Modelling and Structure-Preserving Discretization of the Schrödinger as a Port-Hamiltonian System, and Simulation of a Controlled Quantum Box

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Abstract. The modelling of the Schrödinger Equation as a port-Hamiltonian system is addressed. We suggest two Hamiltonians for the model, one based on the probability of presence and the other on the energy of the quantum system in a time-independent potential. In order to simulate the evolution of the quantum system, we adapt the model to a bounded domain. The model is discretized thanks to the structure-preserving Partitioned Finite Element Method (PFEM). Simulations of Rabi oscillations to control the state of a system inside a quantum box are performed. Our numerical experiments include the transition between two levels of energy and the generation of Schrödinger cat states.

Keywords: port-Hamiltonian systems · open quantum systems

1 Introduction

Over the past two decades, the port-Hamiltonian (pH) theory has continued to develop as a preferential paradigm to describe distributed parameter systems [13]. This formalism is judicious to model and control complex dynamical systems: subsystems communicate *via* ports and the power balance is incorporated within the pH structure. It has been successfully applied to many fields such as structural mechanics, electromagnetism and fluid mechanics (see *e.g.* [3,8,13] and references therein).

Controlling and stabilizing a quantum system in a desired state, such as two-state quantum systems called qubits, is the key of quantum information science [12]. A first attempt in applying the pH theory to quantum systems is proposed in the present work, together with promising numerical experiments.

The modelling of the Schrödinger equation including a control is presented in Sect. 2. In Sect. 3, a discrete (in space) port-Hamiltonian system is obtained by applying PFEM [3,5]. Finally, Sect. 4 ends this work with Rabi oscillations simulation results, *i.e.* controlling the state of a quantum box.

More details, developments and discussions on this work can be found in [14].

Supported by the AID from the French Ministry of the Armed Forces.

F. Nielsen and F. Barbaresco (Eds.): GSI 2023, LNCS 14072, pp. 392–401, 2023.
https://doi.org/10.1007/978-3-031-38299-4_41

2 Port-Hamiltonian Modelling

To take advantage of the distributed port-Hamiltonian paradigm, we adopt the wave function representation $\Psi(\mathbf{r}, t)$ of a quantum system [6]:

$$H\Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t}. \tag{1}$$

This is the Partial Differential Equation (PDE) form of the Schrödinger Equation. The Hamiltonian operator H is given *via*:

$$H\Psi(\mathbf{r}, t) := -\frac{\hbar^2}{2m} \Delta\Psi(\mathbf{r}, t) + V(\mathbf{r}, t)\Psi(\mathbf{r}, t).$$

The control of the wave function $\Psi(\mathbf{r}, t)$ appears in the potential $V(\mathbf{r}, t)$ of the Hamiltonian operator. To build a port-Hamiltonian system, we have to define ports, and especially those composed of controls and observations. Moreover, a Hamiltonian *functional*, a form depending on the *states*, has to be chosen [13].

2.1 Ports: Control and Observation

By splitting the potential $V(\mathbf{r}, t)$ into two terms, one positive and stationary $V_s(\mathbf{r})$ and the other time-dependent $V_c(\mathbf{r}, t)$, we suggest an extension of the Schrödinger Equation. We call this new equation the Controlled Schrödinger Equation:

$$H_s\Psi(\mathbf{r}, t) + i\hbar u(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t}, \tag{2}$$

where $u(\mathbf{r}, t)$ denotes the control. The time-independent part of the Hamiltonian operator is then:

$$H_s\Psi(\mathbf{r}, t) := -\frac{\hbar^2}{2m} \Delta\Psi(\mathbf{r}, t) + V_s(\mathbf{r})\Psi(\mathbf{r}, t).$$

Thanks to this point of view, Ψ follows the Schrödinger Eq. (1) if and only if $u(\mathbf{r}, t) = -\frac{i}{\hbar} V_c(\mathbf{r}, t)\Psi(\mathbf{r}, t)$. Thus, the control u is given by a linear state feedback (see Fig. 2). This imposes the wave function $\Psi(\mathbf{r}, t)$ to be the observation.

