Excitation of time-dependent quantum systems: an application of time-energy uncertainty relations

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Abstract

The conditions under which time-energy uncertainty relations derived by Deffner and Lutz \cite{10} for time-dependent quantum systems minimize the time necessary to excite such systems from their ground state to excited states are examined. The generalized Margolus-Levitin and Mandelstam-Tamm inequalities are worked out for specific fermionic and bosonic systems.

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1 Introduction

Time is an essential concept for the realization of fast electronic devices. As an example, it may be useful to control and minimize the time needed by a two-level quantum system to jump from its ground state to an excited state. This time is constrained by Heisenberg’s time-energy uncertainty relation and bounded by a lower amount known as a quantum speed limit (QSL) time.

The optimization of the time duration of quantum jumps for stationary systems has been the object of numerous theoretical studies starting with Mandelstam and Tamm [1] and pursued up to present time in order to attain the sharper lower bound [2, 3, 4, 5, 6].

A vast literature has been devoted to various aspects of the problem of time dependent systems [7, 8, 9, 10]. Anandan and Aharonov have used alternative geometric derivations to obtain expressions for the Fubini-Study metric where the shortest possible distance between orthogonal states, which is along a geodesic, leads to get implicit bounds for the time of evolution of a quantum system [7, 8]. Other authors have used differential geometric methods to get sharper uncertainty relations for mixed states that can be optimized in the case for fully distinguishable states. Moreover, they characterize the Hamiltonians that optimize the evolution time for finite-level quantum systems [9]. Recently, for arbitrary quantum unitary processes Deffner and Lutz [10] extended the Mandelstam-Tamm (MT) and the Margolus-Levitin (ML) inequalities to time dependent systems which are either intrinsically time-dependent or driven by an external time-dependent perturbation. To this end, they derive the upper bounds for the Bures angle (Bures length) or, rather, for Fisher information [6]. At this stage we optimize the time in the extended ML formulation with respect to a maximum value. Besides, this principle of optimization, that fixes the minimum time, is also applicable for all the estimates presenting an extremum. Another groups have explored the MT bound, which is geometric in nature, to attain the minimum time of evolution in the context of the time-optimal control (time-OC) problem [12, 13, 14, 15]. More specifically, this method seems useful to minimize the decoherence for a system [16]. Further works have been developed for both unitary and non-unitary processes [11, 17, 18].

In practice it is of interest to test the time needed by a quantum system
to be driven from its ground state into excited states. In the present work
the inequalities derived in [10] have been used and worked out in order
to determine the time needed in order to generate quantum transitions. In the
first part of the present work we examine the general conditions under which
the ML inequality is optimized i.e. comes closest to an equality for specific
values of the time interval over which the system evolves. In a second step
the ML and MT relations are applied to fermionic and bosonic systems.

In section 2 the inequalities are explicitly formulated and the conditions
under which the inequalities can be optimized in the ML case are presented
in section 3. Section 4.1 is devoted to a quantitative study of the MT and ML
expressions by applying them to a fermionic 1d quantum chain. In section
4.2 the ML inequality is applied to a simple bosonic system coupled to an
external time-dependent perturbation which can act in a weak or strong
coupling regime.

2 Time-energy inequalities

The general structure of the time-energy inequality can be written as [10]

\[ \tau \geq R(\tau) \tag{1} \]

where \( R(\tau) = \frac{\hbar C_0}{\Delta E(\tau)} \), \( C_0 = \arccos \Omega_0 \), \( \Omega_0 = |\langle \Psi(0)|\Psi(\tau) \rangle| \) is the overlap
between the wave function at time \( t = 0 \) and \( t = \tau \), and \( \Delta E(\tau) \) characterizes
the energy difference acquired by the system between the initial and final
time. In the following \( \hbar = 1 \).

In the Mandelstam-Tamm formulation the energy denominator \( \Delta E(\tau) \) of
Equation (1) is given in terms of the variance of the energy

\[ \Delta E(\tau) = \frac{1}{\tau} \int_0^\tau dt \left[ \frac{<H(t)^2> - <H(t)^2>^2}{\langle \Psi(t)|\Psi(t) \rangle} \right]^{1/2} \tag{2} \]

with

\[ <H(t)^2> = \langle \Psi(t)|H(t)^2|\Psi(t) \rangle \tag{3} \]
In the Margolus-Levitin formulation $\Delta E(\tau) = \langle E(\tau) \rangle - E(0)$ where $E(0)$ is the energy at $t = 0$ and $\langle E(\tau) \rangle = 1/\tau \int E(t) dt$ is the average energy of the system over a time interval $[0, \tau]$.

