Ex–: Dot leaking dynamically into a long chain

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The problem:
Consider an uncoupled occupied dot at $t < 0$, with $\mathcal{E}$ as its self energy on the left of a discrete chain of N sites where the couplings are equal to $-\lambda$.
At time $t = 0$ the dot is coupled to the leftmost site of the chain with coupling $-\lambda_0$.

(1) Calculate the density of states of the chain as function of the energy.

Now assume $\mathcal{E} = 0$.

(2) What is the condition for the chain to have a resonance level to the dot?

Assume such condition holds for the next items.

(3) Calculate the matrix element to the resonant level.

(4) Write the Heisenberg time and the Wigner time.

(5) For the case of $\lambda_0 = \lambda$ calculate the survival probability, the answer should contain a summation.

(6) Sketch numerically different cases of ratio of couplings, write the different time scales on the sketch.

The solution:

(1) The Hamiltonian represntation in the standard basis is:

$$\mathcal{H} = (-1) \cdot \begin{pmatrix} -\mathcal{E} & \lambda_0 & 0 & & \dots & & 0 \\ \lambda_0 & 0 & \lambda & & & & \\ 0 & \lambda & 0 & \lambda & & & \vdots \\ & & \lambda & 0 & \lambda & & \\ \vdots & & & \lambda & \ddots & & 0 \\ & & & & & 0 & \lambda \\ 0 & & \dots & & 0 & \lambda & 0 \end{pmatrix}$$

Considering only the chain, the reduced Hamiltonian will be:

$$\tilde{\mathcal{H}} = -\lambda \cdot \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 0 \\ 0 & 1 & 0 & & \\ \vdots & & & \ddots & 1 \\ 0 & & & 1 & 0 \end{pmatrix}$$

This reduced Hamiltonian is analogous to a 1D potential well of length $L = N$ with Dirichlet boundary conditions.
Hence, the eigenstates and eigenenergies are:

$$|k_n\rangle = \sqrt{\frac{2}{N}} \sum_{x=1}^{N-1} \sin\left(\frac{\pi n x}{N}\right) |x\rangle \qquad ; \qquad E_n = -2\lambda \cos\left(\frac{\pi n}{N}\right)$$

The chain's density of states function is given by:

$$\frac{d\mathcal{E}}{dn} = -2\lambda\frac{\pi}{N}\sin\left(\frac{\pi n}{N}\right) \longrightarrow \rho(\mathcal{E}) = \left|\frac{d\mathcal{E}}{dn}\right|^{-1} = \frac{N}{2\pi\lambda\sin\left(\frac{\pi n}{N}\right)}$$

(2) In order to determine the chain's resonance level condition, we'll require that:

$$E_n = -2\lambda\cos\left(\frac{\pi n}{N}\right) \overset{!}{=} 0$$

The condition is given by:

$$\frac{\pi n}{N} = \frac{\pi}{2} \longrightarrow \; n = \frac{N}{2}$$

which means an odd number of sites.

(3) Represeting the Hamiltonian in the basis which diagonalize $\tilde{\mathcal{H}}$:

$$\mathcal{H}_{new} = T^{-1}\cdot\mathcal{H}\cdot T =$$

$$= \begin{pmatrix} 0 & \sigma_1 & \cdots & \sigma_{\frac{N}{2}+1} & \cdots & \sigma_{N-1} \\ \sigma_1 & E_1 & & & & 0 \\ \vdots & & \ddots & & & \vdots \\ \sigma_{\frac{N}{2}+1} & & & 0 & & \\ \vdots & & & & \ddots & 0 \\ \sigma_{N-1} & 0 & \cdots & & 0 & E_{N-1} \end{pmatrix}$$

Where T is:

$$T = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & | & | & & | \\ \vdots & V_1 & V_2 & \cdots & V_{N-1} \\ 0 & | & | & & | \end{pmatrix}$$

and V_n are the same eigenstates as written before.
From the matrix multiplication it is clear that the matrix element to the resonant level is given by:

$$\sigma \equiv \sigma_{\frac{N}{2}+1} = -\lambda_0\cdot\left\langle 1\middle|V_{\frac{N}{2}+1}\right\rangle = -\sqrt{\frac{2}{N}}\lambda_0\sin\left(\frac{\pi\cdot 1}{N}\cdot\frac{N}{2}\right) = -\sqrt{\frac{2}{N}}\lambda_0$$

