Role of particle interactions in a many-body model of Feshbach-molecule formation in bosonic systems

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(Received 17 July 2008; revised manuscript received 15 September 2008; published 24 February 2009)

We investigate a generalized many-body model of Feshbach molecule formation that includes the atom-atom, atom-molecule, and molecule-molecule interactions. We show that the picture of two-body molecule production depicted by the Landau-Zener model is significantly altered by the particle interactions. In the adiabatic limit, we work out a formula for the ceiling of conversion efficiency when the interaction strength is larger than a critical value. In the sudden limit, we derive a closed equation for the conversion efficiency using stationary phase approximation. Our theory predicts a significant role of the particle interactions in atom-molecule conversion when the atom density is high and the Feshbach resonance width is narrow.

DOI: 10.1103/PhysRevA.79.025602 PACS number(s): 03.75.Mn, 03.75.Hh, 67.60.Bc

The production of ultracold diatomic molecules in bosonic systems is an exciting area of research with important applications ranging from the production of molecular Bose-Einstein condensates (BECs) [1] to the study of chemical reaction dynamics [2]. A widely used production technique involves the association of ultracold atoms into very weakly bound diatomic molecules by applying a time varying magnetic field in the vicinity of a Feshbach resonance [3,4]. The underlying conversion dynamics is usually described by the Landau-Zener (LZ) model [5]. In this model, the Feshbach molecule production is discussed under a two-body configuration where a single pair of atoms is converted to a molecule at an avoided crossing between atomic energy level and molecular energy level while the molecular energy is lifted by an applied linearly sweeping magnetic field. Thus, the molecule production efficiency is expected to be an exponential Landau-Zener type [6,7].

In the above two-body model [6,7] and its some many-body extensions [8–10], however, the interactions between particles such as the atom-atom, atom-molecule, and molecule-molecule interactions, were totally ignored. In this Brief Report, we want to examine the role of particle interactions in the atom-molecule conversion. Our calculations show that the energy levels are significantly distorted and the conversion efficiency is influenced dramatically by these particle interactions. In the adiabatic limit, we work out an explicit formula for the upper bound of conversion efficiency when the interaction strength is larger than a critical value. In the sudden limit, we derive a closed equation for the conversion efficiency using stationary phase approximation. We further point out that these effects might potentially be observable in current experiments.

The two-channel model Hamiltonian that includes the atom-atom, atom-molecule, and molecule-molecule interactions takes the following form [11]:

$$\hat{H} = \frac{u_{aa}}{V}\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a} + \frac{u_{bb}}{V}\hat{b}^\dagger\hat{b}^\dagger\hat{b}\hat{b} + \frac{u_{ab}}{V}\hat{a}^\dagger\hat{a}\hat{b}^\dagger\hat{b} + \epsilon_a\hat{a}^\dagger\hat{a} + \epsilon_b\hat{b}^\dagger\hat{b} + \frac{\omega}{\sqrt{V}}(\hat{a}^\dagger\hat{a}^\dagger\hat{b} + \hat{b}^\dagger\hat{a}\hat{a}). \quad (1)$$

This model has been proposed by Santos *et al.* [11] to investigate the Josephson oscillation and self-trapping phenomena of atom-molecule conversion systems.

In Eq. (1), $\hat{a}^\dagger$ ($\hat{b}^\dagger$) and ϵ_a (ϵ_b) are the creation operator and chemical potential for an atomic (molecular) mode, respectively. In experiments, the magnetic field is linearly swept $B(t)=\dot{B}t$ and crosses the Feshbach resonance at B_0, thus $2\epsilon_a-\epsilon_b=\mu_{co}[B(t)-B_0]$. Here, μ_{co} is the difference between the magnetic moments of a molecule and a pair of separated atoms. $\omega=\sqrt{4\pi\hbar^2 a_{\mathrm{bg}}\Delta B\mu_{co}/m}$ denotes the amplitude for the interconversion of atoms and molecules due to the Feshbach resonance, in which m is the mass of a bosonic atom, a_{bg} is the background scattering length, and ΔB is the width of the resonance. $u_i=2\pi\hbar^2 a_i/m_i$ ($i=aa,bb,ab$) are the particle interactions between atom-atom, molecule-molecule, and atom-molecule. Here a_i and m_i denotes the background scattering length and the reduced mass, respectively, i.e., $a_{aa}=a_{\mathrm{bg}}$, $a_{ab}\approx 1.2a_{\mathrm{bg}}$, $a_{bb}\approx 0.6a_{\mathrm{bg}}$ [12], $m_{aa}=m/2$, $m_{ab}=2m/3$, and $m_{bb}=m$. We introduce N and V to denote the initial atom number and the quantized volume, therefore $n=N/V$ is the mean density of the initial bosonic atoms.

