Phase Coherence in a Driven Double-Well System

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We analyze the dynamics of the molecular field incoherently pumped by the photoassociation of fermionic atoms and coupled by quantum tunnelling in a double-well potential. The relative phase distribution of the molecular modes in each well and their phase coherence are shown to build up owing to quantum mechanical fluctuations starting from the vacuum state. We identify three qualitatively different steady-state phase distributions, depending on the ratio of the molecule-molecule interaction strength to interwell tunnelling, and examine the crossover from a phase-coherent regime to a phase-incoherent regime as this ratio increases.

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The theoretical analysis of interacting quantum fields normally requires the introduction of some approximation schemes that limits the detail with which they can be understood. In the context of many-body theory, these approximations often take the form of a factorization (and possibly linearization) of the higher order correlations for the field operators such as in mean-field theory [1]. There are of course exceptions to this state of affairs, many of them in the realm of quantum optics [2]. One such example is the micromaser, which is amenable to an almost exact quantum description that permits a detailed dynamical understanding of the Maxwell field inside a high-Q microwave resonator [3, 4].

Ultracold matter-wave fields with adjustable interactions [5] are now under remarkable experimental control and are becoming more widely available. This makes them an ideal test bed for detailed dynamical studies of interacting quantum field theories. In this letter, we discuss one such example, a matter-wave analog of coupled micromasers that can be realized using experimental techniques recently developed in the quest for molecular Bose-Einstein condensation [6]. The dynamics of that system is amenable to an essentially exact analysis that shows in particular the build-up of phase coherence between the coupled molecular states. As such, it sheds new light on the dynamics of quantum fields in a system that should soon be amenable to experimental realization.

A major current thrust in atomic, molecular and optical science is the study of molecular Bose-Einstein condensates (BEC) formed via either photoassociation [7, 8] or a Feshbach resonance [9]. These efforts have recently culminated in the realization of molecular condensates of $^{40}$K$_2$ and $^6$Li$_2$ molecules [10].

The formation of molecules by photoassociation in optical lattices has been studied theoretically by several authors [11]. The large energy separations that are possible between the lowest and second Bloch band of the lattice allow one to restrict the center-of-mass states of atoms and molecules to the lowest energy Wannier state of each site, thereby avoiding many of the difficulties associated with free space [12]. Search et al. [13] recently showed that the photoassociation of fermionic atoms into bosonic molecules in a lattice in the Mott-insulator regime [14, 15] can be mapped on to the system of the micromaser, a device that exhibits a number of non-classical features [2].

The present letter extends this model to include interwell tunnelling in a double-well system [16, 17, 18] and analyses the full dynamics of the molecular field. We examine the build-up of the relative phase between the localized molecular states of the wells due to the combined effect of inter-well tunnelling and the incoherent addition of molecules from photoassociation.

We identify three regimes, characterized by different orders of magnitude of the ratio of the two-body collision strength to the inter-well tunnelling coupling [19]. For small values of this ratio the relative phase of the two molecular modes becomes phase locked at a fixed value, while for larger values that phase remains random. This crossover of the non-equilibrium steady state from a phase coherent regime to the phase incoherent regime is reminiscent of the superfluid-Mott insulator transition for the ground state in an infinite lattice [14, 15]. However, in contrast to that system, this behavior occurs now in an open system, with incoherent pumping and damping of the matter-wave field.

We consider the two-photon stimulated Raman photoassociation of fermionic atoms of mass $m_f$ and spin $(σ = 1, 2)$ trapped in a double-well potential into bosonic molecules of mass $m_b = 2m_f$ [7, 8]. We assume that the system is at zero temperature and that the number of fermions of each component that occupy each well is less than or equal to 1 at all times. The fermions, therefore, occupy only the lowest energy level. The molecules are confined in the same potential and occupy only the lowest energy level of each well.

