1D Lattice and Interaction Sums

Marc R. Bourgeois

Department of Chemistry, Northwestern University, Evanston IL 60208

E-mail:

For an infinite 1d NP array with a single NP per unit cell (lattice positions denoted as $\mathbf{r}_n = n\ a\hat{\mathbf{x}}$ with $n \in \mathbb{Z}$), the scattered field at position $\mathbf{r}$ of a phased-array of dipoles with orientation $\mathbf{p}$ (under the condition that $\mathbf{r}$ is not a lattice site) is

$$\mathbf{E}_s(\mathbf{r}) = \overleftrightarrow{\boldsymbol{T}}_{k'}(\mathbf{r}) \cdot \mathbf{p}, \tag{1}$$

where the interaction sum is defined as

$$\overleftrightarrow{\boldsymbol{T}}_{k'}(\mathbf{r}) \equiv \sum_{n=\infty}^{\infty} \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}, \mathbf{r}_n) \mathrm{e}^{\mathrm{i}k'na}. \tag{2}$$

A closely related tensor, called the lattice sum, is defined as

$$\overleftrightarrow{\boldsymbol{S}}_{k'} \equiv {\sum_{\Delta}}' \overleftrightarrow{\boldsymbol{\mathcal{G}}}(|\mathbf{r}_\Delta|) \mathrm{e}^{\mathrm{i}k'\Delta a}. \tag{3}$$

Although the formal definition of the lattice sum appears quite similar to that of the lattice sum, there are two critical distinctions:

- The evaluation point is located ON a lattice site (conventionally defined as $n = 0$).
- The prime above the summation symbol indicates the self-interaction (*i.e.* n=0) term is omitted.

Evaluation of 1D Lattice Sums

A standard approach for handling the infinite sum is the use of polylograthims

$$\mathrm{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}, \tag{4}$$

which have been implemented in standard numerical packages (*e.g.* mpmath for Python). Due to the symmetry of the problem, all of the off-diagonal components of the lattice sum vanish, and the diagonal components are

$$\begin{aligned} S_{xx}(k) = \sum_n{}' \overleftrightarrow{\boldsymbol{\mathcal{G}}}_{xx}(\mathbf{0}, \mathbf{r}_n)\ \mathrm{e}^{\mathrm{i}k_x na} = \frac{2}{4\pi\varepsilon_0 a^3}\Big\{ &\mathrm{Li}_3(e^{\mathrm{i}(k-k_x)a}) + \mathrm{Li}_3(e^{\mathrm{i}(k+k_x)a}) \\ &-ika\big[\mathrm{Li}_2(e^{\mathrm{i}(k-k_x)a}) + \mathrm{Li}_2(e^{\mathrm{i}(k+k_x)a})\big]\Big\}, \end{aligned} \tag{5}$$

$$\begin{aligned} S_{yy}(k) = \sum_n{}' \overleftrightarrow{\boldsymbol{\mathcal{G}}}_{yy}(\mathbf{0}, \mathbf{r}_n)\ \mathrm{e}^{\mathrm{i}k_x na} = -\frac{1}{4\pi\varepsilon_0 a^3}\Big\{ &\mathrm{Li}_3(e^{\mathrm{i}(k-k_x)a}) + \mathrm{Li}_3(e^{\mathrm{i}(k+k_x)a}) \\ &- ika\big[\mathrm{Li}_2(e^{\mathrm{i}(k-k_x)a}) + \mathrm{Li}_2(e^{\mathrm{i}(k+k_x)a})\big] \\ &- k^2a^2\big[\mathrm{Li}_1(e^{\mathrm{i}(k-k_x)a}) + \mathrm{Li}_1(e^{\mathrm{i}(k+k_x)a})\big]\Big\}, \end{aligned} \tag{6}$$

and $S_{yy}(k) = S_{zz}(k)$.

- S_{xx} has been implemented in `pyfunc.py` as `S_diag_1d_long()`. It has been verified that this produces identical output to brute force evaluation of the lattice sum (`TEST_LS.py`).
- $S_{yy/zz}$ has been implemented in `pyfunc.py` as `S_diag_1d_trans()`. It has been verified that this produces identical output to brute force evaluation of the lattice sum (`TEST_LS.py`).
- successfully tested for $kx \neq 0$ and for both real- and complex-valued frequencies.
- defined function `build_S_block()` that returns a 3x3 matrix with diagonal elements calculated using `S_diag_1d_long()` and `S_diag_1d_trans()`.