2.2 The Hamiltonian of the pH System

The choice of the Hamiltonian functional is led by the Ehrenfest Theorem, which provides the evolution of the expectation value of quantum operators (hereafter the identity and H_s), similarly to the evolution equation of observables in classical Hamiltonian mechanics [6]. We define two possible Hamiltonians:

$$\mathcal{H}_{\mathcal{P}} := \int_{\mathbf{r}\in\mathbb{R}^3} |\Psi(\mathbf{r}, t)|^2 d\mathbf{r},$$

$$\mathcal{H}_{\mathcal{N}} := \int_{\mathbf{r}\in\mathbb{R}^3} \frac{\hbar^2}{2m} \|\mathbf{grad}\Psi(\mathbf{r}, t))\|^2_{\mathbb{C}^3} + V_s(\mathbf{r})|\Psi(\mathbf{r}, t)|^2 d\mathbf{r}.$$

The former $\mathcal{H}_\mathcal{P}$ is based on the *probability of presence*: according to Born rule [6], $\mathcal{H}_\mathcal{P} = 1$. The latter $\mathcal{H}_\mathcal{N}$ is based on the *energy*: it is preserved in absence of a time-dependent potential of control. From an analytic point of view, these two Hamiltonians are norms squared of the wave function w.r.t Hermitian inner products. Indeed, $\mathcal{H}_\mathcal{P} = \langle\Psi|\Psi\rangle$ and $\mathcal{H}_\mathcal{N} = \langle\Psi,\Psi\rangle_\mathcal{N}$ with:

- $\langle u|v\rangle := \int_{\mathbf{r}\in\mathbb{R}^3} u(\mathbf{r},.)^* v(\mathbf{r},.)d\mathbf{r}$. We identify the L^2 inner product.
- $\langle u,v\rangle_\mathcal{N} := \int_{\mathbf{r}\in\mathbb{R}^3} \frac{\hbar^2}{2m}\mathbf{grad}u(\mathbf{r},.))^*.\mathbf{grad}v(\mathbf{r},.)) + V_s(\mathbf{r})u(\mathbf{r},.)^* v(\mathbf{r},.)d\mathbf{r}$, which is equivalent to the H^1 inner product if $V_s(\mathbf{r})$ is lower bounded by a positive constant and upper bounded. In keeping with a change in the energy origin, any constant can be added to $V_s(\mathbf{r})$ without changing the quantum system.

The balance equations of these two Hamiltonians can be derived by adapting the Ehrenfest Theorem to the Controlled Schrödinger Eq. (2). For $\langle .,.\rangle \in \{\langle .|.\rangle, \langle .,.\rangle_\mathcal{N}\}$, depending on the choice of the Hamiltonian, we can write canonically the evolution of the Hamiltonian $\mathcal{H} = \langle\Psi,\Psi\rangle$ along the trajectories:

$$\frac{d}{dt}\mathcal{H} = \frac{d}{dt}\langle\Psi,\Psi\rangle = 2\Re(\langle\Psi,\frac{\partial\Psi}{\partial t}\rangle) = 2\Re(\langle\Psi,-i\frac{H_s}{\hbar}\Psi + u\rangle). \tag{3}$$

2.3 Port-Hamiltonian Formulation

The Hamiltonian functional is defined on a complex-valued state, which is the wave function. We define the energy variable of the port-Hamiltonian system $\alpha := \Psi$. Thus, the distributed port-Hamiltonian paradigm has to be extended to complex-valued states. The Hamiltonian functionals of distributed port-Hamiltonian systems are written in the form of an integral on a domain Ω of a real-valued function h:

$$\mathcal{H}[\alpha] = \int_{\mathbf{r}\in\Omega} h(\alpha)d\mathbf{r}.$$

The evolution of the Hamiltonian along the trajectories requires the differentiation of the functional w.r.t the energy variable. Using the $\mathbb{CR}$-calculus, we can consider h as a holormorphic function w.r.t the conjugate coordinates (α,α^*) [7]. Thus the differential rule leads to:

$$\mathcal{H}[\alpha+v] - \mathcal{H}[\alpha] = \int_{\mathbf{r}\in\Omega} 2\Re\left(\frac{\partial h(\alpha,\alpha^*)}{\partial\alpha}v\right)d\mathbf{r} + o(v). \tag{4}$$

Using the inner product $\langle .,.\rangle$ on Ω, we can identify the functional derivative (or variational derivative of the functional), denoted $\delta_\alpha\mathcal{H}$, such that:

$$\int_{\mathbf{r}\in\Omega} \frac{\partial h(\alpha,\alpha^*)}{\partial\alpha}vd\mathbf{r} = \langle\delta_\alpha\mathcal{H},v\rangle.$$

