Non-Hermitian Absorbing Layers for Schrödinger's Smoke: Supplementary Material

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Appendix A: dissipative property of $-i\hat{H}_{damp}$

We demonstrate that our Hamiltonian $-i\hat{H}_{damp}$ can be physically interpreted as velocity damper.

Theorem 1. *If two-component wave function $\boldsymbol{\psi}$ evolves by*

$$i\hbar \frac{\partial}{\partial t}\boldsymbol{\psi} = -i\hat{H}\boldsymbol{\psi}, \tag{1}$$

where $\hat{H}$ is a Hermitian operator whose eigenvalues λ_i satisfy $\lambda_i \geq 0$ and $\min(\lambda_i) = 0$, velocity $u_\alpha(\boldsymbol{x}, t) = Re\left\langle \frac{\partial \boldsymbol{\psi}}{\partial x^\alpha}, i\boldsymbol{\psi} \right\rangle / \rho$ decays exponentially

$$\left| \frac{u_\alpha(\boldsymbol{x}, t)}{u_\alpha(\boldsymbol{x}, 0)} \right| \sim \exp\left(-\hbar\lambda_1 t\right), \tag{2}$$

where λ_1 denotes the second smallest eigenvalue.

Proof. For convenience we re-write ρu_α as

$$\rho u_\alpha = \hbar \mathrm{Re}\left\langle \frac{\partial \boldsymbol{\psi}}{\partial x^\alpha}, i\boldsymbol{\psi} \right\rangle \tag{3}$$

$$=: \mathrm{Re}\left\langle \hat{p}_\alpha \boldsymbol{\psi}, \boldsymbol{\psi} \right\rangle, \tag{4}$$

where $\hat{p}_\alpha$ denote an operator $\hat{p}_\alpha := -i\hbar\frac{\partial}{\partial x^\alpha}$. Recalling that density is $\rho = \langle \boldsymbol{\psi}, \boldsymbol{\psi} \rangle$, velocity u_α is given by

$$u_\alpha = \frac{\mathrm{Re}\left\langle \hat{p}_\alpha \boldsymbol{\psi}, \boldsymbol{\psi} \right\rangle}{\langle \boldsymbol{\psi}, \boldsymbol{\psi} \rangle}. \tag{5}$$

Using the above notation, we derive the temporal evolution of velocity u_α. First, a general solution to the evolution of wave function $\boldsymbol{\psi}$

$$i\hbar \frac{\partial \boldsymbol{\psi}}{\partial t} = -i\hat{H}\boldsymbol{\psi} \tag{6}$$

is given by

$$\boldsymbol{\psi}(t) = \exp(-\hbar\hat{H}t)\boldsymbol{\psi}(0). \tag{7}$$

Therefore, velocity at time t is expressed as a closed-form

$$u_\alpha(t) = \frac{\mathrm{Re}\left\langle \hat{p}_\alpha e^{-\hbar\hat{H}t}\boldsymbol{\psi}(0), e^{-\hbar\hat{H}t}\boldsymbol{\psi}(0) \right\rangle}{\left\langle e^{-\hbar\hat{H}t}\boldsymbol{\psi}(0), e^{-\hbar\hat{H}t}\boldsymbol{\psi}(0) \right\rangle}. \tag{8}$$

Next, without loss of generality, we define $\boldsymbol{\psi}(0)$ as a linear combination of eigenfunctions $\{\boldsymbol{\psi}_i\}$ as

$$\boldsymbol{\psi}(0) = \sum_i c_i \boldsymbol{\psi}_i. \tag{9}$$

Note that the above definition is valid because eigenfunctions are complete since $\hat{H}$ is Hermitian. In the following, we define $\boldsymbol{\psi}_i$ as an eigenfunction associated with an eigenvalue λ_i such that

$$\hat{H}\boldsymbol{\psi}_i(\boldsymbol{x}) = \lambda_i \boldsymbol{\psi}_i(\boldsymbol{x}) \qquad (\lambda_0 \leq \lambda_1 \cdots \leq \lambda_{N-1}), \tag{10}$$

where N denotes the dimension of the linear space associated with the quantum system. For a continuous setting, N is not bounded but we can safely assume that N is bounded because discretization essentially trims dimension (or more simply, numerical simulation approximates the solution space with finite dimensions e.g., N is a number of cells). With this definition, (8) can be re-written as

$$u_\alpha(t) = \frac{\displaystyle\sum_{i,j} e^{-\hbar(\lambda_i+\lambda_j)t}\mathrm{Re}\left(c_i c_j^* \langle \hat{p}_\alpha \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle\right)}{\displaystyle\sum_{i,j} e^{-\hbar(\lambda_i+\lambda_j)t} c_i c_j^* \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle}. \tag{11}$$

Since we assumed that $\lambda_0 = 0$, the denominator of (11) can be arranged to

$$u_\alpha(t) = \frac{\displaystyle\sum_{i,j} e^{-\hbar(\lambda_i+\lambda_j)t}\mathrm{Re}\left(c_i c_j^* \langle \hat{p}_\alpha \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle\right)}{|c_0|^2 \langle \boldsymbol{\psi}_0, \boldsymbol{\psi}_0\rangle + \displaystyle\sum_{\substack{i,j\\(i,j)\neq(0,0)}} e^{-\hbar(\lambda_i+\lambda_j)t} c_i c_j^* \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle}. \tag{12}$$

