

# Tunnelling rates for the nonlinear Wannier-Stark problem

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## Abstract.

We present a method to numerically compute accurate tunnelling rates for a Bose-Einstein condensate which is described by the nonlinear Gross-Pitaevskii equation. Our method is based on a sophisticated real-time integration of the complex-scaled Gross-Pitaevskii equation, and it is capable of finding the stationary eigenvalues for the Wannier-Stark problem. We show that even weak nonlinearities have significant effects in the vicinity of very sensitive resonant tunnelling peaks, which occur in the rates as a function of the Stark field amplitude. The mean-field interaction induces a broadening and a shift of the peaks, and the latter is explained by analytic perturbation theory.

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## 1. Introduction

Quantum dynamics often is intriguing and counter-intuitive. A prominent example thereof is the localisation of a wave packet in a spatially periodic lattice induced by an additional static force: the force can turn an extended Bloch wave (which is a solution of the Schrödinger equation with a periodic potential [1]) to a wave packet which oscillates periodically in (momentum) space [1]. While conceptionally simple, this well-know Wannier-Stark problem is complicated from the mathematical point of view because the system is open, i.e., unbounded, and any initially prepared state will, in the course of time evolution, decay via tunnelling out of the periodic potential wells [2, 3].

Starting from the Bloch bands of the unperturbed problem (i.e., without the static field  $F = 0$ ), the decay can be attributed to tunnelling from the ground state band to the first excited energy band. The celebrated Landau-Zener theory predicts an exponential decay rate (see, for instance, [4, 5] for introductory reviews):

$$\Gamma(F) \propto F e^{-\frac{b}{F}}, \quad (1)$$

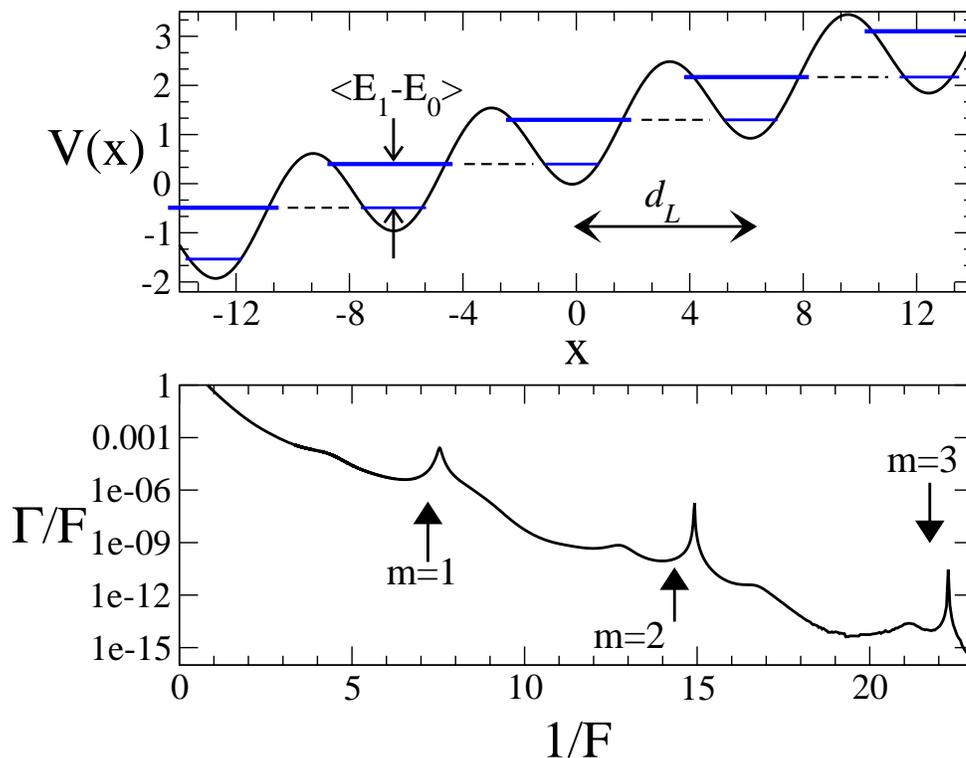
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where  $b$  is proportional to the square of the energy gap between the two lowest energy bands. For experiments with cold atoms, i.e., the scenario on which we focus in this paper, the wave packet decays very quickly by successive tunnelling events, once it has tunneled across the first band gap. This is due to the much smaller gaps of the higher energy bands in a sinusoidal potential [6, 7]. The Landau-Zener formula (1) cannot account for the interaction of the Wannier-Stark levels at adjacent potential wells. Between such adjacent lattice sites nearly degenerate Wannier-Stark levels repel each other, which leads to a strong enhancement of the tunnelling decay. These resonant tunnelling events result in pronounced peaks in the rates as a function of the inverse field amplitude  $1/F$ , on top of the of the global exponential decay described by (1) [5, 8].

