

Optimized geometries for optical lattices

A,¹ B,¹ and C¹

¹Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

This is the abstract.

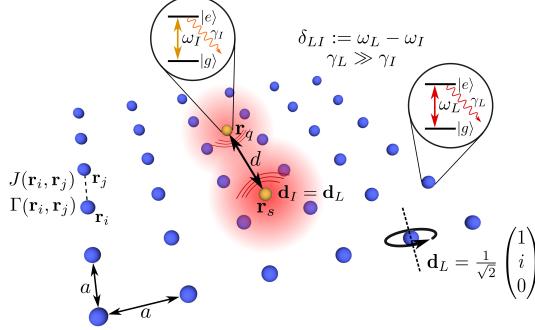


Figure 1. •

I. INTRODUCTION

II. MODEL

[arb. geometry, Green's Tensor, Couplings, Polarizations → Distance dependence, Hamiltonian, Self-energy, Ref. to Taylor's work]

We consider two-dimensional sub-wavelength lattices of quantum emitters which interact via resonant dipole-dipole interactions. The emitters are assumed to be two-level stems with a ground state $|g\rangle$ and an excited state $|e\rangle$ with a transition frequency $\omega_L = ck_L$, such that $k_L = 2\pi/\lambda_L$ denotes the related wavenumber with the resonance wavelength λ_L . Pairwise resonant dipole-dipole interactions among emitters result in collective couplings J_{ij} and collective decay rates Γ_{ij} between emitters i and j at positions \mathbf{r}_i and \mathbf{r}_j , given by

$$J_{ij} = -\frac{3\pi\sqrt{\gamma_i\gamma_j}}{\omega_L} \hat{d}_i^\dagger \cdot \mathbf{Re}[\mathbf{G}(\mathbf{r}_{ij}, \omega_L)] \cdot \hat{d}_j \quad (1a)$$

$$\Gamma_{ij} = \frac{6\pi\sqrt{\gamma_i\gamma_j}}{\omega_L} \hat{d}_i^\dagger \cdot \mathbf{Im}[\mathbf{G}(\mathbf{r}_{ij}, \omega_L)] \cdot \hat{d}_j \quad (1b)$$

where γ_i and γ_j are the decay rates of the individual dipoles i and j , and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ is the displacement vector. $\mathbf{G}(\mathbf{r}_{ij}, \omega_L)$ is the Green's tensor, defined as

$$G_{\alpha\beta}(\mathbf{r}, \omega) = \frac{e^{i\omega r}}{4\pi r} \left[\left(1 + \frac{i}{\omega r} - \frac{1}{\omega^2 r^2} \right) \delta_{\alpha\beta} - \left(1 + \frac{3i}{\omega r} - \frac{3}{\omega^2 r^2} \right) \frac{r_\alpha r_\beta}{r^2} \right] - \frac{\delta(\mathbf{r})}{3\omega^2} \delta_{\alpha\beta} \quad (2)$$

d_i and d_j are the dipole polarizations, which are set to be uniformly circular, so that $\hat{d}_L = \hat{d}_I = \frac{1}{\sqrt{2}} (1 \ i \ 0)^T$

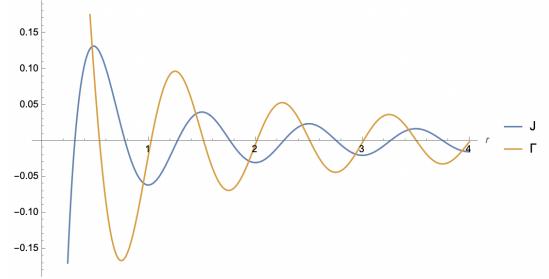


Figure 2. •

where \hat{d}_L is the polarization of the lattice dipoles, and \hat{d}_I is the polarization of any impurities. This polarization ensures that the dynamics of the system depend purely on the relative distances r_{ij} between pairs of dipoles, independent of their relative orientations. As a result, J_{ij} and Γ_{ij} can be written as

$$J_{ij} = -\frac{3}{8\omega_L r_{ij}} \left(\cos(\omega_L r_{ij}) + \frac{\sin(\omega_L r_{ij})}{\omega_L r_{ij}} + \frac{\cos(\omega_L r_{ij})}{(\omega_L r_{ij})^2} \right) \quad (3a)$$

$$\Gamma_{ij} = \frac{3}{4\omega_L r_{ij}} \left(\sin(\omega_L r_{ij}) - \frac{\cos(\omega_L r_{ij})}{\omega_L r_{ij}} + \frac{\sin(\omega_L r_{ij})}{(\omega_L r_{ij})^2} \right) \quad (3b)$$