Using the chain rule, the evolution of the Hamiltonian is the symmetrization of the usual balance (see Fig. 1):

$$\frac{d\mathcal{H}}{dt} = 2\Re(\langle \delta_\alpha \mathcal{H}, \frac{\partial \alpha}{\partial t} \rangle). \tag{5}$$

Focusing on the pH modelling of the Controlled Schrödinger Eq. (2) and using the inner products defined in Sect. 2.2, we can define the co-energy variable $e := \delta_\alpha \mathcal{H} = \Psi$. This leads to the complex-valued distributed pH systems:

$$\begin{cases} \partial_t \alpha = \mathcal{J} e + G u \\ y = G^H e \end{cases} \quad \text{with} \quad \mathcal{J} = -\frac{iH_s}{\hbar} \quad \text{and} \quad G = \mathbf{1}. \tag{6}$$

The structure operator $\mathcal{J}$ is skew-symmetric since H_s is symmetric for both inner products. This property implies that the Hamiltonian balance is achieved *via* the dual controls and observations. Indeed, using (5) (compare with (3)):

$$\frac{d\mathcal{H}}{dt} = 2\Re(\langle \delta_\alpha \mathcal{H}, \mathcal{J} \delta_\alpha \mathcal{H} \rangle + \langle \delta_\alpha \mathcal{H}, G u \rangle) = 2\Re(\langle G^H \delta_\alpha \mathcal{H}, u \rangle) = 2\Re(\langle y, u \rangle).$$

These properties have been identified in [4] to recover the (complex) Stokes-Dirac structure of distributed port-Hamiltonian systems.

Hamiltonian system	**Distributed pH system**
Canonical equations	Stokes-Dirac structure
Hamiltonian functional (typically a quadratic form) $\mathcal{H}[\Psi] = \frac{1}{2}\|\Psi\|^2_{\mathcal{A}}$	Hamiltonian functional (typically a quadratic form) $\mathcal{H}[\Psi] = \frac{1}{2}\|\Psi\|^2_{\mathcal{A}}$
Observable $\mathcal{A}$. $\frac{d\mathcal{A}}{dt} = \{\mathcal{A}, \mathcal{H}\} + \frac{\partial \mathcal{A}}{\partial t}$	Conservation of $\mathcal{H}$ via ports $\frac{d\mathcal{H}}{dt} = \langle \frac{\partial \Psi}{\partial t}, \delta_\Psi \mathcal{H} \rangle$
Quantum mechanics	**Distributed pH system with complex state**
Schrödinger equation / Ehrenfest theorem	(Complex) Stokes-Dirac structure
Hamiltonian operator $\widehat{H} = \frac{\widehat{p}^2}{2m} + \widehat{V}$	Hamiltonian functional $\mathcal{H}[\Psi] = \|\Psi\|^2_{\widehat{A}} = \langle \Psi \| \widehat{A} \| \Psi \rangle$
Observable (operator) $\widehat{A}$. $\frac{d\langle \widehat{A} \rangle_\Psi}{dt} = \frac{1}{i\hbar}\langle [\widehat{A}, \widehat{H}] \rangle_\Psi + \langle \frac{\partial \widehat{A}}{\partial t} \rangle_\Psi$	Conservation of $\mathcal{H}$ via ports $\frac{d\mathcal{H}}{dt} = 2\Re(\langle \frac{\partial \Psi}{\partial t}, \delta_\Psi \mathcal{H} \rangle)$

Fig. 1. The new framework for distributed port-Hamiltonian with complex-valued state as a trade off between quantum mechanics (canonical quantization of the classical Hamiltonian mechanics) and the existing framework for distributed port-Hamiltonian systems with real-valued state.