In the mean-field limit where $N\to\infty$, the quantum fluctuation is negligible. It is appropriate to replace all the quantum operators with c numbers, thus the Heisenberg equations for operators $\hat{a}$ and $\hat{b}$ are casted into the following nonlinear Schrödinger equation:

$$i\frac{d}{dt}\begin{pmatrix} a \\ b \end{pmatrix} = H\begin{pmatrix} a \\ b \end{pmatrix}, \quad (2)$$

where

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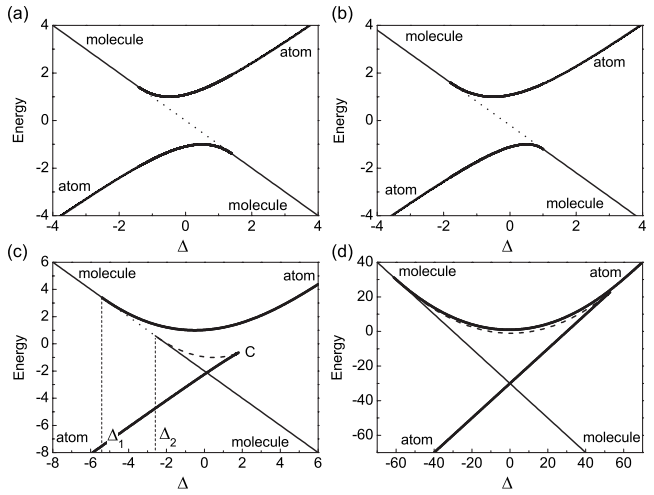

FIG. 1. Adiabatic energy levels for different nonlinear interaction strength: (a) $U=0$, (b) $U=0.2$, (c) $U=2$, and (d) $U=30$. In all cases, $\Omega=1$, the solid lines represent stable eigenstates, and the dotted lines between $\Delta_1=U-\sqrt{2}$ and $\Delta_2=U+\sqrt{2}$ correspond to unstable states. When $U>\sqrt{2}/4$, a loop structure appears at the lower energy level. The loop expands as U increases.

$$H=\begin{bmatrix} 2U(2|b|^2-|a|^2)+\Delta & 4\Omega a^* \\ 2\Omega a & -4U(2|b|^2-|a|^2)-2\Delta \end{bmatrix}, \tag{3}$$

with $U=\frac{n}{4}(\frac{1}{2}u_{ab}-u_{aa}-\frac{1}{4}u_{bb})$, $\Delta=\frac{1}{4}(2\epsilon_a-\epsilon_b+2nu_{aa}-\frac{1}{2}nu_{bb})$, and $\Omega=\frac{\sqrt{n}\omega}{2}$. The total population is normalized to a unit, i.e., $|a|^2+2|b|^2=1$.

We first show how the nonlinear interactions lead to the deformation of the eigenenergy levels. The eigenstates of the system satisfy that

$$H\begin{pmatrix} a \\ b \end{pmatrix}=\begin{pmatrix} \mu & 0 \\ 0 & 2\mu \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}. \tag{4}$$

Notice that a diatomic molecule is composed of two atoms, thus there is a factor 2 before the chemical potential for the molecular mode. Solving the above nonlinear equations together with $|a|^2+2|b|^2=1$, we readily obtain the chemical potential μ and the eigenstate (a,b). The eigenenergies can be derived according to the relationship $\epsilon=\mu/2+\mu|b|^2+\Delta|a|^2/2+4U|b|^4-2U|a|^2|b|^2$. Their dependence on the parameters is plotted in Fig. 1. In the linear case [$U=0$, Fig. 1(a)], the energy levels have a symmetry that they are invariant under a rotation about zero point by 180°. There are only two eigenstates when $|\Delta|$ is large enough, one for atomic mode and the other for molecular mode. When $|\Delta|/\Omega<\sqrt{2}$, there is an additional eigenstate with $S=-1$ represented by the dotted line in Fig. 1. This eigenstate is dynamically unstable. With the appearance of nonlinear interaction, the symmetry of the energy levels breaks down. For the weak nonlinear case $U/\Omega<\sqrt{2}/4$ [see Fig. 1(b)], the energy level structure is very similar to that of the linear case except for a slight shift. However, when $U/\Omega>\sqrt{2}/4$, a loop structure appears at the lower energy level. The loop expands as U increases, and the gap between the upper and lower energy level becomes narrower and narrower. Such deformation of energy levels consequently leads to very different conversion dynamics.