In this way, collective couplings (Fig. ??) and collective decay rates (Fig. ??) depend purely on the relative distances r_{ij} between pairs of dipoles, independent of their relative orientations. Into this lattice, we place one or two lattice impurities with transition frequency $\omega_I \approx \omega_L$. The overall Hamiltonian is $H = H_L + H_{LI} + H_I$, where H_L is the Hamiltonian of the lattice, H_{LI} is the Hamiltonian for the interaction between the lattice and any impurities, and H_I is for the interactions involving just impurities. These Hamiltonians are defined such that

$$H_L = \sum_i^{N_L} \left(\omega_L - \frac{i}{2}\gamma_L \right) \sigma_i^\dagger \sigma_i + \sum_{i,j \neq i}^{N_L} \left(J_{ij} - \frac{i}{2}\Gamma_{ij} \right) \sigma_i^\dagger \sigma_j \quad (4a)$$

$$H_{LI} = \sum_i^{N_L} \sum_j^{N_I} \left[\left(J_{ij} - \frac{i}{2}\Gamma_{ij} \right) \sigma_i^\dagger s_j + \left(J_{ji} - \frac{i}{2}\Gamma_{ji} \right) s_j^\dagger \sigma_i \right] \quad (4b)$$

$$H_I = \sum_j^{N_I} \left(\omega_I - \frac{i}{2}\gamma_I \right) s_j^\dagger s_j + \sum_{i,j \neq i}^{N_I} \left(J_{ij} - \frac{i}{2}\Gamma_{ij} \right) s_j^\dagger s_j \quad (4c)$$

where N_L is the number of lattice atoms, σ_i is the lowering operator for lattice atom i , N_I is the number of impurities, and s_j is the lowering operator for impurity j .

[Then, at some point here or later, explain the role of the detuning delta]

III. SINGLE IMPURITY CASE

[Define lattices, define distances related to lattices, Γ_{eff} , constant area]

The generic form of the Hamiltonian for a given lattice of N atoms along with a single impurity is

$$H = \begin{pmatrix} & C_{LI} \\ H_L & \vdots \\ C_{IL} & \cdots & C_{IL} & H_I \end{pmatrix} \quad (5)$$

where H_L represents the $N \times N$ matrix of terms for the lattice's own Hamiltonian, H_I is the lattice, and C_{IL} along with C_{LI} represent the coupling terms between the lattice atoms and the impurity.

Define the wavefunction such that $\psi = (b_1 \ : \ b_N \ : \ c)^T$, and assume that the lattice occupies a steady state, so that the Schrödinger equation is

$$i\hbar \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \dot{c} \end{pmatrix} = \begin{pmatrix} & C_{LI} \\ H_L & \vdots \\ C_{IL} & \cdots & C_{IL} & H_I \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_N \\ c \end{pmatrix} \quad (6)$$

This can be solved to get

$$\begin{pmatrix} b_1 \\ \vdots \\ b_N \end{pmatrix} = -H_L^{-1} C_{LI} c \quad (7)$$

Putting this back into the Schrödinger equation produces

$$\dot{c} = -i(H_I - C_{IL}^T H_L^{-1} C_{LI})c \quad (8)$$

Recognizing that $H_I - C_{IL}^T (H_L^{-1}) C_{LI} = \Sigma_I - i\frac{\gamma_I}{2}$, we can calculate the impurity's self-energy Σ_I to be

$$\Sigma_I = H_I - C_{IL}^T (H_L^{-1}) C_{LI} + i\frac{\gamma_I}{2} \quad (9)$$

The effective decay rate Γ_{eff} for an impurity in the lattice is related to this self-energy according to

$$\Gamma_{\text{eff}} = \gamma_I - 2 \operatorname{Im}[\Sigma_I] \quad (10)$$

Equipped with these mathematical tools, we consider the full range of non-centered Bravais lattices, for both

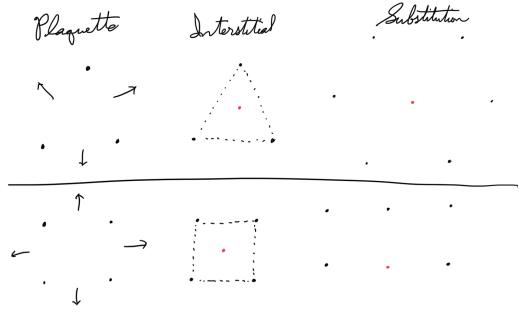


Figure 3. •[Should this be made into one long line and put at the top of a page? Also, maybe draw out the full lattices, all 4x4, and the whole triangular lattice. Or maybe just the triangular lattice?]

interstitial and substitutional impurity positions, as illustrated in Fig. 3. In order to reasonably compare lattices of differing geometries, we ensure, whenever possible, that all plaquettes possess the same area throughout all possible transformations.

