Trajectory tracking for quantum systems: a Lyapounov approach.

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Abstract

A Lyapounov-based approach for trajectory tracking of the Schrödinger equation is proposed. In the finite dimensional case, convergence is analyzed: the connection between the controllability of the linear tangent approximation around the reference trajectory and asymptotic tracking is studied. Closed-loop simulations of a physical example illustrate the interest of such feedback laws for large dimensional systems.

Keywords: nonlinear systems, quantum systems, control Lyapounov function, trajectory tracking.

1 Introduction

Controllability of a finite dimensional quantum system:

$$\imath\dot{\Psi} = (H_0 + u(t)H_1)\Psi$$

where H_0 and H_1 are $n \times n$ Hermitian matrices with coefficients in $\mathbb{C}$, can be studied via the general accessibility criteria proposed in [10] and based on Lie-Brackets. More specific results might be found in e.g. [8] and [11]. In particular, the system is controllable if and only if the Lie algebra generated by the skew-symmetric matrices $H_0/\imath$ and $H_1/\imath$ is $su(n)$. Thus controllability of such systems is well characterized. However, such a characterization does not provide in general a simple and efficient way for control design.

Optimal control techniques (see, e.g., [5] and the reference herein) provides a first set of methods. Another set consists in using feedback: see,e.g., [7] for decoupling techniques, or [12, 2] for Lyapounov based techniques, ...

In this paper we propose a Lyapounov-based technique that can be relevant for trajectory tracking of a system described by a controlled Schrödinger

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equation. The control Lyapounov function is based on the conservation of probability and thus can be used whatever the dimension of the system is. In the finite dimensional case, we show that controllability of the first variation around the reference trajectory is a necessary condition for the global asymptotic convergence. A sufficient condition for asymptotic convergence is also proposed: it is based on an asymptotically persistence of the controllability of the first variation around the reference trajectory. The analysis is based on an adaptation to bilinear quantum systems of the general method proposed in [4] (see also [3]). Our design method is close but different from the one proposed in [12]: our feedback design relies on a control Lyapounov function, deals with tracking of any system trajectory and yields to a convergence characterization related to the controllability of the first variation system.

The paper is organized as follows. In the second section, we describe the control design and give the necessary and sufficient conditions for the asymptotic convergence. Third section is devoted to a short-cut model of large dimension, classical in the physics literature [1], of a discrete state coupled to a continuum.

When the reference trajectory corresponds to an eigen-state of H_0, more detailed convergence results can be found in [6]. The authors thank Gabriel Turinici for many interesting discussions and references and also Laurant Praly for his expertise in LaSalle's invariance principle.

2 Lyapounov-based tracking control

2.1 The design

We consider here, the control of the equation which governs the time evolution of a quantum system. To such a system (supposed to be isolated from the external world for the moment) corresponds an internal Hamiltonian H_0 which is a time independent self-adjoint operator. The dynamic of this system obeys a time dependent Schrödinger equation($\hbar = 1$):

$$\begin{aligned} \iota \tfrac{d}{dt}\Psi &= H_0 \Psi, \\ \Psi|_{t=0} = \Psi_0, &\quad \|\Psi_0\|_{\mathcal{H}} = 1 \end{aligned}$$

where $\| \, . \, \|_{\mathcal{H}}$ is the norm of $\mathcal{H}$, the Hilbert space where Ψ the wave function of the system is defined. The external interaction will be taken as a classical control field amplitude $u(t) \in \mathbb{R}$ coupled to the system through a time independent self-adjoint operator H_1:

$$\begin{aligned} \iota \frac{d}{dt}\Psi &= (H_0 + u(t) H_1)\Psi, \\ \Psi|_{t=0} &= \Psi_0. \end{aligned} \tag{1}$$