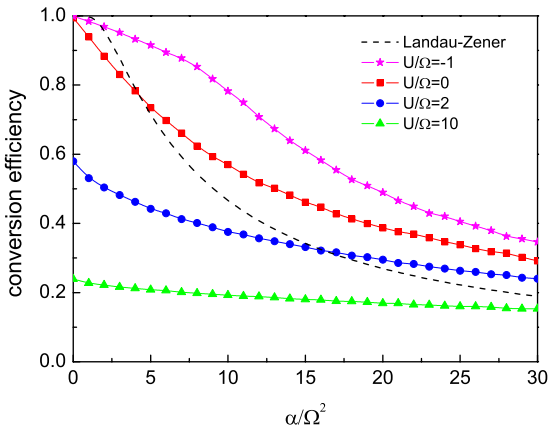

FIG. 2. (Color online) Conversion efficiency as a function of the sweep rate α/Ω^2 for various interaction parameters. For comparison, we also plot the Landau-Zener-type formula $\chi=1-\Gamma_{lz}=1-\exp(-\frac{2\pi\Omega^2}{\alpha})$ [5,9]; here the sweeping rate is defined as $\alpha=\dot{\Delta}=\mu_{co}\dot{B}/4$.

Consider the adiabatic evolution of the system starting from the atomic mode at the left side of the lower energy level. When U is small, e.g., in Fig. 1(a), the evolution of the system follows the solid line, converting all atoms into molecules. However, when $U/\Omega>\sqrt{2}/4$ as in Fig. 1(c), the system moves steadily from the left side to the critical point C. After that, there is no way to go further except to jump to the upper and lower levels. As that fraction of atoms tunnels to the upper level, they are not converted into molecules. The situation becomes even worse when U is very large: the critical point is much closer to the upper level and far away from the lower one, thus the system will jump to the upper level more easily, see Fig. 1(d). As a result, almost all atoms cannot be converted into molecules.

The above simple analysis is confirmed by our numerical results, which are plotted in Fig. 2. In our calculations, the 4–5th Runge-Kutta step-adaptive algorithm is used to solve the nonlinear Schrödinger Eq. (2). The conversion efficiency as a function of the sweep rate α is plotted and shows a monotonous decrease as the sweep rate increases. Even in absence of the particle interactions, i.e., $U/\Omega=0$, the conversion efficiency calculated from our many-body model is quite different from the two-body Landau-Zener theory. For example, in the sudden limit of $\alpha/\Omega^2\gg1$, the former is almost twice that of the latter. In the presence of the particle interactions, the atom-molecule conversion efficiency is further altered. When the dimensionless interaction parameter is positive the atom-molecule conversion is suppressed compared to that of $U/\Omega=0$, while, when this dimensionless parameter is negative, the conversion efficiency turns to be enhanced. From the explicit expression of the effective interaction parameter, we see that the repulsive atomic interaction leads to a negative parameter U/Ω while the attractive atomic interaction corresponds to a positive parameter. For the large positive interaction parameters, even in the adiabatic limit of $\alpha/\Omega^2\to0$, the atoms cannot be totally con-

verted into molecules. The saturation of conversion efficiency has already been discussed qualitatively in Ref. [13] without, however, presenting a quantitative analysis. Below, following the methodology of Ref. [14], we give some analytical calculations in two limit cases, namely, the adiabatic limit and sudden limit, corresponding to $\alpha/\Omega^2 \ll 1$ and $\alpha/\Omega^2 \gg 1$.