[This is just a holding space for this matrix, in case we want to copy and paste it to anywhere. I don't actually intend for it to sit here in this section.]

$$H = \begin{pmatrix} -\frac{i\gamma_L}{2} - \frac{\delta_{LI}}{2} & J(r_{12}) - \frac{i\Gamma(r_{12})}{2} & \dots \\ J(r_{21}) - \frac{i\Gamma(r_{21})}{2} & -\frac{i\gamma_L}{2} - \frac{\delta_{LI}}{2} & \dots \\ \vdots & \ddots & \ddots \end{pmatrix} \quad (11)$$

A. Interstitial

Consider a finite square lattice, with an inter-atomic spacing of $a = 0.2$, defined as a function of the lattice's resonant wavelength. Compare this to the other Bravais lattices, namely a triangular lattice, and monoclinic lattice defined over θ from $\pi/2$ to 0, and a rectangular lattice with a scaling factor μ such that the horizontal sidelength of its rectangular plaquette is μa . [Which variable do we want for scaling? Does μ work?.] To ensure that the plaquettes of all of these lattices have the same area, we set the sidelength of the triangular plaquettes to $\frac{2}{3^{1/4}} a$, the height of monoclinic lattices to a for all θ , and the height of the rectangular lattices to a/μ .

For an interstitial impurity, the position of the impurity in the plaquette along with its detuning relative the lattice's resonant frequency determine its decay properties. Detuning is defined as $\delta_{LI} = \omega_I - \omega_L$. For a given impurity position, δ_{LI} can be chosen to give optimal Γ_{eff} , by minimizing along a curve such as Fig. 5. By conducting this optimization for all positions within a plaquette, a map of the optimal impurity placement can be constructed. The results of this are depicted in Fig. 4. See

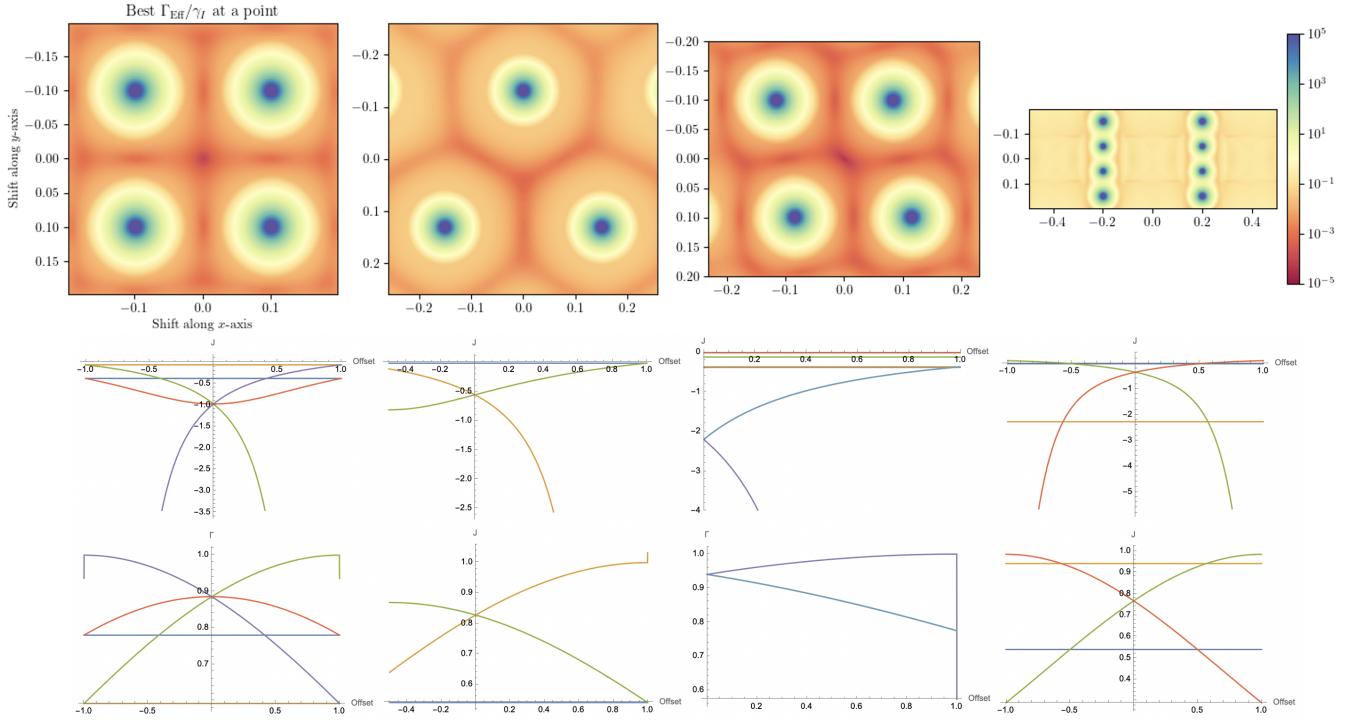


Figure 4. • [To do: 1) Change monoclinic plaquette to something more like theta = 0.4. 2) Change rectangular scaling to something more like 1.5 3) Draw line paths across all the plaquettes, illustrating which paths the plots are graphed over]

