Creating Steady Atom-Molecule Entanglement and Coherent Molecular output by Demkov-Kunike Type Non-adiabatic Transition

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We, based on the photoassociation of fermion atoms into bosonic molecules, propose a scheme to create the steady entanglement between the atom state and the molecule state inside an optical lattice. The stability of entanglement state is guaranteed by sweeping the frequency of Ramman laser beam through resonance according to the second Demkov-Kunike (DK2) nonadiabatic transition model [1,2]. The probability amplitude of each components can be precisely controlled by adjusting the sweeping parameter. Considering the loss of molecule, the steady coherent molecular output can also be obtained in each lattice site.

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In recent years, the photoassociation of fermionic atoms forming bosonic molecules [3–6] has aroused great interest. In this process, two atoms in condensate are illuminated by two Raman laser beams. This atom pair absorbs an photon from one laser beam and emits a photon to another beam. As a result of stimulated Raman effect, there is a transition from the two atom state to a single molecule state. Most recently, there are many experiments to demonstrate this photoassociation process and the Bose-Einstein Condensation (BEC) of molecular has been observed [5]. There also exists another physical mechanism, Feshbach Resonance to create the molecular from the very cold atoms even in situation of BEC. When the external magnetic field of an atomic system is changed, an entrance interaction channel and a closed channel can be resonantly coupled and the population of a two atom bound state, i.e. the molecular state, can be resonantly enhanced. In recent experiments, the disappearance of atoms and the creation of molecules from BEC have been observed [7–9].

In both the two cases, an interesting question is whether one can control exactly the rate of producing the composite particle–molecule and even obtain the coherent output of molecular [10]. If the dissipation mechanism is not considered in this photoassociation process, there must exists a Rabi oscillation between atomic state and molecular state and then there is only a "pulse profile" of molecular productions. In this case, we can not obtain a steady population of atom and molecular state. This phenomenon is very similar to "pulse atomic laser". In the experiment of atomic laser, an crucial technology to overcome this problem is to sweep the frequency of radiation field (r.f) [11] that couples the trapped BEC state to the un-trapped state. This physical mechanism avoiding the pure pulse profile due to Rabi oscillation can be understood in the rotation picture. Within this representation, the sweeping frequency will shift the original energy level of atom. Then the sweeping derives the system to cross the degenerate point of energy level in a non-adiabatic way. Then, the Landau-Zener approximation [12] can be utilized to obtain the steady populations of BEC atoms in the different energy levels. In this article, we will invoke this idea of sweeping frequency to obtain a steady atom-molecule entanglement state, i.e. the coherence superposition of atomic and molecular number states with steady population of molecules produced from the atoms in photoassociation.

We notice that the Landau-Zener model for sweeping the frequency is precisely correct, only when the detuning in the effective two level Rabi model linearly varies with time $t$ from $-\infty$ to $+\infty$. Actually, the linear function of time is only an approximate description of the variation of the realistic detuning, because in practical cases the experimental parameters are always adjusted as smooth functions of time which have finite values in the limit $t \rightarrow \pm \infty$. For instance, in ref. [13], the hyperbolic tangent function is considered as a more practical description of the experimental behavior of the atomic Stark energy difference controlled by laser beams. The validity of the Landau Zener model is also analyzed numerically in the same reference.

In this article, we adopt a feasible sweeping way depicted by the second Demkov-Kunike (DK2) [1,2] model. In this model, the detuning has finite asymptotic values in the limit $t \rightarrow \pm \infty$. When we sweep the detuning in the DK2 way, the finite asymptotic values of detuning are experimentally implementable.

In our study, the model Hamiltonian for the atom-molecule photoassociation inside a single site in a optical lattice can be written as [14]:

$$H = \Omega_b b^\dagger b + \frac{1}{2} U_b b^\dagger b \left[b^\dagger b - 1\right] + \Omega_f \sigma_z + U_x b^\dagger b \sigma_z + \chi b^\dagger \sigma_+ + \chi b \sigma_+.$$  \hspace{1cm} (1)

