Diffusion of Optically Pumped Atoms

Background

We consider an atomic ensemble (i.e., a large number of atoms) confined in a container. Each atom has M internal eigenstates (e.g., quantum mechanical energy levels, usually, denoted by $|\psi_i\rangle$ for $i = 1, 2, \ldots, M$). The overall state of the atomic ensemble is described by a column vector

$$\rho(\mathbf{r}) = [\rho_1(\mathbf{r}), \rho_2(\mathbf{r}), \ldots, \rho_M(\mathbf{r})]^T,$$

where each component $\rho_i(\mathbf{r})$ is the probability for finding an atom at position $\mathbf{r}$ and in the i-th internal state.

We consider the following two processes:

- Quantum evolution. The atoms change from one internal state $|\psi_i\rangle$ to another $|\psi_j\rangle$ at a certain rate. The quantum transition among the M internal states is described by a $M \times M$ matrix G as

$$\left[\frac{\partial \rho}{\partial t}\right]_{\text{transition}} = G(\mathbf{r})\rho.$$

  The matrix element G_{ij} ($i, j = 1, \ldots, M$) is the transition rate from state $|\psi_i\rangle$ to $|\psi_i\rangle$.

- Spatial diffusion. As the atomic state $\rho(\mathbf{r})$ also depends on spatial coordinate $\mathbf{r}$, the atoms will diffuse from the location with higher density to lower density, which is described by a standard diffusion equation with a scalar diffusion constant D

$$\left[\frac{\partial \rho}{\partial t}\right]_{\text{diffusion}} = D\nabla^2\rho.$$

The Problem

Within a three-dimensional domain Ω, the full atomic evolution is governed by

$$\frac{\partial \rho}{\partial t} = D\nabla^2\rho - G(\mathbf{r})\rho, \quad \text{for } \mathbf{r} \in \Omega. \qquad (1)$$

The initial condition is that all the internal states are equally populated, i.e.,

$$\rho(t = 0) = \frac{1}{M}[1, 1, \ldots, 1]^T \equiv \varphi_0, \text{ for all } \mathbf{r} \in \Omega. \qquad (2)$$

The boundary condition, which depends on the physical condition, can be either the Neumann type

$$\hat{\boldsymbol{n}} \cdot \nabla\rho = 0, \quad \text{for } \mathbf{r} \in \partial\Omega, \qquad (3)$$

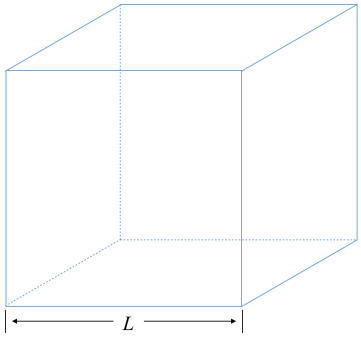
with the unit vector $\hat{\boldsymbol{n}}$ normal to the boundary, or the Dirichlet type

unit normal vector of the boundary

$$\rho(\mathbf{r}) = \varphi_0, \quad \text{for } \mathbf{r} \in \partial\Omega. \qquad (4)$$

Find the solution $\rho(\mathbf{r}, t)$ of Eq.(1), together with the initial condition Eq.(2) and the boundary condition Eq.(3) or Eq.(4), using FEM on a cubic domain (with length of side $L = 1\,\text{cm}$).

建议把所有参数无量纲化
初值条件(2)应该是有量纲的
因为要考虑空间分布，应该用全空间积分来归一化。



The diffusion constant is

$$D = 0.1\,\mathrm{cm}^2/\mathrm{s}. \qquad (5)$$

Consider the atom has $M = 8$ internal states. The 8×8 matrix G can be decomposed as the product of a scalar function $P(\mathbf{r})$ and a constant matrix G_0, i.e. $G(\mathbf{r}) = P(\mathbf{r})G_0$, where $P_0(\mathbf{r})$ describes the inhomogeneity of the matrix $G(\mathbf{r})$

