Investigation of Temperature Effect in Landau-Zener Avoided Crossing

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ABSTRACT— Considering a temperature dependent two-level quantum system, we have numerically solved the Landau-Zener transition problem. The method includes the incorporation of temperature effect as a thermal noise added Schrödinger equation for the construction of the Hamiltonian. Here, the obtained results which describe the changes in the system including the quantum states and the transition probabilities are investigated and discussed. The results successfully describe the behavior of the transition probabilities by sweeping the temperature.

KEYWORDS: Two level system, Landau-Zener, avoided crossing, Temperature effects,

I. INTRODUCTION

Landau-Zener transition problem which describes the population transfer between quantum states in a two level system has many different applications in today's atomic and molecular physics, quantum information science, quantum optics and other related fields [1-6]. This is while, Landau-Zener (LZ) transition model is being used extensively by experimentalists for preparation, manipulation and reading out of quantum states in two level systems (qubits) [2, 6]. The LZ problem which was first considered by L.D. Landau and C. Zener explains the transition of the two energy levels through an avoided crossing by a constant sweeping rate in time [7]. Up to now, many works are devoted to consider different aspects or extensions to this classic problem, e.g. considering different noise models, decay and dissipation or dephasing issues [8-13]. It should be noted that most of the exact solutions to this problem are at zero temperature, however there are studies to investigate the effect of the finite temperature in LZ solution; e.g. in references [2] and [13], the numerical stochastic Schrödinger equation formalism is developed for such calculation.

In this work, we have modified the conventional LZ Hamiltonian with an added stochastic noise term which models the temperature effect. Numerically solving this problem, the dynamics of the system has been investigated and discussed.

II. THEORETICAL MODEL

Here, for the investigation of the quantum system in non-zero temperature, the thermal noise Hamiltonian is added to the LZ Hamiltonian (Eq.(1)) and the non-zero time dependent Schrödinger equation is numerically solved.

$$i\hbar\frac{\partial\psi}{\partial t}=\left(H_{LZ}+H_{th}\right)\psi \tag{1}$$

In this problem, the Hamiltonian of the two level system at zero temperature is:

$$H_{LZ}=\begin{pmatrix}\alpha t/2 & H_{12}\\ H_{12}^{*} & -\alpha t/2\end{pmatrix}, \tag{2}$$

where H_{12} describes the strength of the inter-state interaction and α is the rate of unperturbed energy change [10]. It is evident that the Hamiltonians at different times do not

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commute so the coupled equation should be solved to find the solution.

The second term of the Hamiltonian in Eq.(1) is the thermal noise. The thermal noise could be interpreted as spontaneous changes of energy which its amplitude is proportional to the temperature [13]. Based on this approach, the most general model of thermal noise could be given:

$$\mathbf{H}_{th} = k_B T \boldsymbol{\xi}(t) = k_B T \begin{pmatrix} \xi_1(t) & \xi_3(t) \\ \xi_3(t) & \xi_2(t) \end{pmatrix}, \quad (3)$$

In which the $\xi_i(t)$ are the stochastic functions in the range of [0,1]. The diagonal terms express the fluctuations of the internal energy for each quantum state where we expect them not to have considerable effects on the transition amplitudes. This issue is thoroughly confirmed in our numerical calculations and therefore the diagonal terms are ignored in subsequent models. Substituting the new Hamiltonian H into the Schrödinger Eq.(1) and using the spinor representation for $\boldsymbol{\psi}$, we obtain:

$$\begin{pmatrix} \frac{1}{2}\alpha t & H_{12} + k_B T\,\xi(t) \\ H_{12}^{*} + k_B T\,\xi(t) & -\frac{1}{2}\alpha t \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = i\hbar \begin{pmatrix} \dot{\phi}_1 \\ \dot{\phi}_2 \end{pmatrix}, \quad (4)$$

where ϕ_1 and ϕ_2 are the two states of the systemwhich their absolute square represent the probabilities of finding the system in each state. It is obvious that this equation at zero temperature would be reduced to the conventional Landau-Zener equation [10].