Here, $b$ is the annihilation operator of molecule and $\chi$ is proportional to the two-photon Rabi frequency associated with the two laser beams [14]. Without loss of generality, in the following discussions, we assume $\chi$ to be real. $\Omega_b$ and $\Omega_f$ are defined as.
where $\omega_b$ is the atomic energy, $\omega_f$ is the molecular energy and $\Delta$ the detuning of the two laser beams. The terms contains $U_f$, $U_x$ and $U_b$ denote the energies of two body interactions between atoms, atoms and molecules, and molecules. In the Hamiltonian (1), the Anderson’s quasi-spin maps [15] defined by

$$\sigma_+ = c_1 c_2, \sigma_- = c_1^\dagger c_2^\dagger, \sigma_z = c_1^\dagger c_1 + c_2^\dagger c_2 - 1,$$  

have been used. Here, $c_i$ $(i = 1, 2)$ is the annihilation operator of the atomic state $|i\rangle$. It is easy to see that the operators $\sigma_{\pm}$ are defined as the quasi-spin flips $\sigma_+ = |e\rangle \langle g|$, $\sigma_- = |g\rangle \langle e|$ and $\sigma_z = |e\rangle \langle e| - |g\rangle \langle g|$ where $|g\rangle = |0\rangle_a$ is the atom vacuum state and $|e\rangle = c_1^\dagger c_2^\dagger |0\rangle_a$ is the two atom state. In the mathematical formulism, the Hamiltonian (1) is just a Jaynes-Cummings kind Hamiltonian with a nonlinear detuning [14]. The laser enhanced combination process depicted by the interaction Hamiltonian can be illustrated in Fig 1.

FIG. 1. The photoassociation process of the atoms in optical lattice. In every lattice, the molecule state $|M\rangle$ (the two atom bound state) is coupled with the atom state $|F\rangle$ (the two atom free state) via the two Raman beams $\omega_1$ and $\omega_2$.

In order to use the DK2 model, we assume that the detuning $\Delta$ of the two Raman laser beams varies with time as a hyperbolic tangent function:

$$\Delta (t) = 2\omega_f - \omega_b + U_f - 2k \tanh \left( \frac{t}{T} \right).$$  

It is obviously that the asymptotic values of $\Delta (t)$ in the limit $t = \pm \infty$ are determined by the parameter $k$ and the speed of the variation of $\Delta (t)$ depends on $T$. Therefore, in the limit $t \rightarrow \pm \infty$, the $\Delta$ has finite asymptotic values $2\omega_f - \omega_b + U_f \pm 2k$. Since $|\tanh (\pm 2)| = 0.96 \approx 1$, the practical operational time is about $4T$. Obviously, the subspace expanded by $\{|e, n_b\}, |g, n_b + 1\rangle\}$ is an invariance subspace $V_n$ of $H$ in Eq. (1). In other words, the Hamiltonian can be block-diagonal matrix and an arbitrary superposition of $|e, n_b\rangle$ and $|g, n_b + 1\rangle$ in $V_n$ can only evolve into itself. Here, we define $|e, n_b\rangle = |e\rangle \otimes (n_b\rangle)$ $\otimes b^{n_b} |0\rangle_b$ as the number state corresponding to two atoms and $n_b$ molecules. Here, $|0\rangle_b$ is the molecule vacuum state. $|g, n_b + 1\rangle$ has the similar definition. Then a block of $H$ can be expressed as a $2 \times 2$ matrix:

$$H (n_b, t) = \begin{bmatrix} a + k \tanh \left( \frac{t}{T} \right) |e, n_b\rangle \langle e, n_b| + c |e, n_b\rangle \langle g, n_b + 1| \\ a + k \tanh \left( \frac{t}{T} \right) |g, n_b + 1\rangle \langle e, n_b| + c |g, n_b + 1\rangle \langle g, n_b + 1| \end{bmatrix} / 2,$$

where we have used Eq. (3). Here, $a$ and $c$ are functions of $n_b$ and are defined as $a (n_b) = n_b (U_x - U_b) / 2$, $c (n_b) = \sqrt{n_b} + 1$.