Since an eigenfunction where its eigenvalue is zero is a constant field ($\boldsymbol{\psi}_0 = const.$), applying an operator $\hat{p} = -i\hbar\frac{\partial}{\partial x^\alpha}$ to $\boldsymbol{\psi}_0$ yields zero. Using this relation, the numerator of (12) can be re-written as

$$u_\alpha(t) = \frac{\displaystyle\sum_{i}\sum_{j\neq 0} e^{-\hbar(\lambda_i+\lambda_j)t}\mathrm{Re}\left(c_i c_j^* \langle \hat{p}_\alpha \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle\right)}{|c_0|^2 \langle \boldsymbol{\psi}_0, \boldsymbol{\psi}_0\rangle + \displaystyle\sum_{\substack{i,j\\(i,j)\neq(0,0)}} e^{-\hbar(\lambda_i+\lambda_j)t} c_i c_j^* \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle}. \tag{13}$$

Taking a limit $t \to \infty$ of (13) yields $\frac{0}{|c_0|^2\langle \boldsymbol{\psi}_0, \boldsymbol{\psi}_0\rangle} = 0$. Next, we examine the order of convergence. Using the fact that an expression $e^{-\hbar(\lambda_i+\lambda_j)t}$ is minimized when $i = 0$ and $j = 1$, maximized when $i = j = N-1$, the following inequality holds

$$|u_\alpha(t)| \leq \left| \frac{e^{-\hbar\lambda_1 t}\displaystyle\sum_{i}\sum_{j\neq 0}\mathrm{Re}\left(c_i c_j^* \langle \hat{p}_\alpha \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle\right)}{|c_0|^2 \langle \boldsymbol{\psi}_0, \boldsymbol{\psi}_0\rangle + e^{-2\hbar\lambda_{N-1}t} \displaystyle\sum_{\substack{i,j\\(i,j)\neq(0,0)}} c_i c_j^* \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle} \right|. \tag{14}$$

By multiplying $e^{\hbar\lambda_1 t + 2\hbar\lambda_{N-1}t}$ to both the denominator and numerator, the right-hand side of (14) becomes

$$\left| \frac{e^{2\hbar\lambda_{N-1}t}\displaystyle\sum_{i}\sum_{j\neq 0}\mathrm{Re}\left(c_i c_j^* \langle \hat{p}_\alpha \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle\right)}{e^{\hbar\lambda_1 t+2\hbar\lambda_{N-1}t}|c_0|^2 \langle \boldsymbol{\psi}_0, \boldsymbol{\psi}_0\rangle + e^{\hbar\lambda_1 t} \displaystyle\sum_{\substack{i,j\\(i,j)\neq(0,0)}} c_i c_j^* \langle \boldsymbol{\psi}_j, \boldsymbol{\psi}_i\rangle} \right|. \tag{15}$$

Note that absolute values of the numerator and denominator increase in the order of $O(e^{2\hbar\lambda_{N-1}t})$ and $O(e^{\hbar\lambda_1 t+2\hbar\lambda_{N-1}t})$, respectively. This shows that (15) decays on the order of $O(e^{-\hbar\lambda_1 t})$. □

Corollary 1.1. *Velocity u_α in a system evolved by an operator $-i\hat{H}_{damp}$ damps exponentially where $\sigma(\boldsymbol{x}) \neq 0$.*

Proof. We examine $\int f(\boldsymbol{x})\hat{H}_{\mathrm{damp}} f(\boldsymbol{x})dV$, where $f(\boldsymbol{x})$ is an arbitrary function, to show that $\hat{H}_{damp}$ is a positive semi-definite Hermitian operator. Integrating by parts gives

$$\begin{aligned}\int f(\boldsymbol{x})\hat{H}_{\mathrm{damp}} f(\boldsymbol{x})dV = & \int \nabla f(\boldsymbol{x}) \cdot \Sigma(\boldsymbol{x})\nabla f(\boldsymbol{x})dV \\ - & \oint f(\boldsymbol{x})\Sigma(\boldsymbol{x})\nabla f(\boldsymbol{x}) \cdot \boldsymbol{n}(\boldsymbol{x})dA \qquad (16)\\ = & \int \nabla f(\boldsymbol{x}) \cdot \Sigma(\boldsymbol{x})\nabla f(\boldsymbol{x})dV \qquad (17)\\ = & \int \left|\left|\sqrt{\Sigma}(\boldsymbol{x})\nabla f(\boldsymbol{x})\right|\right|^2 dV \geq 0, \qquad (18)\end{aligned}$$

where

$$\Sigma(\boldsymbol{x}) = \operatorname{diag}\left(\sigma_x\left(\boldsymbol{x}\right), \sigma_y\left(\boldsymbol{x}\right), \sigma_z\left(\boldsymbol{x}\right)\right), \tag{19}$$

$$\sqrt{\Sigma}(\boldsymbol{x}) = \operatorname{diag}\left(\sqrt{\sigma_x}\left(\boldsymbol{x}\right), \sqrt{\sigma_y}\left(\boldsymbol{x}\right), \sqrt{\sigma_z}\left(\boldsymbol{x}\right)\right). \tag{20}$$

In the above we dropped the surface integral term since we assume periodic boundary conditions. Therefore, $\hat{H}_{damp}$ is positive semi-definite. Next, for any constant function e.g., $f(\boldsymbol{x}) = 1$, it holds that $\nabla f = 0$. This shows that

$$\hat{H}_{damp} f(\boldsymbol{x}) = 0. \tag{21}$$

Hence, $f(\boldsymbol{x}) = 1$ is an eigenfunction of $\hat{H}_{damp}$ associated with a zero eigenvalue. Therefore, Corollary 1.1 is proven from Theorem 1. □