It should be noted that, in this model the noise frequency is an important parameter which considerably affect the results. In fact for the thermal equilibrium situation, the noise frequency should be higher than the specific frequency of the system, otherwise for the low frequency noises, the system would be placed in non-equilibrium state.

III. RESULTS AND DISCUSSION

The Eq.(4) is numerically solved with considering the initial condition such that the system is prepared in a pure state (we named it as state 1) at long time ago ($t \rightarrow -\infty$).In this numerical simulation, the time intervals are chosen in such a way that the probabilities could reach to a nearly stable situation. Furthermore the simulation results have been reported for two cases with different set of Hamiltonian parameters. For the first case, H_{12}=0.02 eV and α=1.6 eV/fs and for the second case H_{12}=0.08 eV and α=32 eV/fs.

A. *Transition Probabilities at Zero Temperature*

Figure 1 shows the solution of Eq. (4) for the probability amplitudes of two spinor states $|\varphi_i|^2$, and (in the inset) the Eigen energies of the quantum system versus time through the avoided crossing at zero temperature. This figure reveals that there is a transition from state 1 to state 2 with determined probability. In Fig. 1, the parts (*a)* and (*b)* represent the diagrams for the cases one and two respectively. In this situation the probability of finding the system in the level one and level two at the large times is oscillating around specific values. These values are 0.6 (states one) and 0.4(state 2) for the first case and 0.65 and 0.35 for the second case. The parameters of these two systems (H_{12} and α) are chosen so that the final states become approximately similar. This similarity helps us to compare the temperature effect results more reliable. In the inset of these figures the energy versus time for the both systems are depicted. It is obvious that the energy gap in case 2 at t=0 (that represents the H_{12}) is larger than case 1 but due to the larger time varying magnetic field (proportional to α) the final states of these two systems are approximately similar.

B. *Transition probabilities at non-zero Temperature*

The behavior of the probability versus time for non-zero temperature is declared in Fig. 2.

In this simulation the stochastic function $\xi(t)$ of the Hamiltonian (Eq.(3)) is selected as white noise function for 4 different frequencies which are named as *A, B, C,* and *D* for both cases.

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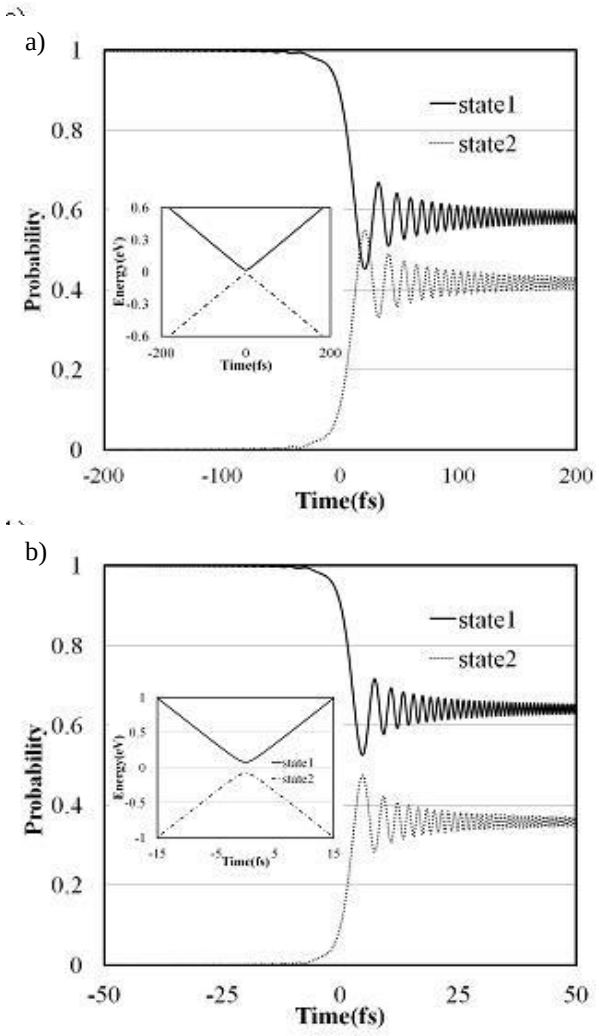

