Chemfarm for collective quantum optics
Tutorial 1: Overview and first steps

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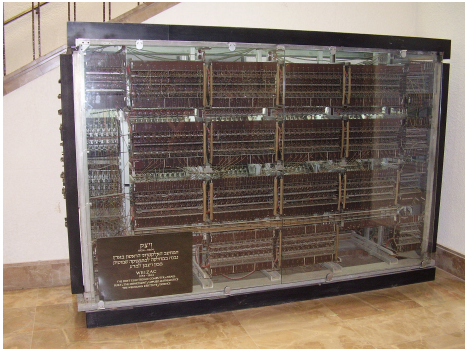
Computers in Weizmann Institute



Weizmann Institute's first computer, Weizac, built in 1954.

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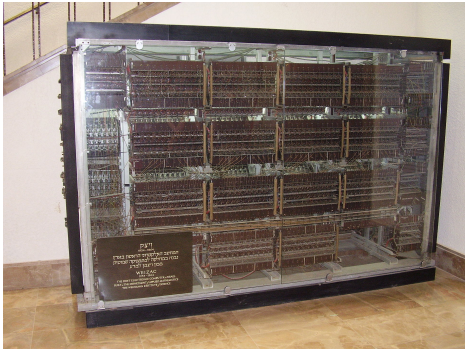

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Now

- WEXAC HPC: 34,000 CPU cores, NVidia GPUs, 11000 TB of storage
- Faculty of Math and Computer Science HPC: 2000 CPU cores, NVidia GPUs (with NVidia A 100, 80 GB of memory)
- **ChemFarm** 31648 CPU cores, 169 TB RAM, 19 nodes with NVidia GPU

Useful links: WEXAC HPC, ChemFarm
Only from WIS Network: ChemFarm Wiki

What do people use HPC for?

HPC (High Performance Computing) is used for computationally intensive tasks, such as:

- Simulating complex physical systems (e.g., quantum optics, molecular dynamics)
- Data analysis and machine learning (e.g., large datasets, training neural networks)
- Computational chemistry (e.g., quantum chemistry calculations, drug discovery)

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What my friends do:

Olga: computational biology (monte carlo simulation of Ising model for decision making)

Rafail and Narek: machine learning for computer vision (Train large model on many pictures using GPU)

Diana: condensed matter physics (running DFT calculations for topological materials)

Dima: machine learning for particle physics (writing code to analyze data from Large Hadron Collider)

What about collective quantum optics?

Solution of Lindblad equation

$$\dot{\rho} = \mathcal{L}\rho$$

Size of ρ grows exponentially with the number of atoms (for N two-level atoms, ρ is a $2^N \times 2^N$ matrix). For $N = 20$, ρ has $2^{40} \approx 10^{12}$ elements, which is too large to store in memory.
We need to solve to find steady states, dynamics, correlation functions, etc.

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Mean-field equations

Experiments $N \sim 10^4 - 10^6$ atoms, so we need to solve mean-field equations for N atoms, which is a system of $3N$ coupled nonlinear ODEs. Even at mean-field level computations can be challenging + some new methods (e.g., cluster mean-field, cumulant expansion) require solving even larger systems of equations.

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Large matrix diagonalization

Finding ground states and first excited states of many-body Hamiltonians, which is a large matrix diagonalization problem. $N = 20$ two-level atoms $\Rightarrow 2^{20} = 10^6$
Liouvivillian diagonalization: $4^N \times 4^N$ matrix. For $N = 10$ $\Rightarrow 2^{20} = 10^6$ $4^{10} = 10^6$
GPUs can be used..

