Energy relaxation in the mean-field description of polariton condensates

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Abstract. We introduce a dissipation term in the Gross–Pitaevskii equation that describes the stimulated relaxation of condensed bosons due to scattering with different types of particles. This situation applies to Bose–Einstein condensates of quasi-particles in the solid state, such as magnons and excitons. Our model is compatible with the phenomenology of superfluidity: supercurrents are stable up to a critical speed and decay when they are faster. We apply our model to a description of the relaxation of polariton condensates in a shallow trap.

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1. Introduction

The Gross–Pitaevskii equation (GPE) provides an excellent description of an isolated dilute Bose gas at low temperature. For example, the GPE accurately describes the density profiles and frequencies of elementary excitations of trapped ultracold atomic Bose gases [1].
Figure 1. Schematic illustration of the relaxation of polaritons due to scattering with phonons. Several modes in a random potential are macroscopically occupied. Where they spatially overlap, relaxation takes locally place from the high- to the low-frequency modes, as indicated by the arrows.

Systems featuring Bose–Einstein condensation (BEC) of quasi-particles in the solid state, such as (exciton-) polaritons [2] and magnons [3], are however not so well isolated from their environment as the atomic gases. In semiconductor microcavities for example, the polaritons that form a Bose–Einstein condensate undergo scattering with lattice phonons and with high-energy excitons. These interactions allow the polaritons to relax toward lower energy. The Boltzmann equation is the easiest way of modeling these scattering dynamics theoretically [4]. The semiclassical approximation involved in this approach becomes, however, problematic when the polariton gas enters the condensed phase. Most importantly, supercurrents, which are a gradient of the phase of the polariton field, are missed. This precludes e.g. the description of vortices in polariton condensates [5], which appear naturally in the GPE.

In order to allow for a simultaneous description of supercurrents and of the relaxation due to interactions with the environment, we will present here a dissipation term that can be added to the GPE. This term models the transitions between components of the GPE field at different frequencies (see figure 1). For specificity, we will use in the following the terminology of ‘polaritons’ relaxing through ‘phonon scattering’, but our formalism is applicable to any dilute Bose gas that dissipates energy into the environment.

The same model has already been applied to the description of the relaxation of currents in polariton nanowires [13] in the paper [14]. Here, we will discuss in general the properties of extensions of the GPE that include dissipation. In particular, an important requirement of the theory is compatibility with superfluidity. According to the Landau criterion [1], the superflow cannot relax due to phonon scattering as long as the superfluid velocity is below the critical speed. A Boltzmann description that includes phonon scattering violates this requirement: a Bose gas with initially all the particles at finite momentum $k = k_c$ will relax to a state with the majority of particles in the ground state $k = 0$. We will show below that our GPE-based model for phonon relaxation is instead fully in agreement with the Landau criterion for the stability of superflow slower than the critical speed. In addition, it provides a dynamical model for the dissipation of superflow when the speed exceeds the critical one.
The outline of the paper is as follows. In section 2, we will derive the dissipation term that can be added to the GPE. As a first example, it is applied to the simple case of two coupled traps (Josephson junction) in section 3. In the next section, we consider the homogeneous Bose gas, for which we investigate the damping of the elementary excitations. Finally, in section 5, we turn to a more complex example of nonresonantly excited polaritons that relax in a quadratic trapping potential. The conclusions are presented in section 6.

2. The model

The states in sketch 1 can be labeled by their frequencies \( \omega \). This involves a coarse graining of the time, analogous to the coarse graining of space used in the semiclassical Boltzmann equation \[6\]. We will use the following definition of the time-dependent spectrum of the Bose field \( \psi(x, t) \):

\[
\psi_{\omega}(x, t) = \frac{1}{T} \int_{t-T}^{t} e^{i \omega t'} \psi(x, t') dt',
\]

(1)

where \( T \) is the coarse graining time step. The inverse transform reads

\[
\psi(x, t) = \sum_{\omega} e^{-i \omega t} \psi_{\omega}(x, t).
\]

(2)

We will derive the classical field equation that describes relaxation between the states at different frequencies in two different ways. First, we will start from a rate equation model that we rewrite as a field equation. The second derivation will be more fundamental and start from the Heisenberg equations of motion for the Bose field that interacts with a localized phonon bath.