Note that the wave function Ψ is evolving on the unit sphere of $\mathcal{H}$ (conservation of the probability):

$$\|\Psi(t)\|_{\mathcal{H}} = \|\Psi_0\|_{\mathcal{H}} = 1 \qquad \forall t \geq 0.$$

Our purpose here, is to do trajectory tracking. Consider a reference trajectory $t \mapsto (\Psi_r(t), u_r(t))$ of (1):

$$\imath \frac{d}{dt}\Psi_r = (H_0 + u_r(t)H_1)\ \Psi_r.$$

Set $\Delta\Psi = \Psi - \Psi_r$ and $\Delta u = u - u_r$. Then

$$\imath \frac{d}{dt}\Delta\Psi = (H_0 + u_r(t)H_1)\ \Delta\Psi + \Delta u\ H_1\Psi. \tag{2}$$

Take the following time varying function $V(\Delta\Psi)$:

$$V(\Psi, t) = \langle \Delta\Psi \mid \Delta\Psi \rangle \tag{3}$$

where $\langle .|. \rangle$ denotes the hermitian product in $\mathcal{H}$. V is positive for all $\Delta\Psi \in \mathcal{H}$ and vanishes when $\Delta\Psi = 0$. Simple computations show that V is a control Lyapounov function:

$$\frac{d}{dt}V = -2\Delta u \Im(\langle H_1\Psi(t) \mid \Psi_r \rangle) \tag{4}$$

where $\Im$ denotes the imaginary part. By choosing Δu with the same sign as $\Im(\langle H_1\Psi(t) \mid \Psi_r\rangle)$, V will decrease along the trajectories. Any time varying feedback of the form

$$u = u_r + K\left(t, \Im(\langle H_1\Psi(t) \mid \Psi_r \rangle)\right) \tag{5}$$

where K is a smooth function such that for all $t > 0$ and $s \in \mathbb{R}$,

$$sK(t,s) \geq 0, \quad K(t,s) = 0 \Leftrightarrow s = 0,$$

ensures $dV/dt \leq 0$: with such feedback, the distance between the systems trajectory $\Psi(t)$ and the reference trajectory $\Psi_r(t)$ decreases.

As a particular case, one may consider the reference trajectory, $\Psi_r = e^{-\imath\lambda t}\phi$ and $u_r = 0$, where ϕ is an eigen-state of the free Hamiltonian H_0 corresponding to the eigen-value $\lambda \in \mathbb{R}$. Trivially $(\Psi_r = e^{-\imath\lambda t}\phi, u_r = 0)$ is a trajectory of the system (1). Using the Lyapounov based method for this case, we can try to steer the initial state Ψ_0 to the pure state corresponding to the eigen-state ϕ of H_0.

Convergence of the method for this special case and when the system is of finite dimension, has been studied in [6]. Here, the wave function is an element of $\mathbb{C}^n$ and H_0 and H_1 are $n \times n$ Hermitian matrices. It has been shown when the eigenvalues of H_0 are distinct, that the ω-limit set is the intersection of the unit sphere of $\mathbb{C}^n$ and the vector space spanned by ϕ and the eigen-vectors φ of H_0 such that $\langle H_1\phi \mid \varphi\rangle = 0$. It has also been proved that the trajectories of such a closed-loop system converge to span(ϕ), if and only if the linear tangent system around ϕ on the unit sphere of $\mathbb{C}^n$ is controllable. In the next subsection the same convergence analysis is done for an arbitrary reference trajectory.