I believe there are much more and we should discuss

Plan for today

- Look through the ChemFarm wiki and documentation to understand the available resources and how to access them
- Show examples of HPC usage in Mean-Field with Green Function
- Outline future directions and opportunities for collaboration

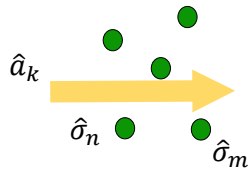
ChemFarm Wiki

- ChemFarm Wiki (Weizmann Network) is the main source of information about ChemFarm, including documentation, tutorials, and user guides.
- It contains information on how to access ChemFarm, how to use the job scheduler, and how to run different types of jobs (e.g., CPU, GPU).
- It also has a section with available software ()

Connect to cluster: ssh terminal command: `ssh <username>@chemfarm.weizmann.ac.il` (need to be on WIS network or use VPN); VS Code Remote SSH extension; JupyterHub; We will try OpenOnDemand, JupyterHub, and VS Code Remote SSH today.

Model: atoms + photon modes

$$H = H_A + H_P + H_{AP}$$



"atoms": two-level emitters $n = 1, \dots, N$ at positions $\mathbf{r}_n$

$$H_A = \hbar\omega_a \sum_{n=1}^{N} \hat{\sigma}_n^\dagger \hat{\sigma}_n \qquad \hat{\sigma}_n = |g\rangle_n\langle e| \qquad = \quad \omega_a \;\; \begin{matrix} \text{——} \; |e\rangle \\ \text{——} \; |g\rangle \end{matrix}$$

"photons" = continuum of photon modes $\hat{a}_k$ (modes defined by geometry) $\{k\}$ = mode index

$$H_P = \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k$$

"atom-photon": dipole interaction (+rotating wave approx.)

$$H_{AP} = -\sum_n \hat{E}(\mathbf{r}_n)\hat{\sigma}_n^\dagger d + h.c. \qquad \hat{E}(\mathbf{r}_n) = -i\sum_k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0}}\, u_k(\mathbf{r}_n)\hat{a}_k$$

mode profile

Heisenberg-Langevin approach

[see Lehmberg PRA 2, 883 (1970) for a full derivation]

$$H = \hbar\omega_a \sum_{n=1}^{N} \hat{\sigma}_n^\dagger \hat{\sigma}_n + \sum_k \hbar\omega_k \hat{a}_k^\dagger \hat{a}_k - \sum_n \left[\hat{E}(\mathbf{r}_n)\hat{\sigma}_n^\dagger d + h.c.\right]$$

$$\hat{E}(\mathbf{r}_n) = -i \sum_k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0}} u_k(\mathbf{r}_n)\hat{a}_k$$

$$\hat{\sigma}_n = |g\rangle_n\langle e|$$

Heisenberg Eq. for atom n:

$$\partial_t \hat{\sigma}_n = \frac{i}{\hbar}[H, \hat{\sigma}_n]$$

Use: $[\hat{\sigma}_n^\dagger, \hat{\sigma}_n] = \hat{\sigma}_n^z$ $\quad \hat{\sigma}_n^z = |e\rangle_n\langle e| - |g\rangle_n\langle g|$

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n - i\frac{d}{\hbar}\hat{\sigma}_n^z \hat{E}(\mathbf{r}_n)$$

Now wish to find Eq. for field $\hat{E}(\mathbf{r}_n)$ and insert it into the above

Heisenberg Eq. for field = Maxwell's Eqs. (=Hamilton's Eq. for field...)

$$\nabla \times \hat{E}(r,t) = -\partial_t \hat{B}(r,t) \qquad \nabla \times \hat{B}(r,t) = \frac{1}{c^2}\partial_t \left[\hat{E}(r,t) + \frac{1}{\varepsilon_0}\hat{P}(r,t)\right]$$

Polarization density
= dipoles (of atoms) per volume

$$\hat{P}(\mathbf{r},t) = \sum_n \hat{d}_n(t)\delta(\mathbf{r}-\mathbf{r}_n)$$

$$\hat{d}_n = d\hat{\sigma}_n + \text{h.c.}$$

Freq. domain $\partial_t \to -i\,\omega$

$$\nabla \times \hat{E}(r,\omega) = i\,\omega \hat{B}(r,\omega) \qquad \nabla \times \hat{B}(r,\omega) = -i\frac{\omega}{c^2}\left[\hat{E}(r,\omega) + \frac{1}{\varepsilon_0}\hat{P}(r,\omega)\right]$$