the appendix for the values of δ_{LI} corresponding to these impurity positions.

In all cases, geometric symmetries determines where the points of minimal Γ_{eff} lie. The paths of minimal Γ_{eff} follow the geometry of a Voronoi diagram where the lattice atoms are taken to be ...

Whichever geometry one examines, the center of the plaquette is either the optimal position, or at least one of the better positions. For highly symmetric lattices, such as the square lattice and the triangular lattice, it is unequivocally the optimal position, while for lattices where some symmetries are broken by a variable parameter, such as the monoclinic and rectangular lattices, other points can have slower decay rates than the center.

The role of symmetry is particularly clear once the coupling terms between pairs of particles are plotted over paths through the plaquette space.

In particular, the points at which the values of coupling terms coincide match the points of geometric symmetry. This is to be expected,

(as with a square lattice and a triangular lattice)

(as with the monoclinic lattice and the rectangular lattice)

Fig. 4 depicts the optimal value of Γ_{eff}

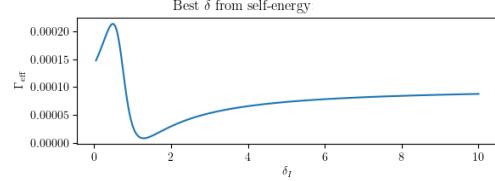


Figure 5. •

B. Substitutional

C. Square vs. triangular

Consider a finite square lattice, with an inter-atomic spacing of $a = 0.2$, defined as a function of [that characteristic wavelength].

Compare this to a triangular lattice with the same plaquette area, and hence, a side-length of (...) [fill in these details]

[Put a diagram of all the Bravais lattices, as a part of this one.]

See Fig. 3.

1. Interstitial

[Interstitial which imposes one more length scale -> refer to analytics, numerics -> impurity position] Now, consider an impurity atom placed within a plaquette. For the square case, we implemented this arrangement using a 4×4 lattice, so that the impurity was centered within the lattice.

Likewise, for the triangular case, we placed the impurity at the center of a [12 atom?] lattice, with the following arrangement.

By placing the impurity at the center of a plaquette, only one additional length scale is introduced.

After attempting to place the impurity off-center,

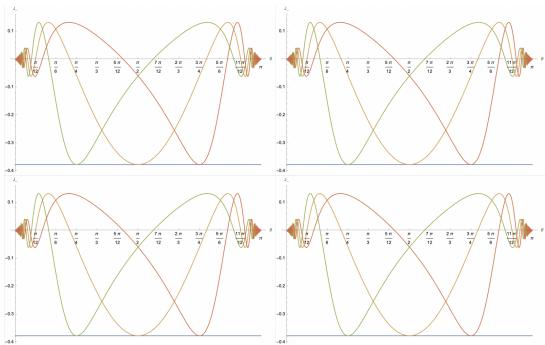
[Either one or both of these plots, perhaps for some different range of values. Also, can this be fully in-line, or should it be given a caption?] [Have a single graph, from the analytics]

[Should the plots in Fig. 6 and Fig. 7 be separate?] [Take out optimal delta values, and put it in the appendix. Change to Stefan's recommendation, with square and triangle side-by-side, and the minimal lineplots directly below]

it is clear that the point at which the impurity atom experiences minimal decay is at the center of the plaquette.