2.4 Adaptation of the Model to Simulation

The wave function that represents the quantum system extends to infinity. However, the dynamics of the quantum system is simulated in a *bounded* domain $\Omega \subset \mathbb{R}^3$ only. A *virtual* system has to be defined, such that its solution is the restriction of the wave function to Ω. Let us denote $\partial\Omega$ the boundary, and $\mathbf{n}$ its outward normal. We consider the *restricted* inner products $\langle u|v \rangle$ and $\langle u, v \rangle_{\mathcal{N}}$:

– $\langle u, v \rangle_\Omega := \int_{\mathbf{r} \in \Omega} u(\mathbf{r}, .)^* v(\mathbf{r}, .) d\mathbf{r}$,
– $\langle u, v \rangle_{\mathcal{N}\Omega} := \int_{\mathbf{r} \in \Omega} \frac{\hbar^2}{2m} \mathbf{grad} u(\mathbf{r}, .)^* . \mathbf{grad} v(\mathbf{r}, .) + V_s(\mathbf{r}) u(\mathbf{r}, .)^* v(\mathbf{r}, .) d\mathbf{r}$.

The corresponding Hamiltonians are $\mathcal{H}^\Omega_\mathcal{P} := \langle \Psi, \Psi \rangle_\Omega$ and $\mathcal{H}^\Omega_\mathcal{N} := \langle \Psi, \Psi \rangle_{\mathcal{N}\Omega}$. The formulation of the port-Hamiltonian systems is the same. H_s becomes formally symmetric for these inner products. Thus, a boundary contribution now takes place in the Hamiltonian balance. Defining the speed operator by $\mathbf{v}\Psi(\mathbf{r}, t) := -i\frac{\hbar}{m} \mathbf{grad} \Psi(\mathbf{r}, t)$, we can derive the equation of probability conservation by integrating by parts (3):

$$\frac{d}{dt} \mathcal{H}^\Omega_\mathcal{P} = 2\Re(\langle \Psi, u \rangle_\Omega) - \Re\left(\int_{\partial\Omega} \Psi^*(\mathbf{r}, t)(\mathbf{v}\Psi(\mathbf{r}, t).\mathbf{n}) d\gamma \right). \tag{7}$$

The first term is the expected flow from the model $2\Re(\langle y, u \rangle_\Omega)$. It is zero when Ψ follows the Schrödinger Equation with potential $V(\mathbf{r}, t)$. The second term is the probability flows across the boundary. Indeed, denoting the real-valued probability current $\mathbf{J} := \frac{i\hbar}{2m}(\Psi \mathbf{grad} \Psi^* - \Psi^* \mathbf{grad} \Psi)$ then $\mathbf{J} = \Re(\Psi^* \mathbf{v} \Psi)$.

The energy balance for $\mathcal{H}^\Omega_\mathcal{N}$ is more difficult to interpret. This is the reason why the pH system based on $\mathcal{H}^\Omega_\mathcal{P}$ is chosen for the sequel of this work.

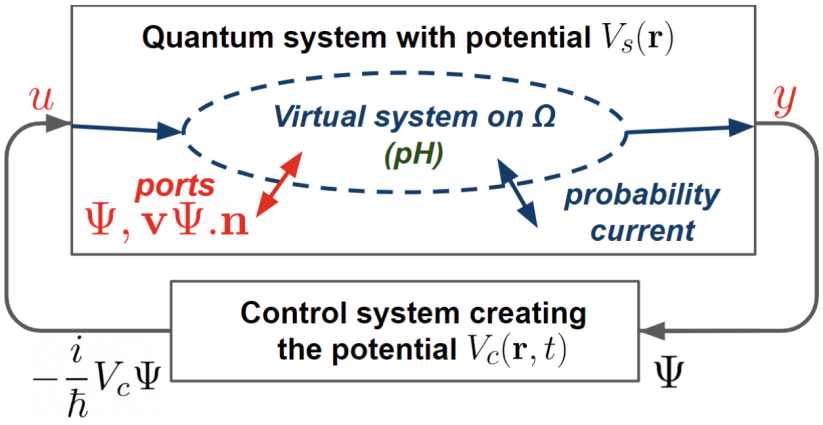

Fig. 2. The Schrödinger Equation as a pH model controlled by a linear state feedback from a control system. The pH model of the virtual system is the restriction of the pH model describing the Controlled Schrödinger Equation to a bounded domain.

3 Structure-preserving Discretization

In this part we apply the PFEM to build a discrete pH representation of the model [3,5]. Let ϕ be a sufficiently smooth complex-valued test function. Writing the weak formulation of (6) with the inner product $\langle ., . \rangle_\Omega$ and integrating by parts, one gets:

$$\langle \phi, \partial_t \Psi \rangle_\Omega = -\frac{i}{\hbar}\langle \phi, \Psi \rangle_{\mathcal{N}\Omega} + \langle \phi, u \rangle_\Omega - \frac{1}{2}\int_{\partial\Omega} \phi^* (\underbrace{-i\frac{\hbar}{m}\mathbf{grad}\Psi}_{\mathbf{v}\,\Psi}.\mathbf{n}) d\gamma. \tag{8}$$

The normal speed boundary condition is identified.

