BOSE-EINSTEIN CONDENSATION BEYOND MEAN FIELD: MANY-BODY BOUND STATE OF PERIODIC MICROSTRUCTURE

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Abstract. In Bose-Einstein condensation, integer-spin atoms (Bosons) occupy macroscopically a one-particle quantum state, called condensate. We study time-independent quantum fluctuations of a mean field limit in trapped, dilute atomic gases of repulsively interacting Bosons at zero temperature. Our goal is to describe quantum-mechanically the *lowest macroscopic many-body bound state* consistent with a microscopic Hamiltonian that accounts for spatial inhomogeneity in the particle scattering processes. In the mean field limit, the wave function, $\Phi(t,x)$, of the condensate satisfies a defocusing cubic nonlinear Schrödinger-type equation (NSE), the Gross-Pitaevskii equation. We include macroscopic consequences of *pair excitation*, i.e., the scattering of particles in pairs from the condensate to other states, proposed in [Wu, *J. Math. Phys.*, 2 (1961), pp. 105–123]. From a microscopic Hamiltonian with spatially varying interaction strength, we derive a Φ-dependent integro-partial differential equation for the pair collision kernel, K. For a scattering length with periodic microstructure of subscale ϵ, we describe the effective many-body lowest bound state in terms of Φ and K up to second order in ϵ. If the external potential $V_{\rm e}$ is slowly varying, $V_{\rm e}(x) = U(\check{\epsilon}\, x)$, we solve the homogenized equations to leading order in $\check{\epsilon}$ via boundary layer theory. As an application of the perturbation program, we describe the partial depletion of the condensate.

Key words. Bose-Einstein condensation, homogenization, many-body perturbation theory, two-scale expansion, singular perturbation, mean field limit, bound state

AMS subject classifications. 81V45, 81Q15, 81V70, 82C10, 76M50, 35Q55, 45K05

1. Introduction.

A far-reaching advance in physics in 1995 was the first observation of Bose-Einstein condensation (BEC) in trapped dilute atomic gases [1,15]. In BEC, particles with integer spin (Bosons) occupy a macroscopic one-particle quantum state, usually referred to as the "condensate". This possibility was first predicted for non-interacting particles over 80 years ago [6,16,17]. Many recent experimental observations have stimulated theoretical research in systems without translation symmetry, particularly when an external potential spatially confines the atoms.

Modeling dilute atomic gases involves at least three length scales: (i) the de Broglie wavelength, l_{dB}, for the wavelike nature of particles; (ii) the mean interparticle distance, l_d; and (iii) the scattering length, a, where $a \ll l_d \ll l_{dB}$. In the absence of an external potential, $l_d = \rho^{-1/3}$ and $l_{dB} = (\rho a)^{-1/2}$ where ρ is the gas density and $\rho a^3 \ll 1$. With a trapping potential, another length is the typical size of the trap which may be larger than or comparable to l_{dB}. A known mean field limit involves a cubic nonlinear Schrödinger-type equation (NSE) (or Gross-Pitaevskii equation) for the one-particle wave function, Φ, of the condensate [33,34,54,68]. This description is adequate for many experimental situations, but does *not* capture the partial depletion of the condensate as particles scatter from it to other states [70].

In this article, we apply perturbation theory to study static effects beyond the NSE in the BEC of trapped atomic gases with a varying positive scattering length at zero temperature. We focus on the lowest many-particle bound state. This state encompasses the condensate as well as coherent superpositions of particle states amounting to the scattering of atoms from the condensate *in pairs*. For non-translation invariant settings, this *pair excitation* formalism is due to Wu [68, 69] on the basis of

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the work by Lee, Huang and Yang on periodic systems [44]. The pair excitation is described by the pair collision kernel, K, a function of two spatial variables. From a microscopic Hamiltonian with a confining potential, we (i) derive partial differential equations (PDEs) for Φ and K; (ii) homogenize these equations for an interaction strength with a periodic microstructure; and (iii) describe the condensate depletion.

A novelty of our work lies in its focus on the interplay of a periodic scattering length and trapping potential for estimating the condensate depletion. In [68, 69] no explicit connection is made of an external potential to the fraction of particles out of the condensate. Here, we show heuristically how the condensate depletion can be influenced by spatial oscillations of the scattering length combined with a trap. For this purpose, we revisit the pair excitation formalism in a reasonably general setting; and extend this formalism to scattering lengths of periodic microstructure.

The physical motivation for our work comes from experimental efforts to relate properties of ultracold atomic gases to the superfluidity of liquid Helium [11, 42, 70]. The Helium system is characterized by strong particle interactions, with a significant fraction of particles leaving the condensate to occupy other states; and, thus, is less amenable to a systematic theory. A plausible way to influence condensate depletion in atomic gases would be to control the scattering length, e.g., near a Feshbach resonance [10, 12, 40, 62], or using an optical lattice [70]. We study an aspect of the former possibility, aiming to understand the effects of inhomogeneous scattering processes, namely, a spatially varying scattering length, on the many-particle bound state. In contrast to an actual Feshbach resonance, in which particle interactions can switch sign, the atomic interactions remain repulsive throughout our analysis.