Fig. 1. The amplitude probabilities of states 1 and 2 versus time through avoided crossing at zero temperature for a) H_{12}=0.02 eV and α=1.6 eV/fs and b) H_{12}=0.08 eV and α=32 eV/fs. The insets are the Eigen energies of the quantum system as a function of time at zero temperature.

In simulation *A*, The maximum noise frequency is set to N/T=[50000/(4×10^{-13}s)]=1.25×10^{17} Hz, where N is the number of mesh points andT is the time period. The noise frequencies of the simulations *B*, *C*, and *D* are set to 1.25×10^{16}Hz, 1.25×10^{15}Hz and 1.25×10^{14}Hz respectively. It should be mentioned that the characteristic frequency of the system is $f_0=\alpha T/\hbar$~2×10^{15}Hz, so the high or low frequencies are defined in comparison to this frequency. The frequencies much larger than $f_0$are called the high frequencies and the other ones are the low frequencies. Therefore the cases *A* and *B* are considered as high frequency noise regimes and *C* and *D* as the low frequency regimes.

As mentioned before, the results of the calculation for diagonal noise components which are not presented here, confirm that such noises do not change the probability of the states in Landau-Zener problem.

The probability amplitudes for the temperatures of 200K and 700K which are related to simulations 1-*A* and 1-*D* are shown in Figs. 2(*a*) and 2(b) respectively. The Eigen energies are not depicted because they do not change significantly from zero temperature case. It should be noted that the resulting probabilities has been averaged over 10 samples.At high frequency regime the averaging over different samples does not considerably change the probability behavior. The reason is that in these cases, the results of different samples are almost the same. However for low frequency noise cases, the probability amplitudes for each sample is considerably different to the others and so averaging over the samples significantly changes the amplitude probabilities.

Figure 2(*a*) shows that by increasing the temperature in sample 1-A with the mentioned noise frequency, the probability of transition accordingly increase.

Figure 2(b) shows the same increasing behavior of the transition probability for sample 1-D by increasing the temperature. However in this case, at higher temperature the transition probability of crossing is smaller than the case with higher frequency. As expected, for low frequency noises the probability of states without averaging (that is not presented here) fluctuates severely. In fact such noise sources guide the system into non-equilibrium situations, however the high frequency noise sources because of numerous interactions with the system keep it in the equilibrium situation.

These figures clearly show that the probability of transition from state 1 to 2 significantly increase by increasing the temperature. This

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behavior is in match with physical common sense which we expect that by increasing the temperature, the quantum fluctuations increase and therefore the transitions would be facilitated. The obtained results are also in agreement with other works in [12] and [13], where they have reported similar behaviors.