2.2 Convergence analysis

First result of this section may be presented as:

Theorem 1. *Take* $\imath\frac{d}{dt}\Psi = (H_0 + uH_1)\Psi$ *with* H_0 *and* H_1*,* $n \times n$ *Hermitian matrices and* u *a real control of dimension* 1 *defined as*

$$u = u_r + c\ \Im(\langle H_1\Psi(t)|\Psi_r\rangle)$$

where $[0, +\infty) \ni t \mapsto (\Psi_r(t), u_r(t))$ *is a reference trajectory of the system which is analytic with respect to* t*:*

$$\imath\frac{d}{dt}\Psi_r = (H_0 + u_r H_1)\Psi_r, \quad |\Psi_r(t)| = 1,$$

and where c *is positive real constant. Then* $\mathbf{A}_1$ *implies* $\mathbf{A}_2$ *where:*
$\mathbf{A}_1$*: All the trajectories of the closed-loop system with any initial condition converge to the reference trajectory* (Ψ_r, u_r) *as* $t \to +\infty$*.*
$\mathbf{A}_2$*: the linear tangent system around* Ψ_r*:*

$$\imath\frac{d}{dt}\delta\Psi = (H_0 + u_r H_1)\delta\Psi + \delta u H_1 \Psi_r$$

seen as a system defined on the tangent space to the unit sphere of $\mathbb{C}^n$ *at* $\Psi_r(t)$*,* $\mathbf{T}^n(t) = \{v \in \mathbb{C}^n \mid \Re(\langle v|\Psi_r(t)\rangle) = 0\}$*, is controllable.*

A multi-input version can be performed without difficulties.

Proof of theorem 1:

Let's denote ($\Re$ and $\Im$ stand for real part and imaginary part, respectively):

$$\widetilde{\Psi} = (\Re(\Psi), \Im(\Psi))^T, \qquad \widetilde{\Psi}_r = (\Re(\Psi_r), \Im(\Psi_r))^T, \qquad \widetilde{\Delta\Psi} = \widetilde{\Psi} - \widetilde{\Psi}_r$$
$$G_0 = \begin{pmatrix} \Im(H_0) & \Re(H_0) \\ -\Re(H_0) & \Im(H_0) \end{pmatrix}, \qquad G_1 = \begin{pmatrix} \Im(H_1) & \Re(H_1) \\ -\Re(H_1) & \Im(H_1) \end{pmatrix}.$$

G_0 and G_1 are thus, real anti-Hermitian matrices. Equation (2) reads:

$$\frac{d}{dt}\widetilde{\Delta\Psi} = (G_0 + u_r(t)G_1)\widetilde{\Delta\Psi} + \Delta u\ G_1\widetilde{\Psi}, \tag{6}$$

where,

$$\Delta u = c\ \Im(\langle H_1\Psi(t) \mid \Psi_r\rangle) = c\ \langle G_1\widetilde{\Delta\Psi(t)} \mid \widetilde{\Psi}_r\rangle_{\mathbb{R}^{2n}},$$

with $\langle . \mid . \rangle_{\mathbb{R}^{2n}}$ the Euclidean product in $\mathbb{R}^{2n}$. So from now on, we are simply dealing with real systems.
Let's note $A(t) = G_0 + u_r(t)\ G_1$ and $b(t) = G_1\widetilde{\Psi}_r(t)$. Then the linear tangent system around the reference trajectory $(\widetilde{\Psi}_r, u_r)$ reads:

$$\frac{d}{dt}\widetilde{\delta\Psi} = A(t)\widetilde{\delta\Psi} + \delta u\ b(t). \tag{7}$$

where $\widetilde{\delta\Psi}$ evolves in the tangent space to the unit sphere of $\mathbb{R}^{2n}$ and thus, $\widetilde{\delta\Psi}(t)$ is an element of $\widetilde{\mathbf{T}}^{2n-1}(t) = \{v \in \mathbb{R}^{2n} \mid \langle v \mid \widetilde{\Psi}_r(t)\rangle_{\mathbb{R}^{2n}} = 0\}$, $\forall t$.