Evaluating the 1D Interaction Sum

The interaction sums can be expressed in terms of the Lerch transcendent, defined as

$$\Phi(z, s, \nu) = \sum_{k=0}^{\infty} \frac{z^k}{(k+\nu)^s}, \tag{7}$$

which reduces to the polylogarithm when $\nu = 0$. The procedure for doing so is covered in this section.

As shown in Eq. (2)

$$\overleftrightarrow{\boldsymbol{T}}(k_x) = \sum_n \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_n, \mathbf{r}_e) \mathrm{e}^{\mathrm{i}k_x n a} = \sum_n \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_e, \mathbf{r}_n) \mathrm{e}^{\mathrm{i}k_x n a}, \tag{8}$$

which is the field evaluated at $\mathbf{r}_e$ (located in the unit cell specified by $n = 0$) due to a periodic array of sources located at $\mathbf{r}_n = na\hat{x}$.

Specializing first to the case where $\mathbf{r}_e = t\hat{x}$, which is considered in ref.[1] Recalling from above that

$$\overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_e, \mathbf{r}_n, \omega) = \frac{k^2}{\varepsilon_0 \varepsilon r} \left[\left(1 + \frac{i}{kR} - \frac{1}{(kR)^2} \right) \overleftrightarrow{\boldsymbol{I}} + \left(-1 - \frac{3i}{kR} + \frac{3}{(kR)^2} \right) \hat{\mathbf{R}}\hat{\mathbf{R}} \right] \frac{\mathrm{e}^{ikR}}{4\pi R}, \tag{9}$$

where $R = |\mathbf{r}_e - \mathbf{r}_n|$ and $\hat{\mathbf{R}}\hat{\mathbf{R}}$ is the dyadic product.

xx-Component (Longitudinal Coupling)

Considering the xx component of the interaction sum explicitly

$$\overleftrightarrow{\boldsymbol{T}}_{xx}(k_x) = \sum_{n=-\infty}^{\infty} \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_e, \mathbf{r}_n) \mathrm{e}^{\mathrm{i}k_x n a} = \sum_{n=-\infty}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r} \, \mathrm{e}^{ikR} \, \mathrm{e}^{\mathrm{i}k_x n a} \left[\frac{1}{R^3} - ik \frac{1}{R^2} \right]. \tag{10}$$

At this point, two cases must be considered.

CASE 1

If $(\mathbf{r}_e - \mathbf{r}_n)\cdot\hat{x} > 0$, then

$$R = \begin{cases} t - na, & \text{if } n \le 0 \\ \\ na - t, & \text{if } n > 0 \end{cases}. \tag{11}$$

This allows Eq. (10) to be written as

$$\begin{aligned}
\overleftrightarrow{\boldsymbol{T}}_{xx}(k_x) = &\sum_{n=-\infty}^{0} \frac{2}{4\pi\varepsilon_0\varepsilon_r}\, \mathrm{e}^{ik(t-na)}\, \mathrm{e}^{\mathrm{i}k_x na}\left[\frac{1}{(t-na)^3} - ik\frac{1}{(t-na)^2}\right] \\
&+ \sum_{n=1}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r}\, \mathrm{e}^{ik(na-t)}\, \mathrm{e}^{\mathrm{i}k_x na}\left[\frac{1}{(na-t)^3} - ik\frac{1}{(na-t)^2}\right] \\
\\
= &\sum_{n=0}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r a^3}\, \mathrm{e}^{ikt}\left[\mathrm{e}^{i(k-k_x)a}\right]^n \left[\frac{1}{(t/a+n)^3} - ika\frac{1}{(t/a+n)^2}\right] \\
&+ \sum_{m=0}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r a^3}\, \mathrm{e}^{-ikt}\mathrm{e}^{i(k+k_x)a}\left[\mathrm{e}^{i(k+k_x)a}\right]^m \left\{\frac{1}{[m+(1-t/a)]^3} - ika\frac{1}{[m+(1-t/a)]^2}\right\} \\
\\
= &\frac{2}{4\pi\varepsilon_0\varepsilon_r a^3}\left\{\mathrm{e}^{ikt}\left[\Phi(\mathrm{e}^{i(k-k_x)a}, 3, t/a) - ika\ \Phi(\mathrm{e}^{i(k-k_x)a}, 2, t/a)\right] + \mathrm{e}^{-ikt}\mathrm{e}^{i(k+k_x)a}\right. \\
&\left.\times\left(\Phi\left[\mathrm{e}^{i(k-k_x)a}, 3, (1-t/a)\right] - ika\ \Phi\left[\mathrm{e}^{i(k-k_x)a}, 2, (1-t/a)\right]\right)\right\}.
\end{aligned} \tag{12}$$

Note that Eq. (12) is in agreement with the expression given in Eq. 7 of the SI of ref.[1] (lower sign convention).

