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A PHYSICALLY REALIZABLE TERM-CROSSING MODEL FOR COLD ATOM ASSOCIATION

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The mean-field dynamics of ultracold molecule formation via Demkov-Kunike level-crossing field configuration is studied. Analyzing the fast sweep regime of strong coupling limit, a highly accurate two-term ansatz describing the temporal dynamics of the process is suggested. Examining the role of different terms in this approximation, we prove that in the fast sweep regime the atom-molecule conversion effectively consists of a process of resonance crossing governed by a first-order nonlinear limit equation, followed by atom-molecular coherent oscillations which are basically described by a solution of the linear problem, associated with the considered nonlinear one.

The Landau-Zener term-crossing model [1] describes a well appreciated quantum paradigm when two states of a quantum system are coupled by an external field of constant amplitude and a variable frequency which is linearly changed in time. This is a seminal approximation that serves as a prototype of all the resonance-crossing quantum models. However, this situation has some drawbacks; it is unrealistic to have a constant coupling that never turns off or infinite energies at $t \to \pm\infty$. However, there exists a model that has all the virtues of the Landau-Zener model and is free from its shortcomings. Such a model is the first Demkov-Kunike quasi-linear level-crossing model of a bell-shaped pulse (vanishing at $t \to \pm\infty$) and finite detuning [2]. Thus, the Demkov-Kunike (DK) model can be considered as a *physically realizable generalization* of the Landau-Zener model.

In the mean-field two-mode approximation, the dynamics of ultracold molecule formation is described by the nonlinear semiclassical time-dependent two-state model [3]:

$$i\frac{da_1}{dt} = U(t)e^{-i\delta(t)}\overline{a}_1 a_2, \quad i\frac{da_2}{dt} = \frac{U(t)}{2}e^{i\delta(t)}a_1 a_1, \tag{1}$$

where t is the time, a_1, a_2 are the atomic and molecular state probability amplitudes, $\overline{a}_1$ is the complex conjugate of a_1, the Rabi frequency $U(t)$ is proportional to the amplitude of the associating field, and the real function $\delta(t)$ is the integral of the frequency detuning δ_t (the alphabetical index denotes differentiation with respect to the corresponding variable). System (1) possesses the first integral $|a_1|^2 + 2|a_2|^2 = 1$ that reflects the particle number conservation during the interaction. We suppose that the system starts from the all-atomic state.

The DK field configuration is defined as

$$U = U_0 \operatorname{sech}(t), \quad \delta_t = 2\delta_0 \tanh(t). \tag{2}$$

Following the general scheme [4], we make the transformation of the independent variable $z(t) = \int_0^t (U/U_0)dt'$ and apply the following exact equation for the function $p = |a_2|^2$:

$$p_{zzz} - \frac{\delta^*_{zz}}{\delta^*_z}p_{zz} + \left[\delta^{*2}_z + 4\lambda(1-3p)\right]p_z + \frac{\lambda}{2}\frac{\delta^*_{zz}}{\delta^*_z}\left(1 - 8p + 12p^2\right) = 0, \tag{3}$$

where the effective detuning δ_z^* is defined as $\delta_z^*(z(t)) = \sqrt{\lambda}\,\delta_t(t)/U(t)$ with $\lambda = U_0^2$. For the DK model under consideration we have $\delta_z^* = 2\delta_0 \sinh(t)$.

Since in the large sweep rate regime of the strong interaction limit the parameters λ and δ_0 are supposed to be large, in Ref. [5] the approximate solution of the exact equation for the molecular state probability (3) has been proposed by trying to compensate the two higher order derivate terms by a term of the form $A\delta_{zz}^*/\delta_z^*$, where A is an adjustable parameter. Thus, the zero-order approximation to the problem has been chosen as a solution of the following nonlinear differential equation of the first order:

$$\left[\delta_z^{*2} + 4\lambda(1-3p_0)\right]p_{0z} + \frac{\lambda}{2}\frac{\delta_{zz}^*}{\delta_z^*}\left(1-8p_0+12p_0^2\right) - A\frac{\delta_{zz}^*}{\delta_z^*} = 0. \tag{4}$$