Since $\chi$ is proportional to the Rabi frequency which is slowly varying with the frequency of the Raman beams, it is reasonable to assume $2847701 \times 10^{-22} J^{-1} e (n_b) = \chi \sqrt{n_b + 1} \mp 1$ to be a time-independent constant. The instantaneous eigenvectors of the matrix $H (n_b, t)$ can be noted as $|\Phi_+ (n_b, t)\rangle$ and $|\Phi_- (n_b, t)\rangle$. It is apparently that in the limit $t \rightarrow \pm \infty$, the matrix $H (n_b, t)$ has asymptotic expressions

$$H (n_b, \pm \infty) = [a (n_b) \pm k] |e, n_b\rangle \langle e, n_b| + c (n_b) |e, n_b\rangle \langle g, n_b + 1| - [a (n_b) \pm k] |g, n_b + 1\rangle \langle g, n_b + 1| + c (n_b) |g, n_b + 1\rangle \langle g, n_b + 1|$$

Therefore, the eigenvectors $|\Phi_\pm (n_b, t)\rangle$ also have asymptotic expressions when $t \rightarrow \pm \infty$. We note them as $|\Phi_\pm (n_b, \pm \infty)\rangle$. Generally speaking, $|\Phi_\pm (n_b, \pm \infty)\rangle$ are superposition states of $|e, n_b\rangle$ and $|g, n_b + 1\rangle$. It can be seen in the following discussion that we are only interested in the special cases that $|\Phi_\pm (n_b, \pm \infty)\rangle$ can be approximated as $|e, n_b\rangle$ or $|g, n_b + 1\rangle$. Then the general expression of $|\Phi_\pm (n_b, t)\rangle$ is not needed here.

The instantaneous state $|\Psi (n_b, t)\rangle$ of the quantum system is the solution of the Schrodinger equation

$$i \frac{d}{dt} |\Psi (n_b, t)\rangle = H (n_b, t) |\Psi (n_b, t)\rangle,$$

and it can be expanded as the superposition of $|\Phi_\pm (n_b, t)\rangle$:

$$|\Psi (n_b, t)\rangle = \sum_{i=+,-} D_i (n_b, t) |\Phi_i (n_b, t)\rangle.$$

Obviously, $|D_\pm (n_b, t)|^2$ are the populations in the states $|\Phi_\pm (n_b, t)\rangle$ at any instantaneous. In practical cases, the asymptotic value $|D_\pm (n_b, \pm \infty)|^2$ in the limit $t \rightarrow \pm \infty$ is usually of interest. If the quantum system is initially prepared in the state

$$|\Psi (n_b, -\infty)\rangle = |\Phi_+ (n_b, -\infty)\rangle,$$

the values of $|D_\pm (+\infty)|^2$ can be obtained with direct calculations [1,2]:

$$D_- (+\infty)|^2 = \frac{\sinh [\pi T E_a] \sinh [\pi T E_c]}{\pi T E_a \sinh [\pi T E_c]},$$

$$D_+ (+\infty)|^2 = 1 - |D_- (+\infty)|^2,$$

where the complicated notations $E_a$, $E_c$ and $E_\pm$ are defined as functions of the physical parameters $a$, $b$ and $k$:

$$E_a (a, k, c) = \left[ (a - k)^2 + c^2 \right]^{1/2},$$

$$E_c (a, k, c) = \left[ (a + k)^2 + c^2 \right]^{1/2},$$

$$E_\pm = \frac{E_c - E_a}{2}.$$
In the above calculations, we have referred to the main result in the DK2 model.

To create the atom-molecule entanglement state from the direct product of the atomic and molecular number state \( |e, n_b\rangle \), we assume the amplitude \( k \) is large enough so that the conditions \( k \pm a(n_b) \gg e(n_b) \) are satisfied. Since \( a \) is proportional to \( n_b \) and \( c \) is proportional to \( \sqrt{n_b} \), this condition implies that \( n_b \) is small enough. In this case, when \( t = \pm \infty \), since \( k \pm a(n_b) \gg c(n_b) \), the diagonal terms of \( H(n_b, \pm \infty) \) is much larger than the off diagonal terms. The eigenstates of \( H(n_b, \pm \infty) \) can be approximated as

\[
|\Phi_+(n_b, -\infty)\rangle \simeq |\Phi_-(n_b, +\infty)\rangle \simeq |e, n_b\rangle \\
|\Phi_-(n_b, -\infty)\rangle \simeq |\Phi_+(n_b, +\infty)\rangle \simeq |g, n_b + 1\rangle
\]

This is an analogy of large detuning case when a two level atom interact with a classical radiation field. Therefore, in the limit \( t \to \pm \infty \), there is almost no atom-molecule transition and the mode of the probability amplitudes of the states \( |e, n_b\rangle \) and \( |g, n_b + 1\rangle \) do not change with time. This phenomenon has been shown in the experiment of photoassociation [5]. The mixing of the two states mainly happens in the nearby of the “resonance point” where \( |a + k \tanh(t/T)| \ll c \).