3 Extrema in the Margolus-Levitin expression

In the case of a time-independent system the realization of eq.(1) as a strict equality can be of great practical interest since it leads to the determination of the minimum time needed by the system starting from its ground state to excited states. This question has been successfully answered in [5, 7].

The question may also be raised in the case where the hamiltonian dynamics are time-dependent when it is of interest to find out the minimal time interval $[0, \tau]$ needed in order to realize the equality. It comes out that an analytic solution has not been found yet. A priori a less ambitious empirical answer might correspond to $C_{0\tau} = 0$ and a minimum of the energy denominator $\Delta E(\tau)$.

A rigorous answer to the optimization of the inequality towards an equality consists in a determination of the maximum of $R(\tau)$ which brings the r.h.s. of the expression closest or equal to $\tau$.

The first derivative of this quantity with respect to $\tau$ leads to

$$dR(\tau)/d\tau = \frac{\hbar[\Delta E(\tau)dC_{0\tau}/d\tau - C_{0\tau}d\Delta E(\tau)/d\tau]}{\Delta^2 E(\tau)}$$

An extremum is reached if $dR(\tau)/d\tau = 0$ which leads to

$$\frac{dC_{0\tau}/d\tau}{C_{0\tau}} = \frac{d\Delta E(\tau)/d\tau}{\Delta E(\tau)}$$

This extremum is a maximum if, for the corresponding value of $\tau$

$$\Delta E(\tau)d^2 C_{0\tau}/d\tau^2 - C_{0\tau}d^2 \Delta E(\tau)/d\tau^2 < 0$$
A consequence of Eq.(5) can be observed if $C_0\tau$ is maximized. This corresponds to $\Omega_0\tau = |\langle \Psi(0)|\Psi(\tau)\rangle| = 0$, the vectors $|\Psi(\tau)\rangle$ and $|\Psi(0)\rangle$ are orthogonal to each other. Then $dC_0\tau/d\tau = 0$ and induces $d\Delta E(\tau)/d\tau = 0$ if $\Delta E(\tau) \neq 0$. But, in the ML formulation

$$
d\Delta E(\tau)/d\tau = \frac{E(\tau)}{\tau} - \frac{< E(\tau)>}{\tau} = 0
$$

which leads back to the expression of $\Delta E(\tau)$ if $E(0) = 0$. Hence the stationarity of $\Delta E(\tau)$ is correlated with the orthogonality of the vectors $|\Psi(\tau)\rangle$ and $|\Psi(0)\rangle$. The stationary point $\tau$ can be an inflexion point or an extremum. Then $C_0\tau = \pi/2 \mod (k\pi)$ and

$$
\tau \geq \frac{\hbar \pi/2}{\Delta E(\tau)}
$$

Whether or not this limit can be reached and $\geq$ replaced by a strict equality depends on the system.

4 Models and applications

4.1 Fermionic 1d chain

In a first step the time-energy inequality is applied to the time-dependent 1d chain with even periodic boundary conditions already introduced in [19, 20]

$$
H_0 = J/2(1+\gamma) \sum_{(i)} \sigma_i^x \sigma_{i+1}^x + J/2(1-\gamma) \sum_{(i)} \sigma_i^y \sigma_{i+1}^y - h_0 \sum_{(i)} \sigma_i^z
$$

where $\sigma_i^z$ is the $x$ component of the Pauli matrix and similarly for the $y$ and $z$ components. The system is integrable and the wave function is given as a product of single particle wave functions with corresponding energies [21]. The time dependence is generated by a local excitation of the last spin by an external magnetic field

$$
H_1^{(N)}(t) = h_1 \exp(-t/\tau_H) S_N^z
$$
with $S_N^z = \sigma_N^z/2$ \[21\].

The wave function of the system is obtained perturbatively, up to second order in the interaction which works as a perturbation and leads to the expression of the overlap

$$
\Omega_{\alpha \tau} = |\langle \Psi(0) | (1 + U^{(1)}(0, \tau) + U^{(2)}(0, \tau)) | \Psi(0) \rangle | \tag{11}
$$

where $|\Psi(0)\rangle$ is the wave function at $t = 0$ and $U^{(1)}(0, \tau), U^{(2)}(0, \tau)$ are the first and second order contribution to the evolution operator $U(0, \tau) = \exp[-i(H_0 \tau + \int_0^\tau dt H_1^{(N)}(t))]$. A justification for the neglect of higher order contributions used in the numerical application is given in the Appendix.