This point also possesses the highest symmetry, suggesting that additional symmetries lead to slower decay rates. This hypothesis is supported by the behavior of the coupling constants for various positions of the impurity away from the center

[a diagram of this description, which has not been made yet. Or perhaps two diagrams, one moving from the center to a lattice point, and another moving from the center to the midpoint between two lattice points. Actually, four diagrams, because these two should be made for both the square and triangular cases. See placeholder below]



[This is a placeholder. again, should this be given a caption?] [Consolidate into the two big pictures of this section, as Stefan's outline shows]

2. Substitution

[Does NOT(!) impose another length scale as long as it is not away from the center -> refer to analytics, -> always at band edge, numerics -> impurity position]

Now, considering substituting a lattice atom for an impurity, so that, in effect, the impurity takes up a vacancy in the lattice. For the square lattice, we used this 5×5 geometry for our analysis:

[diagram. Or is this unnecessary? Probably not]

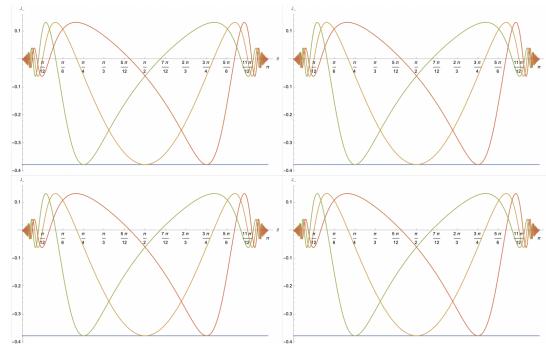
and for the triangular lattice, we used this geometry

[Don't mind the spacing error, that will be fixed. Also, caption or not? Also, make sure to redo simulations with specifically this geometry]

Performing this substitution on the lattice introduces no additional length scales, as long as the impurity is placed at the center of the vacancy. If it is placed off-center, the best possible values of Γ_{eff} are

Once again, the point with the highest symmetry experience minimal decay rates.

[Maybe include another analytic plot showing how symmetry changes coupling constants? Just do this for square lattice.]



[placeholder. Also, should this be combined with the other couplings plot? To give a kind of plot of symmetries? Then there will be 3 pages of large plots.]