The effective Hamiltonian for the atom-molecule system in the lowest energy level of the wells is

$$H = \sum_{i=1,2} (H_{0i}+H_{1i}) + H_T,$$

where $H_{0i} = \hbar (\omega_b + \delta) \hat{n}_i + \hbar U_f (\hat{n}_{1i} + \hat{n}_{2i}) + \frac{1}{2} \hbar U_b (\hat{n}_{1i} - \hat{n}_{2i}) + \hbar U_i (\hat{n}_{1i} \hat{n}_{2i} + \hat{n}_{1i} + \hat{n}_{2i}) + \hbar U_j \hat{n}_{1i} \hat{n}_{2i} + \hbar \chi(t) \hat{b}_i \hat{c}_1 \hat{c}_2 + h.c.$, and $H_T = -\hbar J \hat{b}_i \hat{b}_r - \hbar J_f (\hat{c}_1 \hat{c}_1 + \hat{c}_2 \hat{c}_2 + h.c.)$. Here $\hat{c}_r$ and $\hat{b}_i$ are the annihilation operators of fermionic atoms and bosonic
molecules in the left or right wells, \( i = l, r \), respectively. The corresponding number operators \( \hat{n}_i = \hat{b}_i^\dagger \hat{b}_i \) and \( \hat{n}_{\sigma i} = \hat{c}_{\sigma i}^\dagger \hat{c}_{\sigma i} \) have eigenvalues \( n_i \) and \( n_{\sigma i} \), respectively; and \( \omega_b \) and \( \omega_f \) are the energies of the molecules and atoms in the isolated wells (\( J_{b,f} = 0 \)). The terms proportional to \( U_b, U_x, \) and \( U_f \) in \( \hat{H}_0 \) describe onsite two-body interactions between molecules, atoms, and molecules, and atoms, respectively. The parameters \( J_b \) and \( J_f \) in the tunnelling Hamiltonian, \( \hat{H}_T \), are the single molecule and atom tunnelling rates. The interaction Hamiltonian, \( \hat{H}_I \), describes the conversion of atoms into ground-state molecules via two-photon stimulated Raman photoassociation. The photoassociation coupling constant \( \chi(t) \) is proportional to the far-off-resonant two-photon Rabi frequency associated with two nearly co-propagating lasers with frequencies \( \omega_1 \) and \( \omega_2 \), and \( \delta \) is the two-photon detuning between the lasers and the energy difference of the atom pairs and molecules.

The dynamics of the molecular field in the double-well system is governed by four mechanisms: (1) The injection of pairs of fermionic atoms inside the double-well during time interval \( T \) when \( \chi = 0 \), after which the atoms in each well are in the state \( |e_i\rangle = |c_{\sigma l}^\dagger c_{\sigma l} |0\rangle \) with unit probability [13]; (2) The unitary time evolution of the molecular field subject to the Hamiltonian \( \hat{H}_b \) during the time interval \( T \), with

\[
\hat{H}_b = -\hbar J_b (\hat{b}_l^\dagger \hat{b}_l + \hat{b}_r^\dagger \hat{b}_r) + \hbar (U_b/4)(\hat{n}_l - \hat{n}_r)^2.
\]