Figure 1(a) shows two Wannier-Stark levels on each lattice site. The levels within either of the two ladders are separated by  $mFd_L$  in energy, where  $d_L \equiv 2\pi$  denotes the lattice period and the integer  $m$  counts the number of sites in-between two energy levels of the same ladder [1, 2]. The decay rates for non-interacting particles in the periodic potential  $V(x) = V_0 \sin^2(x/2) + Fx$  can be computed from the Wannier-Stark spectrum, e.g., by using the numerical method described in [5]. Figure 1(b) presents the rate  $\Gamma$  as a function of  $1/F$ . The maxima occur when  $mFd_L$  is close to the difference in energy  $\langle E_1 - E_0 \rangle$  between the first two energy bands (averaged over the fundamental Brillouin zone in momentum space) of the unperturbed ( $F = 0$ ) problem [5, 9]. The actual peak positions are slightly shifted with respect to this simplified estimate [marked by arrows in Fig. 1(b)], owing to a field-induced level shift close to the avoided crossings of the levels [8].

Exceptional experimental control is possible nowadays with Bose-Einstein condensates (BEC) whose initial conditions in coordinate and momentum space can be adjusted with unprecedented precision. With the help of a BEC, sensitive tunnelling phenomena were studied in time-dependent systems [10], as well as in static potentials [11]. Here we are interested in tunnelling in the Wannier-Stark problem where the impact of the intrinsic atom-atom interactions in the BEC has been studied in several recent experiments [7, 12, 13, 14]. In those experiments, the difficulty in understanding quantum transport processes, such as coherent tunnelling, originates from the complex interplay between classical transport in the underlying phase space, quantum interference effects, and the many-particle interactions.

In a typical experiment with a BEC, where the number of atoms in the condensate is large and the atom-atom interaction is rather small, the Gross-Pitaevskii equation (GPE) describes the condensate in very good approximation [15]. Recently, some of us proposed a concrete experimental scenario to measure the impact of a mean-field interaction potential (which in the GPE takes into account of the atomic collisions) on the tunnelling in the Wannier-Stark problem [16]. More specifically, the interaction-induced modification of the resonant tunnelling peaks was studied, and it was found that the peaks [such as the ones in Fig. 1(b)] are washed out for a large enough – but still experimentally feasible – interaction strength. As discussed in [16], for a finite mean-field nonlinearity, the concept of decay rates is not as well defined as in the case



**Figure 1.** (a) Schematic sketch of nearly degenerate Wannier-Stark levels (thin line: ground state levels; thick line: first excited levels in each well) in a potential of the form  $V(x) = V_0 \sin^2(x/2) + Fx$ . (b) tunnelling rates  $\Gamma$  for  $V_0 = 2$  as a function of the inverse Stark field amplitude  $1/F$ . The resonant tunnelling leads to the pronounced peaks, which lie approximately at  $F \approx \langle E_1 - E_0 \rangle / (2\pi m)$  (with integer  $m$ ). These estimates (marked by the arrows) are slightly modified by field-induced level shifts.

of non-interacting particles. The reason is that the weight of the nonlinear term, which is proportional to the condensate density, varies in time. Hence, the probability that an initially prepared state will stay in the preparation region does not follow a simple exponential law. In other words, the nonlinear interaction decreases as the condensate escapes via tunnelling and, as a consequence, the decay rates can be defined only locally in time.

In this paper we want to discuss how the problem of defining proper decay rates can be solved. One way to define a time-independent, global tunnelling rate is to renormalise the density of the condensate in the preparation region (e.g., in the central potential well of the periodic lattice) continuously, such that the average density remains constant in time. For experimentally realisable nonlinearities [7, 12, 13, 17], this approach results in a mono-exponential decay of the survival probability, and in consequence in a reasonable definition of the decay rate. The corresponding resonance states are characterised by their stationary asymptotics, much in the same way as the stationary solutions of a linear scattering problem (i.e, described by the linear Schrödinger equation) [5]. We solve numerically the well-posed problem of finding the resonance states, using the method

of complex scaling. The theoretical background to treat the nonlinear interaction in the GPE in a consistent way was recently laid in [18]. We use a modified version of this method, with crucial extensions on the algorithmic side, which proved necessary to stabilise the computations for more complicated potentials than the single-well potential exemplarily treated in [18].

We review the defining equations of the nonlinear Wannier-Stark problem and the complex scaling technique of [18] in the following section 2, where we also describe our numerical algorithm in detail, c.f., subsection 2.2. Section 3 presents our central results on the decay rates in the vicinity of the resonant tunnelling peaks for experimentally relevant nonlinearities. Section 4 finally concludes the paper.