As u_r and $\widetilde{\Psi}_r$ are analytic functions of t, so are $A(t)$ and $b(t)$. Thus, using the generalized Kalman criteria for analytic time-dependent linear systems [9], controllability of (7) is equivalent to:

$$\operatorname{span}\left(\left[A(t) - \frac{d}{dt}\right]^i b(t); i \in \mathbb{N}\right) = \widetilde{\mathbf{T}}^{2n-1}(t) \quad \forall t \geq 0, \tag{8}$$

Now let prove that not($\mathbf{A}_2$) $\Rightarrow$ not($\mathbf{A}_1$): if the linear tangent system is not controllable, there exists a vector $v \in \mathbb{R}^{2n}$, $v \neq 0$, and $t_0 > 0$ such that:

$$\begin{aligned}
&\langle v \mid \widetilde{\Psi}_r(t_0)\rangle_{\mathbb{R}^{2n}} = 0 \\
&\langle v \mid b(t_0)\rangle_{\mathbb{R}^{2n}} = 0 \\
&\langle v \mid (A(t_0) - \frac{d}{dt})b(t_0)\rangle_{\mathbb{R}^{2n}} = 0 \\
&\langle v \mid (A(t_0) - \frac{d}{dt})^2 b(t_0)\rangle_{\mathbb{R}^{2n}} = 0 \\
&\ldots
\end{aligned}$$

One can always assume that $\|v\| = 1$. Let us prove that the solution χ of

$$\frac{d}{dt}\chi = (G_0 + u_r G_1)\chi \qquad \chi|_{t=t_0} = v.$$

corresponds to a closed-loop trajectory. The map

$$t \mapsto \langle G_1 \chi \mid \widetilde{\Psi}_r\rangle_{\mathbb{R}^{2n}}$$

is analytic and all its derivatives at $t = t_0$ vanish. Thus it is identically zero and the closed-loop control u coincides with u_r. Since $\|\chi\| = 1$ and

$$\chi(t) \perp \widetilde{\Psi}_r(t) \qquad \forall t \geq t_0,$$

this closed-loop trajectory does not converge to Ψ_r. $\square$

In general $\mathbf{A}_2$ without any assumption regarding the behavior of the controllability when $t \to +\infty$, does not imply $\mathbf{A}_1$: we can not perform a direct analysis using the LaSalle's invariance principle when the reference trajectory is not stationary nor periodic.

Theorem 2. *Take the same system as in theorem 1 with the same reference trajectory. Assume (with the same notations as in the proof of theorem 1) that:*
$\mathbf{A}_3$*:*

$$\forall i \in \mathbb{N}, \qquad \sup_{t \geq 0} | u_r^{(i)}(t) | < +\infty.$$

$\mathbf{A}_4$*: ("asymptotic controllability of the first variation") There exists a sequence* $\{t_k\}_{k=1}^{\infty}$ *with* $t_k \to \infty$ *such that:*

$$\begin{aligned}
\forall i \in \mathbb{N}, \qquad (A(t) - \frac{d}{dt})^i\, b(t)|_{t=t_k} &\to v_i^{\infty} \in \mathbb{R}^{2n} \quad \textit{when} \quad k \to \infty \\
\widetilde{\Psi}_r(t_k) &\to \widetilde{\Psi}_r^{\infty} \in \mathbb{R}^{2n} \quad \textit{when} \quad k \to \infty
\end{aligned} \tag{9}$$

and that:

$$span\left(\{\widetilde{\Psi}_r^\infty\} \cup \{v_i^\infty\}_{i\in\mathbb{N}}\right) = \mathbb{R}^{2n}. \tag{10}$$

Then the trajectories of the closed-loop system with any initial condition converge to the reference trajectory (Ψ_r, u_r) as $t \to +\infty$.