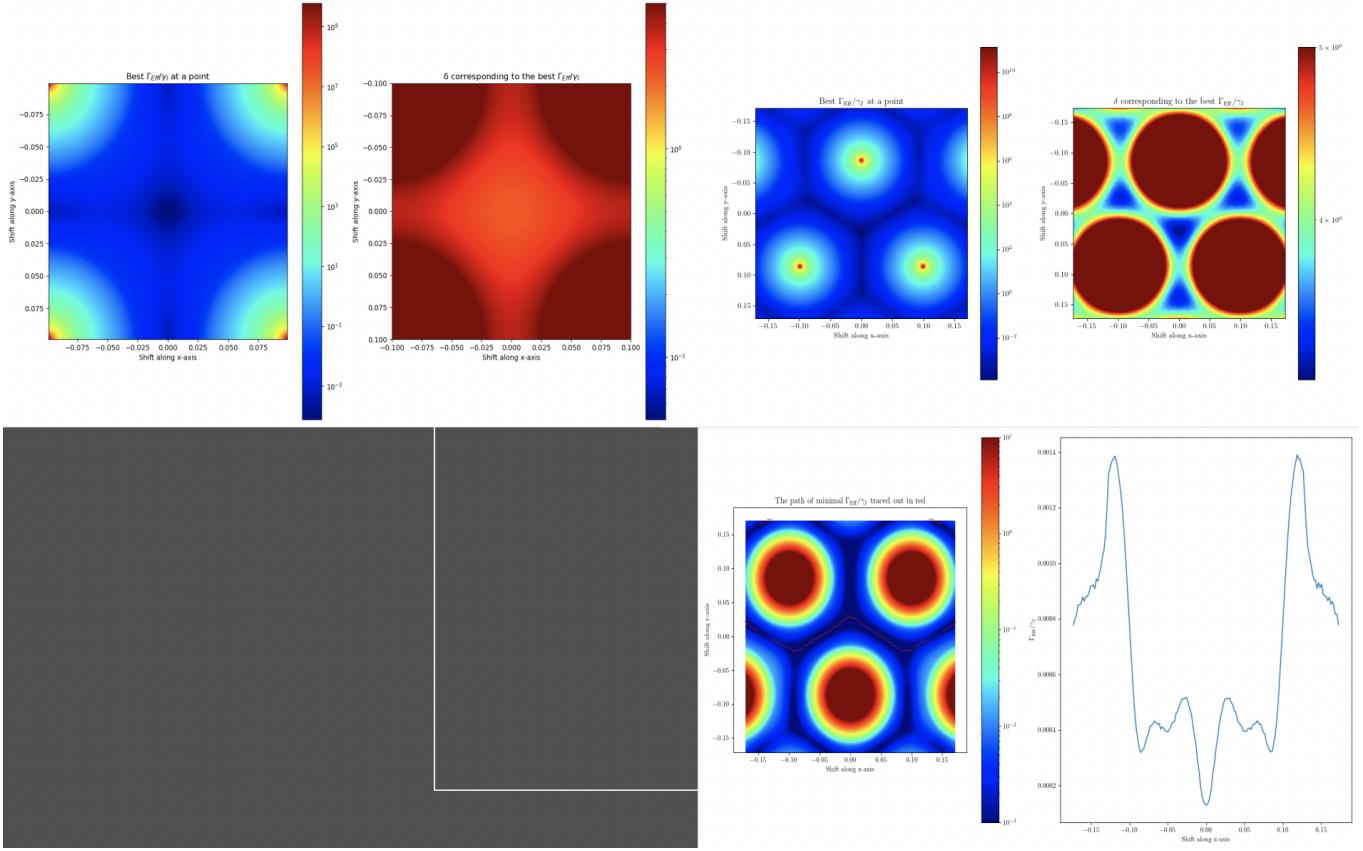


Figure 6. •

D. Monoclinic vs. rectangular lattice

[similar arguments]

Now, consider the Bravais lattices defined by variable parameters.

In particular, consider a monoclinic lattice defined by θ , such that at $\theta = \frac{\pi}{2}$ we recover the square lattice case with an inter-atomic spacing of 0.2. By maintaining a constant vertical distance between the layers of the lattice, we ensure that the area of the plaquettes remains constant over the range $0 < \theta \leq \frac{\pi}{2}$.

[diagram of this geometry]

1. Interstitial

2. Substitution

3. Varying scaling factors

[justify why we use interstitial in the following]

IV. TWO IMPURITY CASE

[Q-factor, analyze different lattices -> discuss the most important figures, constant distance]

Γ_{eff} for a lattice with two impurities is calculated in a manner analogous to the single-impurity case, starting with the Schrödinger equation for the two-impurity Hamiltonian, for which

$$i\hbar \begin{pmatrix} 0 \\ \vdots \\ 0 \\ \dot{c} \\ \dot{d} \end{pmatrix} = \begin{pmatrix} H_L & C_{L1} & C_{L2} \\ & \vdots & \vdots \\ & C_{L1} & C_{L2} \\ C_{1L} & \cdots & C_{1L} & H_1 & C_{12} \\ C_{2L} & \cdots & C_{2L} & C_{21} & H_2 \end{pmatrix} \begin{pmatrix} b_1 \\ \vdots \\ b_N \\ c \\ d \end{pmatrix} \quad (12)$$