Part of our results concern deviations from the usual mean field description of the NSE because of pair excitation in a reasonably general setting of inhomogeneous scattering with periodic microstructure. Such quantum fluctuations (defined in section 3) cannot be avoided in BEC; for example, these are considered responsible for phonon creation [44, 68]. We simplify the particle model by removing complications that are not absolutely essential for a fundamental treatment; for instance, the particles are taken to be spinless. We consider *weakly interacting* atoms and non-periodic trapping potentials, leaving periodic potentials for future work; see [38, 61] for the NSE.

The present approach has been inspired by and forms an extension of work by Fibich, Sivan and Weinstein on the (one-particle) bound states of the focusing NSE [25]. In our case, an additional complication stems from the spatial *nonlocality* inherent to couplings of the PDE for the kernel K with the condensate wave function, Φ.

The mathematical context of our study is quantum many-body perturbation theory and homogenization via two-scale expansions. At the level of the many-particle Hamiltonian, perturbations are applied to many-body operators in a Hilbert space via heuristics. In the context of macroscopic equations, periodic homogenization, in the spirit of Bensoussan, Lions and Papanicolaou [2,51], is applied to PDEs with nonlinear couplings. We seek sufficiently regular solutions of the effective equations via singular perturbations for traps that vary slowly in the spatial variable. The convergence and strict legitimacy of the related asymptotic expansions is not addressed. It is hoped that our investigations will serve as an invitation to more rigorous studies.

Because the pair-excitation approach is not used widely in applied mathematics, we introduce some germane elementary concepts first, and then study their implications. For broad reviews of BEC in trapped atomic gases, the reader may consult, e.g., [7, 11, 13, 42, 46, 53, 56].

1.1. Particle model. An assumption throughout this article is that the number of particles at state Φ remains $\mathcal{O}(N)$, where N is the total (conserved) number of atoms. This hypothesis is consistent with the Bose-Einstein condensation.[1]

The starting point is the Hamiltonian, H_N, of N Bosons. This H_N encompasses three major effects: (i) the repulsive pairwise particle interaction, $\mathcal{V}$; (ii) the spatially varying scattering length, $a(x)$; and (iii) the confining potential, $V_{\rm e}(x)$:

$$H_N = \sum_{j=1}^{N}[-\Delta_j + V_{\rm e}(x_j)] + \sum_{i<j}\mathcal{V}(x_i,x_j) \qquad (x_j \in \mathbb{R}^3)\ , \tag{1.1}$$

where the units are chosen so that $\hbar = 2m = 1$ ($\hbar$: Planck's constant, m: atomic mass) and x_j are particle positions. In the above, $V_{\rm e}$ is a positive, smooth trapping potential with $V_{\rm e}(x) \to \infty$ as $|x| \to \infty$, e.g., $V_{\rm e}(x) = |x|^2$; and $\mathcal{V}(x_i,x_j)$ is a positive, symmetric, short-range interaction, which may not be translation invariant. We represent $\mathcal{V}$ by the Fermi pseudopotential for many-body problems, following Huang, Yang and Luttinger [36]. This pseudopotential comes from an effective operator that reproduces the low-energy far field in 2-body scattering [4]:[2]

$$\mathcal{V}(x_i,x_j)f(x_i,x_j) = g(x_i)\ \delta(x_i-x_j)\frac{\partial}{\partial x_{ij}}\big[x_{ij}f(x_i,x_j)\big] \qquad (i \neq j)\ , \tag{1.2}$$

where f is any 2-body wave function, $g(x) := 8\pi a(x) > 0$, $x_{ij} := |x_i - x_j|$, $\delta(x)$ is the Dirac mass in $\mathbb{R}^3$, and a is the scattering length. A rigorous definition of constant a can be found, e.g., in [22]. By omission of $(\partial/\partial x_{ij})x_{ij}$, we use [68, 69]

$$\mathcal{V}(x_i,x_j) \Rightarrow V(x_i,x_j) = g(x_i)\ \delta(x_i-x_j)\ . \tag{1.3}$$

An alternate approach is to employ a regularized interaction potential, which would be properly scaled by N [20–22]: $V = N^{3b}g(x_i,x_j)\ V_1(N^b(x_i-x_j))$ where V_1 can be chosen to be compactly supported and smooth, and $b > 0$.