$\mathbf{A}_3$ implies up to extraction of a subsequence (in fact one has to use a diagonal extraction method) that there exists a sequence $\{t_k\}_{k=1}^\infty$ with $t_k \to \infty$ such that (9) is satisfied. But $\mathbf{A}_3$ together with $\mathbf{A}_2$ do not imply $\mathbf{A}_4$ in general. Although by assumption $\mathbf{A}_2$ we have

$$\text{span}\left(\{\widetilde{\Psi}_r(t_k)\} \cup \{(A(t_k) - \frac{d}{dt})^i\ b(t_k)\}_{i\in\mathbb{N}}\right) = \mathbb{R}^{2n} \qquad \text{for} \quad k \in \mathbb{N} \tag{11}$$

problems appear at infinity. Passing to the limit when $k \to \infty$ the vectors may tend to be co-linear asymptotically and so we eventually will lose the property (10) of $\mathbf{A}_4$. So we are obliged in general to add hypothesis $\mathbf{A}_4$ to avoid this situation. Now, let's prove the theorem. This proof is based on an iterative use of Barbalat's lemma recalled below:

Lemma 1. *Assume $f(t) : \mathbb{R} \to \mathbb{R}$ to be uniformly continuous and suppose that:*

$$\int_0^\infty f(s)\ ds = C < \infty$$

then $f(t) \to 0$ when $t \to \infty$.

Proof of theorem 2:

As V is definite positive and decreasing on the trajectories of the system it converges toward some constant $c_1 < \infty$ as $t \to \infty$. Let's define:

$$f_1(t) = \frac{dV}{dt} = -c\ \langle \widetilde{\Delta\Psi}(t) \mid b(t) \rangle^2_{\mathbb{R}^{2n}}$$

Thus:

$$\int_0^\infty f_1(s)\ ds = \lim_{t\to\infty} V(t) - V(0) = c_1 - V(0) < \infty$$

Trivially $f_1(t)$ is a regular function of t. Moreover using the fact that the functions $\widetilde{\Psi}(t)$ and $\widetilde{\Psi}_r(t)$ evolve on the unit sphere of $\mathbb{R}^{2n}$ and that the function $u_r(t)$ is a bounded function of t we have:

$$\mid \frac{d}{dt} f_1(t) \mid < c_2$$

for a constant $c_2 < \infty$, which implies uniform continuousness of $f_1(t)$. So Barbalat's lemma yields to:

$$f_1(t) \to 0 \qquad \text{when} \quad t \to \infty$$

and thus:

$$\langle \widetilde{\Delta\Psi}(t) \mid b(t) \rangle_{\mathbb{R}^{2n}} \to 0 \qquad \text{when} \quad t \to \infty$$

Now let's define:

$$f_2(t) = \frac{d}{dt}\langle \widetilde{\Delta\Psi}(t) \mid b(t)\rangle_{\mathbb{R}^{2n}} = \langle \widetilde{\Delta\Psi}(t) \mid (\frac{d}{dt} - A(t))b(t)\rangle_{\mathbb{R}^{2n}}$$

We have:

$$\int_0^\infty f_2(s)\ ds = \lim_{t\to\infty} f_1(t) - f_1(0) = -f_1(0) < \infty$$

Similarly as $\widetilde{\Psi}$ and $\widetilde{\Psi}_r$ evolve on the unit sphere of $\mathbb{R}^{2n}$ and $u_r(t)$ and its derivative are bounded we have:

$$\mid \frac{d}{dt} f_2(t) \mid < c_3$$

and so we can still apply Barbalat's lemma and so:

$$f_2(t) \to 0 \qquad \text{when} \quad t \to \infty$$

Let's define for all $i \in \mathbb{N}$:

$$f_i(t) = \langle \widetilde{\Delta\Psi}(t) \mid (\frac{d}{dt} - A(t))^{i-1} b(t)\rangle_{\mathbb{R}^{2n}}$$