As will be seen in Sect. 4.1, Dirichlet boundary condition is essential to model a quantum box. Following [3], such a control can be imposed by using Lagrange multipliers. Splitting the boundary into two distinct and complementary parts $\partial\Omega = \Gamma_N \cup \Gamma_D$, one can distinguish between Dirichlet controls u^D imposed via the Lagrange multipliers $\lambda^D = -\frac{1}{2}(\mathbf{v}\,\Psi).\mathbf{n}|_{\Gamma_D}$ on Γ_D, and Neumann control $u^N = -\frac{1}{2}(\mathbf{v}\,\Psi).\mathbf{n}|_{\Gamma_N}$ on Γ_N.

Let us define the finite real approximation spaces $\overline{W} = \text{span}((\phi_n)_n)$ and $\overline{B} = \text{span}((b_n)_n)$ to discretize the variables defined on Ω and on $\partial\Omega$ respectively. Let us denote $\Psi(\mathbf{r}, t) \approx \psi^d(\mathbf{r}, t) = \sum_{n=1}^{\dim\overline{W}} \psi_n(t)\phi_n(\mathbf{r}) = \underline{\phi}(\mathbf{r})^T \underline{\psi}(t)$ and similarly for other quantities.

Defining the skew-symmetric complex matrix $(J)_{m,n} = -\frac{i}{\hbar}\langle \phi_m, \phi_n \rangle_{\mathcal{N}\Omega}$ of size $\dim\overline{W} \times \dim\overline{W}$, the symmetric real matrices $(M)_{m,n} = \langle \phi_m, \phi_n \rangle_\Omega$ of size $\dim\overline{W} \times \dim\overline{W}$, $(M^D)_{m,n} = \langle b_m, b_n \rangle_{\Gamma_D}$ and $(M^N)_{m,n} = \langle b_m, b_n \rangle_{\Gamma_N}$ of size $\dim\overline{B} \times \dim\overline{B}$, and the real matrices $(G^D)_{m,n} = \langle \phi_m, b_n \rangle_{\Gamma_D}$ and $(G^N)_{m,n} = \langle \phi_m, b_n \rangle_{\Gamma_N}$ of size $\dim\overline{W} \times \dim\overline{B}$, the discrete counterpart of (8) reads:

$$M\frac{d}{dt}\underline{\psi} = J\underline{\psi} + G\underline{u} + G^N\underline{u^N} + G^D\underline{\lambda^D}.$$

The discretized Dirichlet algebraic constraint is:

$$G^D\underline{u^D} = (B^D)^H\underline{\psi}.$$

The discretized Neumann boundary observation (of the wave function) is:

$$M^N\underline{y^N} = (G^N)^H\underline{\psi}.$$

The discretized Dirichlet boundary observation (of the normal speed), through the Lagrange multipliers, is:

$$M^D\underline{y^D} = (B^D)^H\underline{\lambda^D}.$$

And finally, the distributed observation is:

$$M^\Omega\underline{y} = G^H\underline{\psi}.$$

Note that $M = G = M^\Omega$ and $M^D = B^D$ in this work, although this is not mandatory (using *e.g.* different spaces of approximation for controls and observations).

Altogether, denoting $\mathbb{E} := \text{diag}(M, 0, M^\Omega, M^N, M^D)$ leads to:

$$\mathbb{E}\begin{pmatrix} \frac{d}{dt}\underline{\psi} \\ \frac{d}{dt}\underline{\lambda^D} \\ -\underline{y} \\ -\underline{y^N} \\ -\underline{y^D} \end{pmatrix} = \begin{pmatrix} J & G^D & G & G^N & 0 \\ -(G^D)^H & 0 & 0 & 0 & B^D \\ -(G)^H & 0 & 0 & 0 & 0 \\ -(G^N)^H & 0 & 0 & 0 & 0 \\ 0 & -(B^D)^H & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{\psi} \\ \underline{\lambda^D} \\ \underline{u} \\ \underline{u^N} \\ \underline{u^D} \end{pmatrix}. \tag{9}$$

This Differential Algebraic Equation (DAE) respects the Dirac structure, known as the algebraic structure describing finite-dimensional port-Hamiltonian systems [4,10,13].