CASE 2

If $(\mathbf{r}_e - \mathbf{r}_n)\cdot\hat{x} < 0$, then

$$R = \begin{cases} -t - na, & \text{if } n < 0 \\ \\ na + t, & \text{if } n \ge 0 \end{cases}. \tag{13}$$

This allows Eq. (10) to be written as

$$\begin{aligned}
\overleftrightarrow{\boldsymbol{T}}_{xx}(k_x) &= \sum_{n=-\infty}^{-1} \frac{2}{4\pi\varepsilon_0\varepsilon_r}\, \mathrm{e}^{-ik(t+na)}\, \mathrm{e}^{\mathrm{i}k_x na}\left[\frac{1}{(-t-na)^3} - ik\frac{1}{(-t-na)^2}\right] \\
&\quad + \sum_{n=0}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r}\, \mathrm{e}^{ik(t+na)}\, \mathrm{e}^{\mathrm{i}k_x na}\left[\frac{1}{(na+t)^3} - ik\frac{1}{(na+t)^2}\right] \\
&= \sum_{m=0}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r a^3}\, \mathrm{e}^{-ikt}\mathrm{e}^{i(k-k_x)a}\left[\mathrm{e}^{i(k-k_x)a}\right]^m \left\{\frac{1}{[m+(1-t/a)]^3} - ika\frac{1}{[m+(1-t/a)]^2}\right\} \\
&\quad + \sum_{n=0}^{\infty} \frac{2}{4\pi\varepsilon_0\varepsilon_r a^3}\, \mathrm{e}^{ikt}\left[\mathrm{e}^{i(k+k_x)a}\right]^n \left[\frac{1}{(t/a+n)^3} - ika\frac{1}{(t/a+n)^2}\right] \\
&= \frac{2}{4\pi\varepsilon_0\varepsilon_r a^3}\Big\{\mathrm{e}^{ikt}\left[\Phi(\mathrm{e}^{i(k+k_x)a}, 3, t/a) - ika\ \Phi(\mathrm{e}^{i(k+k_x)a}, 2, t/a)\right] + \mathrm{e}^{-ikt}\mathrm{e}^{i(k-k_x)a} \\
&\qquad \times \left(\Phi\left[\mathrm{e}^{i(k-k_x)a}, 3, (1-t/a)\right] - ika\ \Phi\left[\mathrm{e}^{i(k-k_x)a}, 2, (1-t/a)\right]\right)\Big\}.
\end{aligned} \tag{14}$$

Note that Eq. (14) is in agreement with the expression given in Eq. 7 of the SI of ref.[1] (upper sign convention).

yy/zz-Component (Transverse Coupling)

$$\overleftrightarrow{\boldsymbol{T}}_{yy}(k_x) = \sum_{n=-\infty}^{\infty} \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_e, \mathbf{r}_n)\mathrm{e}^{\mathrm{i}k_x na} = \sum_{n=-\infty}^{\infty} \frac{1}{4\pi\varepsilon_0\varepsilon_r}\, \mathrm{e}^{ikR}\, \mathrm{e}^{\mathrm{i}k_x na}\left[k^2\frac{1}{R} + ik\frac{1}{R^2} - \frac{1}{R^3}\right]. \tag{15}$$

Following the same procedure as done above for the xx-component (splitting the sum into 2 parts and re-writting each in terms of the Lerch transcendent) produces Eq. 8 of the SI of ref.[1]

Testing – $\mathbf{r}_e$ on $\hat{x}$

- T_{xx} and $T_{yy/zz}$ have been implemented in `pyfunc.py` as `T_1d_long()` and `T_1d_trans()`, respectively. It has been verified that they produces identical output to brute force evaluation of the interaction sum components for both $k_x \neq 0$ and $n \neq 1.0$ (`TEST_LS.py`).

- NOTE: Form of interaction sum is ONLY valid for $\mathbf{r}_e$ positioned on the 1D chain axis!

Example: Site Space Description with Nearest Neighbor Approx.

