Macroscopic Quantum Self-Trapping in Dynamical Tunnelling

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It is well-known that increasing the nonlinearity due to repulsive atomic interactions in a double-well Bose-Einstein condensate suppresses quantum tunnelling between the two sites. Here we find analogous behaviour in the dynamical tunnelling of a Bose-Einstein condensate between period-one resonances in a single driven potential well. For small nonlinearities we find unhindered tunnelling between the resonances, but with an increasing period as compared to the non-interacting system. For nonlinearities above a critical value we generally observe that the tunnelling shuts down. However, for certain regimes of modulation parameters we find that dynamical tunnelling re-emerges for large enough nonlinearities, an effect not present in spatial double-well tunnelling. We develop a two-mode model in good agreement with full numerical simulations over a wide range of parameters, which allows the suppression of tunnelling to be attributed to macroscopic quantum self-trapping.

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The transition from the classical to the quantum world is a subject of intense interest. In particular, the topic of quantum chaos studies systems which exhibit chaotic dynamics in the classical limit of $\hbar \to 0$. An important phenomenon in driven one-dimensional quantum systems is dynamical tunnelling, first identified by Heller and Davis [6]. This is a classically forbidden process whereby particles trapped in a regular region of phase space may quantum-mechanically tunnel to another. The behaviour of such systems has provided important insights into the quantum-classical transition [7–14]: in particular, the period of the dynamical tunnelling is strongly affected by a number of subtle effects [11–14]. Dynamical tunnelling has mostly been studied in the single-particle regime [7, 12–19], and has been demonstrated experimentally with ultra-cold atoms in modulated optical lattice potentials [20, 21]. Recently it has been shown in [14] that atomic interactions in trapped Bose-Einstein condensates (BECs) can have a detectable effect for experimentally realistic parameters.

Here we investigate the effect of repulsive atomic interactions on the dynamical tunnelling of a trapped BEC through the variation of the nonlinearity, $U$. A priori, the effect of nonlinearity on a given dynamical system is not clear. It has been shown to suppress transport in the kicked rotor and oscillator [22–25], Landau-Zener tunnelling in optical lattices [26], but in contrast enhance transport in quantum ratchets [27].

We find that dynamical tunnelling also occurs for the interacting system with $U > 0$ up to a critical interaction strength $U_{\text{crit}}$. Beyond $U_{\text{crit}}$ we find that dynamical tunnelling mostly ceases. We connect the dynamical tunnelling suppression to the phenomenon of macroscopic quantum self-trapping (MQST) using a two-mode model based on Floquet tunnelling states. It allows us to predict the critical nonlinearity $U_{\text{crit}}$ from knowledge of the noninteracting system, and to understand the increase of the tunnelling period with $U$ that we find numerically. While previous work reported detrimental effects of nonlinearities on dynamical tunnelling [28], a connection with MQST was not made. Surprisingly, at higher nonlinearities with $U > U_{\text{crit}}$ we find some parameter ranges where dynamical tunnelling reappears. This effect has no analogue in bosonic Josephson junctions, where MQST has been extensively studied [29, 31, 32] and demonstrated experimentally [33].

We begin by reviewing the dynamical tunnelling of ultra-cold atoms. For classical atoms in a one-dimensional (1D) potential to exhibit chaotic dynamics, the potential must be both driven and anharmonic. The experiments demonstrating dynamical tunnelling used a modulated sinusoidal potential provided by an optical lattice [20, 21]. Here we instead consider the dimensionless classical Hamiltonian

$$H = \frac{p^2}{2} + V(x,t) \equiv \frac{p^2}{2} + \kappa [1 + \epsilon \cos(t)] \sqrt{1 + x^2},$$

where $\kappa$ is the potential strength, $\epsilon$ the amplitude of the modulation, and $x$ and $p$ are position and momentum coordinates respectively. Potentials $V(x, t)$ as in Eq. (1) can be realised on atom-chip traps in the radial direction [14]. This potential has the conceptual advantage of not being periodic in space; however, the physics we describe below will be generic for any one-dimensional potential where dynamical tunnelling is realised.