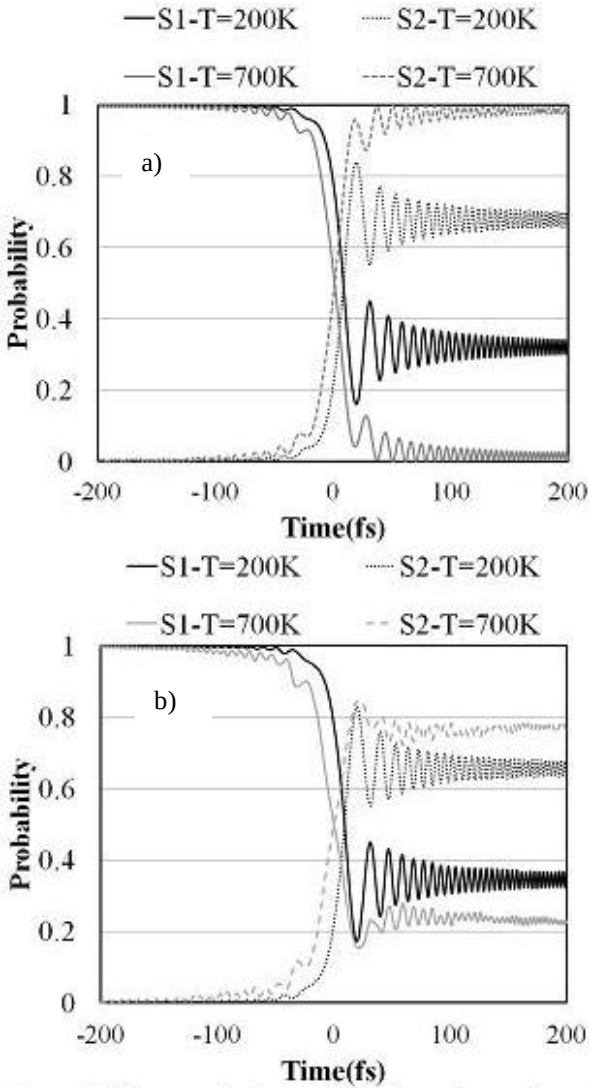

Fig. 2.The amplitude probabilities of states 1 and 2 versus timethrough avoided crossing at a) Simulation 1-*A*, b) Simulation 1-*D*.

Figure 3 shows the same simulation result of case 2-A and 2-D for two different temperatures of 400°K and 1000°K. This figure also shows that by increasing the temperature, the probability of system transition from state 1 into state 2 after applying magnetic field has been increased. In comparison with Fig. 2, it is clear that the temperature effect on the first case is more significant than the second case. This is because that in the second case the energy gap is significantly larger than the energy gap of the first case, and so the environment fluctuation is faced to higher barrier to change the states of the system. Comparing these figures, it is expected that for the barrier H_{12} about 1ev the temperature effect could not be observed in the room temperature.

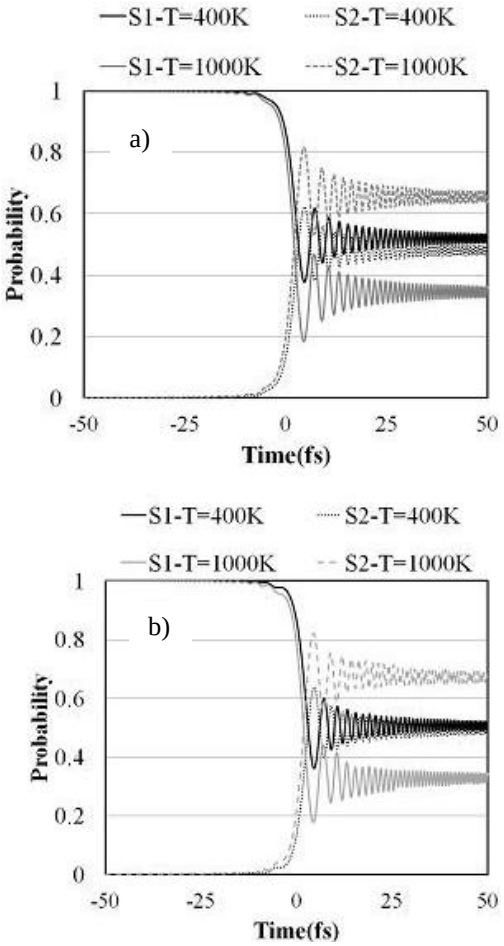

Fig. 3. The probability amplitudes of states 1 and 2 versus time through avoided crossing at a) simulation 2-A, b) simulation 2-D.