Derive wave equation:

$$\nabla \times \nabla \times \hat{E} = i\,\omega \nabla \times \hat{B} = \frac{\omega^2}{c^2}\left[\hat{E} + \frac{1}{\varepsilon_0}\hat{P}\right]$$

$$\nabla \times \nabla \times \hat{E}(\mathbf{r},\omega) - \frac{\omega^2}{c^2}\hat{E}(\mathbf{r},\omega) = \frac{\omega^2}{c^2}\frac{1}{\varepsilon_0}\hat{P}(\mathbf{r},\omega) = \frac{\omega^2}{c^2}\frac{1}{\varepsilon_0}\sum_n \delta(\mathbf{r}-\mathbf{r}_n)d\hat{\sigma}_n(\omega)$$

Heisenberg Eq. for field: formal solution (1)

$$\underbrace{\nabla \times \nabla \times \hat{E}(\mathbf{r},\omega) - \frac{\omega^2}{c^2}\hat{E}(\mathbf{r},\omega)}_{\text{Linear operator (\sim "Helmholtz" Eq. for the field)}} = \underbrace{\frac{\omega^2}{c^2}\frac{1}{\varepsilon_0}\sum_n \delta(\mathbf{r}-\mathbf{r}_n)d\hat{\sigma}_n(\omega)}_{\text{point sources ("dipoles") @ atom positions}}$$

→ Solution to point source (=dipole) @ $\mathbf{r}_n$ – Green's function: $G(\mathbf{r}-\mathbf{r}_n)$

$$\hat{E}(\mathbf{r},\omega) = \hat{E}_0(\mathbf{r},\omega) + \underbrace{\frac{\omega^2}{c^2}\frac{d}{\varepsilon_0}\sum_n G(\mathbf{r}-\mathbf{r}_n,\omega)\hat{\sigma}_n(\omega)}_{\text{Field from all "dipole" sources (=radiating atoms)}}$$

Total field

"Source free" solution
= "free" field (in the absence of atoms)
= vacuum fluctuations + incident laser

field propagator = Green's function $G(\mathbf{r}_1,\mathbf{r}_2) = \mathbf{e}_d{}^{\dagger}\cdot\overline{\overline{\boldsymbol{G}}}(\mathbf{r}_1,\mathbf{r}_2)\cdot\mathbf{e}_d$

$$\mathbf{e}_i{}^{\dagger}\cdot\overline{\overline{\boldsymbol{G}}}(\mathbf{r}_1,\mathbf{r}_2)\cdot\mathbf{e}_j = G_{ij}(k,\mathbf{r}_1,\mathbf{r}_2) = \frac{e^{ikr}}{4\pi r}\left[\left(1+\frac{ikr-1}{k^2r^2}\right)\delta_{ij} + \left(-1+\frac{3-3ikr}{k^2r^2}\right)\frac{r^i r^j}{r^2}\right]$$

with $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, $r = |\mathbf{r}|$ and $r^i = \mathbf{e}_i \cdot \mathbf{r}$.

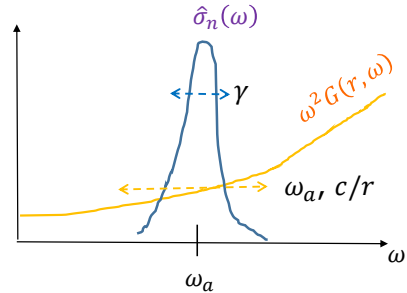
$k = \omega/c$

Heisenberg Eq. for field: formal solution (2)

$$\hat{E}(\mathbf{r},\omega) = \hat{E}_0(\mathbf{r},\omega) + \frac{\omega^2}{c^2}\frac{d}{\varepsilon_0}\sum_n \hat{\sigma}_n(\omega) G(\mathbf{r}-\mathbf{r}_n,\omega)$$