For our quantum treatment of the system we consider a BEC subjected to this single-particle Hamiltonian. We assume that mean-field theory is valid and the BEC is well described by the wave function $\psi \equiv \psi(x)$ that evolves according to the Gross-Pitaevskii equation (GPE) [33]:

$$i \hbar_\text{eff} \frac{\partial}{\partial t} \psi = [H + U|\psi|^2] \psi,$$

with $\int dx |\psi|^2 = 1$. Here $p$ of Eq. (1) becomes $p = -i \hbar_{\text{eff}} \frac{\partial}{\partial x}$, and consequently $[x, p] = \hbar_{\text{eff}}$. $U$ parametrizes the nonlinearity, stemming from s-wave interactions, and $\hbar_{\text{eff}}$ denotes the effective
Planck’s constant. It arises naturally when rescaling all variables in the GPE to be dimensionless \[\hbar\alpha\] and indicates how “quantum” the system is, with \(\hbar\alpha \to 0\) being the classical limit.

The classical system \(H_0\) is integrable for \(\epsilon = 0\). The Kolmogorov-Arnold-Moser (KAM) theorem \[2\] states that regular regions of motion persist in phase-space for \(\epsilon > 0\), but become increasingly destroyed as \(\epsilon\) is increased \[1,4\]. An example is shown in the Poincaré section of Fig. 1(a), where co-ordinates of classical motion from a large range of initial conditions are plotted stroboscopically, i.e. at times \(t = 2\pi n\) for \(n \in \mathbb{N}\). A key feature is the two large period-one islands of regular motion \(I_{\pm}\), traced by trajectories of atoms moving in phase with the modulation of the potential \[21\]. The KAM theorem forbids classical motion connecting these islands.

Quantum mechanics, however, allows tunnelling to occur between these islands. Consider the linear Schrödinger equation \((U=0)\) obtained from the quantized form of the Hamiltonian \[1\]. To relate the quantum dynamics of the modulated system to the classical phase-space, we use Floquet states \[2\], denoted \(|u_n\rangle\), that are invariant up to a phase under time evolution through one modulation of period \(T\), and can hence be found as eigenvectors of the time evolution operator: 
\[
U(0,T)|u_n\rangle = \exp[ -i\lambda_n T/\hbar\alpha ]|u_n\rangle.
\]

The operator \(U(0,T)\) evolves the wave function from time \(t = 0\) to \(t = T\). As \(U\) is unitary, the quasi-energy \(\lambda_n\) is real. The period-one islands of regular motion occur in the Floquet spectrum as a pair of states that are even/odd respectively under the transformation \(p \to -p\), and have support on both islands, as shown by the phase space Husimi function in Fig. 1(b). We will label these linear tunnelling states \(|u_\pm\rangle\) (even) and \(|u_0\rangle\) (odd).

An atomic wavepacket that is initially localized on a single period-one island is a superposition of tunnelling states: 
\[
|u_{\pm}(0)\rangle = |u_\pm(0)\rangle \pm i|u_0(0)\rangle,
\]
where \(|u_\pm\rangle\) is located on the island with \(p > 0\). Using the time evolution of Floquet states, we have 
\[
U(0,nT)|u_{\pm}(0)\rangle = e^{-i\lambda_n nT/\hbar\alpha} \left[ |u_\pm(0)\rangle \pm i e^{(\lambda_e - \lambda_\pm)nT/\hbar\alpha} |u_0(0)\rangle \right].
\]

This gives rise to quantum tunnelling. Its experimental signature is a classically forbidden periodic reversal of the stroboscopically sampled atomic momentum as observed in \[21\]. The quasi-energy splitting of the odd and even tunnelling states determines the linear period of dynamical tunnelling: \(T_{\text{lin}} = 2\pi \hbar\alpha/|\lambda_e - \lambda_\pm|\).