## 2. The nonlinear Wannier-Stark problem

We use the one-dimensional GPE to model the temporal evolution of a BEC loaded into a spatially periodic optical lattice potential and subjected to an additional static force  $F$ :

$$i \frac{\partial}{\partial t} \psi(x, t) = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V_0 \sin^2 \left( \frac{x}{2} \right) + Fx + g |\psi(x, t)|^2 \right] \psi(x, t). \quad (2)$$

$\psi(x, t)$  represents the condensate wave function, and we used the dimensionless quantities  $V_0 = V_{\text{SI}}/E_B$ ,  $F = F_{\text{SI}}d_L/(2\pi E_B)$ ,  $g = g_{\text{SI}}d_L N/(2\pi E_B)$ . The characteristic length scale is the lattice period  $d_L$ , i.e.,  $x = x_{\text{SI}}2\pi/d_L$ , the Bloch energy is  $E_B = (\pi\hbar/d_L)^2/M$ , with atomic mass  $M$ , the number of atoms  $N$ , and the (from three to one spatial dimensions) rescaled nonlinearity parameter  $g_{\text{SI}}$  (see [19] for a definition of  $g_{\text{SI}}$ , where also the regime of validity of the one-dimensional approximation is discussed in detail).

Since  $V(x) = V_0 \sin^2(x/2) + Fx \rightarrow -\infty$  for  $x \rightarrow -\infty$ , any state initially prepared in the optical lattice will escape via tunnelling. We search for the resonance state  $\psi_g$  which solves the stationary version of Eq. (2)

$$H[\psi_g]\psi_g = E_g\psi_g, \quad (3)$$

for the eigenvalue  $E_g = \mu_g - i\Gamma_g/2$ , and the Hamiltonian

$$H[\psi] = -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V(x) + g|\psi(x)|^2 \quad (4)$$

To render the problem posed by Eq. (3) meaningful we demand that the condensate wave function remains normalised around the initially prepared state, i.e., around  $x \approx 0$ :

$$\int_{-x_n}^{x_n} dx |\psi_g(x)|^2 = 1. \quad (5)$$

The boundaries  $x_n$  must be chosen in a reasonable way, and we chose  $x_n = \pi$  (so the probability to stay in the central well around  $x = 0$  remains one [20]). We verified that slightly different choices of the boundary  $\pi \lesssim x_n < 3\pi/2$  led to eigenvalues which did not change on the significant digits given below in section 3.

We discuss now the renormalisation condition (5) and its consequences. In practice such a condition may be realised by the presence of a source term which constantly supplies a condensate flow [21]. Experimentally such a scenario could be achieved by constantly reloading the central well with coherent BEC matter. Transport experiments of such kind could be realised with the help of optical tweezers [22], atomic conveyor belts [23], or microscopic guides for ultracold atoms [24]. Any realisation may introduce additional modifications in the temporal evolution of the decaying system, which go beyond our simplified assumption of renormalisation. Such modifications, e.g., the relaxation of added particles in the periodic lattice potential, depend on the specific realisation. We expect, however, that the asymptotic decay will be hardly affected by such processes, the time scales of which should be relatively short and of the order of the period of oscillations in the potential wells.

On the other hand, if the condensate wave function tunnels out of the central well without sudden changes of its shape, the time-dependent atomic population  $N(t)$  inside the well decays according to the relation [18, 25]

$$\frac{dN(t)}{dt} = -\Gamma_{g(t)}N(t) . \quad (6)$$

Assuming that the decay rate adiabatically adjusts itself to the time-dependent value  $\Gamma_{g(t)}$ , with  $g(t) \propto N(t)$ , Eq. (6) can be solved for a given initial number of atoms  $N(0)$  in the condensate. Knowing the “local” rates  $\Gamma_{g(t)}$  for  $0 \leq |g| \leq |g(0)|$  allows us then to compute the actual survival probability in the central well, which in [16] was obtained differently by a brute force integration of the time-dependent GPE (2).

We emphasise that the setup studied in Ref. [16] bears some crucial differences to the problem posed here, which is based on condition (5). In [16] the short time behaviour of the relaxed ground state (for  $F = 0$  in the periodic potential and in the presence of additional harmonic confinements) was predicted for the three dimensional Wannier-Stark problem. The approach presented here is capable to determine, via Eq. (6), the decay only for *single* resonance states according to the above arguments. Although such resonance states are typically distributed over many lattice sites, they do not provide a prediction for the decay of a general initial state (which could be composed of contributions from many adjacent wells), simply because the superposition principle does not apply for the nonlinear GPE (2).

In this paper we want to compute *directly* the precise decay rates  $\Gamma_g$  of a single resonance state using the complex scaling method, which is described in the following subsection.

### 2.1. Complex scaling

For the linear problem with  $g = 0$ , one of the standard techniques to compute resonance states numerically is the complex scaling method (which goes back to [26], and is reviewed, for instance, in [27]). Applying the renormalisation condition (5) allows us to use this method to find the stationary eigenstates and the corresponding eigenvalues,

see Eq. (3). Without this condition, the nonlinear interaction term would vary in time, and a stationary state would not exist because of the tunnelling decay.