Spontaneous scattering is a quantum feature that is difficult to describe with a classical field model such as the GPE. We therefore, restrict the relaxation to the stimulated processes, which are described by the rate equation

\[
dn_{\omega}(x, t) = n_{\omega}(x, t) \sum_{\omega'} r(\omega, \omega') n_{\omega'}(x, t) dt,
\]

(3)

where \( r(\omega, \omega') \) is the net scattering rate from the mode at frequency \( \omega' \) to the mode at \( \omega \). In order to conserve particle number, the relaxation rate should change sign under exchange of \( \omega \) and \( \omega' \): \( r(\omega, \omega') = -r(\omega', \omega) \). The first term in the expansion of the rate as a function of the frequency difference is therefore

\[
r(\omega, \omega') = \kappa (\omega' - \omega),
\]

(4)

where the relaxation constant \( \kappa \) has the dimension of an inverse density. Equation (4) is, for example, the form of the scattering rate obtained with the golden rule for the relaxation of quantum well excitons due to scattering with acoustic phonons [7].

The rate equations (3) describe transitions between states that are characterized by their position and energy. We have chosen a dissipation mechanism that is local in real space. The validity of this assumption depends on the specific system under study. It is expected to be a good approximation when the coherence length of the ‘phonon bath’ is much shorter than the characteristic length scale of the Bose system. This is for example the case for the relaxation of polaritons through scattering with high-energy excitons.
Under the change of the density (3), the wave function varies as

$$\psi^{\omega}(x, t) + d\psi^{\omega}(x, t) = \sqrt{n^{\omega}(x, t) + dn^{\omega}(x, t)/n^{\omega}(x, t)} \psi^{\omega}(x, t),$$

(5)

where we used the fact that a stimulated relaxation process does not change the phase of $\psi$. Expanding equation (5) to first order in $dn^{\omega}$, we obtain for the change of the wave function

$$\frac{d}{dt} \psi^{\omega}(x, t) = \left( \frac{1}{2n^{\omega}(x, t)} \frac{dn^{\omega}(x, t)}{dt} \right) \psi^{\omega}(x, t).$$

(6)

Substituting into equation (6) equations (3) and (4) and using the inverse transform (2), one obtains for the relaxation dynamics of the wave function

$$\frac{\partial}{\partial t} \psi(x, t) \bigg|_{\text{relax}} = \frac{\kappa \bar{n}(x, t)}{2} \left[ \bar{\mu}(x, t) - \frac{i \partial}{\partial t} \right] \psi(x, t).$$

(7)

In the derivation, boundary terms in the partial integration that scale as $1/T$ were neglected, because we consider the limit of a large coarse graining time where $1/T$ is smaller than any other relevant frequency scale. In equation (7), $\bar{n}$ and $\bar{\mu}$ are the time-averaged density and chemical potential, respectively:

$$\bar{n}(x, t) = \frac{1}{T} \int_{t-T}^{t} |\psi(x, t')|^2 dt',$$

(8)

$$\bar{\mu}(x, t) = \frac{1}{\bar{n}(x, t)} \text{Re} \left[ \frac{1}{T} \int_{t-T}^{t} \psi^*(x, t') \frac{i \partial}{\partial t} \psi(x, t') dt' \right].$$

(9)

The real part is taken in equation (9), because it is readily shown with the Madelung transformation $\psi = \sqrt{\bar{n}} e^{i \theta}$ that the imaginary part of the integral in equation (9) scales as $1/T$. Equation (7) gives the term that was sought to describe the stimulated relaxation of a classical Bose field due to local scattering with phonon-like particles. The appearance of the effective chemical potential in equation (7) should not be confused with its appearance in the usual GPE. In this case, it gives rise to an exponential variation of the field amplitude and does not give a mere phase factor.

Let us now rederive equation (7) starting from a Hamiltonian that couples the Bose field to a phonon bath. For a localized phonon bath, the coupling can be described by

$$H_p = \sum_{x,i} g_i \psi^\dagger(x) \psi(x) \{b^\dagger_i(x) + b_i(x)\},$$

(10)

which describes the interaction of the bosonic field $\psi$ with localized phonons $b_i$, whose frequency we denote by $\omega_i$. Because we are deriving a mean-field theory, we replace the quantum field $\psi$ by classical field in the following derivation.