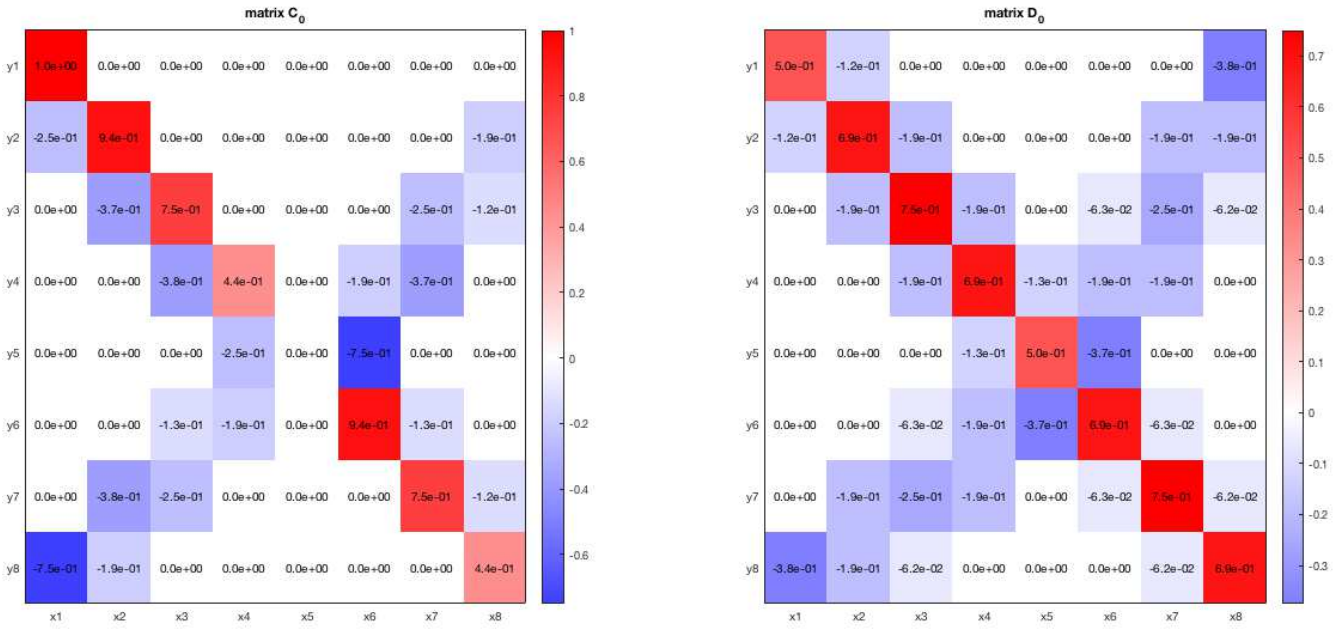
$$P(\mathbf{r}) = P_0 \exp\left[-\frac{x^2 + y^2}{w^2}\right], \qquad (6)$$

with typical values $P_0 = 1\,\mathrm{s}^{-1}$, and $w = 0.2\,\mathrm{cm}$.

The constant matrix G_0 consists of two components C_0 and D_0,

$$G_0 = C_0 + \alpha D_0, \qquad (7)$$

where $\alpha > 0$ is a real variable with the typical value $\alpha = 0.5$. The matrices $C_0$and D_0 have the following form



These matrices are stored in a matlab data file ('DifussionFEM.mat'), and you can load them by executing the command

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load('DiffusionFEM.mat');
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Task

Solve the following problems step-by-step, with increasing degree of difficulty

1. Neglect the spatial dependence of G [assuming $w \to +\infty$ in Eq.(6)], and consider the steady-

(1)假设G可以正交对角化，则这个稳态解不一定存在。因为把G对角化以后，这个问题相当于一个给定了本征值的本征值问题。而矩阵G的本征值不一定刚好就是拉普拉斯算子的本征值。
(2)C0并不是对称的，所以G不一定能正交对角化，解析不会算。

state solution ($\partial\rho/\partial t = 0$). Solve the problem using FEM, and compare the numerical results with the exact solution by separation of variables method;

条件(3)好像不够定稳态解，要加一个归一化条件。

2. Find the steady-state solution ($\partial\rho/\partial t = 0$) of Eq.(1) with parameters $L = 1\,\mathrm{cm}$, $D = 0.1\,\mathrm{cm^2/s}$, $P_0 = 1\,\mathrm{s^{-1}}$, $w = 0.2\,\mathrm{cm}$, and $\alpha = 0.5$, under different boundary conditions Eq.(3) or Eq.(4);
3. Solve the full evolution problem under boundary condition Eq.(3) and Eq.(4), respectively;
4. Compare the computation efficiency of the h-version and p-version FEM on solving above problems.

Possible Extensions

1. **Different geometry**: in real experiments, the domain can be of various shape, like cubic, sphercial, cylindrical, pyramidical, or even more complicated shape. The p-version FEM may not so convenient as in the case of a cubic domain. Some commercial software may be useful in solving realistic problems. Try to build a model in, e.g., Comsol Multiphysics, and compare the results in the cubic domain obtained above;
2. **Non-linear problem**: in realistic problems, the matrix $G(\mathbf{r})$ in Eq.(1) can be much more sophisticated than that we defined in Eq.(7). Indeed, the value of G depends on the value of ρ, i.e., $G = G[\mathbf{r}, \rho(\mathbf{r})]$. In this case, Eq.(1) becomes a non-linear equation. The exact form of $G[\mathbf{r}, \rho(\mathbf{r})]$ was dicussed in S. Appelt, et. al., Physical Review A **58**, 1412 (1998) [see Eq. (96)]. We have developed numerical code, according to this reference, for calculating the explicit values of $G[\mathbf{r}, \rho(\mathbf{r})]$. Come to us if you want to try the non-linear problem.