An additional problem when dealing with the nonlinear term in the GPE arises from the method of complex scaling itself. The problem of defining the complex conjugate of the wave function  $\psi(x)$  is described in [18, 28], and was solved in [18]. Usually, the scaling transformation is defined as follows

$$\psi(x) \rightarrow \psi^\theta(x) \equiv \hat{R}(\theta)\psi(x) \equiv e^{i\theta/2}\psi(xe^{i\theta}), \quad (7)$$

where the pre-factor is just a phase depending on the dimensionality of the problem (here we treat only the one-dimensional case).  $\theta$  is a real rotation angle, and the eigenvalues should not depend on it [26, 27], which is a useful fact for testing convergence. To evaluate the nonlinear term  $|\psi|^2 = \psi^*\psi$  away from the real coordinate (or  $x$ ) axis, we need to define a generalised complex conjugate  $\bar{\psi}$  which reduces to  $\bar{\psi}(x) = \psi(x)^*$  for  $x \in \mathbb{R}$ . Applying the complex scaling transformation to  $\bar{\psi}$

$$\overline{\psi(x)} \rightarrow \bar{\psi}^\theta(x) \equiv \hat{R}(\theta)\bar{\psi}(x) \equiv e^{i\theta/2}\bar{\psi}(xe^{i\theta}), \quad (8)$$

we see that  $\bar{\psi}^\theta$  can be obtained from  $\psi^\theta$  via the relation:

$$\bar{\psi}^\theta(x) = \hat{R}(\theta) \left( \hat{R}(-\theta)\psi^\theta \right)^* (x). \quad (9)$$

The analytic continuation of Eq. (3) to the complex domain can now be stated as

$$H^\theta[\psi_g^\theta]\psi_g^\theta = E_g\psi_g^\theta, \quad (10)$$

with

$$H^\theta[\psi_g^\theta] = -\frac{1}{2}\frac{\partial^2}{\partial x^2}e^{-i2\theta} + V(xe^{i\theta}) + g_\theta\bar{\psi}_g^\theta(x)\psi_g^\theta(x). \quad (11)$$

The nonlinear interaction strength is defined here as  $g_\theta = ge^{-i\theta}$  to compensate for the two identical phase factors  $e^{i\theta/2}$  of  $\psi^\theta$  and  $\bar{\psi}^\theta$ .

## 2.2. Numerical solution and propagation algorithm

In the linear case with  $g = 0$ , the complex eigenvalue problem of the form Eq. (10) is usually solved by representing the complex-scaled Hamiltonian in a suitable basis and final matrix diagonalisation [29]. For  $g \neq 0$ , the corresponding problem to find the eigenvalues can be solved only by implicit methods, since  $H^\theta[\psi^\theta]$  explicitly depends on the wave function.

We solved Eq. (10) by searching for the ground-state solution in a self-consistent manner. Starting with an initial guess for the wave function  $\psi^\theta(x, t = 0)$ , we evolved in real-time the grid representation of  $\psi^\theta(x, t)$ , i.e.,

$$\psi^\theta(x, t) = \sum_{j=-n}^n c_j(t)\chi_j(x), \quad (12)$$

with the box functions

$$\chi_j(x) = \begin{cases} 1/\Delta_x & , \quad |x/\Delta_x - j| < 1/2 \\ 0 & , \quad \text{otherwise} , \end{cases} \quad (13)$$

and a suitable grid spacing  $\Delta_x$ .

The time-propagation was performed by a sequential application of two different integration methods. First, we used a sequence of Crank-Nicholson steps [30], i.e.,

$$(1 + iH^\theta \Delta t/2) \psi^\theta(x, t + \Delta t/2) = (1 - iH^\theta \Delta t/2) \psi^\theta(x, t - \Delta t/2). \quad (14)$$

The Crank-Nicholson method has the advantage of preserving the norm of the wave function, but the disadvantage that it treats all modes equally. Since we are interested in the ground state, we iterated in a second stage the explicit relation

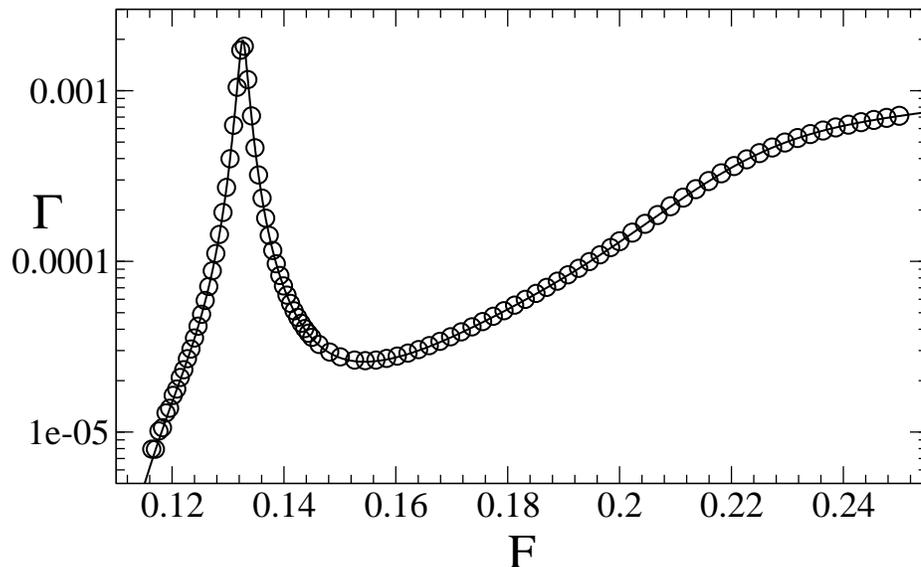
$$\psi^\theta(x, t + \Delta t) = (1 - iH^\theta[\psi^\theta]\Delta t) \psi^\theta(x, t). \quad (15)$$