Treating the effect of $H_p$ as a perturbation on the equation of motion for the bosons, we have to first order in the coupling constant $g_i$

$$[\delta\psi(x, t) - \psi(x, t = 0)]_{\text{relax}} = \left( \sum_i \int dt' e^{-i\omega_i(t-t')} \psi^\dagger(x, t') \psi(x, t') \right) \psi(x, t).$$

(11)
Using the Fourier expansion (2), we can rewrite to lowest order the relaxation contribution to the dynamics as

\[
[\delta \psi(x, t) - \psi(x, t = 0)]_{\text{relax}} = \sum_{\omega, \omega_1, \omega_2} \left( \sum_i |g_i|^2 \int_0^t \frac{d\tau'}{\tau'} e^{-i\omega_2(\tau' - \tau) - i(\omega_2 - \omega_1)\tau'} \psi_{\omega_1}^\dagger(x, \tau') \psi_{\omega_2}(x, \tau') \right) \psi_{\omega_1}(x, t).
\]

(12)

We now assume that the temporal Fourier components at different frequencies have no fixed phase relation. This means that only the terms with \(\omega_1 = \omega_2\) and \(\omega_1 = \omega\) contribute. The former implies that the phonon frequency \(\omega_i = 0\), while the latter contribution describes a relaxation process where a particle from the mode at frequency \(\omega\) relaxes to the mode at frequency \(\omega_1\). For phase matching conditions \(\omega_i = \omega_2 - \omega\), the time integral in equation (12) rises linearly with \(t\), giving

\[
[\delta \psi(x, t) - \psi(x, t = 0)]_{\text{relax}} = t \sum_{\omega_2} r(\omega_2) e^{-i\omega_2t} |\psi_{\omega_2}(x, t)|^2 \psi_{\omega_2}(x, t).
\]

(13)

Under assumption (4), we obtain again equation (7).

The right-hand side of equation (7) resembles the frequency-dependent amplification term that was introduced in [9] to describe an energy-dependent gain mechanism:

\[
\frac{\partial \psi}{\partial t} = (P/\Omega_k)[\Omega_k - i\partial/\partial t] \psi.
\]

(14)

Two main differences should be emphasized. First, here the relaxation term is proportional to the polariton density \(\bar{n}\), whereas in [9], the relaxation is proportional to the gain from the reservoir \(P\). The second important difference is that the gain cut-off frequency \(\Omega_k\) is replaced by the average frequency \(\bar{\mu}\). As a consequence, particle loss and gain balance each other and there is no net gain in equation (7). The modes with frequency \(\omega > \bar{\mu}\) experience loss, whereas the ones with \(\omega < \bar{\mu}\) are amplified. Phonon absorption is thus not included in our model. The relaxation (7) is due to the interaction with an environment that is effectively at zero temperature.

Our dissipation term also resembles the one that was phenomenologically introduced by Pitaevskii [8] for liquid helium and investigated by Choi et al for cold atoms [22] and reads

\[
\frac{d\psi(x, t)}{dt} \bigg|_{\text{relax}} = -\Lambda \frac{i\partial}{\partial t} \psi.
\]

(15)

In the case of ultracold atoms, where the bosons are extremely well isolated from any environment, the relaxation processes are due to the interaction of the condensate with the thermal atoms. Microscopic calculations considering such interactions that lead to an equation of the form (15) can be found in [20].

Despite the similarity between equations (7) and (15), there are several differences. Firstly, the relaxation rate in equation (15) does not depend on the condensate density, but it does in equation (7). Physically, stimulated relaxation however accelerates the relaxation when the density is higher. Secondly, the model (15) does not conserve the number of particles. This is remedied in practice by restoring the norm of the wave function in the numerical integration of the dynamics after each relaxation step by a global normalization of the wave function. Such a normalization may affect the density in regions where no relaxation has taken place at all. In
Figure 2. Dynamics of the relative phase ($\Delta \theta$) and density on the first well ($n_1$) for two wells coupled by tunneling and dissipating through the emission of phonons. The initial condition was taken to be $\psi_{1,2} = e^{\pm 0.05}$. Inset: the decay of the projection of the wave function on the excited state from the full model (16) (full line) is excellently reproduced by the exponential decay $\exp(-2J\kappa n_1 t)$ obtained from equation (3) (dashed line). The phonon relaxation constant was taken as $\kappa = 0.05$ and the coarse graining time scale $T = 20J^{-1}$.

this sense, the model (7) is more satisfactory from a physical point of view, because the particle number is locally conserved.