The energy of the system over a time interval $[0, \tau]$ reads

$$
E(\tau) = 1/\tau \int_0^\tau \langle \Psi(t) | H(t) | \Psi(t) \rangle / \langle \Psi(t) | \Psi(t) \rangle - E(0) \tag{12}
$$

where $|\Psi(t)\rangle$ is the perturbed wave function evaluated up to order 2 and $E(0)$ the initial energy of the system.

4.1.1 General considerations concerning the application of the model

The present external magnetic field on an unique spin state of the chain has been explicitly chosen to produce a weak effect on the chain in order to allow for a perturbative treatment. Under these conditions and for fixed $J = 1$ it comes out that the wave function overlaps are not very sensitive to the strength of the magnetic fields, neither $h_0$ nor $h_1$ as long as these quantities stay in the range of unity. The same is true in the case of variations of the asymmetry parameter $\gamma$ which are fixed in the interval $[0, 1]$. In all applications the length of the chain is $N = 100$.

4.1.2 Application of the Mandelstam-Tamm expression

Typical results concerning the r.h.s. of the MT expression are shown in Figure 1 as function of $\gamma$ with $\tau = 100, h_0 = 1, h_1 = 1$. The results show that $R(\tau)$ keeps very small when compared with $\tau$. 

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4.1.3 Application of the Margolus-Levitin expression

Using the ML expression leads to the results shown in Table 1 for \( R(\tau) \). Here \( \tau = 100, h_0 = 1, h_1 = 1 \) in lines (1-2), \( h_0 = 1, h_1 = 2 \) in line 3. \( R(\tau) \) keeps again quite small when compared with \( \tau \).

4.1.4 General comments

As a consequence of the perturbative nature of the time dependence of the total Hamiltonian \( H(t) = H_0 + H_1^{(N)}(t) \) the overlap between the wave functions at \( t = 0 \) and \( t = \tau \) staying in the numerator of \( R(\tau) \) keeps relatively sizable, hence \( C_{0r} \) never gets close to its maximum \( \pi/2 \) which would correspond to orthogonal states.

The energy denominators in both the MT and ML expressions are at least an order of magnitude larger that the numerator so that \( R(\tau) \) gets a small quantity in every investigated case. Since the external excitation is confined to a small time interval the evolution of this quantity reaches quickly a quasi-stationary value after a very short number of time steps. The time-energy inequality is strictly verified.

4.2 Bosonic model

As a second application consider a simple time-dependent bosonic system with 0 and 1 quantum excitation. The Hamiltonian is given by the expression

\[
H = A(a^+a + 1/2) + V^*(t)a^+ + Va 
\]

where \( V(t) = V_0e^{i\omega t} \) is an external perturbation. The wave function obeys the time-dependent Schroedinger equation and it is written as

\[
|\Psi(t)\rangle = \sum_n c_n(t)e^{-iE_n t}|n> 
\]

Here one keeps two states, the ground state \( |n> = |0> \) and an oscillator quantum excitation \( a^+|0> \). Then the normalized amplitudes \( c_n(t) \) can be determined analytically as solutions of a system of two coupled first order differential equations
\[
\begin{align*}
\frac{dc_0(t)}{dt} &= -ie^{-i\omega t}V(t)c_1(t)/\hbar \\
\frac{dc_1(t)}{dt} &= -ie^{i\omega t}V^*(t)c_0(t)/\hbar 
\end{align*}
\] (15)

The second order differential equation obtained for \(c_0(t)\) shows three types of solutions depending on the sign of the determinant

\[
\Delta = 4V_0^2/\hbar^2 - (\omega - A)^2.
\]

The amplitudes \(c_0(t)\) and \(c_1(t)\) show an oscillatory behaviour if \(\Delta < 0\) or equal 0 and a product of an exponential and oscillatory behaviour when \(\Delta > 0\).

The knowledge of the time-dependent wave function

\[
|\Psi(t)\rangle = \bar{c}_0(t)e^{-iE_0t}|0\rangle + \bar{c}_1(t)e^{-iE_1t}a^+|0\rangle
\] (16)

where \(E_0 = A/2\), \(E_1 = 3A/2\) and \(\bar{c}_0(t)\), \(\bar{c}_1(t)\) are the normalized amplitudes. The overlap \(C_{0\tau}\) and energy \(E(\tau)\) can be determined for any value of \(\tau\)

\[
\langle \Psi(0)|\Psi(\tau)\rangle = (R_0(0, \tau) + iI_0(0, \tau))e^{-iE_0\tau} + (R_1(0, \tau) + iI_1(0, \tau))e^{-iE_1\tau} \quad (17)
\]

where \(R_0(0, \tau)\) and \(I_0(0, \tau)\) are the real and imaginary parts of \(\bar{c}_0^\dagger(0)\bar{c}_0(\tau)\) and similarly for \(R_1(0, \tau)\) and \(I_1(0, \tau)\). Then the expression of the energy reads

\[
E(\tau) = 1/\tau \int_0^\tau \mathcal{A}(|\bar{c}_1(t)|^2 + 1/2) + 2Re[V^*(t)\bar{c}_1^\dagger(t)\bar{c}_0(t)e^{i(E_1-E_0)t}dt] - E(0) \quad (18)
\]