In Eq. (11), we have neglected terms that are functions only of \( \hat{n}_l + \hat{n}_r \). This is justified as long as the initial density matrix is diagonal in the total number of molecules in the two wells (see below); (3) The molecular damping at rate \( \gamma \) during the intervals \( T \); modelled by a master equation with a Liouvillean \( \mathcal{L}_j \rho_0 = -(\gamma/2)[\hat{b}_l^\dagger \hat{b}_l \rho_0 - 2\hat{b}_l \rho_0 \hat{b}_l^\dagger + \rho_0 \hat{b}_l^\dagger \hat{b}_l] \) for each well, \( \rho_0 \) being the reduced density operator for the molecules; (4) The switching on of the photoassociation lasers in a train of short pulses of duration \( \tau \) and period \( T + \tau \). We assume that \( \tau \) is much shorter than all other time scales in this model, \( \tau \ll J_b^2 \gamma^{-1} \), so that damping and tunnelling may be ignored while the photoassociation fields are on. The atom-molecule conversion is described by \( F_i(t)\rho_0 \equiv \text{Tr}_a [\mathcal{U}_i(t)\rho_{ab}(t)\mathcal{U}_i^\dagger(t)] \), where \( \rho_{ab} \) is the total density operator and \( \mathcal{U}_a \) denotes the trace over the atomic variables, \( \mathcal{U}_i(t) = \exp(-i\hat{H}_a t/\hbar) \) being the evolution operator for the Jaynes-Cummings-like Hamiltonian of each well. It describes the interaction between the molecular field and a fictitious two-state system for fermionic atoms \( |e_i\rangle \) and \( |g_i\rangle = |0\rangle \) [13].

\[
\hat{h}_i = \hbar (\omega_b + U_x) \hat{n}_i + \hbar (\omega_f + U_x \hat{n}_i) \sigma_{zi} + \frac{\hbar}{2} U_x \hat{n}_i (\hat{n}_i - 1)
\]

where \( \sigma_{zi} = \sigma_{zi}^\dagger = |g_i\rangle \langle e_i| \) and \( \sigma_{zi} = |e_i\rangle \langle e_i| - |g_i\rangle \langle g_i| \).

In Eq. (2), we have dropped constant terms and made the redefinitions \( \omega_b + \delta \rightarrow \omega_b \) and \( \omega_f + U_f/2 \rightarrow \omega_f \). For \( \chi = \text{const} \), Eq. (2) can be solved within the two-state manifolds of each well \( \{|e_i, n_i\}, |g_i, n_i + 1\} \).

Within each manifold, the resulting dynamics is in the form of quantized Rabi oscillations at frequency \( \mathcal{R}_n = \sqrt{2\omega_f - \omega_b + (2U_x - U_b)n_i^2 + 4|\chi|^2(n_i + 1)} \).

The photoassociation of atoms into molecules during the intervals \( \tau \) leads to the build-up of the molecular field. The coarse-grained master equation for the reduced molecular density operator, valid for \( T \gg \tau \), is given by

\[
\dot{\rho}_0 = \sum_{j=l,r} \left[ \mathcal{L}_j + T^{-1} \{ F_j(\tau) - I \} \right] \rho_0 - \frac{i}{\hbar} [\hat{H}_b, \rho_0].
\]

(3)

The density operator for the molecular field in the number representation for the left and right wells is given by \( \rho_0 = \sum_{n_l, n_r, m_l, m_r} \rho(n_l, n_r; m_l, m_r | n_l | n_r) \langle m_l | m_r \rangle \). The initial condition for the molecules is taken to be the vacuum state. Because the molecular pumping and decay is the same in both wells, \( \rho \) remains diagonal in the total number of molecules in the two wells, \( N = n_l + n_r = m_l + m_r \), for all times. Consequently, the only nonzero terms in \( \rho(n_l, n_r; m_l, m_r) \) are those with \( n_l + n_r = m_l + m_r \).

The master equation (3) depends on six independent parameters: the pump parameter, \( \Theta = \sqrt{\mathcal{N}_{xx} \chi \tau} \); the number of photoassociation cycles per lifetime of the molecule, \( \mathcal{N}_{xx} = 1/\gamma T \); the two-body collision strength and tunneling coupling strength per decay rate, \( \omega_0 = U_b/\gamma \) and \( \gamma_f = J_b/\gamma \); and finally, the (non-)linear detuning parameters, \( \eta \equiv (2\omega_f - \omega_b)/2|\chi| (\beta \equiv (2U_x - U_b)/2|\chi|) \) from \( \mathcal{R}_n \). In the following, we consider for simplicity only exact resonance, \( \eta = \beta = 0 \), and fixed \( \mathcal{N}_{xx} = 10 \). The results presented below do not depend in any qualitative manner on the specific value of these parameters.