3. Decay of Josephson oscillations

As a first application, we add the dissipation term (7) to the GPE for noninteracting particles in two coupled levels. In the context of polariton condensation, the coupled two-level system describes, for example, the situation of spatially distinct potential wells [10] or the polarization degree [11]. The full dynamics is

$$i \frac{\partial}{\partial t} \psi_j(t) = -J \psi_{3-j} + \frac{\kappa \bar{n}_j(t)}{2} \left[ \hat{\mu}_j(t) - i \frac{\partial}{\partial t} \right] \psi_j(t)$$  \hspace{1cm} (16)

for $j = 1, 2$, where $J$ is the coupling energy. Figure 2 shows the time evolution of the densities in the two states, obtained from the numerical integration of equation (16). The initial wave function is taken to have equal amplitudes on the two states and a small phase difference between them. Due to the dissipation, the Josephson oscillations are damped. Note that the time evolution (16) drives the system automatically into the ground state and that the eigenstates of the Hamiltonian were not explicitly needed to compute the phonon scattering rates. The contribution of the excited state $|\psi_A\rangle$ to the wave function is shown in the inset of figure 2. Its exponential decay predicted by equation (16) (solid line) is excellently reproduced with the rate obtained from equation (3) (dashed line).

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We have numerically checked that the dissipative dynamics conserves particle number in the limit of a small time step in the numerical integration. We correct the residual deviation by restoring the norm of the wave function after each application of the dissipation operator.

4. The homogeneous Bose gas and superfluidity

In extended systems, the macroscopic phase coherence of the Bose gas leads to the appearance of superfluid properties. A specific manifestation is the stability of condensate superflows. When a condensate is created with a finite momentum $k_c$, it will maintain this momentum even when it can scatter with the environment.

The original discussion by Landau of this stability of the supercurrents was based on thermodynamic considerations for the creation of excitations on top of the condensate. When the low-energy dispersion of the excitations is linear $\omega(k) = ek$, it is energetically not favorable to create excitations when the condensate speed $v_c = k_c/m$ is below the speed of sound $c$ [1]. This results in a dissipationless flow of the condensate. For the case when the excitations are nonzero when $v_c < c$, this force is indeed found to vanish, whereas it is nonzero when $v_c > c$.

The GPE description of the effect of inelastic scattering with the environment, such as dissipation by phonon emission, is the subject of the discussion below. The GPE for the homogeneous interacting Bose gas supplemented with the phonon-scattering term reads

$$\frac{i}{\hbar} \frac{\partial}{\partial t} \psi = \left[-\frac{\nabla^2}{2m} + g|\psi|^2 + \frac{\kappa n}{2} \left(\tilde{\mu} - \frac{i}{\hbar} \frac{\partial}{\partial t}\right)\right] \psi. \quad (17)$$

The usual steady-state solution $\psi_0(x, t) = \sqrt{n_c} e^{-i\mu t + ik_c x}$ is still a solution to equation (17) with $\mu = k_c^2/2m + gn_c$, where $k_c$ is the condensate momentum, $g$ the interaction constant and $n_c$ the condensate density. This solution describes a superflow. In order to find out whether it is dynamically stable, we linearize the GPE around this solution. The excitations on top of the condensate can be described by the wave function $\psi(x, t) = \psi_0(x, t)[1 + u e^{ikx - i\omega t} + v^* e^{-ikx + i\omega t}]$. Linearizing the equations of motion in $u$ and $v$ is not more difficult than in the standard case, because to first order in $u$ and $v$, the average density $\bar{n}$ and frequency $\bar{\mu}$ do not change. The spectrum of the elementary excitations is given by the eigenvalues of the matrix

$$B = \begin{pmatrix} (k_c^2/2 + kk_c)/m + gn_c & gn_c \\ 1 + i\kappa n_c/2 & 1 + i\kappa n_c/2 \\ -gn_c & (-k_c^2/2 + kk_c)/m + gn_c \\ 1 - i\kappa n_c/2 & 1 - i\kappa n_c/2 \end{pmatrix}. \quad (18)$$