The latter method, which still corresponds to a real-time integration of the complex scaled Gross-Pitaevskii equation, tends to suppress the higher modes [30] and leads to a faster stabilisation of the numerical solution of Eq. (10) in comparison with the Crank-Nicholson method (14). For *each* time step  $t \mapsto t + \Delta t$ , we self-consistently solved Eq. (15) by using the left side of Eq. (15) to approximate the nonlinear term  $g\theta \overline{\psi}^\theta \psi^\theta$ . Three to five such self-consistent iterations proved sufficient for a stable and reliable time propagation. The second derivative appearing in  $H^\theta$  was approximated by a finite difference representation (in other words we applied the “forward time centred space” representation [30] to solve the GPE). This leads to a tridiagonal Hamiltonian matrix, which significantly simplifies the implementation of both propagators (14) and (15).

For evaluating  $\overline{\psi}^\theta(x, t)$ , we used the method described in detail in [18], which produced reliable numerical results also for our Wannier-Stark problem. Briefly speaking, we represent  $\psi^\theta(x, t)$  in a basis set of Gaussians with increasing variance for increasing  $|x|$ . The Gaussian basis is thus well-behaved at the boundaries of our grid, which allows us a numerically stable back-rotation to the real domain in  $x$ . At the end,  $\overline{\psi}^\theta(x, t)$  is re-expressed again in the grid basis. The necessary matrix-vector multiplications are fast since the number of vectors in the Gaussian set can typically be chosen much smaller than the number of grid points in the spatial domain. Furthermore, the transformation matrices are effectively banded, which reduces the numerical effort (note that we computed  $\overline{\psi}^\theta(x, t)$  from  $\psi^\theta(x, t)$  for *each* time step  $t \mapsto t + \Delta t$  to ensure stable convergence).

### 3. Results and discussion

In the following, we present our results on the tunnelling rates of resonance states [c.f. Eq. (10)] in the Wannier-Stark problem as sketched in Fig. 1(a). Without loss of generality we kept fixed the potential depth  $V_0 = 2$  in Eq. (2), which corresponds to an optical lattice with a maximal amplitude of 16 photon recoil energies [6, 7]. We were particularly interested in studying the impact of the nonlinear term in Eq. (2) on the resonant tunnelling peaks of Fig. 1(b). Using the method described in the previous section we chose  $\theta = 0.01 \dots 0.02$  (where we found stable eigenvalues which are not dependent on  $\theta$  in this range), and a grid spacing  $\Delta_x = 0.02 \dots 0.05$  for  $-100 \leq x \leq 100$ .



**Figure 2.** Comparison between the tunnelling rates around the first resonant tunnelling peak from Fig. 1(b), obtained for  $g = 0$  by direct diagonalisation of the problem (solid line) and by our complex scaling algorithm (circles).

The integration time step was  $\Delta t = 2.5 \times 10^{-3}$  for  $|g| < 0.2$  and reduced to  $\Delta t = 2 \times 10^{-3}$  for larger  $|g| \geq 0.2$  and the region of small  $F < 0.2$ , while the maximal integration time for finding one eigenvalue was  $t_{\max} = 300$ .

As expected, it is very difficult to find the correct eigenvalue close to a resonant tunnelling peak because of two reasons: (i) the rates  $\Gamma$  vary dramatically around the peak due to the close degeneracy of the Wannier-Stark levels in adjacent wells, and (ii) the rates are rather small  $10^{-13} < \Gamma \lesssim 2 \times 10^{-3}$  at small fields  $0.05 < F < 0.2$ .

Therefore, we focused on the first (i.e., with  $m = 1$ ) peak in Fig. 1(b), where the rates remain  $\Gamma \gtrsim 10^{-5}$ . Moreover, we improved the stability of the integration by starting with parameters in a stable regime (where we easily found stable, fast converging eigenvalues) and adiabatically changing the two parameters  $F$  and  $g$  into less stable parameter regimes. In our case, for  $V_0 = 2$ , the stable regime is above  $F > 0.25$  for not too large nonlinearities  $|g| \lesssim 0.5$  (with optimal stability properties for  $g = 0$ ).

We tested our results in three different and independent ways. First, we compared them for  $g = 0$  with the spectra of the linear Wannier-Stark problem, which can be computed by a standard diagonalisation of  $H_{g=0}^\theta$  [5, 29]. Figure 2 shows the good agreement between the data set obtained by our integration of the complex scaled, linear version of Eq. (2) and the data presented already in Fig. 1(b).