Back to time-domain – perform IFT:

$$\hat{E}(\mathbf{r},t) = \hat{E}_0(\mathbf{r},t) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t}\hat{\sigma}_n(\omega)\ \omega^2 G(\mathbf{r}-\mathbf{r}_n,\omega)$$



- Dominant "free" dynamics: oscillations at ω_a
- Slow dynamics due to radiation ~ decay/shift γ

Wide function around ω_a
Width ~ $\omega_a,\ c/r$

Markov approximation: $\omega_a,\ c/r \gg \gamma$

$$\hat{E}(\mathbf{r},t) \approx \hat{E}_0(\mathbf{r},t) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n {\omega_a}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi} e^{-i\omega t}\hat{\sigma}_n(\omega)$$

$$= \hat{E}_0(\mathbf{r},t) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n {\omega_a}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\hat{\sigma}_n(t)$$

Heisenberg-Langevin Eq. for atoms (1)

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n - i\frac{d}{\hbar}\hat{\sigma}_n^z \hat{E}(\mathbf{r}_n)$$

We got for field: $\hat{E}(\mathbf{r}) = \hat{E}_0(\mathbf{r}) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n {\omega_a}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\hat{\sigma}_n$

→ Field "felt" by **atom** n, $\mathbf{r} = \mathbf{r}_n$:

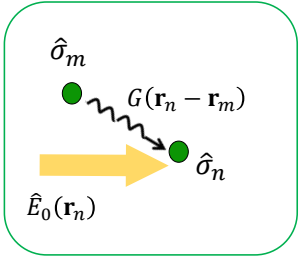
$$\hat{E}(\mathbf{r}_n) = \hat{E}_0(\mathbf{r}_n) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_m {\omega_a}^2 G(\mathbf{r}_n-\mathbf{r}_m)\hat{\sigma}_m$$

= "free" field (in the absence of atoms)
= vacuum fluctuations + incident laser

$$\hat{E}_0(\mathbf{r}_n) = -i\sum_k \sqrt{\frac{\hbar\omega_k}{2\varepsilon_0}} u_k(\mathbf{r}_n)\hat{a}_k(0)e^{-i\omega_k t}$$

Field from all "dipole" sources (=radiating atoms)

field propagator = $G(\mathbf{r}_n - \mathbf{r}_m)$



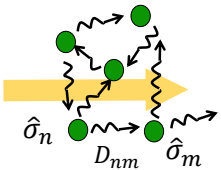
Heisenberg-Langevin Eq. for atoms (2)

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n - i\hat{\sigma}_n^z \frac{d}{\hbar}\left[\hat{E}_0(\mathbf{r}_n) + \frac{{\omega_a}^2}{c^2}\frac{d}{\varepsilon_0}\sum_m G(\mathbf{r}_n - \mathbf{r}_m)\hat{\sigma}_m\right]$$

$$D_{nm} = -i\frac{3}{2}\gamma\lambda G(\mathbf{r}_n - \mathbf{r}_m) \qquad \gamma = \frac{{d^2\omega_a}^3}{3\pi\varepsilon_0\hbar c^3}$$

$$\lambda = 2\pi c/\omega_a$$

$$\partial_t \hat{\sigma}_n = -i\omega_a \hat{\sigma}_n + \hat{\sigma}_n^z\left[\hat{F}_n + \sum_m D_{nm}\,\hat{\sigma}_m\right]$$



→ Collective response

(= multiple scattering
= dipole-dipole)

quantum noise (vacuum) + incident laser

$$\hat{F}_n = -i\frac{d}{\hbar}\hat{E}_0(\mathbf{r}_n) = -d\sum_k \sqrt{\frac{\omega_k}{2\varepsilon_0\hbar}}u_k(\mathbf{r}_n)\hat{a}_k(0)e^{-i\omega_k t}$$