Introducing the angular momentum representation \( J_x = J_x^l + J_x^r \) and \( J_y = J_y^l \) for \( J_z = (\hat{b}_l^\dagger \hat{b}_l - \hat{b}_r^\dagger \hat{b}_r)/2 \), and \( J^z = (N/2)(N/2 + 1) \) where \( N = n_l + n_r \) is the total number operator, we have that \( \langle J_z \rangle = \langle J_z \rangle^* = \sum_{n_l, n_r} \sqrt{(n_l + 1)n_r \rho(n_l, n_r; n_l + 1, n_r - 1)} \), \( \langle J_z \rangle = \sum_{n_l, n_r} \rho(n_l, n_r; n_l, n_r)/2 \). Since the initial state of the molecules in each well and \( \hat{H}_0 \) is invariant with respect to the interchange \( l \leftrightarrow r \), the density matrix is invariant with respect to \( n_l \leftrightarrow n_r \) and \( m_l \leftrightarrow m_r \). As a result, the reduced density matrices for the left and right wells are identical. This leads to the same single-well molecule statistics for the two wells. The symmetry of the density matrix with respect to the two wells furthermore implies that \( \langle J_z \rangle \equiv \langle J^z \rangle = 0 \).

Figure (H) shows the normalized steady-state first-order coherence \( \langle \hat{n}_i \rangle / \langle \hat{n}_i \rangle \) as a function of \( \omega_0/\gamma_f \) for \( \Theta = \pi \) and \( \gamma_f = 2.5 \). \( \langle \hat{n}_i \rangle \) is suppressed in both the weak and the strong two-body coupling limits, and has an extremum at \( |\omega_0|/\gamma_f \sim 0.6 \). In the strong coupling regime,
FIG. 1: (a) \(\langle \hat{J}_x \rangle/(n_j)\) and (b) \(g_{\ell r}^{(2)}\) versus \(u_0/t_J\) for \(\Theta = \pi\) and 
\(t_J = 2.5\).

|\(u_0|/t_J \gg \langle \hat{N} \rangle \sim 10\), the nonlinearity in \(\hat{H}_b\) dominates and reduces the coherence between the localized states of each well. We note that the average occupation numbers for each well are relatively unaffected by \(u_0/t_J\), with 
\(\langle \hat{n}_j \rangle = \langle \hat{N} \rangle/2 = 4.78 - 4.87\) for \(|u_0|/t_J = 10^2 - 10^{-2.5}\).

The origin of the mutual coherence between the two molecular modes can be determined from the equation of motion for \(\langle \hat{J}_x \rangle\),

\[
\begin{align*}
\langle \hat{J}_x \rangle & = \sum_{n_l, n_r} \sqrt{(n_l + 1)n_r} \rho_R(n_l, n_r; n_l + 1, n_r - 1) \\
& = -U_b\langle \hat{J}_y \hat{J}_x + \hat{J}_z \hat{J}_y \rangle - \gamma \langle \hat{J}_x \rangle \\
& + 2T^{-1} \sum_{n_l, n_r} \sqrt{n_l n_r} \rho_R(n_l, n_r; n_l + 1, n_r - 1),
\end{align*}
\]