A simple computation shows that:

$$\frac{d}{dt} f_i(t) = f_{i+1}(t) \tag{12}$$

As $\widetilde{\Delta\Psi}$ and $\widetilde{\Psi}_r$ are bounded in $\mathbb{R}^{2n}$ and as all the derivatives of u_r are bounded, the functions $f_i(t)$ for $t \in \mathbb{N}$ have bounded derivatives and so they are uniformly continuous. Thus using (12) and Barbalat's lemma:

$$f_i(t) \to 0 \qquad \text{implies} \qquad f_{i+1}(t) \to 0$$

So:

$$\langle \widetilde{\Delta\Psi}(t) \mid (\frac{d}{dt} - A(t))^{i-1} b(t)\rangle_{\mathbb{R}^{2n}} \to 0 \quad \forall i \in \mathbb{N} \qquad \text{when} \qquad t \to \infty. \tag{13}$$

Let's suppose that the trajectory of the system does not converge toward the reference trajectory; i.e. $\|\widetilde{\Delta\Psi}\|(t)$ does not converge to 0. But, as $\|\widetilde{\Delta\Psi}\|(t)$ is a decreasing function of t this implies that there exists a constant $\alpha > 0$ such that $\|\widetilde{\Delta\Psi}\|(t) > \alpha$ for all $t > 0$. Now, take the sequence $\{t_k\}$ introduced in $\mathbf{A}_4$. $\widetilde{\Delta\Psi}(t)$ is bounded in $\mathbb{R}^{2n}$ and so we may extract a subsequence of $\{t_k\}$ (which for simplicity sakes will still numerated as $\{t_k\}_{k=1}^\infty$) such that $\widetilde{\Delta\Psi}(t_k) \to \widetilde{\Delta\Psi}_\infty$ when $k \to \infty$. Trivially we must have $\|\widetilde{\Delta\Psi}_\infty\| \geq \alpha > 0$.

Now passing to the limit in (13) when $n \to \infty$, we obtain:

$$\langle \widetilde{\Delta\Psi}_\infty \mid v_i^\infty \rangle_{\mathbb{R}^{2n}} = 0 \quad \forall i \in \mathbb{N}.$$

Thus using $\mathbf{A}_4$ this is equivalent to $\widetilde{\Delta\Psi}_\infty = \widetilde{\Psi}^\infty - \widetilde{\Psi}_r^\infty = \beta\widetilde{\Psi}_r^\infty$, where $\beta \in \mathbb{R}$ is a real constant. As $\|\widetilde{\Delta\Psi}_\infty\| \geq 0$ and $\|\widetilde{\Psi}_r^\infty\| = 1$ we deduce that $|\beta| \geq \alpha$. This implies that:

$$\|\widetilde{\Psi}^\infty\| = |(1+\beta)|\|\widetilde{\Psi}_r^\infty\| = |1+\beta| \neq 1$$

which contradicts the fact that $\widetilde{\Psi}^\infty$ is the limit of $\widetilde{\Psi}(t_k) \in \mathbb{S}^{2n-1}$. □

Remark 1. *When the reference trajectory* (Ψ_r, u_r) *is periodic, assumption* $\mathbf{A}_2$ *implies* $\mathbf{A}_3$ *and* $\mathbf{A}_4$*. Thus by theorem 2 we have the asymptotic convergence.*

3 A discrete state coupled to a quasi-continuum

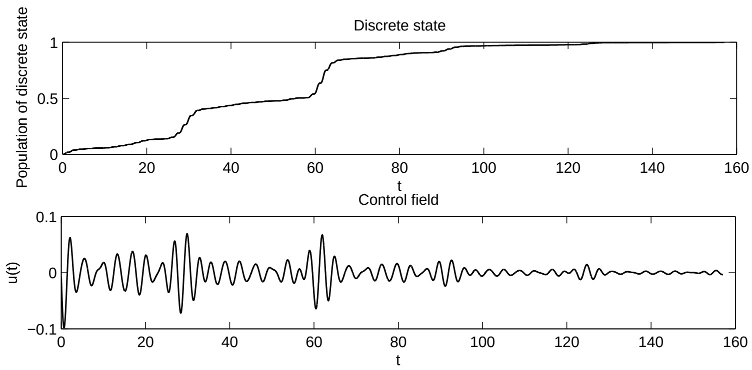

Figure 1: the first plot shows the projection of $\Psi(t)$ on the "discrete state" with the feedback (14) and the second one gives the control(laser) field u.