For \(U > 0\) the problem is nonlinear, and we cannot construct the operator \(\hat{U}\) from the evolution of a set of basis states. Instead, we find nonlinear Floquet states \[31\] that are solutions \(\phi_n\) of
\[
\left[ \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) + U|\phi_n|^2 - i\hbar\alpha \frac{\partial}{\partial t} \right] \phi_n = E_n \phi_n,
\]
periodic in the time dimension: \(\phi_n(x,t) = \phi_n(x,t+2\pi)\) and vanishing for \(x \to \pm\infty\). A state \(\phi_n(x,0)\) will reform after one driving period of evolution with the GPE, up to a phase \(-E_n T/\hbar\alpha\), analogous to the linear case \[34\].

We only consider the even (odd) nonlinear Floquet states localized on the islands, labelled \(\phi_e\) (\(\phi_o\)).

Using \(|\phi_{e/o}\rangle\) we simulate dynamical tunnelling with the GPE and \(U > 0\). For illustration we choose \(\kappa = 2.4\), \(\epsilon = 0.3\) and \(\hbar\alpha = 0.5\), solving for nonlinear Floquet states up to \(U = 4 \times 10^{-3}\). We begin simulations in the state \(|\Psi\rangle = |\phi_e\rangle = i|\phi_o\rangle\), and evolve it with the GPE for 1100 modulation periods. We sample the momentum space wave function of the BEC once every driving period \(T\), with the results shown in Fig. 2.
Before 100 modulation periods with $U = 0.7 \times 10^{-3}$ the momentum distribution is little changed [Fig. 2(a)]. However, on longer time-scales we observe a complete reversal of the system momentum after about 500 modulation periods, demonstrating dynamical tunnelling. As the nonlinearity is increased to $U = 2.7 \times 10^{-3}$ the effective tunnelling period $T_{DT}$ increases [Fig. 2(b)]. For $U > 3 \times 10^{-3}$ complete momentum reversal no longer takes place, and the population becomes trapped in phase-space [Fig. 2(c)]. This phenomenon is analogous to the cessation of inter-well tunnelling due to MQST in a bosonic Josephson junction [29, 32].

For the system in Fig. 2 tunnelling remains suppressed as $U$ is further increased. However, we have discovered parameter regimes where trapping occurs for a finite range of $U$, but tunnelling returns for larger $U$, as shown in Fig. 3(a). Dynamical tunnelling can then persist to high nonlinearity — an effect that is not seen in the bosonic Josephson junction.

To understand these results, we derive a two-mode model based on the nonlinear Floquet states. We assume that the time-dependent solution of the GPE can be approximated by $\psi(x,t) = c_+^*(t)\phi_+(x,t) + c_-(t)\phi_-(x,t)$ or equivalently $\psi(x,t) = c_+(t)\phi_+(x,t) + c_-(t)\phi_-(x,t)$. Members of both pairs are orthogonal by symmetry. Inserting the latter expansion into the GPE, using Eq. (2), projecting out the equations of motion for $c_+$ and $c_-$, and finally changing basis to $c_+(t)$ and $c_-(t)$, we obtain:

$$i\hbar \frac{\partial}{\partial t} c_\pm = \bar{E} c_\pm + \Delta E c_\mp \mp$$

$$+ \Re\{A_{eo}\} c_+^2 c_\mp - i\Im\{A_{eo}\} c_+ c_\mp c_\mp$$

$$+ [U_{eo} - \Re\{A_{eo}\}/2 - U_{ee}/4 - U_{oo}/4] c_+^2 c_\mp$$

$$+ [\Im\{A_{eo}\}/2 - U_{ee}/4 + U_{oo}/4] c_\mp^2 c_\mp$$

$$+ [U_{ee}/4 + U_{oo}/4 - U_{eo} - \Re\{A_{eo}\}/2] c_+^2 c_\pm$$

$$+ [\Im\{A_{eo}\}/2 - U_{ee}/4 + U_{oo}/4] c_\mp^2 c_\pm.$$  (3)