where \(\rho_R(n_l, n_r; n_l + q, n_r - q)\) with \(q\) odd couple only to themselves and to the imaginary part of \(\rho(n_l, n_r; n_l + p, n_r - p)\) with \(p\) even. For wells incoherently pumped at equal rates, this implies that 
\(\rho_R(n_l, n_r; n_l + 1, n_r - 1) = 0\) for all times. Alternatively, this can be understood by noting that the expectation value \(\langle \hat{J}_x \rangle\) corresponds to the difference in occupation numbers between the in-phase, \(\hat{b}_a = (\hat{b}_l + \hat{b}_r)/\sqrt{2}\), and out-of-phase, \(\hat{b}_q = (\hat{b}_l - \hat{b}_r)/\sqrt{2}\), states of the localized states of each well, \(\hat{J}_x = \hat{b}_a^\dagger \hat{b}_q - \hat{b}_q^\dagger \hat{b}_a\). These states are equally populated since the bandwidth of the photoassociation pulse is larger than their energy splitting, 
\(1/\tau \gg J_b\). Hence \(\langle \hat{J}_x \rangle = 0\) for \(U_b = 0\), and the creation of cross-coherence between the two wells is due solely to two-body collisions. We also remark that a semiclassical treatment in which \(\langle \hat{J}_y \hat{J}_x + \hat{J}_z \hat{J}_y \rangle\) is factorized as 
\(2\langle \hat{J}_y \rangle \langle \hat{J}_z \rangle\) results in \(\langle \hat{J}_x \rangle = 0\) for all times and all values of \(u_0/t_J\). Hence, the buildup of \(\langle \hat{J}_x \rangle\) is a purely quantum-mechanical effect due to quantum fluctuations.

The pump and decay mechanisms act identically on the in-phase and out-of-phase states, hence the fact that \(\langle \hat{J}_x \rangle\) has the sign of \(U_b\) results from the unitary time evolution from \(\hat{H}_b\), which gives 
\(\langle \hat{J}_x(t) \rangle = \langle u_0/2t_J \rangle \langle \hat{J}_x(0) \rangle\), if 
\(\langle \hat{J}_x(0) \rangle = 0\) \(\Rightarrow \langle \hat{J}_x \rangle = 0\). Since \(\langle \hat{J}_x^2 \rangle \geq 0\), it follows that the sign of \(\langle \hat{J}_x \rangle\) is determined by that of \(U_b\).

Figure 1(b) shows the steady-state second-order correlation function, 
\(g_{\ell r}(2) = \langle \hat{n}_l \hat{n}_r \rangle/(\langle \hat{n}_l \rangle \langle \hat{n}_r \rangle)\) as a function of 
\(|u_0|/t_J\) for \(\Theta = \pi\) and \(t_J = 2.5\). It is related to the variance of the relative number difference, such that 
\(\langle \Delta J_x \rangle^2 = (\langle \Delta n_l/2 \rangle^2 - \langle \hat{n}_l \rangle \langle \hat{n}_r \rangle)(g_{\ell r}(2) - 1)/2 + (\langle n_l \rangle^2/2)\).

In the strong two-body coupling limit, the molecular states are uncorrelated, 
\(g_{\ell r}(2) = 1\), and \(\langle \Delta J_x \rangle^2\) becomes a sum of variances for independent localized states of the molecules. In the weak coupling region, 
\(|u_0|/t_J \ll \langle \hat{N} \rangle^{-1}\), the two molecular states are anti-correlated, 
\(g_{\ell r}(2) < 1\), and the variance \(\langle \Delta J_x \rangle^2\) is greater than that of uncorrelated states. The enhancement of relative number fluctuations indicates the locking of the relative phase between the two wells.

To investigate the relative phase distribution of the molecular field in the two wells, we consider the difference of the two single-mode Pegg-Barnett phase operators \(20\). Specifically, we introduce the \((s+1)^2\) orthonormal phase states

\[
\theta_l |\theta_r \rangle = \frac{1}{(s+1)} \sum_{n_l=0}^s \sum_{n_r=0}^s e^{i n_l \theta_l} e^{i n_r \theta_r} |n_l, n_r\rangle,
\]