(4) The level spacing is given by:

$$\Delta(\mathcal{E}) = \frac{1}{\rho(\mathcal{E})}$$

calculating for $\mathcal{E} = 0$:

$$\Delta(\mathcal{E} = 0) = \frac{1}{\rho(n = \frac{N}{2})} = \frac{2\pi\lambda}{N}$$

computing Heisenberg's time gives:

$$t_H = \frac{2\pi}{\Delta} = \frac{N}{\lambda}$$

Finally, according to FGR, Wigner's time is given by:

$$t_\Gamma = \frac{1}{\Gamma} = \frac{\Delta}{2\pi\sigma^2} = \frac{\lambda}{2\lambda_0^2}$$

(5) In the case where $\lambda_0 = \lambda$ the Hamiltonian is:

$$\mathcal{H} = -\lambda \cdot \begin{pmatrix} 0 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 0 \\ 0 & 1 & 0 & & \\ \vdots & & & \ddots & 1 \\ 0 & & & 1 & 0 \end{pmatrix}$$

As before, the system can be considered as a 1D potential well with dirichlet boundry conditions, only this time of length $L = N + 1$.
Hence, the eigenstates and eigenenergies will be:

$$|k_n\rangle = \sqrt{\frac{2}{N+1}} \sum_{x=1}^{N} \sin\left(\frac{\pi n x}{N+1}\right) |x\rangle \qquad ; \qquad E_n = -2\lambda \cos\left(\frac{\pi n}{N+1}\right)$$

The initial state represented in the momentum basis is:

$$|\psi(t=0)\rangle = |1\rangle = \sum_{n=1}^{N} \langle k_n|1\rangle \, |k_n\rangle$$

Therfore, the time dependent state is:

$$|\psi(t)\rangle = \sum_{n=1}^{N} \langle k_n|1\rangle \, |k_n\rangle \, e^{-iE_n t}$$

The probability $P(t)$ to find the particle in the first site after time t is:

$$P(t) = |\langle 1|\psi(t)\rangle|^2 = \left| \sum_{n=1}^{N} |\langle k_n|1\rangle|^2 e^{-iE_n t} \right|^2$$

(6) All sketches were done for N=300.

a. For $\lambda_0 = 0.01\lambda$ and λ=1:

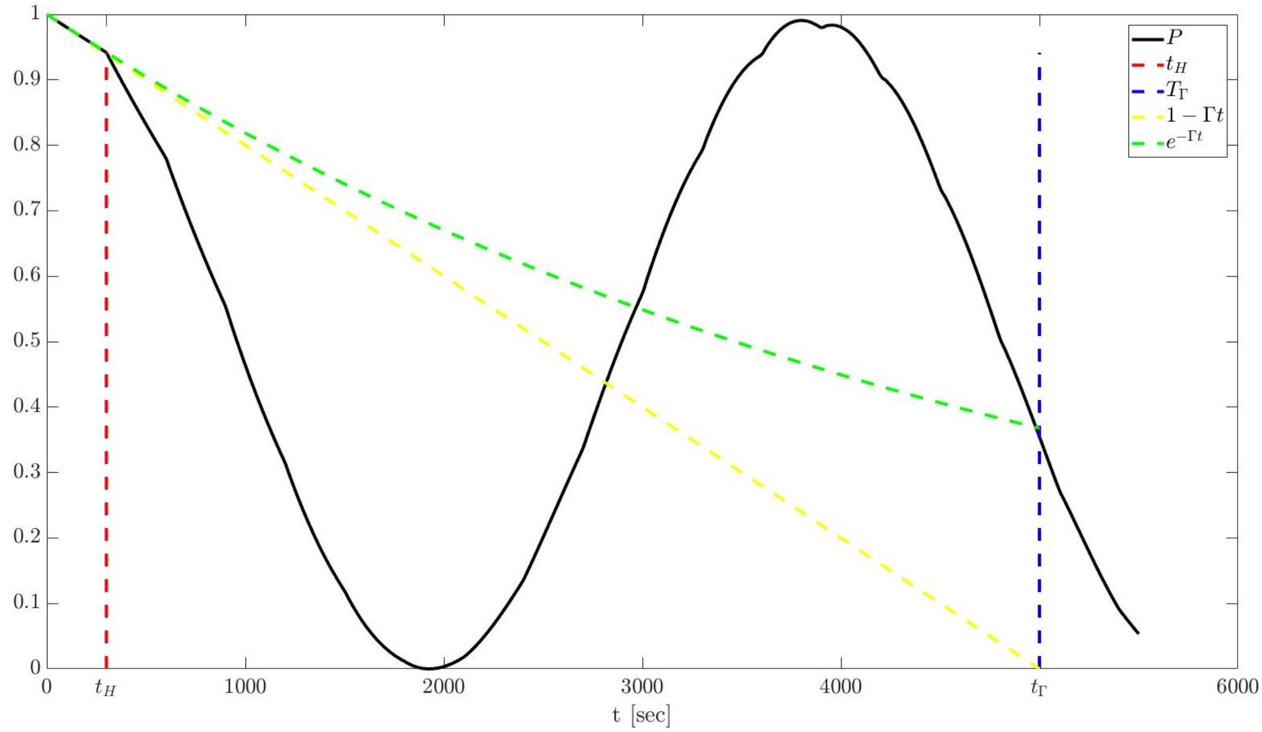

Figure 1: Weak coupling between the dot and the chain

b. For λ_0=0.1λ and λ=1:

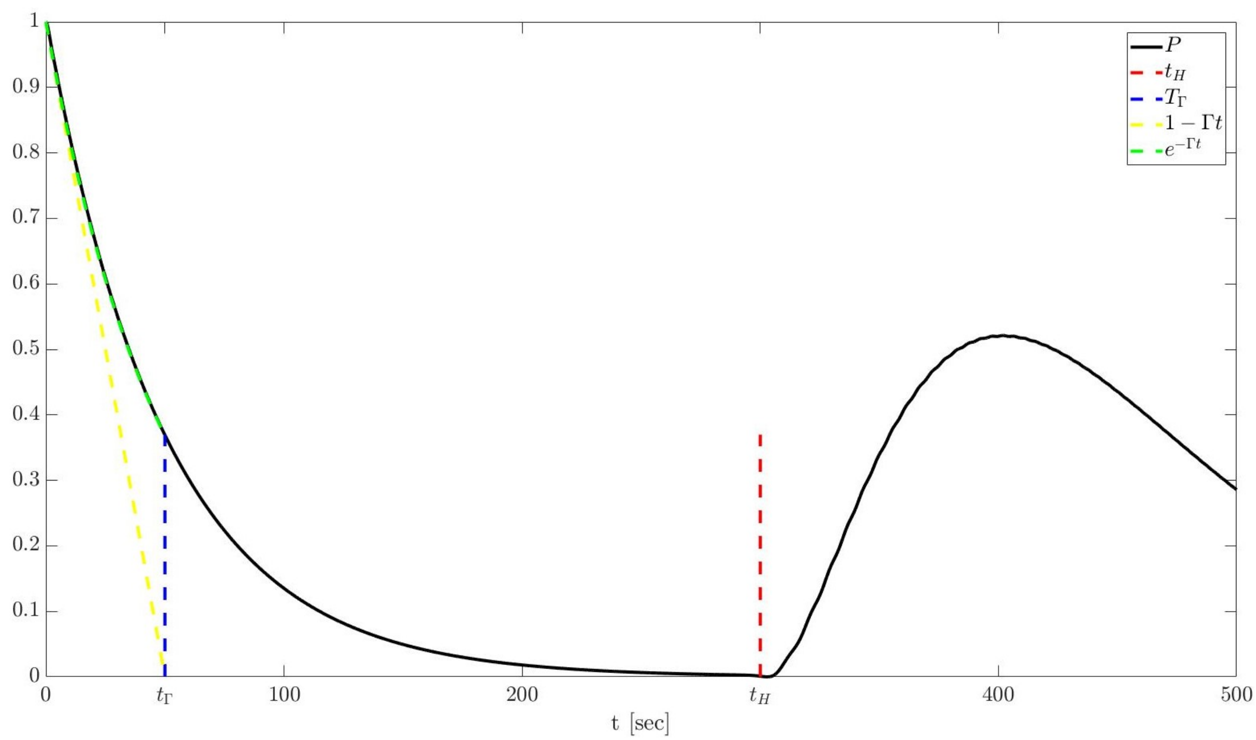

Figure 2: Medium coupling between the dot and the chain

c. For λ_0=λ=1:

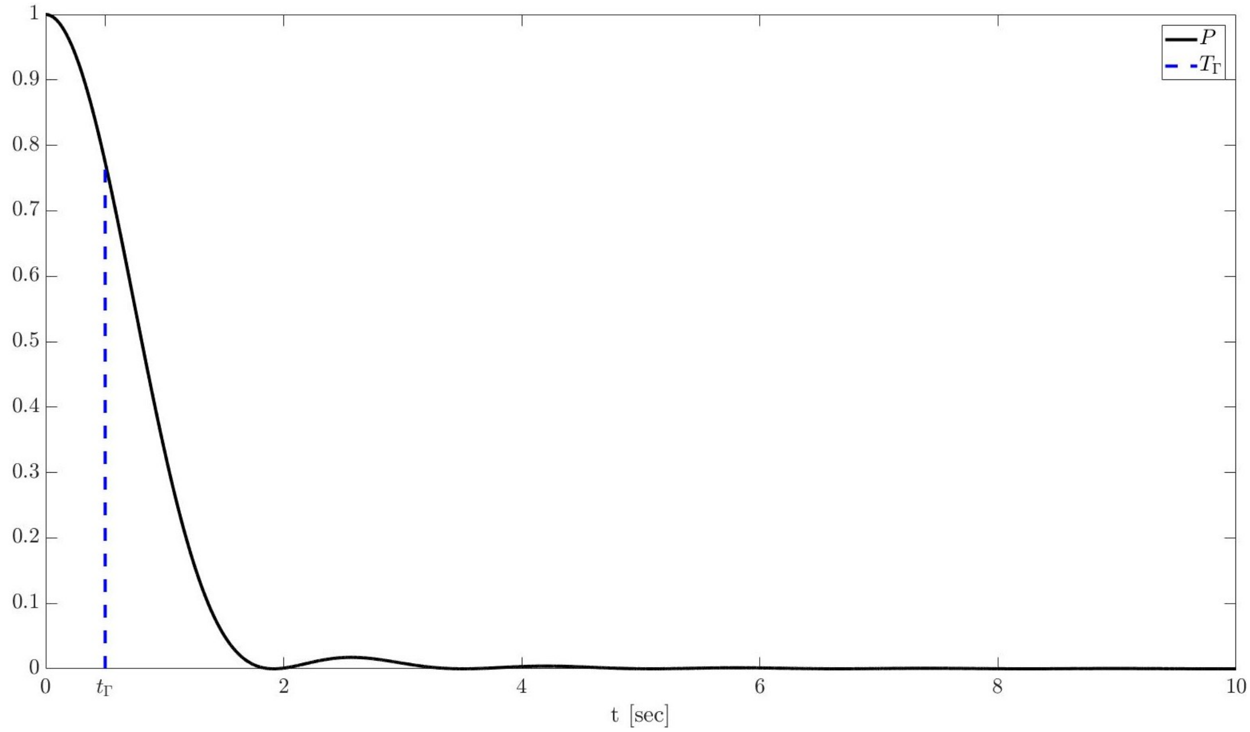

Figure 3: Strong coupling between the dot and the chain

Notice, in figure 3 $t_H = 300$ sec and it is not shown.