Dipole-dipole coupling (with all atomic dipoles)

$$D_{nm} = \gamma_{nm}/2 + i\Delta_{nm}$$

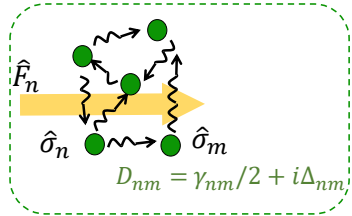
dipole-dipole kernel
(photon Green's function)

$$\partial_t \hat{\sigma}_n = -\left(i\omega_a + \frac{\gamma}{2}\right)\hat{\sigma}_n + \hat{\sigma}_n^z\left[\hat{F}_n + \sum_{m\neq n} D_{nm}\,\hat{\sigma}_m\right]$$

$$\mathrm{Re}\; D_{nn} = \gamma/2$$

$$\mathrm{Im}\; D_{nn} + \omega_a \rightarrow \omega_a$$

Many-body physics of quantum emitters (atoms)



Heisenberg-Langevin Eq. for atoms:

$$\partial_t \hat{\sigma}_n = \frac{i}{\hbar}[H_{\text{eff}}, \hat{\sigma}_n] + \hat{\sigma}_n^z \hat{F}_n$$

Effective Hamiltonian (non-Hermitian): **collectivity**

$$H_{\text{eff}} = \hbar\left(\omega_a - i\frac{\gamma}{2}\right)\sum_{n=1}^{N}\hat{\sigma}_n^\dagger\hat{\sigma}_n + \hbar\sum_{n=1}^{N}\sum_{m\neq n}\left(\Delta_{nm} - i\frac{\gamma_{nm}}{2}\right)\hat{\sigma}_n^\dagger\hat{\sigma}_m$$

Quantum noise
(has to exist due to dissipation)

$$\hat{F}_n = -d\sum_k \sqrt{\frac{\omega_k}{2\varepsilon_0\hbar}}\, u_k(\mathbf{r}_n)\hat{a}_k(0)e^{-i\omega_k t}$$

Dipole-dipole interaction
(reversible excitation exchange)

Collective radiation
(dissipation)

Equivalent description: quantum master equation $\partial_t\hat{\rho} = -\frac{i}{\hbar}\left(H_{\text{eff}}\hat{\rho} - \hat{\rho}H_{\text{eff}}^\dagger\right) + \sum_{n,m}\gamma_{nm}\hat{\sigma}_n\hat{\rho}\hat{\sigma}_m^\dagger$

Output light $\hat{E}(\mathbf{r}) = \hat{E}_0(\mathbf{r}) + \frac{1}{c^2}\frac{d}{\varepsilon_0}\sum_n \omega_a{}^2 G(\mathbf{r}-\mathbf{r}_n,\omega_a)\hat{\sigma}_n$

Quantum noise: "jump term"

Mean-Field in waveguide QED or atomic array/cloud

Denoting $s_n = \langle \sigma_n^- \rangle$ and $s_n^z = \langle \sigma_n^z \rangle$ and neglecting quantum correlations, we get the following system of equations for N atoms:

$$\begin{cases} \dot{s}_n = -\frac{\gamma}{2} s_n + s_n^z \left[\frac{\gamma_{1D}}{2} \sum_{m \neq n} D_{nm} s_m + i\Omega e^{ikz_n} \right] \\ \dot{s}_n^z = -\gamma(s_n^z + 1) - 2\left[s_n^* \left(\frac{\gamma_{1D}}{2} \sum_{m \neq n} D_{nm} s_m + i\Omega e^{ikz_n} \right) + c.c. \right] \end{cases} \tag{1}$$

Geometry information: $D_{nm} = -i\frac{3\gamma}{2} \lambda G(\boldsymbol{r}_n - \boldsymbol{r}_m)$

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Problem statement: solve the system depending on the geometry. Find $s_n(t)$ and $s_n^z(t)$ for $n = 1, ..., N$ depending on Ω, initial conditions.

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Where HPC comes in: big memory ($N \sim 10^3$), NumPy for Greens Function, parallelization for parameter scans.