With introducing the canonical transformation $S=|a|^2-2|b|^2$ and $\theta=2\theta_a-\theta_b$, where $\theta_a=\arg a$ is the phase of the atomic mode and $\theta_b=\arg b$ is the phase of the molecular mode, the quantum system is equivalent to the following classical Hamiltonian:

$$\mathcal{H} = -2US^2 + 2\Delta S + 2\Omega(1+S)\sqrt{1-S}\cos\,\theta. \tag{5}$$

The canonical variables satisfy $\frac{dS}{dt}=-\frac{\partial \mathcal{H}}{\partial \theta}$ and $\frac{d\theta}{dt}=\frac{\partial \mathcal{H}}{\partial S}$. The above Hamiltonian is the same as that obtained in [11]. As pointed out by Ref. [13], it contains some properties distinguished from the "standard" nonlinear Landau-Zener Hamiltonian of Ref. [14]. First, the nonlinearity in Hamiltonian (3) is not only caused by the particle interactions but also from the fact that two atoms are needed to form a molecule. In addition, the mean-field motion is restricted on a "tear-drop" shaped surface [13,15], rather than the surface of a Bloch sphere. As we will show later, the interplay of these features leads to a very different conversion dynamics.

In the adiabatic limit where the external field varies slowly compared with the intrinsic motion of the system, the conversion dynamics is entirely determined by the phase-space structure evolution of the classical Hamiltonian (5), see, for example Refs. [11,13]. The fixed points (i.e., the energy extrema of the classical Hamiltonian) on the phase space correspond to the quantum eigenstates. According to the adiabatic theory [16,17], when the energy bias Δ changes adiabatically, a closed orbit in the phase space remains closed and the action $I=\frac{1}{2\pi}\oint S d\theta$ stays invariant in time. The action equals the phase-space area enclosed by the closed orbit and is zero when the orbit shrinks to a fixed point.

For the case of $U/\Omega<\sqrt{2}/4$, the initial state is prepared at an elliptical point on the phase space. It evolves, following the elliptical point, from the boundary line of $S=1$ to $S=-1$ as Δ increases. This means all the atoms are converted into molecules, i.e., the conversion efficiency is $\chi=1$.

However, for the case of $U/\Omega>\sqrt{2}/4$, the elliptical point will collide with a saddle point when $\Delta=\Delta_c$. After this collision, the system enters a new orbit with $\mathcal{H}=\mathcal{H}_c$, and evolves adiabatically for $\Delta>\Delta_c$ according to the rule of constant action, which is now nonzero. This orbit eventually evolves into a straight line of constant S. With these considerations, we can obtain the conversion efficiency in the adiabatic limit, $\chi=1-\frac{1}{2}I_c$.

To work out the explicit expression of χ, we first need to determine the critical point C. For this purpose, we notice that point C (with $\theta=\pi$) is a double root of $\dot{\theta}=0$, thus $\frac{\partial \dot{\theta}}{\partial S}|_{S_c}=-4U+\Omega\frac{5-3S_c}{2(1-S_c)^{3/2}}=0$. Once S_c is obtained, the critical energy bias Δ_c and orbit energy $\mathcal{H}_c$ can also be easily determined through their explicit expressions given in the foregoing paragraphs. The whole orbit passing through the critical point is given by $\cos\,\theta=f(S)=\frac{\mathcal{H}_c+2US^2-2\Delta_c S}{2\Omega(1+S)\sqrt{1-S}}$. Thus

$$I_c = \frac{1}{\pi}\int_{S_{\min}}^{S_c}\left[\pi - \arccos\left(\frac{\mathcal{H}_c + 2US^2 - 2\Delta_c S}{2\Omega(1+S)\sqrt{1-S}}\right)\right]dS + 1 + S_{\min}. \tag{6}$$

Here, $S_{\min}$ can be determined by $f(S_{\min})=1$. The above formula can be further simplified at the critical point of $U/\Omega\to\frac{\sqrt{2}}{4}$ and in the asymptotic regime of $U/\Omega\to\infty$ as following,

$$\chi = \begin{cases} 1-2.4\left(\dfrac{U}{\Omega}-\dfrac{\sqrt{2}}{4}\right)^2, & \dfrac{U}{\Omega}\to\dfrac{\sqrt{2}}{4} \\ 1.2\left(\dfrac{U}{\Omega}\right)^{-2/3}, & \dfrac{U}{\Omega}\gg 1 \end{cases} \tag{7}$$

Notice that in the nonlinear Landau-Zener model which describes the tunneling of BEC in a double-well potential [14], the expressions of the tunneling rate at the critical point and in the asymptotic regime are different. At the critical point, the exponent of the power law is 3/2. While in the asymptotic regime, the prefactor of the power law is 3/2 and the exponent stays the same.