In this case, if the system is initially prepared in the state \( |e, n_b\rangle \) when \( t = -\infty \) and \( \Delta \) is changed with time according to condition (3), the system will evolve into the superposition state

\[
D_1(n_b)|e, n_b\rangle + D_2(n_b)|g, n_b + 1\rangle
\]

when \( t = +\infty \). Apparently, this quantum state can be considered as a atom-molecule entanglement state. It follows from Eq. (5) that

\[
|D_1(n_b)|^2 \approx \frac{\sinh [\pi T E_+ (a, k, c)] \sinh [\pi T E_- (a, k, c)]}{\sinh [\pi T E_0 (a, k, c)] \sinh [\pi T E_\pm (a, k, c)]}
\]

(8)

where the functions \( E_0(a, k, c) \), \( E_+ (a, k, c) \) and \( E_\pm (a, k, c) \) are defined in Eq. (6). The probability of creating one molecule from two atoms can be expressed as \( P = 1 - |D_1|^2 \). Especially when \( n_b = 0 \), \( P \) describes the molecular vacuum production.

It is easy to prove that when \( k \) is large enough so that \( e^{Tk} >> 1 \), \( |D_1(n_b)|^2 \) in Eq. (8) can be approximated as

\[
|D_1(n_b)|^2 \approx \exp \left[ -\frac{\pi}{k} \frac{T \nu^2}{(1 - \frac{\nu^2}{T^2})} \right]
\]

(9)

\[
= \exp \left[ -2\pi \frac{c^2}{\pi} \frac{1}{2k \tanh \left( \frac{t}{T} \right)} \right]_{t=t_0}
\]

Here, \( t_0 \) which satisfies \( a + k \tanh \left( t_0/T \right) = 0 \) is the cross point of the diagonal elements of the Hamiltonian in Eq. (4). Therefore, the approximated expression of \( |D_1(n_b)|^2 \) in Eq. (9) is just the result given by Landau Zener formula.

Now we are in a position to analyze the influence of the parameters \( T, n_b, k, U_x \) and \( U_b \) on the molecular probability \( P \). It is convenient to express the probability \( P \) as \( P = 1 - f \) where \( f = \frac{\sinh [\pi T E_+]}{\sinh [\pi T E_0]} \) and \( g = \frac{\sinh [\pi T E_-]}{\sinh [\pi T E_0]} \). Using the simple relationships

\[
E_a - E_- = E_e - E_+ = \frac{E_e + E_a}{2} - k > 0
\]

(10)

we can prove \( df/dT < 0 \) and \( dg/dT < 0 \) with the inequality \( y \tanh x < x \tanh y \) when \( x > y > 0 \). Then we have \( dP/dT > 0 \). With straightforward calculations, it is also proved that under the condition \( k \pm a(n_b) >> c(n_b) \), we have \( dP/dn_b > 0 \) [16]. Therefore, the molecular probability \( P \) increases with \( T \) and the molecular number \( n_b \). Therefore, in order to obtain a high molecular probability \( P \), the speed of the variation of the detuning \( \Delta \) should be low enough. In Fig. 2, the behavior of \( P \) as a function of \( T \) is shown. It can be seen from this figure that when \( n_b = 0 \) and \( T \) is larger than \( 25 \chi^{-1} \), \( P \) is approximately unit and a molecule is created with unit probability from two atoms. However, when \( n_b = 5 \), we have \( P \approx 1 \) when \( T \) is larger than \( 5 \chi^{-1} \).

FIG. 2. The molecular probability \( P \) as a function of \( T \) in case the molecular number \( n_b = 0, 2 \) and 5. Here, we have assumed \( k = 20 \chi, (U_x - U_b/2) = 0.5 \chi \) and the unit of \( T \) is \( \chi^{-1} \). It is obviously that \( P \) increases with \( T \) and \( n_b \).