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Solution step: calculate Green function using vectorized code, solve ODEs using `scipy.integrate.solve_ivp` (parallelization for parameter scans), run on chemfarm

Parallel solver function

```python
def solve_system_wrapper(args):
    """Wrapper for parallelization."""
    return solve_system_prop(*args)


def parallel_solve_omega(N, gamma, Dnm, Gnm, Omega_n_values, t_span, y0, n_workers=4):
    """Parallelized execution for solving ODEs across different Omega values."""
    with mp.Pool(processes=n_workers) as pool:
        results = list(tqdm(
            pool.imap(
                solve_system_wrapper,
                [(N, gamma, Dnm, Gnm, Omega_n, t_span, y0) for Omega_n in Omega_n_values],
                chunksize=2
            ),
            total=len(Omega_n_values),
            desc="Solving ODE sweep"
        ))
    return results
```

n_workers - number of parallel processes to use

Vectorized 1D Greens function

```python
def create_1d_gnm_matrix_vectorized(positions, gamma1D=1):
    """Creates the Green's function matrix for 1D lattice using vectorized operations."""
    N = len(positions)

    # Compute all pairwise displacement vectors in 1D
    r_vec = positions[:, np.newaxis] - positions[np.newaxis, :]
    # Compute Euclidean distances
    R = np.abs(r_vec)
    # Set diagonal elements to avoid division by zero
    np.fill_diagonal(R, 1.0)
    # Compute kr
    kr = 2 * np.pi * R
    # Compute the 1D Green's function
    g1 = gamma1D / 2 * np.exp(1j * kr)
    np.fill_diagonal(g1, 0)

    gnm = 2 * np.real(g1)
    dnm = np.imag(g1)

    return gnm, dnm
```

3D lattice with numpy

```python
#create an 3D array with x,y,z lattice with lattice spacing a_x, a_y, a_z
def create_lattice(nx, ny, nz, a_x, a_y, a_z):
    """Creates a 3D lattice of points with given dimensions and spacings."""
    x = np.arange(-nx/2, nx/2) * a_x
    y = np.arange(-ny/2, ny/2) * a_y
    z = np.arange(-nz/2, nz/2) * a_z
    xv, yv, zv = np.meshgrid(x, y, z, indexing='ij')
    lattice = np.stack((xv, yv, zv), axis=-1).reshape(-1, 3)
    return lattice
```

3D Greens function with numpy

```python
def create_gnm_matrix_vectorized(positions):
    """Creates the Green's function matrix using vectorized operations."""
    N = len(positions)

    # Compute all pairwise displacement vectors using broadcasting
    # Shape: (N, N, 3)
    r_vec = positions[:, np.newaxis, :] - positions[np.newaxis, :, :]

    # Compute Euclidean distances
    # Shape: (N, N)
    R = np.linalg.norm(r_vec, axis=2)

    # Set diagonal elements to a non-zero value to avoid division by zero
    np.fill_diagonal(R, 1.0)
    kr = 2 * np.pi * R

    # Create e_0 vector (polarization)
    e_0 = (1 / np.sqrt(2)) * np.array([1, 1j, 0])
    #e_0 = np.array([0, 0, 1])
    # Compute dot products between e_0 and all displacement vectors
    # Shape: (N, N)
```

```
    # Shape: (N, N)
    dot_products = np.sum(e_0 * r_vec, axis=2)

    # Compute cos^2(theta)
    # Shape: (N, N)
    cos2_theta = np.abs(dot_products / R) ** 2

    # Compute the Green's function
    g1 = np.exp(1j * kr) / kr * (
        (1 + (1j * kr - 1) / kr**2) + cos2_theta * (-1 + (3 - 3 * 1j * kr) / kr**2))

    # Set diagonal elements to zero (no self-interaction)
    np.fill_diagonal(g1, 0)

    # Compute gnm and dnm
    dnm = -3/4 * np.real(g1)
    gnm = 3/2 * np.imag(g1)
    #dnm = np.zeros((N,N))

    return gnm, dnm
```