In this way,

$$b = -(H_L)^{-1}(C_{L1}c + C_{L2}d) \quad (13)$$

Putting this result back into the Schrödinger equation

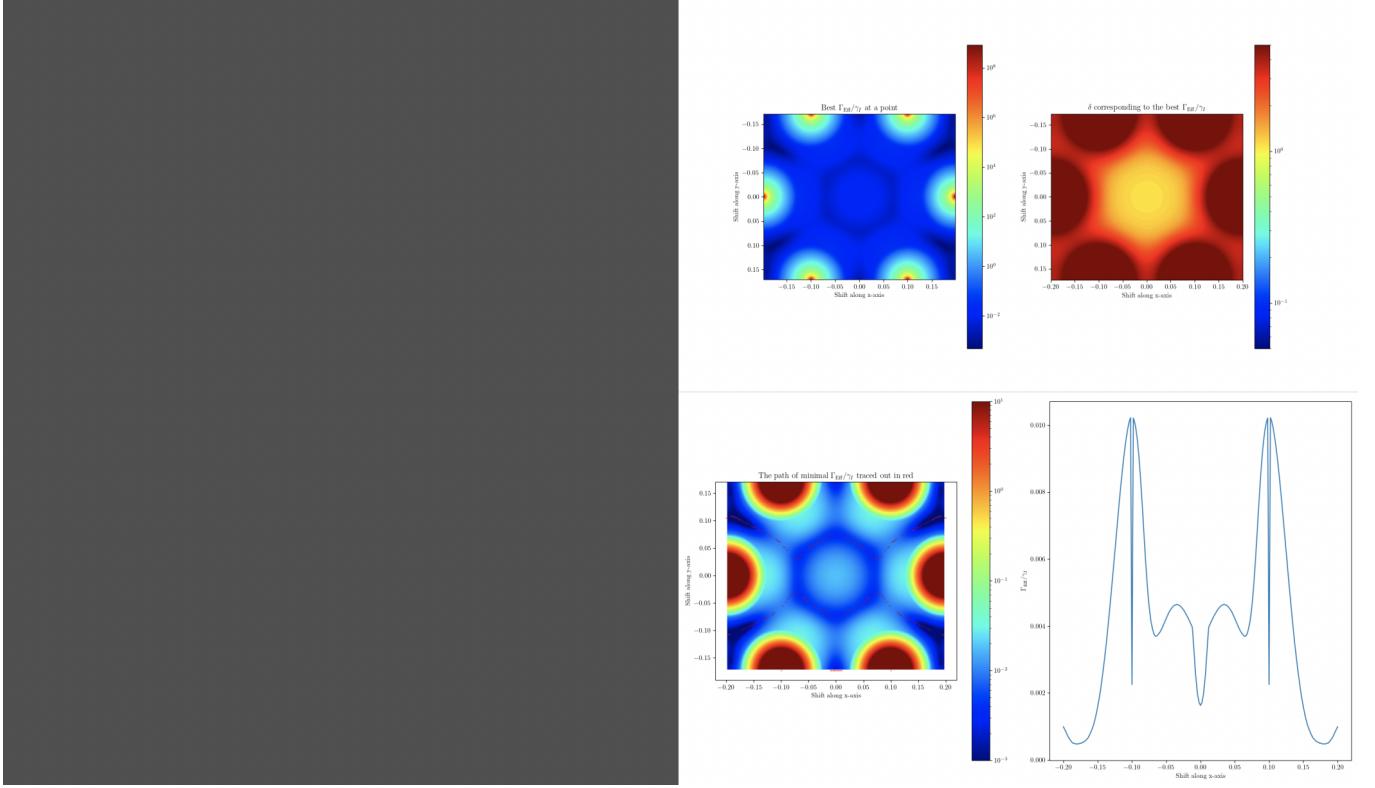


Figure 7. •

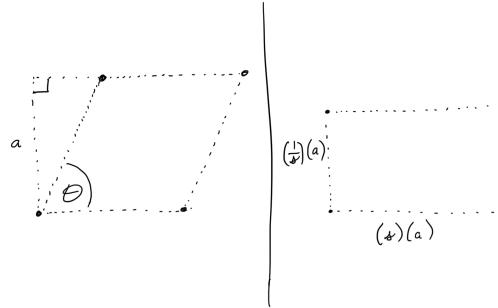


Figure 8. •

gives

$$\begin{aligned} \dot{c} &= -i \left[H_1 - C_{1L}^T (H_L)^{-1} C_{L1} \right] c \\ &\quad - i \left[C_{12} - C_{1L}^T (H_L)^{-1} C_{L2} \right] \end{aligned} \quad (14a)$$

$$\begin{aligned} \dot{d} &= -i \left[H_2 - C_{2L}^T (H_L)^{-1} C_{L2} \right] c \\ &\quad - i \left[C_{21} - C_{2L}^T (H_L)^{-1} C_{L1} \right] d \end{aligned} \quad (14b)$$

Let $\dot{c} = -i[\Sigma_1 - \frac{i\gamma_1}{2}]c - i\kappa_1 d$ and $\dot{d} = -i[\Sigma_2 - \frac{i\gamma_2}{2}]d - i\kappa_2 c$, where κ_1 and κ_2 are ‘‘effective couplings.’’ Solving for

these and the self-energies results in

$$\Sigma_1 = H_1 - C_{1L}^T (H_L)^{-1} C_{L1} + \frac{i\gamma_1}{2} \quad (15a)$$

$$\Sigma_2 = H_2 - C_{2L}^T (H_L)^{-1} C_{L2} + \frac{i\gamma_2}{2} \quad (15b)$$

$$\kappa_1 = C_{12} - C_{1L}^T (H_L)^{-1} C_{L2} \quad (15c)$$

$$\kappa_2 = C_{21} - C_{2L}^T (H_L)^{-1} C_{L1} \quad (15d)$$

The impurities’ effective decay rates are determined by $\Gamma_{\text{eff},i} = \gamma_i - 2 \text{Im}[\Sigma_i]$, where i stands for either the first or second impurity. Likewise, we define the Q-factor as a function of the effective decay rate and the effective coupling, so that $Q_i = \frac{\text{Re}[\kappa_i]}{\Gamma_{\text{eff},i}}$ for each of the two impurities.