The exact solution of this equation, satisfying the imposed initial condition $p_0(t=-\infty)=0$, is given as a solution of the following polynomial equation of the fourth order:

$$\frac{\lambda}{\delta_z^{*2}(z(t))} = \frac{p_0(p_0-\beta_1)(p_0-\beta_2)}{9(p_0-\alpha_1)^2(p_0-\alpha_2)^2}, \tag{5}$$

where

$$\alpha_{1,2} = \frac{1}{3} \mp \frac{1}{6}\sqrt{1+\frac{6A}{\lambda}}, \quad \beta_{1,2} = \frac{1}{2} \mp \sqrt{\frac{A}{2\lambda}}. \tag{6}$$

When $0 < A < \lambda/2$, the limit solution $p_0(z(t), A)$ is a monotonically increasing function that starts from zero at $t=-\infty$, reaches the value $p_0(0) = \alpha_1 < 1/6$ at $t=0$ and tends to the finite positive value $p_0(+\infty) = \beta_1 < 1/2$ at $t \to +\infty$.

In Ref. [5], an analytical expression for the parameter A has been suggested. However, in the present development we do not specify the value of A to consider it as a ***variational parameter***. To proceed, we now try to construct the first-order approximation to the problem using the limit function p_0 as a zero-order approximation. To do that, we make the change of the dependent variable $p = p_0 + u$ in the exact equation for the molecular state probability (3). This change leads to the following exact equation for the correction term u:

$$\left(\frac{d}{dz} - \frac{\delta_{zz}^*}{\delta_z^*}\right)\left(u_{zz} + 4\lambda(1-3p_0)u + p_{0zz} - A - 6\lambda u^2\right) - \delta_z^{*2}u_z = 0. \tag{7}$$

Since the function p_0 is supposed to be a good approximation for the molecular state probability p, the correction u is supposed to be small. Hence, if we neglect the nonlinear term $-6\lambda u^2$, the exact equation (7) for u will be linearized. By comparing the resultant linear equation with that obeyed by the second state probability P_{DK}, calculated within the linear theory of nonadiabatic transitions, we see that if we consider p_0 as a constant, the solution of the constructed linearized equation will be given as a scaled solution to the *linear* DK problem with modified parameters. This observation gives an argument to make a conjecture that the exact solution of Eq. (7) can be approximated as $u \sim P_{DK}(\lambda^*, \delta_0^*, t - t_{ph})$, where $P_{DK}(\lambda^*, \delta_0^*, t)$ is the solution to the linear DK problem with effective parameters λ^*, δ_0^*, and t_{ph} being an extra temporal shift.

Thus, we arrive at the following principal conjecture: an approximation describing the time evolution of the molecular state probability can be written as a sum of a solution of the limit equation (4) and a scaled solution to the *linear* DK problem with *modified* parameters (note that a similar ansatz has previously been suggested for the Landau-Zener model [6]):

$$p = p_0(A,t) + C^* \frac{P_{DK}(\lambda^*, \delta_0^*, t - t_{ph})}{P_{DK}(\lambda^*, \delta_0^*, \infty)} , \qquad (8)$$

This conjecture is well confirmed by numerical analysis. The numerical simulations show that one can always find A, C^*, λ^*, and t_{ph} such that the function (8) accurately fits the numerical solution of the exact equation for the molecular state probability (3). Furthermore, the simulations indicate that there is no need to modify the detuning parameter δ_0. It also turns out that we may put $t_{ph} = 0$. Further numerical analysis shows that the absolute error of formula (8) is typically less than $5 \cdot 10^{-6}$ for the final transition probability. For arbitrary times, its absolute error is commonly of the order of $10^{-5} - 10^{-4}$, and for the points of the first few maxima and minima of the function $p(t)$ (at certain values of the input parameters λ and δ_0) the deviation may increase up to $\sim 10^{-3}$.

Examining the role of the two terms in the approximate expression for the molecular state probability (8), we see that the first term, being a solution of the nonlinear equation (4), effectively describes the process of the molecule formation while the second one, being the scaled solution to the *linear* DK problem, describes the oscillations which arise some time after the system has passed through the resonance (see Fig. 1). From this, one can conclude that in the strong coupling limit the dynamics of the atom-molecule conversion effectively consists of the nonlinear resonance crossing followed by atom-molecular coherent oscillations that are principally of linear nature. The possibility to make such decomposition is not trivial since the governing set of equations (1) does not indicate this.