where \(\theta_l = 2\pi l/(s+1)\) and \(\theta_r = 2\pi r/(s+1)\) \((l, r = 0, 1, \ldots, s)\) are phase variables and \(s\) is a finite value. Projection onto these phase eigenstates gives the quantum phase distribution for the two wells, 
\(P(\theta_l, \theta_r) = \text{Tr} \{ |\theta_l, \theta_r \rangle \langle \theta_l, \theta_r | \rho_b \}\). Since the density matrix is diagonal in the total number of molecules, \(n_l + n_r = m_l + m_r\), the phase distribution depends only on the relative phase, 
\(\phi_{lr} = \theta_l - \theta_r\), which has a width of \(4\pi\) in the phase coordinate. In order to obtain a mod(2\(\pi\)) distribution for the relative phase, we average over the total phase coordinate, \(\theta_l + \theta_r\), and map the mod(4\(\pi\)) distribution into a mod(2\(\pi\)) one following the method of Ref. 21. Using a redefined relative phase variable, \(\phi_n = 2\pi n/(s+1) - \pi\) \((n = 0, 1, \ldots, s)\) gives the mod(2\(\pi\)) distribution

\[
P(\phi_n) = \frac{1}{s+1} \sum_{n_l=0}^s \sum_{n_r=0}^s e^{-i k \phi_n} \rho(n_l, n_r; n_l + k, n_r - k).
\]

Figure 2 shows the evolution of the relative phase distribution \(P(\phi_n)\) in three different regimes (a) \(u_0/t_J = 0.0032\), (b) \(u_0/t_J = 0.5623\), (c) \(u_0/t_J = 56.23\), for \(\Theta = \pi\), \(t_J = 2.5\), and \(s = 40\). Since the vacuum state is taken as the initial state, the relative phase at \(t = 0\) is randomly distributed, 
\(P(\phi_n) = 1/(s+1)\). For \(|u_0|/t_J \ll \langle \hat{N} \rangle\), corresponding to Figs. 2(a) and (b), 
\(P(\phi_n)\) develops a peak around 0 and/or \(\pm \pi\) in the characteristic time \(\gamma^{-1}\) needed to reach a steady state 23. As previously discussed, for weak two-body interaction the in-phase and
out-of-phase modes have equal population. This leads to the bimodal phase distribution with peaks around both 0 and ±π. For moderate \( u_b/t_j \), the relative phase locks in time around 0 (±π), for repulsive (attractive) two-body interactions, see Fig. 2(b). In contrast to these two regimes, when \( |u_b|/t_j \gg \langle N \rangle^{-1} \), the relative phase distribution becomes almost random, and the localized modes in the two wells evolve independently of each other. The steady-state phase variance, \((\Delta \phi)^2\), is shown in Fig. 2(d) as a function of the ratio \( u_b/t_j \). Consistently with Fig. 2(a-c), it exhibits large fluctuations due to the bimodal phase distribution in the case of \( u_b/t_j < \langle N \rangle^{-1} \), and becomes narrow in the region \( \langle N \rangle^{-1} < u_b/t_j < \langle N \rangle \). When \( u_b/t_j > \langle N \rangle \), the variance approaches the value \((\Delta \phi)^2 = \pi^2/3\) corresponding to a uniformly distributed phase \((s \to \infty)\).

The three regimes of phase distributions correspond to different orders of magnitude of the ratio \( u_b/t_j \), which characterizes the behavior of the double-well system. The crossover of the non-equilibrium steady state from a phase-coherent regime to the random-phase situation is reminiscent of the superfluid-Mott insulator phase transition for the ground state of an optical lattice. Since we consider just two sites, however, there is no sharp transition between these regimes.

In this paper, we have studied the quantum dynamics of the bosonic molecules in a double-well system in the presence of both incoherent pumping and damping. We have shown that the phase coherence of initially independent molecular states builds up due to quantum mechanical fluctuations. We identified three qualitatively different phase distributions for the non-equilibrium steady states. The crossover from the phase coherent regime to phase incoherent regime occurs as the ratio \( |u_b|/t_j \) increases, similar to the superfluid-Mott insulator phase transition in an optical lattice.

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