This classical model is a finite order approximation for the coupling of a discrete state with a continuum described by set of n-tightened discrete states [1]. In its simplest version, the matrices H_0 and H_1 read

$$H_0 = \begin{pmatrix} -1 & 0 & & \dots & 0 \\ 0 & \epsilon & 0 & & \\ & 0 & 2\epsilon & 0 & \vdots \\ \vdots & & & \ddots & 0 \\ 0 & & \dots & 0 & n\epsilon \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & 1 & & \dots & 1 \\ 1 & 0 & 0 & & \\ & 0 & 0 & 0 & \vdots \\ \vdots & & & \ddots & 0 \\ 1 & & \dots & 0 & 0 \end{pmatrix}$$

where $0 < \epsilon \ll 1$. As a first experience, let's suppose a particle trapped in the discrete state of energy -1. Using the Fermi's golden rule, one does not have much problem to make the particle leaving this stationary state toward the continuous part of the spectrum. Indeed, it suffices to use a laser field having for frequency ω such that $\hbar\omega \geq 1$. It is much more difficult to trap our particle in the first state of energy -1 corresponding to ϕ^0. In coordinates, Ψ

corresponds to the vector $(\Psi_1, ..., \Psi_{n+1})$ and ϕ^0 to $(1, 0, ..., 0)$. Since (* means complex conjugate)

$$\Im(\langle H_1 \Psi | \Phi^0(t) \rangle) = \Im\left(\sum_{i=1}^{n} \Psi_{i+1}^\star \exp(\iota t)\right)$$

we choose the following time varying feedback

$$u = c\, \Im\left(\sum_{i=1}^{n} \Psi_{i+1}^\star \exp(\iota t)\right) \qquad (14)$$

where c is a positive constant. Simulations of figure 1 correspond to $n = 20$, $\epsilon = 0.1$, and $c = 0.05$. The initial state for Ψ is associated to a Gaussian distributed population centered around energy $n\epsilon/2$ with arbitrary phases (figure 2).

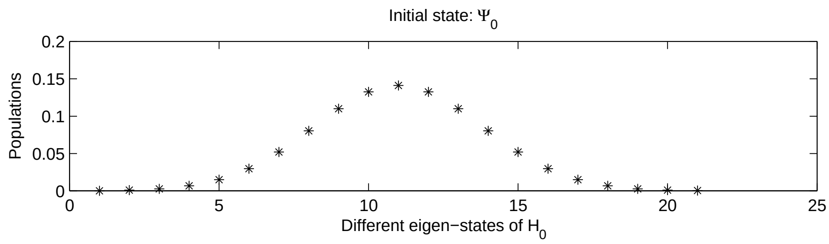

Figure 2: This figure shows the distribution of populations for the initial state Ψ_0.

It appears that our Lyapounov based technics is quite efficient for this case since the linear tangent system around ϕ on the unit sphere of $\mathbb{C}^n$ is controllable. Furthermore, the same method may be used for any number of states in the quasi-continuum part and the energy steps ϵ of very small sizes. This is an approximative model for a system of one particle in a one dimensional potential well shown by $V(x)$; here, the depth and the height of the well are chosen such that the Hamiltonian $H_0 = -\frac{1}{2}\triangle + V(x)$ has just one discrete state. The next section has for goal to test numerically such Lyapounov feedback on a more realistic and infinite dimensional model.

4 Conclusion

In section 2.2 we have shown, in the finite dimensional case, that controllability of the first variation around the reference trajectory is strongly related to asymptotic convergence. A natural question is the following: is such convergence characterization via the controllability of the linear tangent system still true in the infinite dimensional case.

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