The influences of the amplitude \( k \) of the detuning and the atomic scattering coefficient \( (U_x - U_b/2) \) on the molecular probability \( P \) is shown in Fig. 3. It can be seen that with the same operation time \( T \) and molecular number \( n_b \), as the amplitude \( k \) increases, the molecular probability \( P \) decreases. On the other hand, when the scattering strength is small enough so that \( (U_x - U_b/2) / \chi \ll 10 \), \( P \) has almost the same value with respect to different values of \( (U_x - U_b/2) \), i.e. the effect of atomic scattering can be ignored. When \( (U_x - U_b/2) \) becomes larger, \( P \) increases with \( (U_x - U_b/2) \). It is pointed out that in Fig. 3 we assume \( k \sim 10^2 \) and \( T \sim 10^{-4} \) so that \( e^{kT} < 1 \). Therefore, the figure is drawn in the domain where the Landau-Zener formula is not applicable. In case of larger \( k \) or \( T \), the same conclusion can be obtained with the expression of \( P \) in Eq. (9) given by Landau-Zener formula.

FIG. 3. The molecular probability \( P \) as a function of \( k \) with different value of \( (U_x - U_b/2) \). In the figure, we note \( m = (U_x - U_b/2) \). We assume \( n_b = 1 \) and \( T = 10^{-2} \chi^{-1} \). The unit of \( m \) and \( k \) are all \( \chi \). The unit of \( P \) is \( 10^{-3} \).

Apparently, the quantum state in Eq. (7) can also be considered as a atom-molecule entanglement state writ-
each in interval $\tau$, there are two plus used in our system. We assume in state $|\psi\rangle$ before the Raman beams are turned on, the transition $\Delta$ is adiabatically changed into state $|\psi',\psi\rangle$ during each time interval $\tau$. Therefore, we have $|D_2(n-1)|^2 \approx 1$ which do not depend on both $\tau$ and $n$. In this case the molecular distribution $p_n$ in Eq. (13) is proportional to $N_{ex}/n!$. It is apparently that $p_n$ is just the Possion distribution which is just the population distribution of a molecular coherent state. The average molecular number $\langle n \rangle$ is just $N_{ex}$ which can be controlled easily. Then we can obtain a coherent output of molecule with the nonadiabatic transition method. The coherence of the output molecular field can be described by the line width $D$. This line width can be calculated with the standard method as in the laser theory [17] and we have the result $D \approx 9\gamma/N_{ex}$. On the other hand, when the parameter $T$ is not very large, it can be obtained with numerical simulation that we have $\langle n \rangle < N_{ex}$ and the Mandel $Q$ factor is larger than 1. Therefore, we can get superpossession distribution in this case.

In this paper we have shown that in the photoassociation process, we can create the atom-molecule entanglement state with steady atomic and molecular probability by varying the detuning of the Raman laser beams. The influence of the variation parameters of the detuning on the molecular probability $P$ have also been investigated. As we have shown, if we want to create a high probability $P$, the operation time (4T) should be long enough. However, it can be seen from Fig. 4 that to obtain the maximal entanglement state in Eq. (11), the operation time needed is much shorter than the one needed to create a pure molecule state. We have also shown that steady coherent output with Possion or superpossession molecular distribution can be obtained by turning on and off the Raman laser beams for many times. It is pointed out that, since in photoassociation process the Rabi frequency $\chi$ is much larger than the molecular dissipation rate $\gamma$ [14], the condition that the time interval $\tau \ll 10^2\chi^{-1}$ can be realized. Therefore, the scheme in our paper can be used in the atom-molecule wave function engineering.

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It is easy to prove that $E_e, E_a$ and $E_\pm$ satisfy $dn_b/d(E_e + E_a) > 0$ and $E_\pm dE_e/dn_b > E_e dE_\pm/dn_b$. Considering Eq. (10) and the inequality $y \tanh x < x \tanh y$ when $x > y > 0$, it can be seen that these inequalities lead to the results $df/dn_b < 0$ and $dg/dn_b < 0$. Then we have the result $dP/dn_b > 0$. 

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