4.2.1 General considerations concerning the model

Here the strength of the coupling in the time-dependent part of the Hamiltonian can be weak as well as strong:

Three different regimes can be generated. They correspond to \(\Delta > 0\), \(\Delta = 0\), \(\Delta < 0\).
4.2.2 Analysis of the Margolus-Levitin inequality in these different regimes

Here the initial conditions are fixed as \( c_0(0)=1, \frac{dc_0}{dt}=0 \).

- If \( \Delta < 0 \) (weak coupling) one can come close to the maximum of \( C_{0r} \) which leads also closest to a state which is not far from being orthogonal to the initial state \( |\Psi(0)\rangle \). Calculations indicate that \( R(\tau) \) reaches a maximum when \( C_{0r} \) gets to a maximum. This is in qualitative agreement with the considerations of section 3 about the fact that the denominator \( \Delta E(\tau) \) of \( R(\tau) \) can reach an extremum when its numerator is maximum.

Some values of \( R(\tau) \) are shown in Figure 2. Here \( A = 1, \omega = 2, V_0 = 0.475 \). The oscillations are due to the oscillating nature of the external perturbation.

- If \( \Delta \geq 0 \) (intermediate and strong coupling) the situation is similar to the one observed in the fermionic chain system. The final state \( \Psi(\tau) \) reaches a maximum of \( \pi/4 \), \( C_{0r} \) and \( R(\tau) \) reach very quickly a stationary value. This can be explained by the structure of the wave function which stabilizes to a final value due to an exponential time component that multiplies an oscillatory term.

Some values of \( R(\tau) \) are shown in Figure 3. Here \( A = 6, \omega = 4, V_0 = 3 \).

In all cases the time-energy inequality is numerically verified.

5 Conclusions

The extension of the Margolus-Levitin and Mandelstam-Tamm time-energy inequality to time-dependent systems has been investigated on hand of two models, a fermionic 1d chain and a two-state bosonic system. The numerical calculations are in agreement with the analytical expressions, a fixed time interval is always larger than the r.h.s. of the inequality expressions.

In the case of the Margolus-Levitin formulation it has been shown that the minimum overlap between the wave function at the initial time and the
time evolved wave function reaches a minimum when the r.h.s. of the inequality is itself at an extremum. Numerical calculations confirm this point in the case where this extremum corresponds to an exact orthogonality or not.

6 Appendix

The perturbation induced by the external perturbation given in eq. (10) is essentially governed by the relaxation time $\tau_H$ and the field strength $h_1$. To first order the strength of the perturbation is fixed by $\tau_H h_1$. At second order the magnitude of the different contributions are governed by the strength factors

\begin{align}
S_1 &= h_1^2 \tau_H^2 \\
S_2 &= h_1^2 (1/D^2) \\
S_3 &= h_1^2 / (\tau_H D) \\
D &\sim (1/\tau_H^2 + \Delta \epsilon^2)
\end{align}

where $\Delta \epsilon \sim \epsilon^{(i)} - \epsilon^{(j)}$, $(i, j)$ corresponding to single particle ground or excited states. The single particle state energies are of the order of unity. In the numerical applications $h_1$ is chosen to be of the same order of magnitude and $\tau_H$ is two to three orders of magnitude smaller. As a consequence the second order contributions are two to three orders of magnitude smaller than the zeroth order ones. This justifies the cut-off of the expansion at order 2.

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Figure 1: $R(\tau)$ as a function of $\gamma$ for $\tau=100$.

Table 1: $R(\tau)$ as a function of $\gamma$ and time $\tau_H$

| $\gamma$ | $\tau_H$ | $R(\tau)$ |
|----------|----------|-----------|
| 0.1      | 0.01     | 0.16      |
| 0.2      | 0.01     | 0.34      |
| 0.5      | 0.01     | 0.04      |
Figure 2: $R(\tau)$ as a function of $\tau$. The numerical values between parentheses in the figure correspond to $C_{0\tau}$ (weak coupling case).

Figure 3: $R(\tau)$ as a function of $\tau$ where $C_{0\tau} = 0.79$ (strong coupling case).