.

**S-III. Simulations of Scheme-2 with \( N = 30 \)**

It is argued that the ratio \( r_\beta = \Delta \omega/(\beta \gamma_{\text{ex}}) \) with \( \Delta \omega = \Re \alpha_2/(N\delta)^2 \) determines the visibility of the free-fermion feature. However, in the main text, results are presented only for \( N = 20 \). Calculations with identical parameters but \( N = 30 \) show that a larger \( N \) leads to a smaller energy gap between the eigenstates and hence blurs the visibility of the free-fermion states. The simulation is restricted to the Hilbert space of \( n_e \leq 3 \), and obtained by averaging over 150 samplings of Monte Carlo quantum trajectories.

Comparing Fig. S2(a) with Fig. (2a) of the main text, we see that now for \( \beta = 1/25 \) the steady states are apparently closer to the free-boson state \( |B_{0,0}\rangle \); and for \( \beta = 1/150 \), the steady states are closer to but not perfectly described by \( |F_{1,2}\rangle \). As in Fig. (2a) of the main text, the red solid and dotted curves match better than the blue curves. This is because \( |B_{0,0}\rangle \) has overlap with states \( |F_{\xi_1,\xi_2}\rangle \) that are not close to \( k_{\text{ex}} = 0 \), for which our “toy model” becomes less precise.

In Fig. S2(b) we plot \( \log_{10} G(k_1,k_2) \) for \( 0 \leq k_1, k_2 \leq 0.2\pi/d \). The arrangement of the subplots is same as in the main text. It can be seen that patterns of suppressed coincidence are different for \( |B_{0,0}\rangle \) and \( |F_{1,2}\rangle \): the former is featured by four upright crossings, which are absent in the latter. The two states of \( \beta = 1/25 \) clearly display the crossings, while for \( \beta = 1/150 \) the crossings are deformed. Comparing them with the plot of \( |F_{1,2}\rangle \) we can see that the character of the free-fermion state is not clear, demonstrating that a larger \( N \) reduces the visibility.

In Fig. S2(c) we plot the diagonal lines of the subplots of Fig. S2(b). In the insert we see that the blue solid and dashed lines for \( |B_{0,0}\rangle \) feature two regions of suppressed coincidences (\( \beta = 1/25 \)). The curves for \( \beta = 1/150 \) (red lines) unambiguously show the first reduced coincidence, at about \( k = 0.1\pi/d \), a little bit towards larger \( k \) compared with those of \( |B_{0,0}\rangle \) and the values for \( \beta = 1/25 \). However, the second region with suppressed coincidences is flattened for \( |F_{1,2}\rangle \) (the red curves).

It is important to emphasize that the eigenstates of the system become better and better approximated by the fermionic states for large \( N \). What we have shown here is only that the reduced level spacing for larger \( N \) makes it more difficult to prepare and detect the fermionic states by optical means.

![Figure S2. Detection scheme-2 with \( N = 30 \). (a) Fidelities between the two-excitation components of the steady states (normalized) and the bosonic state \( |B_{0,0}\rangle \) (blue) and \( |F_{1,2}\rangle \) (red), with solid lines and dotted lines defined as in Fig. 2 of the main text. (b) \( \log_{10} G(k_1,k_2) \) evaluated from the steady states, with the three rows defined as in Fig. 2 of the main text. The color map belongs to the 1st and 2nd rows. The color map of the 3rd row is not shown. (c) \( \log_{10} G(k,k) \), i.e., the diagonal lines of the plot in (b).](image-url)