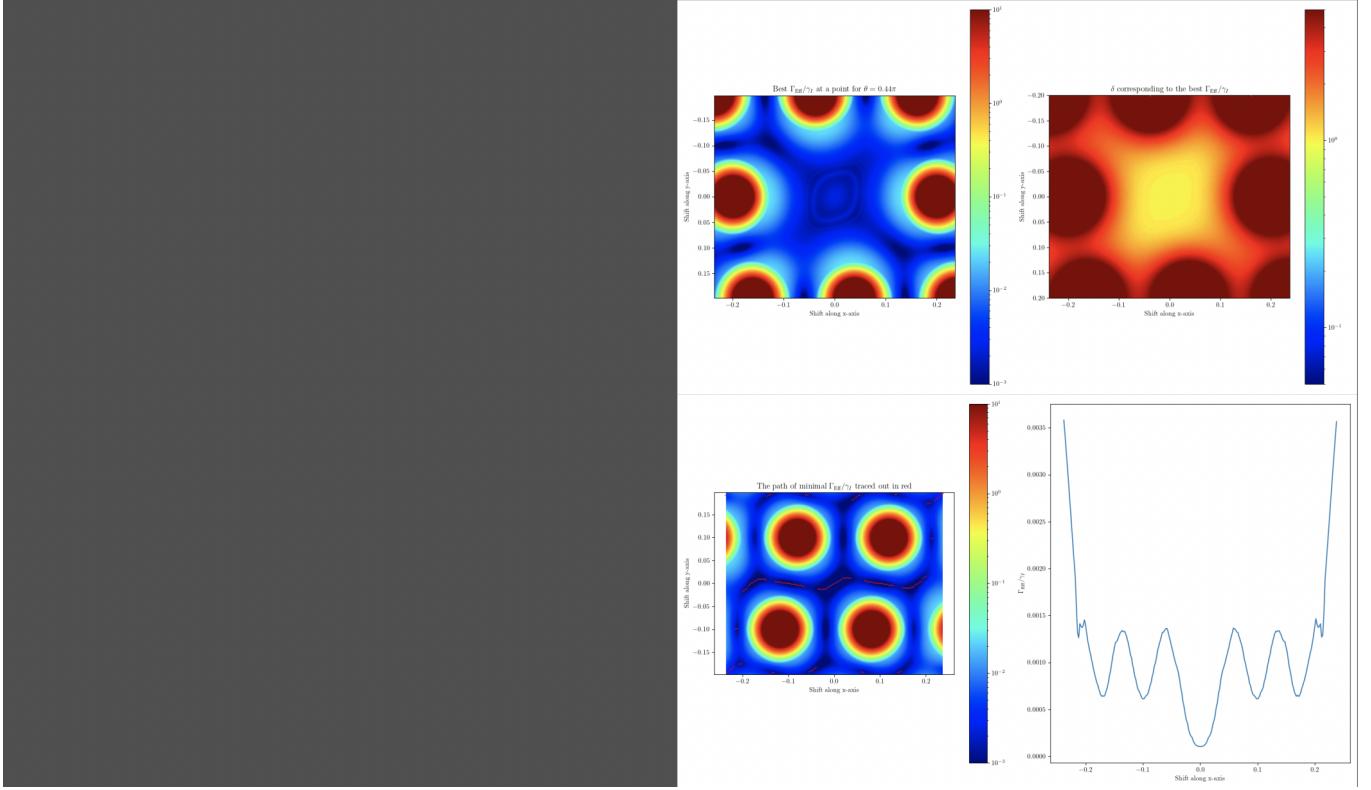


Figure 9. •

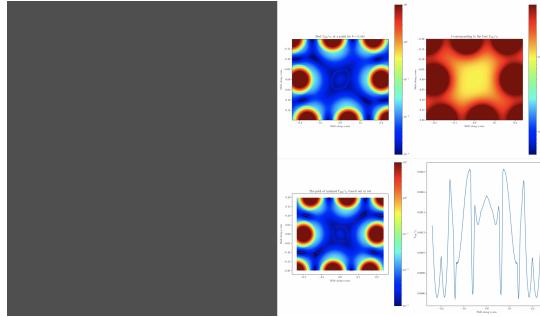


Figure 10. •

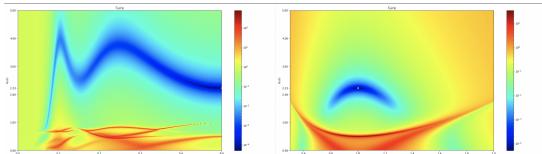


Figure 11. •

Because the first and second impurities occupy symmetric positions in the lattice, we find that $\Gamma_{\text{eff},1} = \Gamma_{\text{eff},2}$ and $Q_1 = Q_2$. We thus consolidate these variables, so that we may speak of the impurities' effective decay rate Γ_{eff} and overall quality factor Q .

A. Monoclinic lattice

B. Rectangular lattice

V. CONCLUSIONS AND OUTLOOK

These are the Conclusions.

Acknowledgments. We would like to thank [add people]. This work was supported by [add funding sources]

The numerical simulations were performed with the open-source framework `QuantumOptics.jl` [1].

-
- [1] S. Krämer, D. Plankensteiner, L. Ostermann, and H. Ritsch, QuantumOptics.jl: A Julia framework for simulating open quantum systems, *Computer Physics Communications* **227**, 109 (2018).