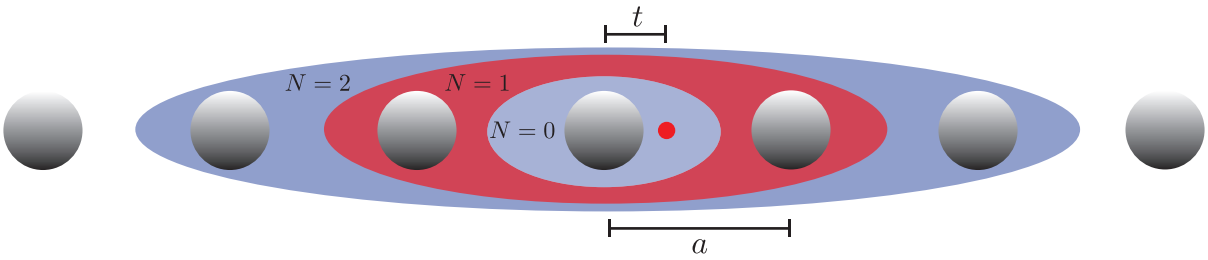

Figure 1: Schematic representation of site space representation under the nearest-neighbor approximation, with the order denoted by N. The red dot represents the emitter.

This section describes an example of what can be done using the `SLRpy_1d` code. A site space coupled dipole description of the coupling between a single defect dipole (representing a classical emitter) coupled to a 1d NP chain under the nearest-neighbor approximation (where N designates the number of nearest neighbors) is given by

$$\begin{aligned} \mathbf{p}_n &= \overleftrightarrow{\boldsymbol{\alpha}} \cdot \sum_{n'}{}' \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_n, \mathbf{r}_{n'}) \cdot \mathbf{p}_{n'} + \overleftrightarrow{\boldsymbol{\alpha}} \cdot \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_n, \mathbf{r}_d) \cdot \mathbf{d} \\ \mathbf{d} &= \overleftrightarrow{\boldsymbol{\beta}} \cdot \sum_{n} \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}_d, \mathbf{r}_n) \cdot \mathbf{p}_n, \end{aligned} \tag{16}$$

where $n \in [-N, N]$.

The above set of equations can be compactly expressed as $\overleftrightarrow{\boldsymbol{M}} \cdot \mathbf{P} = \mathbf{E}$, where

$$\begin{aligned}
\mathbf{P}^T &= [\ \mathbf{d}\ \mathbf{p}_{-N}\ \ldots \mathbf{p}_N\ ] \\
\mathbf{E}^T &= [\ \mathbf{E}_d\ \mathbf{E}_{-N}\ \ldots \mathbf{E}_N\ ] \\
\overleftrightarrow{\boldsymbol{M}} &= \begin{pmatrix}
\overleftrightarrow{\boldsymbol{\beta}}^{-1} & -\overleftrightarrow{\boldsymbol{\mathcal{G}}}_{d-N} & \ldots & -\overleftrightarrow{\boldsymbol{\mathcal{G}}}_{dN} \\
-\overleftrightarrow{\boldsymbol{\mathcal{G}}}_{-Nd} & \overleftrightarrow{\boldsymbol{\alpha}}_{-N}^{-1} & & \\
\vdots & & \ddots & \\
-\overleftrightarrow{\boldsymbol{\mathcal{G}}}_{Nd} & & & \overleftrightarrow{\boldsymbol{\alpha}}_{N}^{-1}
\end{pmatrix}.
\end{aligned} \tag{17}$$

The emitter dipole alone can be driven by choosing $\mathbf{E}^T = [\ \hat{\mathbf{d}}\ \mathbf{0}\ \ldots \mathbf{0}\ ]$. The moments induced at each site are then $\mathbf{P} = \overleftrightarrow{\boldsymbol{M}}^{-1} \cdot \mathbf{E}$. Once the induced moments at each site are determined, the total scattered field at position $\mathbf{r}$ is given by

$$E_s(\mathbf{r}) = \sum_{n=-N}^{N} \overleftrightarrow{\boldsymbol{\mathcal{G}}}(\mathbf{r}, \mathbf{r}_n) \cdot \mathbf{p}_n, \tag{18}$$

where the components of $\mathbf{p}_n$ can be taken from the elements of $\mathbf{P}$. In particular, the Purcell factor for the nearest-neighbor model can then be calculated using Eq. (18) with the evaluation point $\mathbf{r} = \mathbf{r}_d$

$$\mathrm{F_P} = 1 + \frac{6\pi\varepsilon_0\varepsilon_r}{|\mathbf{d}|^2\ k^3}\mathrm{Im}\big(\mathbf{d}^* \cdot \mathbf{E}_s(\mathbf{r}_d)\big). \tag{19}$$