In the small dissipation limit $\kappa n \ll 1$, the frequencies of the elementary excitations read

$$\omega(k) = \pm \sqrt{\omega_B^2(k) - (g\kappa n_c^2/2)^2 + kk_c/m - i\frac{\kappa n_c}{2} \left[k_c^2/2m + gn_c\right]} [\omega_B(k) \pm kk_c]. \quad (19)$$

Note that the correction quadratic in $\kappa n_c$ to the usual Bogoliubov dispersion $\omega_B(k) = \sqrt{gn_c k_c^2/m + k^4/4m}$ under the square root on the first line in equation (19) is necessary to satisfy the Goldstone theorem that requires at least one branch of elementary excitations to have exactly zero real and imaginary parts of the frequency for $k \rightarrow 0$.
Importantly, for a condensate wave vector below the critical one \( k_{\text{crit}} = \min[\omega_B(k)/k] \), the elementary excitations have a negative imaginary part and the condensate is dynamically stable against decay into a lower-energy state. As soon as \( k_c > k_{\text{crit}} \), the imaginary part of the excitations becomes positive and the condensate becomes unstable with respect to decay toward a lower momentum. In agreement with the thermodynamical considerations of Landau \[1\], the phonon scattering is able to dissipate the supercurrent only when the condensate velocity is above the critical speed. In the present dynamical model \[17\], the energetic instability gives rise to a dynamical one, because the dissipative environment is explicitly included and describes the kinetics of the supercurrent’s decay.

A natural question is whether the decay rate of the excitations \[19\] that follows from the extended classical GPE is reproduced by a quantum calculation for the decay of Bogoliubov excitations. To this end, we compute with the golden rule the decay rate of Bogoliubov excitations due to the interaction Hamiltonian \[10\].

When there is a condensate, the dominant contribution comes from the terms in which one component of the Bose field is at \( k = 0 \),

\[
H_P \approx \sqrt{n_c} \sum_{x,i} g_i [\delta \psi^\dagger(x) + \delta \psi(x)][b_i(x) + b_i^\dagger(x)],
\]

(20)
in linear approximation in the field fluctuations, defined as \( \psi(x) = \sqrt{n_c} + \delta \psi(x) \).

With the golden rule, the decay rate is proportional to the square of the matrix element

\[
| M |^2 \sim (u_k + v_k)^2 = \frac{k^2/2m + 2gn_c}{\omega_B(k)}.
\]

(22)

This matrix element is of the same form as the factor in square brackets in equation \(19\), but the interaction term in the numerator is multiplied by a factor of two. The same expression as in equation \(19\) would be obtained when equation \(22\) would read \( | M |^2 \sim u^2 + v^2 \), suggesting that the classical approximation involved in the GPE does not retain the coherence between the normal and the anomalous component of the Bogoliubov excitations. The incoherence of the waves at different frequencies was indeed an assumption in the transition between equations \(12\) and \(13\).

In the context of ultracold atoms in optical lattices, the connection between the Landau critical velocity and the decay rate of excitations was investigated with a dissipative GPE in \[21\]. The origin of the damping was in this case the Landau damping of the condensate due to collisions with atoms in the thermal cloud \[1\]. They also found that the decay rate changes sign when the superfluid velocity exceeds the Landau critical velocity.

5. Relaxation in polariton traps

As a last illustration, we describe the relaxation of polaritons in a harmonic trap as observed in \[12\]. When polaritons were created off-center, relaxation toward the lower-energy state...
in the middle of the trap was observed. This experimental configuration is illustrated in figure 3. Another striking evidence of the relaxation mechanism modeled here is the very recent experimental result reported by Wertz et al [13, 14].

In polariton condensates, a steady state can be reached when new particles are continuously injected by optical excitation. In order to avoid the pinning of the condensate phase by the excitation laser, the additional particles are created at a frequency different from the condensate
one (nonresonant excitation). In the case of a far detuned laser, the excitation creates free electron hole pairs that relax to form an excitonic reservoir. Further relaxation of the excitons into the lower polariton branch then provides a gain for the condensate. A steady state is reached when gain and losses compensate for each other. The stimulated part of the scattering into the lower polariton branch can be modeled by introducing a gain term in the GPE [15, 16].

