III. FOURIER MODE REPRESENTATION

The lattice has discrete translational symmetry, and we can hence simplify the above Hamiltonian (12) and reset operator (20) by transforming to Fourier space, which we do in this section.

A. Mode operators

The Fourier mode operators $s_{\mathbf{p}}$, $b_{\mathbf{p}\alpha}$ are labelled by a wavevector $\mathbf{p}$, which runs over the first Brillouin zone $-\pi/a < p_\alpha \leq \pi/a$, where a is the lattice spacing. They are defined in terms of the single site electronic excitation and phonon operators S_i, $B_{i\alpha}$ by

$$\begin{aligned} s_{\mathbf{p}} &= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{X}_i} S_i \,, \\ b_{\mathbf{p}\alpha} &= \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{X}_i} B_{i\alpha} \,, \end{aligned} \tag{21}$$

where N is the total number of atoms and we assume periodic boundary conditions. The creation operators $s^\dagger_{\mathbf{p}}$, $b^\dagger_{\mathbf{p}\alpha}$ are given by the Hermitian conjugates of Eq. (21). As before, α denotes the direction of vibration of the atoms and can assume the values x, y, and z.

These operators create or destroy collective excitations spread over all the atoms. The internal atomic excitations are hardcore bosons (no more than one can exist on any one atom), and hence $s_{\mathbf{p}}$, $s^\dagger_{\mathbf{p}}$ do not exactly obey normal bosonic commutation relations, but in the limit of small excitation density the difference can be neglected [26, 27]. (We cannot use the Jordan-Wigner transformation to turn them into fermions, as their number is not conserved.) The collective phonons described by $b_{\mathbf{p}\alpha}$ are ordinary bosons, as in the deep lattice limit one atom can have any number of phonons. As we shall see below, the electronic excitations propagate by photon exchange, while the phonons do not propagate to zeroth order in η_α.

B. The conditional Hamiltonian

The definitions (21) can be inverted to give the single site operators S_i, $B_{i\alpha}$ in terms of the Fourier mode operators $s_{\mathbf{p}}$, $b_{\mathbf{p}\alpha}$. We now substitute this into the conditional Hamiltonian Eq. (12), and make a Lamb-Dicke expansion up to second order in η_α, using Eqs. (16)-(18). Introducing the notation

$$H_{\mathrm{cond}} = H^{(0)}_{\mathrm{cond}} + H^{(1)}_{\mathrm{cond}} + H^{(2)}_{\mathrm{cond}} \,, \tag{22}$$

where the superscripts indicate the order of each term with respect to η_α, we obtain

$$\begin{aligned} H^{(0)}_{\mathrm{cond}} &= \frac{1}{2}\hbar\sqrt{N}\Omega(s_{\mathbf{k}_\mathrm{L}} + s^\dagger_{\mathbf{k}_\mathrm{L}}) - \sum_{\mathbf{p}} \frac{\mathrm{i}}{2}\hbar c(\mathbf{p})\, s^\dagger_{\mathbf{p}} s_{\mathbf{p}} + \sum_{\mathbf{p},\alpha} \hbar\nu_\alpha b^\dagger_{\mathbf{p}\alpha} b_{\mathbf{p}\alpha} \,, \\ H^{(1)}_{\mathrm{cond}} &= \sum_{\mathbf{p},\alpha} \frac{\mathrm{i}}{2}\, \hbar\eta_\alpha \Omega\, \hat{k}_{\mathrm{L}\alpha}(b_{\mathbf{p}\alpha} + b^\dagger_{-\mathbf{p}\alpha})(s^\dagger_{\mathbf{k}_\mathrm{L}+\mathbf{p}} - s_{\mathbf{k}_\mathrm{L}-\mathbf{p}}) - \sum_{\mathbf{p},\mathbf{q},\alpha} \frac{\mathrm{i}\hbar}{2\sqrt{N}}[d_\alpha(\mathbf{q}) - d_\alpha(\mathbf{p}+\mathbf{q})](b_{\mathbf{p}\alpha} + b^\dagger_{-\mathbf{p}\alpha}) s^\dagger_{\mathbf{p}+\mathbf{q}} s_{\mathbf{q}} \,, \\ H^{(2)}_{\mathrm{cond}} &= -\sum_{\mathbf{p},\mathbf{q},\alpha,\beta} \frac{\hbar}{4\sqrt{N}}\, \eta_\alpha\eta_\beta\Omega\, \hat{k}_{\mathrm{L}\alpha}\hat{k}_{\mathrm{L}\beta}(b_{\mathbf{p}\alpha} + b^\dagger_{-\mathbf{p}\alpha})(b_{\mathbf{q}\beta} + b^\dagger_{-\mathbf{q}\beta})(s^\dagger_{\mathbf{k}_\mathrm{L}+\mathbf{p}+\mathbf{q}} + s_{\mathbf{k}_\mathrm{L}-\mathbf{p}-\mathbf{q}}) \\ &\quad + \sum_{\mathbf{p},\mathbf{q},\mathbf{r},\alpha,\beta} -\frac{\mathrm{i}\hbar}{2N}[e_{\alpha\beta}(\mathbf{r}+\mathbf{q}) - 2e_{\alpha\beta}(\mathbf{r}) + e_{\alpha\beta}(\mathbf{r}-\mathbf{p})](b_{\mathbf{p}\alpha} + b^\dagger_{-\mathbf{p}\alpha})(b_{\mathbf{q}\beta} + b^\dagger_{-\mathbf{q}\beta}) s^\dagger_{\mathbf{r}+\mathbf{q}} s_{\mathbf{r}-\mathbf{p}} \,, \end{aligned} \tag{23}$$

where addition of wavevectors is defined mod the Brillouin zone. Here the coefficients $c(\mathbf{p})$, $d_\alpha(\mathbf{p})$, $e_{\alpha\beta}(\mathbf{p})$ are given by

$$\begin{aligned} c(\mathbf{p}) &= \sum_i \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{X}_i} C(\mathbf{X}_i) \,, \\ d_\alpha(\mathbf{p}) &= \sum_i \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{X}_i} D^\alpha(\mathbf{X}_i) \,, \\ e_{\alpha\beta}(\mathbf{p}) &= \sum_i \mathrm{e}^{-\mathrm{i}\mathbf{p}\cdot\mathbf{X}_i} E^{\alpha\beta}(\mathbf{X}_i) \,. \end{aligned} \tag{24}$$

These are the discrete Fourier transforms of the constants C_{ij}, D^α_{ij} and $E^{\alpha\beta}_{ij}$ in Eqs. (19) and (18), with the single atom terms $\hbar(\Delta - \frac{\mathrm{i}}{2}\Gamma)$ absorbed into them by allowing $i = j$ and defining

$$C(\mathbf{0}) \equiv \Gamma + 2\mathrm{i}\Delta \quad \text{and} \quad D^\alpha(\mathbf{0}) \equiv 0 \,. \tag{25}$$

They are functions of wavevector $\mathbf{p}$, and also depend on the lattice spacing and orientation; they are plotted against $\mathbf{p}$ in Fig. 9(d) for a few example settings.

The main advantage of changing into the Fourier space is that the zeroth order term (in η_α) $C(\mathbf{X})$ in the dipole-