Here $\bar{E} = (E_e + E_o)/2$, $\Delta E = E_e - E_o$ and the coupling coefficients are defined as: $U_{ij}(t) = U \int dx |\phi_i(x,t)|^2 |\phi_j(x,t)|^2$ with $\{i,j\} \in \{e,o\}$ and $A_{eo}(t) = U \int dx \phi_{e}^*(x,t) \phi_{o}^2(x,t)$. These coefficients are periodic in time with period $T$. Since the tunnelling oscillations usually take place on much longer timescales, we replace the coefficients by their average over one period, e.g. $U_{ij}(t) \to \bar{U}_{ij} = \frac{1}{T} \int_0^T U_{ij}(t) dt$.

To test the model, we extract the amplitudes $a_{\pm}(t) = \int dx \phi_{\pm}^2(x,t)\phi_0^2(x,t)$ from the simulations of the GPE, and compare them with those obtained using Eq. (3). In Fig. 2(d-f) we find excellent agreement between the two mode model and the full numerical solution of the GPE.

To analyse self-trapping, we consider the population imbalance $z = N_+ - N_-$ and relative phase $\varphi = \theta_+ - \theta_-$, where $c_\pm = \sqrt{N_\pm e^{i\theta_\pm}}$ with $N_\pm, \theta_\pm \in \mathbb{R}$, following [29]. Note that $N_+ + N_- = 1$. We find $\Im\{A_{eo}\}$ is zero for all simulations and henceforth neglect this quantity. The equations of motion for $z$ and $\varphi$ from Eq. (3) are then the Euler-Lagrange equations of the effective Hamiltonian

$$H_{eff} = \frac{\Lambda}{2}(1 - \zeta) + \alpha \zeta^2 \cos(\varphi) + \beta \zeta \cos(2\varphi).$$  (4)

where $\zeta = 1 - z^2$ and $\Lambda = (U_{ee} + U_{oo})/4 + 3\Re\{A_{eo}\}/2 - U_{eo}$, $\alpha = (U_{ee} - U_{oo})/2 - \Delta E$, $\beta = U_{eo}/2 - (U_{ee} + U_{oo})/8 + 3\Re\{A_{eo}\}/4$. For $\alpha = 1$ and $\beta = 0$ Eq. (4) simplifies to the Hamiltonian of Ref. [29], which analysed MQST for a BEC in a spatial double-well potential.

Following [29] we can find Hamiltonian parameters for which dynamical tunnelling cannot occur. Starting from $z(0) = 1$, energy conservation requires that for $z(t) = 0$ to occur there must exist a solution to

$$\frac{1}{2}\Lambda = \alpha \cos[\varphi(t)] + \beta \cos[2\varphi(t)].$$  (5)

The atoms are self-trapped when this equation cannot be fulfilled for any $\varphi(t)$. If we assume $|\Delta E| \gg |\beta|$ and $|\Delta E| \gg |(U_{ee} - U_{oo})/2|$, empirically justified in most cases, we find that tunnelling is impossible if $U > U_{crit} = 2|\Delta E|/|\Lambda_0|$. Here $\Lambda_0 = \Lambda/U$ is an overlap integral between Floquet states that no longer explicitly depends on $U$, but implicitly through the shape of $|\phi_+(x,t)|^2$. We can then estimate the critical nonlinearity for self-trapping from the linear Floquet states, as they are generally very similar to the nonlinear Floquet states for $U < U_{crit}$. As long as the simple expression $U_{crit} = 2|\Delta E|/|\Lambda_0|$ is justified, $U_{crit}$ decreases rapidly for smaller $\hbar_{eff}$ and larger $\kappa$ or $\epsilon$, owing to a decrease in $|\Delta E|$ [14].