Secondly, for moderate nonlinearities  $|g| \leq 0.5$ , we computed for the *un-scaled* problem (2) the survival probability

$$P_{\text{sur}}(t) \equiv \int_{-p_c}^{\infty} dp |\hat{\psi}(p, t)|^2 \approx N(t), \quad (16)$$

with  $p_c \gtrsim 3$  photon recoils (such as to cover the support in momentum space of the initial

$g$	$F$	$\Gamma_{\text{fit}}$	$\Gamma_{\text{CS}}$
0	0.5	$1.94 \pm 0.01 \times 10^{-2}$	$1.941 \times 10^{-2}$
0.1	0.5	$2.18 \pm 0.01 \times 10^{-2}$	$2.180 \times 10^{-2}$
0	0.25	$7.2 \pm 0.1 \times 10^{-4}$	$7.2 \times 10^{-4}$
0.1	0.25	$8.4 \pm 0.1 \times 10^{-4}$	$8.4 \times 10^{-4}$
0.2	0.25	$9.7 \pm 0.1 \times 10^{-4}$	$9.7 \times 10^{-4}$
0.25	0.25	$1.04 \pm 0.02 \times 10^{-3}$	$1.04 \times 10^{-3}$
0.5	0.25	$1.45 \pm 0.03 \times 10^{-3}$	$1.48 \times 10^{-3}$
0.2	0.15	$3.0 \pm 0.2 \times 10^{-5}$	$2.9 \times 10^{-5}$
0.2	0.13125	$5.7 \pm 0.3 \times 10^{-5}$	$5.7 \times 10^{-5}$

**Table 1.** Comparison between the tunnelling rates for  $V_0 = 2$  obtained by the complex scaling method ( $\Gamma_{\text{CS}}$ ) and by the integration of the GPE ( $\Gamma_{\text{fit}}$ ; integration time up to 100 Bloch periods; the integration was performed on a large grid that covered the full extension of the tunnelled and subsequently accelerated part of the wave function, without the use of any cutoff or absorbing boundary conditions). Because of the restriction in the integration time,  $\Gamma_{\text{fit}}$  carries the shown error, whilst the complex scaling method allows us to compute the rates  $\Gamma_{\text{CS}}$  with an absolute accuracy of at least  $10^{-6}$  for  $F \geq 0.15$ , and  $10^{-5}$  for  $F$  down to  $\gtrsim 0.12$ .

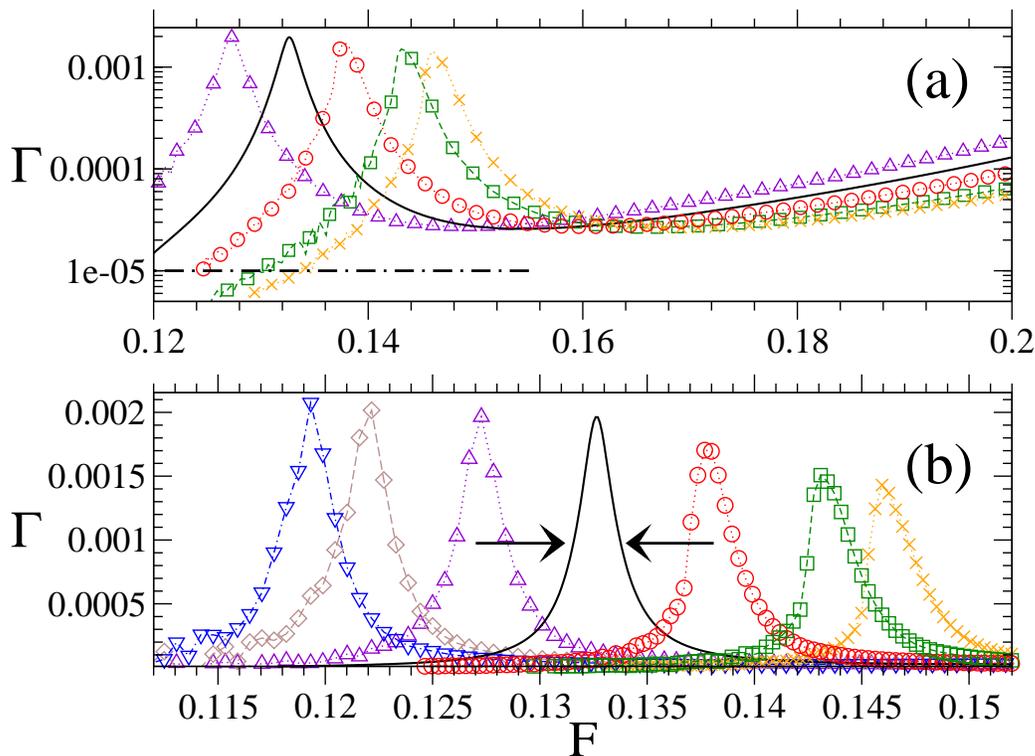
state prepared in the spatially periodic lattice potential).  $P_{\text{sur}}(t)$  was introduced for the Wannier-Stark problem in [16] and characterises the out-coupled loss in momentum space, which corresponds to the part of the condensate which has tunnelled through the potential. We integrated Eq. (2) constantly applying the renormalisation condition (5), and computed the survival probability (16) with the wave function