Numerical Results

Figure 2 compares the Purcell factors calculated for an individual emitter coupled to a single NP (red) and to an infinite 1d NP chain (blue dashed). Panel (a) shows that the single-NP and chain $\mathrm{F_P}$s are nearly identical when the emitter is oriented along the chain axis (longitudinal) – physically, this behavior occurs because the emitter radiation lobes are orthogonal to the chain axis in this case. In contrast, when the emitter is oriented transverse to the chain axis (Figure 2b), the radiation lobes are along the chain axis and deviations

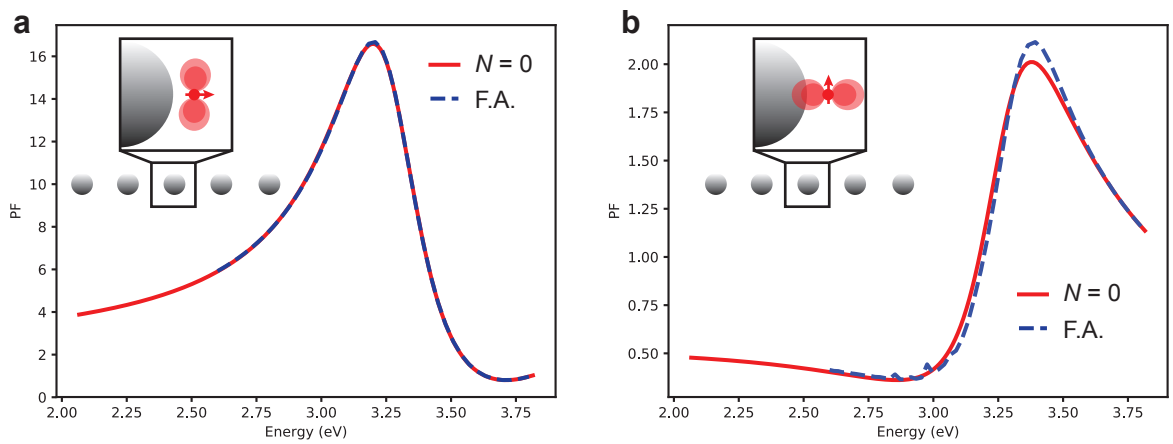

Figure 2: Comparison of single-NP and chain Purcell Factors. a) Red curve is longitudinally oriented dipole coupled to single NP with $d = 20$ nm (reproduced from Figure **??** above). Blue-dashed curve is Purcell factor for a single emitter coupled to an infinite 1d chain calculated using the self-propagator in Eq. (**??**). b) Same as panel (a), but for transversely oriented dipole. Parameters: 80 nm diameter Ag NPs, $a = 400$ nm chain periodicity, dipole spaced 20 nm from NP surface, $n = 1$.

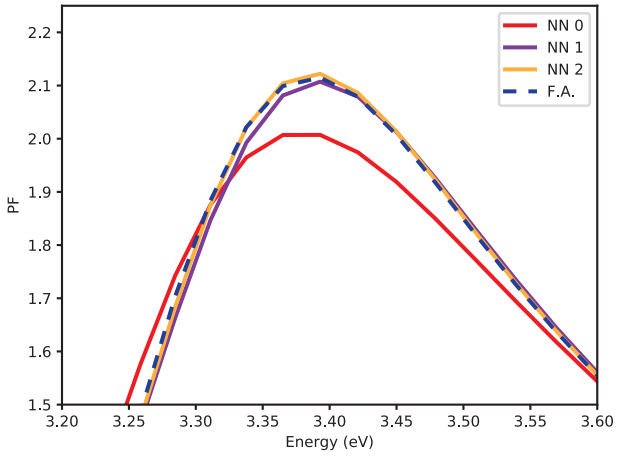

Figure 3: Comparison of Nearest-Neighbor and Fano Anderson Purcell Factors for transversely oriented emitter displaced 20 nm along the chain axis.

between the single-NP and chain Purcell factor spectra are observed. Interestingly, based on these observations, it is expected that the largest deviations of the chain $\mathrm{F_P}$ from that of the single NP occur when the emitter is displaced along the z-direction and oriented along $\hat{z}$. Unfortunately, writing the interaction sum in terms of the Lerch transcendent, which enables efficient evaluation, can only be done when the evaluation point is located on the chain axis (*i.e.* $\mathbf{r}_e = t\hat{\mathbf{x}} + 0\hat{\mathbf{y}} + 0\hat{\mathbf{z}}$).

References

(1) Pocock, S. R.; Xiao, X.; Huidobro, P. A.; Giannini, V. Topological Plasmonic Chain with Retardation and Radiative Effects. *ACS Photonics* **2018**, *5*, 2271–2279.