The Schrödinger Equation is embedded into the system by considering the time-dependant linear feedback from the control system that generates $V_c(\mathbf{r},t)$. We introduce the symmetric real matrix $(V_c^d)_{m,n} = \langle \phi_m, V_c \phi_n \rangle_\Omega$ of size $\dim\overline{W} \times \dim\overline{W}$. Then the discretization of the feedback associated to the Schrödinger Equation leads to:

$$M^\Omega \underline{u} = -\frac{i}{\hbar} V_c^d(t) \underline{y}. \tag{10}$$

Let us denote $\mathcal{H}_\mathcal{P}^d(t) := \mathcal{H}_\mathcal{P}^\Omega[\psi^d] = \langle \psi^d, \psi^d \rangle_\Omega = \underline{\psi}^H M \underline{\psi}$ the Hamiltonian of the discretized system. Thanks to the Dirac structure enlightened in (9), the corresponding balance follows:

$$\frac{d}{dt}\mathcal{H}_\mathcal{P}^d = 2\Re\left(\underline{y}^H M^\Omega \underline{u} + (\underline{y^D})^H M^D \underline{u^D} + (\underline{y^N})^H M^N \underline{u^N}\right).$$

This equality is the discrete counterpart of (7). Similarly to the continuous equation, the first term is equal to zero in the case of the Schrödinger Eq. (10), because the feedback matrix $-\frac{i}{\hbar}V_c^d(t)$ is always skew-symmetric.

To conclude, thanks to the application of the PFEM to the complex-valued distributed pH system, both Dirac structure and probability conservation (Hamiltonian balance) have been preserved at the discrete level.

4 Numerical Experiments

4.1 One-Dimensional Quantum Box

The quantum system is entirely in the domain of the box Ω. We impose a homogeneous Dirichlet condition on the boundary $\partial\Omega$. For $x \in \Omega = [0, L]$, in absence of potential, the stationary states $\Psi_n(x,t)$ are the states of energies $E_n = \frac{\hbar^2 k_n^2}{2m} = \hbar\omega_n = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}$ $(n \in \mathbb{N}^\star)$. These states $\Psi_n(x,t) = \sqrt{\frac{2}{L}}\sin(k_n x)\exp(-i\omega_n t)$, analogous to oscillating modes, form an ortho-normal basis of conservative states [6].

For our simulations, the spatial structure-preserving discretization of (6) is performed as in (9), using Lagrange finite elements of order 1. Then, the resulting DAE is solved in time by the *Matlab* DAE solver *ode23t*. Let us point out that defining time schemes for finite-dimensional (real-valued) port-Hamiltonian DAE is a current topic of research, see *e.g.* [9,10] and references therein.

In Table 1, we reproduce the propagation of the first modes for a sufficiently fine discretization (sampling of oscillations). The Hamiltonian balance is well respected.

Table 1. Results of the simulation of conservative systems over a period T_f. N_x is the number of points of discretization. N_{osc} is the number of temporal oscillations of the analytical solution. N_t is the number of instants at which the numerical solution is computed. The L^2-error corresponds to the maximum in space of the L^2-error between the numerical solution of the wave function and the analytical solution over the time span. The relative error on $\mathcal{H}_{\mathcal{P}}^d$ compares the value at T_f to the initial value.

Initial state	N_x	T_f	N_{osc}	N_t	L^2 error	Relative error on $\mathcal{H}_{\mathcal{P}}^d$
State 1 : Ψ_1	51	$2\pi/\omega_1$	1	43	9.7×10^{-3}	4.9×10^{-4}
State 2 : Ψ_2	51	$2\pi/\omega_1$	4	160	1.6×10^{-2}	4.9×10^{-4}
State 3 : Ψ_3	51	$2\pi/\omega_1$	9	357	5.7×10^{-2}	4.9×10^{-4}
States 1 + 2 : $(\Psi_1 + \Psi_2)/\sqrt{2}$	51	$2\pi/\omega_1$	1	203	4.0×10^{-3}	6.8×10^{-7}

4.2 Rabi Oscillations: Control of the Energy Levels and Generation of Schrödinger Cat States

Applying an electric field of amplitude $\mathcal{E}_0$ and angular frequency ω_E on a dipole of charge q results in a potential $V_c(x,t) = -qx\mathcal{E}_0 \sin(\omega_E t)$ [1]. If the initial state of the system is the superposition of the states 1 and 2 and if $\omega_E \approx \omega_2 - \omega_1$, then the system oscillates between state 1 and state 2 at the Rabi period T_{Rabi} that can be computed analytically for the quantum box. The probability of measuring the state n is $P_n = |\langle \Psi_n, \Psi \rangle_\Omega|^2$.