$$\hat{\psi}(p, t) \approx \frac{\hat{\psi}_{\text{renorm}}(p, t)}{\prod_{j=1}^K \int_{-\pi}^{\pi} dx |\psi(x, jt/K)|^2},$$

for the discretised times  $jt/K$  ( $j = 1, 2, \dots, K$ ) and large  $K \in \mathbb{N}$ . Here  $\psi(x, jt/K)$  denotes the propagated wavefunction immediately before applying the renormalisation ( $\psi(x, jt/K)$  is renormalised afterwards and propagated up to time  $(j+1)t/K$ ).  $\hat{\psi}_{\text{renorm}}(p, t)$  represents the Fourier transform of the renormalised wavefunction at the end of the complete propagation. The decay rates  $\Gamma_{\text{fit}}$  were obtained by a direct mono-exponential fit to the temporal decay of  $P_{\text{sur}}(t)$ . Table 1 highlights the good agreement with the rates computed by the complex-scaling method.

As a final test of our results, we constantly monitored the quality of the computed eigenvalues by evaluating  $|(H^\theta[\psi^\theta] - E)\psi^\theta|$ , which in all cases had to be  $\lesssim 10^{-8}$  for not rejecting the eigenvalue. This boundary was chosen such as to be more than two orders of magnitude smaller than the smallest tunnelling rates which we computed.

Our central results are reported now in Fig. 3. There we observe two effects which are induced by the presence of the nonlinear interaction term in Eq. (2): (I) the resonant tunnelling peak shifts systematically with increasing  $g$  as a function of the Stark field amplitude  $F$ . (II) the peak width slightly increases as  $|g|$  increases away from zero.



**Figure 3.** Decay rates  $\Gamma$  obtained for  $V_0 = 2$  and the range of nonlinearities  $-0.25 \leq g \leq 0.25$  as a function of the Stark field amplitude  $F$  [(a) logarithmic and (b) linear scale on y-axis]:  $g = -0.25$  (crosses),  $g = -0.2$  (squares),  $-0.1$  (circles),  $0$  (solid line),  $0.1$  (pyramids),  $0.2$  (diamonds; only in (b)), and  $0.25$  (inverse pyramids; only in (b)). The nonlinearity systematically shifts the peak centres and slightly broadens the peaks. Their width we defined as the full peak width at half maximum, which is marked by the arrows in (b) for the  $g = 0$  peak. The dot-dashed line in (a) shows the lower bound for converged  $\Gamma \gtrsim 10^{-5}$  on the left side of the resonant tunnelling peaks, i.e., for very small  $F \lesssim 0.12$ , where convergence is very hard to achieve even at small  $g \simeq 0.1$  (in this parameter range, i.e., at the left side of the peaks where  $\Gamma$  changes abruptly by about two orders of magnitude, the propagation according to Eqs. (14) and (15) becomes unstable).

The slight broadening goes along with a small increase in the height of the peaks with increasing nonlinearity  $g$ . Such a destabilisation of the condensate for  $g > 0$ , more precisely of the decay in the survival probability  $P_{\text{sur}}(t)$ , has already been observed in [16]. The ratio of the difference in the height and the difference in the peak width (measured at the half of the peak height, see Fig. 3) is roughly constant as a function of the nonlinearity  $0 < g \lesssim 0.25$ . The broadening and the change in height of the peak are caused by two different, but simultaneously acting mechanisms. The nonlinear mean-field term in Eq. (2) partially lifts the degeneracy of the Wannier-Stark levels [as sketched in Fig. 1(a)] by smearing them out. This qualitatively explains the slight broadening of the peak with increasing  $|g|$ . In addition, the peak maximum becomes systematically larger as  $g$  increases in Fig. 3, because the condensate is destabilised (stabilised) by an increasingly repulsive (attractive) nonlinearity.

The shift of the peak maximum can be estimated by first-order perturbation theory, which predicts the following shift in energy of the levels with respect to the linear case with  $g = 0$ :

$$\Delta E \approx g \int_{-x_c}^{x_c} dx |\psi_g|^2 |\psi_{g=0}|^2 . \quad (17)$$