For better investigation of the temperature effect on the intra state transition, a new parameter is defined as the average of the probability at the 5% of the final time interval. This quantity simply shows the probability of each state at the end of time interval (we have called it Averaged Final Probability (AFP)). Furthermore we define the LZ crossing probability as the absolute difference of the AFPs that determines the probability of crossing between states 1 and 2. The AFP for

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both states and all four simulations of both cases versus temperature are depicted in Fig. 4.

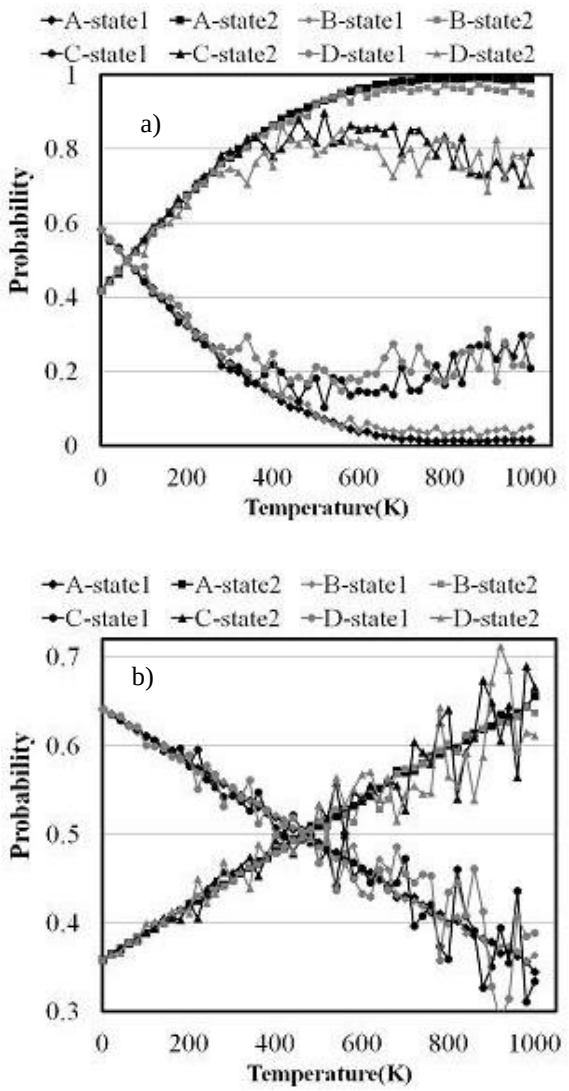

Fig. 4. The averaged probability amplitudes (averaged in the 5% of end time interval)of the states 1 and 2 versus temperature for different thermal noise frequencies. *a*) Case one *b*) case two.

The results for the first case is depicted in Fig. 4-*a*. This figure reveals that by increasing the temperature, the probability of the crossing would be increased significantly. The AFP of LZ crossing probability for the two high frequency simulations 1-*A* and 1-*B* is smoothly increasing so that for the temperature 1000°k this value approaches to 1, but for the low frequency simulations 1-*C* and 1-*D*, the increasing of LZ crossing probability include some fluctuations and the final values does not approach to 1. The results of the similar calculations for the second case is showed in Fig. 4-b. In this case the LZ crossing probability increase by the increasing of temperature, however in comparison with the first case, the temperature effect is much smaller. In addition, the smooth increasing behavior of the probabilities for high frequency samples and non-smooth increasing of the probabilities for low frequency samples is obvious in Fig. 4. It is expected that by increasing the temperature the fluctuation would increases that is also clearly evident in Fig. 4.

IV. CONCLUSION

Here we have investigated the effect of temperature on the Landau-Zener transitions. The results quantitatively show the increasing behavior of the transition amplitudes by increasing the system temperature. This is while the temperature effect decrease by increasing the barrier potential H12. Furthermore in our stochastic approach, for the low frequency noises, large fluctuations in probability amplitude are observed which cannot be seen for the high frequency noises. We believe that this is because of the fact that for high frequency noises the energy is transferred to the system in the large number of interactions, but in the low frequency regime, the energy transfer is abrupt.

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