Equation (5) does not always predict self-trapping. For
\( \beta \ll \alpha \) (usually fulfilled) the self-trapping condition is

\[
1 < \left| \frac{A}{2\alpha} \right| = \left| \frac{(\bar{U}_{ee} + \bar{U}_{oo})/4 - \bar{U}_{ee} + 3\Re \{\bar{A}_{ee}\}/2}{\bar{U}_{ee} - \bar{U}_{oo} - \Delta E} \right|. \tag{6}
\]

Aside from \( \Delta E \) in the denominator, all terms in the fraction on the RHS are proportional to the nonlinearity \( U \). For \( U \gg \Delta E \) the nonlinearity then cancels out, and the condition (6) depends only on the overlap integrals \( \bar{U}_{ij}/U \) and \( \bar{A}_{oo}/U \). These again are only weakly dependent on the nonlinearity \( U \) through the shape of \( |\phi_i(x,t)|^2 \). In particular for parameters where \( \phi_i(x,t) \) and \( \phi_e(x,t) \) have a significant difference in mean interaction energy, \( |\bar{U}_{ee} - \bar{U}_{oo}| \), we will expect to see a reappearance of tunnelling at large \( U \). This occurs for values of \( \kappa \gtrsim 2 \); we find for \( \kappa \gtrsim 2 \) that \( \bar{U}_{ee} \approx \bar{U}_{oo} \) [35]. An example without trapping at large \( U \) is illustrated in Fig. 5. The reappearance of tunnelling, a striking difference to the spatial double-well case, arises because the nonlinearity here affects both the self-energy of each tunnelling mode and the effective mode coupling.

The 1D nonlinearity \( U \) can be related to experimental parameters by accounting for the details of the confinement geometry [14]. For \( \kappa = 2.3, \epsilon = 0.3 \) we find \( U_{\text{crit}} = 0.004 \) (onset of trapping) for \( N = 8 \) atoms. However, tunnelling will occur for \( U = 2 \) with \( \kappa = 1.3 \), corresponding to \( N = 4590 \) atoms [28]. These disparate values for \( N \) highlight the importance of our results for any experimental realisation of dynamical atom-chip tunnelling. We note that the large \( h_{\text{eff}} \) used here would require very tight trapping potentials [14, 56].

For the set of parameters in Fig. 5, the two-mode model correctly predicts the tunnelling period at small \( U \) and the first range of MQST. In fact, for many parameter regimes the simplified two-mode dynamics of Eq. (3) makes accurate predictions when \( \Delta E, U_{ij}, \) and \( A_{oo} \) are calculated using the linear tunnelling states, i.e. \( \phi_i \rightarrow u_i \) (inset of Fig. 5). For larger nonlinearities, the model correctly predicts tunnelling but with a period that is too long for \( U \gtrsim 0.05 \). We find that in this region the two-mode approximation begins to break down, with \( |d_+|^2 + |d_-|^2 \) as low as 0.8 for the full dynamics.

In summary, we have demonstrated the analogue of macroscopic quantum self-trapping in a bosonic Josephson junction for the dynamical tunnelling of BECs. However, we have discovered parameter regimes where MQST is lifted for large nonlinearities. We have shown that most of these features are reproduced by the dynamics of a simple two-mode model. An interesting extension of our work would be to consider the quantum many-body two-mode model, as considered for double-well tunnelling in Refs. [37, 38], or considering heating effects that can result from nonlinearities in the presence of driving [39].

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scribed in [14], the total 3D atom number is
\[ N = \frac{L_z U}{(2\sqrt{2\pi a_s h/\hbar})^{3/2} \kappa^{1/4}} \sqrt{\omega_x / \omega_y}, \]
where \( a_s \) is the three-dimensional scattering length, \( \omega_x \) the strength of the
chip trap, \( \omega_y \) the potential strength in the frozen \( y \)-dimension and \( L_z \) the condensate size in the long, uni-
form \( z \)-direction (see [14]). For the \( N \) quoted, we assume
\( L_z = 50 \mu \text{m}, \omega_x = (2\pi) \times 10 \text{ kHz}, \omega_y = 5\omega_x \) and \( a_s = 5.5 \text{ nm (}^{87}\text{Rb)}.\)
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