For the moderate nonlinearities realised in experiments [7, 17, 31], i.e.,  $|g| \lesssim 0.5$ , the overlap integral is nearly independent of  $g$ , and the major contribution comes from the central potential well where the condensate is localised initially. Hence we approximate further

$$\Delta E \approx g \int_{-\pi}^{\pi} dx |\psi_{g=0}|^4 , \quad (18)$$

which in turn leads to a shift in the position on the  $F$  axis corresponding to  $\Delta E \approx 2\pi\Delta F$ . Taking into consideration that the probability in the central well remains normalised [condition from Eq. (5)], Eq. (18) corresponds to the energy shift induced by the nonlinearity which was baptised “frequency pulling” in [32], because it leads to a phase dispersion of the Bloch oscillations in the wells. With (18) we arrive at the general result that the following ratio is approximately constant:

$$\frac{2\pi\Delta F}{|g|} \approx \int_{-\pi}^{\pi} dx |\psi_{g=0}|^4 \approx 0.37 . \quad (19)$$

This estimate proved to be valid with a maximal relative deviation of less than 18% with respect to the shifts observed in Fig. 3. Since the integral  $\int_{-\pi}^{\pi} dx |\psi_g|^4$  is constant up to the third digit for all  $|g| \leq 0.25$ , we conclude that the first-order perturbation correction is not enough to describe the shifts more quantitatively.

While a repulsive mean field ( $g > 0$ ) enhances the tunnelling rate far away from the  $g = 0$  peak, an attractive interaction ( $g < 0$ ) stabilises the decay sufficiently far away from all the peaks. This is the case, e.g., for  $F > 0.16$  in Fig. 3(a), where  $\Gamma$  systematically decreases with decreasing  $g$ . The symmetric displacement of the peak with respect to the sign of  $g$  reflects the symmetry of the Bloch band model, in which tunnelling from the first excited band back to the ground band can be interpreted as the converse process but with a sign change in  $g$  [13]. The same qualitative behaviour of enhancement ( $g > 0$ ) and stabilisation ( $g < 0$ ) was observed in the short-time evolution of the three dimensional Wannier-Stark problem [16]. Apart from the conceptual difficulty of decomposing a solution of the nonlinear GPE (2) into contributions from many adjacent wells (see discussion in section 2), the observed washing out of the peak structure in Ref. [16] is a direct consequence of an effectively moving peak as  $|g|$  diminishes monotonously (c.f. Fig. 3) with decreasing density in the wells.

To conclude this section, we briefly compare our results to other recent works which investigated the impact of a mean-field interaction of the GPE type on quantum mechanical decay processes. We emphasise, however, that such a comparison can only be qualitative, since such works [25, 28, 33, 34] typically treat much simpler model potentials than our Wannier-Stark problem with close level degeneracies. The common

feature of our work and the results presented in [25, 28, 33, 34] is that an increasing nonlinearity typically enhances the decay in the one-dimensional problem. Systematical shifts in the chemical potential of resonance states (induced by the interaction term) were analytically studied in [34] for a delta-shell potential. Such shifts correspond to our perturbative estimate in Eqs. (18) and (19).

Particularly, we compared the results obtained from our method (see section 2) with the description of [28] where a nonlinear equation was introduced which differs from ours [see Eq. (11)] in the treatment of the nonlinear term. In [28] the nonlinearity is of the form  $g_\theta(\psi^\theta)^3$ , and we found that such a nonlinear term leads to *different* decay rates than the ones we computed from either our complex scaling method or from the real-time integration of the un-scaled GPE (2) and subsequent fits to  $P_{\text{sur}}(t)$ . We conclude that a treatment based on complex scaling – for a condensate within the standard GPE description and generally complex-valued wave functions – makes it necessary to use the explicit form of  $\overline{\psi^\theta}$  as presented in section 2.

There is a growing literature of works on Landau-Zener tunnelling in the presence of a mean-field nonlinearity and its impact on the Bloch oscillation problem, see, e.g., [13, 35]. In such works a similar systematical stabilisation (for  $g < 0$ ) or destabilisation (for  $g > 0$ ) was predicted (and also measured, see [13]) for a *single* Landau-Zener tunnelling event with various approximative models. This corresponds to our results on the decay rates which describe directly the initial decay of the condensate via tunnelling, i.e., the behaviour of  $P_{\text{sur}}(t)$  at short times that are not much larger than one Bloch period. At and close to the resonant tunnelling peaks the problem is, however, more subtle because of the strong interaction of Wannier-Stark levels [see Fig. 1(a)], and such a case was not treated in [13, 35].

#### 4. Conclusion

To summarise, we presented a method to numerically compute precise decay rates for tunnelling problems within the framework of the Gross-Pitaevskii equation. We adapted and improved the technique developed by one us in [18] for the more complicated scenario of resonant tunnelling in the Wannier-Stark problem. We showed that the mean-field nonlinearity leads to experimentally observable modifications in the tunnelling of resonance states from the periodical potential wells, even in a regime where the kinetic and the periodic potential terms still dominate the dynamics. The broadening and the shift of the resonant tunnelling peaks define clear signatures for nonlinearity induced effects.

Our method can be extended – with further system-specific improvements in the propagation algorithm – to treat even more complicated problems appearing in experiments with Bose condensates, e.g., the transport of coherent matter within atomic wave guides. Finally, we can readily extend the proposed method to three spatial dimensions, with the only drawback of much larger numerical effort.

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