In the following numerical experiment, we apply the control of pulsation $\omega_E = \omega_2 - \omega_1$ on a time interval $[t_{\text{start}}, t_{\text{stop}}]$ of period $T_{\text{Rabi}}/2$ (Fig. 3). We correctly reproduce the Rabi oscillations and we identify the expected high frequency oscillations of period π/ω_E (Fig. 3 on the right). Thanks to the control, we switch from state 1 to state 2. Balanced Schrödinger cat states are reached by applying the control on a period $T_{\text{Rabi}}/4$ (blue dot on Fig. 3). Note that the Hamiltonian balance accuracy is clearly driven by the precision of the time scheme as soon as the control is switched on (Fig. 3 on the left).

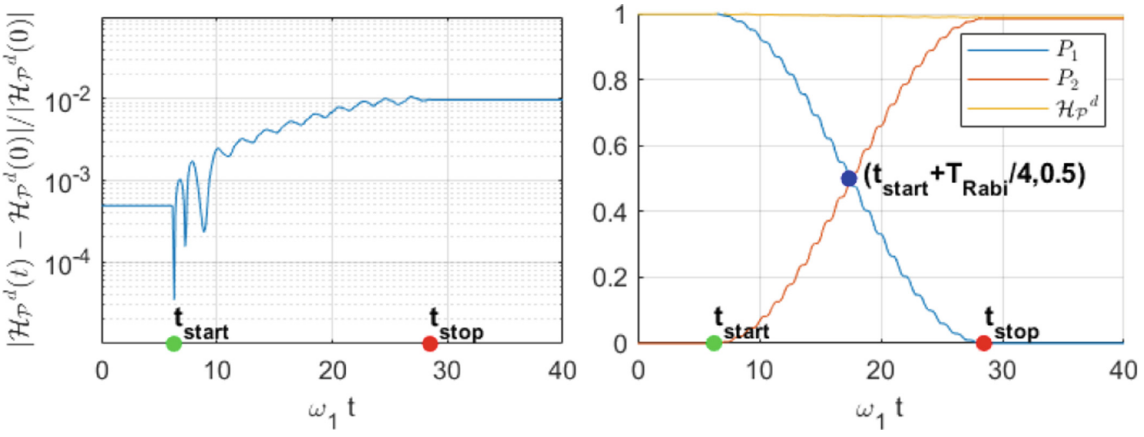

Fig. 3. Simulation of Rabi oscillations and transition from the state 1 to the state 2. $N_x = 51$, $N_t = 1346$. The values of q and $\mathcal{E}_0$ are taken arbitrarily.

5 Conclusion

In this work, we modelled the PDE form of the Schrödinger Equation as a distributed pH system. We proposed a (space-)discretization preserving the probability of presence balance equation at the discrete level. Our numerical experiments show that it is possible to apply simple controls on quantum systems to manipulate their states.

Compared to our real-valued modelling approach [14], the framework we suggested here for modelling distributed port-Hamiltonian systems with complex-valued states describes the system in a more compact way and better emphasizes the formalism used in quantum mechanics.

The interaction of the quantum system with a system of control has been interpreted as the feedback of a potential of control. Thus the system of control is represented by a black box. However, the port specifications of the model remain robust to further pH modelling, *e.g.* the Schrödinger-Newton Equation could be tackled by coupling the model with the Poisson Equation [2].

Modelling interacting quantum systems in the port-Hamiltonian framework is still challenging. It cannot only be the interconnection of individual quantum systems. Indeed, without considering the system dynamics, the space of states of interacting systems is the tensor product of the individual space of states, which deeply restrains the system decomposition [6,11].

Acknowledgements. The authors would like to thank Pr. S. Massenot for his useful advice on the choice of quantum mechanics numerical experiments.

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