The full dynamics of the polariton gas including trapping, nonresonant pumping and relaxation is given by

$$i \frac{\partial}{\partial t} \psi = -\left[ \frac{\hbar \nabla^2}{2m} + V_{\text{eff}} - \frac{i}{2} \left[ \gamma - R(n_R) \right] + g |\psi|^2 + \frac{i \kappa n}{2} \left( \bar{\mu} - \frac{i \partial}{\partial t} \right) \right] \psi. \quad (23)$$

Here $\gamma$ is the loss rate and the function $R(n_R)$ describes the gain of the lower polariton branch thanks to stimulated scattering from the nonresonantly excited excitons in the reservoir with density $n_R$. The exciton density can be described by the rate equation

$$\frac{d}{dt} n_R = -\gamma_R n_R - R(n_R) |\psi|^2 + P, \quad (24)$$

where $\gamma_R$ is the reservoir relaxation rate and $P$ the nonresonant pumping rate. The effective potential $V_{\text{eff}} = V_{\text{trap}} + V_{\text{exc}}$ consists of the trapping potential $V_{\text{trap}}$ and the blue shift due to the high-energy excitons, proportional to the pumping term $V_{\text{exc}} = G P$ [17].

It is worth pointing out that equation (23) actually describes two relaxation mechanisms: (i) from the excitonic reservoir into the lower polariton branch and (ii) from high- to low-energy polariton states. Only the second relaxation process is modeled with the new dissipation mechanism derived here (the term on the second line of equation (23)).

In the absence of the relaxation term, the model (23) and (24) predicts a condensate at a single frequency (see figure 3(a)). The frequency of the condensate coincides with the potential energy at the center of the pumping spot. Away from the pumping spot, the potential energy is converted into kinetic energy.

On the other hand, when the relaxation is included (figure 3(b)), a condensate also appears at an energy close to the bottom of the trap. It is important to highlight that the steady-state solution consists of two condensates at well-defined frequencies. As our mean-field model only describes the coherent part of the bosonic field and neglects the fluctuations due to spontaneous scattering and losses, the condensate line width vanishes. To make them visible in the figure, the linewidths of the states in the figures are numerically enhanced.

Physically, it is likely that a large contribution to the relaxation within the lower polariton branch comes from the scattering of polaritons with reservoir excitons. Indeed, estimates based on the golden rule for exciton–phonon scattering [7] yield a relaxation constant of the order of $\kappa \approx 10^{-4} \mu \text{m}^2$. Our numerical simulations show relaxation toward the bottom of the lower polariton branch for $\kappa n > 0.1$. If exciton–phonon scattering was the only relaxation mechanism, it would require a polariton density $n = 10^3 \mu \text{m}^{-2}$, much larger than the experimental estimates [12].

Figure 2(b) is fully in agreement with the experimental observations in [12]. Differently from our simulations however, in experiments polariton luminescence was observed at all frequencies between the pump region and ground state [12]. In the theoretical simulations, this intermediate energy luminescence appears when a disorder potential is added to the global quadratic trapping potential. In experiments, disorder acting on polaritons is present mainly due to fluctuations in the distance between the microcavity mirrors. Figure 2(c) shows the steady state for a simulation where a disorder potential was included. Between the polaritons in the

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pumped region and at the bottom of the trap, a state at intermediate energy appears. The disorder enhances the occupation of states at energies between the pumped region and the bottom of the external potential. The relaxation now occurs in a cascaded way.

6. Conclusions

We have presented a number-conserving relaxation term for the GPE that describes the stimulated relaxation of a Bose gas due to its interaction with the environment. We have applied this model to study the damping of the elementary excitations of the homogeneous Bose gas. The damping rate is found to change sign when the condensate reaches the critical velocity. Above this speed, the condensate becomes unstable, in agreement with the Landau criterion. When the relaxation term is added to the generalized GPE for driven-dissipative condensates, we are able to describe the relaxation of a nonresonantly pumped polariton condensate in a shallow trapping potential.

Further applications of the relaxation in the description of polariton condensates include the relaxation of nonresonantly excited polariton condensates in periodic potentials [18] and the interplay of phonon relaxation with parametric scattering [19].

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