The sudden limit corresponds to nonadiabatic conversion. The conversion efficiency is not strongly related to the structure of the energy levels. In this limit, we can derive the analytical expression of the conversion efficiency using the stationary phase approximation (SPA) [14]. With the variable transformation,

$$a = a'\,\exp\left\{-i\int_0^t [\Delta + 2U(2|b|^2-|a|^2)]dt\right\}, \tag{8}$$

$$b = b'\,\exp\left\{i\int_0^t [2\Delta + 4U(2|b|^2-|a|^2)]dt\right\}, \tag{9}$$

we get

$$b' = -2i\Omega\int_{-\infty}^{t} dt\,\exp\left\{-i\int_0^t [4\Delta + 8U(4|b|^2-1)]dt\right\}. \tag{10}$$

The dominant contribution to the integral comes from the stationary point t_0 of the phase around which we have

$$4\Delta + 8U(4|b|^2-1) = \bar{\alpha}(t-t_0). \tag{11}$$

Substitute Eq. (11) into Eq. (10) and calculate the integral self-consistently, we finally get

$$\frac{1}{\chi} = \frac{\alpha}{4\pi\Omega^2} + \frac{2U}{\pi\Omega}\sqrt{\chi}, \tag{12}$$

where $\chi=2|b|^2_{+\infty}$. We have used Eq. (12) to calculate the conversion efficiencies and compared them with the numerical results obtained by directly integrating the Schrödinger Eq. (2), and find a good agreement between them. Interestingly, when $\alpha/\Omega^2\gg 1$, the second term on the right-hand side of Eq. (12) can be neglected, thus we get $\chi=4\pi\Omega^2/\alpha$. This result from our many-body mean-field theory is twice that

obtained from the standard two-body Landau-Zener formula. This many-body effect is consistent with the theoretical analysis based on a renormalized Landau-Zener formula in Ref. [9] that has been used to explain the experimental data [18].

Our above discussions are restricted to the attractive interaction case. Nevertheless, it is easy to extend the above discussion to the repulsive interaction case. In the latter case, the adiabatic energy levels are the 180° angular rotation of the levels presented in Fig. 1, accordingly, the conversion from atoms to molecules started from the upper level at the right side in the repulsive case is equivalent to the atom-molecule conversion started from the lower level at the left side in the attractive case while the sweeping direction of the magnetic field is reversed. Our calculation in Fig. 2 already showed that for both repulsive and attractive cases, the atom-molecule conversion efficiency is significantly affected by the particle interactions when $|U/\Omega|$ is comparable with or larger than the critical value of $\sqrt{2}/4$.

The effects of particle interactions discussed in our Brief Report for bosonic systems are not observed until now. Such effects might potentially be observable in current experiments suppose the atom density is high and the Feshbach resonance is narrow. That is because the effective interaction parameter U/Ω is related to the physical quantities of the Feshbach resonance and the atom cloud through following explicit expression, $|\frac{U}{\Omega}| \approx 0.3\sqrt{|\frac{4\pi\hbar^2 n a_{\mathrm{bg}}}{m\Delta B \mu_{co}}|}$. It is proportional to the square root of the density and inversely proportional to the square root of the resonance width. So, the effects of the particle interactions are expected to be observable in the experiments with high atom density and narrow Feshbach resonance width. As an example, we consider the MIT experiment parameters with ^{23}Na condensate [19], where the mean density of the condensate is $n \sim 10^{15}$ cm^{-3}, and the parameters for the Feshbach resonance at $B_0 = 853$ G are $\Delta B = 0.0025$ G, $a_{\mathrm{bg}} = 3.38$ nm, and $\mu_{co} = 3.47 \times 10^{-23}$ J T^{-1} [4,6], which gives $U/\Omega = 0.36$. The interaction parameter is beyond the critical value, therefore, it offers a good ground to test our theoretical predictions.

This work was supported by National Natural Science Foundation of China (Grants No.10725521 and No. 10604009) and the National Fundamental Research Programme of China under Grants No. 2006CB921400 and No. 2007CB815103.

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