One of the essential virtues of Eq. (8) is that it provides a simple expression for the final transition probability written in terms of the variational parameters A and C^*:

$$p(+\infty) = p_0(+\infty) + C^* . \qquad (9)$$

To study the asymptotic behavior of the involved variational parameters in the limit $\lambda \to \infty$, we substitute the trial function (8) into the exact equation for the molecular state probability (3) and consider the behavior of the remainder

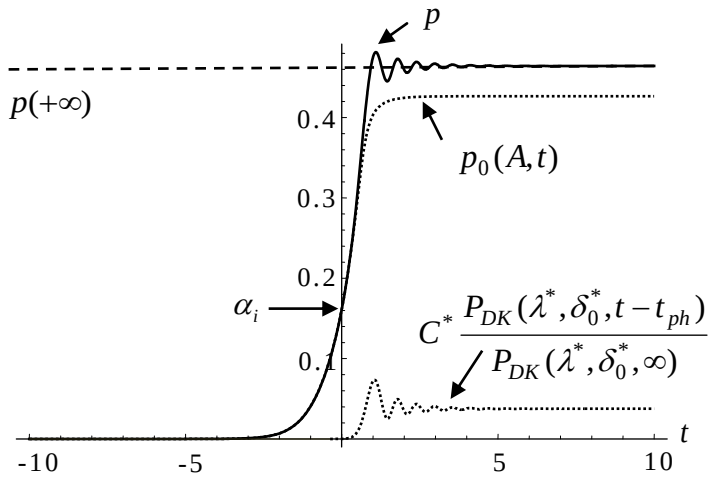


Fig. 1. Molecular state probability p, the limit solution p_0 determined from Eq. (5), and the scaled solution to the linear DK problem with modified parameters ($\lambda = 49$ and $\delta_0 = 5.5$).

$$R=\left(\frac{d}{dz}-2\csc(2z)\right)\Bigg\{4\Big[\lambda(1-3p_0)-\lambda^*\Big]C^*\,\frac{p_{DK}(\lambda^*,z(t))}{p_{DK}(\lambda^*,z(+\infty))}+C^*\,\frac{2\lambda^*}{p_{DK}(\lambda^*,z(+\infty))}$$
$$+\left(p_{0zz}-A\right)-6\lambda C^{*2}\,\frac{p_{DK}^2(\lambda^*,z(t))}{p_{DK}^2(\lambda^*,z(+\infty))}\Bigg\}. \tag{10}$$

It is seen that for $\lambda>>1$ the first term of the remainder is highly suppressed if we choose the variational parameter λ^* as

$$\lambda^*=\lambda(1-3p_0(+\infty)). \tag{11}$$

It is clear that for $\lambda>>1$, when $p_0\sim 1$, λ^* is a *negative* parameter. Regarding the two last terms of Eq. (10), one should minimize them with respect to the parameter C^*. This implies the condition

$$\frac{\partial(R/C^*)}{\partial C^*}=\left(\frac{d}{dz}-2\csc(2z)\right)\left(-\frac{1}{C^{*2}}\left(p_0''-A\right)-6\lambda\,\frac{P_{DK}^2(\lambda^*,z(t))}{P_{DK}^2(\lambda^*,z(+\infty))}\right)=0. \tag{12}$$

Since the last term is proportional to (large) λ and $P_{DK}(\lambda^*,t)$ is an increasing function of time, the "worst" point is $t=+\infty$. Hence, we look for a minimization at $t=+\infty$. This immediately leads to the following value for C^*:

$$C^*=\sqrt{\frac{A}{6\lambda}}. \tag{13}$$

Thus, we have examined, in the mean-field approximation, the strong interaction limit of the nonlinear DK problem for coherent molecule formation in an atomic Bose-condensate via two-mode one-color photoassociation or a sweep across a Feshbach resonance. We have shown that the approximate expression for the molecular state probability can effectively be represented as a sum of two distinct terms. The first term is defined as a solution of a limit first-order *nonlinear* differential equation while the second one is a scaled solution to the *linear* DK problem with modified parameters. The constructed solution incorporates three variational parameters, A, C^*, and λ^*, the appropriate choice of which ensures that it provides an accurate approximation (the graphs of the approximate and numerical solutions are practically indistinguishable for almost whole time range). We have also derived approximate expressions for the parameters λ^* and C^* (as functions of A) for the case of strong laser field intensities.

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