The N-particle wave function $\Psi_N(t,\vec{x})$, $\vec{x} = (x_1, \ldots, x_N)$, is a crucial quantity, since it can generate all observable properties of the atomic gas. For Bosons, this Ψ_N is symmetric with respect to arbitrary permutations of the N atoms, and satisfies

$$i\partial_t\Psi_N = H_N\Psi_N \qquad (i^2 = -1)\ . \tag{1.4a}$$

For many applications, it is reasonable to consider the initial data

$$\Psi_N(0,\vec{x}) = \prod_{j=1}^{N}\Phi(x_j)\ , \tag{1.4b}$$

where $\Phi(x)$ corresponds to the condensate at $t = 0$. Bound states of Ψ_N are particular solutions to (1.4a) of the form $\Psi_N = e^{-iE_Nt}\Theta(\vec{x})$ where E_N is the total energy.

In the (simplest) case with $\mathcal{V} \equiv 0$, the wave function can be the tensor product

$$\Psi_N(t,\vec{x}) = \Psi_N^0 := \prod_{j=1}^{N}\Phi(t,x_j)\ , \qquad \Phi(0,x_j) = \Phi(x_j)\ , \tag{1.5}$$

[1] A formal definition of Bose-Einstein condensation invokes the appropriate projection operator for the condensate; see Penrose and Onsager [52].

[2] The scattering length, $a(x)$, enters our description as an ad hoc function. In contrast, in recent works by Elgart, Erdős, Schlein and Yau [18, 20–22] the (constant) scattering length emerges as an effective parameter from the mean field limit of many-particle quantum dynamics.

where $\Phi(t,x)$ obeys a *linear* Schrödinger equation on $(0,\infty)\times\mathbb{R}^3$. A nontrivial $\mathcal{V}$ in H_N (i) introduces *nonlinearities*, and (ii) spoils the tensor product (1.5) because of particle *correlations*. It is a remarkable feature of the quantum dynamics that, as $N\to\infty$, (1.5) still holds in an appropriate sense [22].

1.2. Mean field limit. The simulation of the particle model by (1.1)–(1.4) becomes impractical for $N\gg 1$. The many-body Schrödinger equation needs to be replaced by PDEs for macroscopic variables of interest in lower dimensions. One such variable is the condensate wave function, Φ. More generally, it is desirable to formulate a macroscopic theory that appropriately encapsulates the N-body dynamics, particularly the scattering of atoms in pairs, for finite yet large N.

The NSE results heuristically from the substitution of (1.5) into (1.4a) [68, 69]. Alternatively, consider the L^2-variation of the energy functional [13, 33, 34, 46, 54]

$$\mathcal{E}[u,u^*]=\int\limits_{\mathbb{R}^3}\mathrm{d}x\ \{|\nabla u|^2+(g/2)|u|^4+V_{\mathrm{e}}(x)|u|^2\}\ . \tag{1.6}$$

The condensate wave function, Φ, satisfies

$$i\partial_t\Phi(t,x)=\frac{\delta\mathcal{E}[u,u^*]}{\delta u^*}\bigg|_{(\Phi,\Phi^*)}=[-\Delta+V_{\mathrm{e}}(x)+g|\Phi||^2]\Phi\ ,\qquad g=8\pi a\ . \tag{1.7}$$

The time-translation invariance and global gauge symmetry (by $u\mapsto e^{i\theta}u$) of (1.6) entail that the energy, $\mathcal{E}$, and mass, $\|\Phi\|_{L^2}^2$, are conserved. For one-particle bound states, one seeks solutions $\Phi(t,x)=e^{-i\mu t}\phi(x)$ where $\mu\in\mathbb{R}$ is the particle 'chemical potential'. If $g<0$ (focusing case), bound states exist even if $V_{\mathrm{e}}\equiv 0$. This case was studied at the level of NSE in [25], inspiring our work. We consider the defocusing case ($g>0$) with attention to the lowest many-body bound state in a trapping V_{e}.

1.3. Pair excitation. It is worthwhile mentioning the case with periodic boundary conditions and constant scattering length, where the condensate is the state of zero momentum. This case is more transparent to physical interpretation since it is amenable to the Fourier transform on a lattice; the variables are (discrete) momenta.

Bogoliubov [5] addressed the problem of the particle energy spectrum for this setting by invoking a manipulation of the Hamiltonian. His approach, discussed in [45, 46], makes use of many-body operators in the Fourier space. The idea of pair excitation was placed on a firmer basis ten years later by Lee, Huang and Yang [44], who systematically considered the scattering of atoms from the condensate to states of nonzero momenta. By diagonalizing an approximate matrix representation of the Hamiltonian, these authors derived a formula for the N-particle wave function, Ψ_N, that distinctly deviates from the usual tensor product form: their formula expresses excitation of particles from zero momentum to *pairs of opposite momenta* [44].

The periodic case serves as a paradigm for the use of operators in pair excitation. We do not further elaborate on this case, focusing on the implications of an external potential (which removes the translation invariance). For details on the periodic case, the reader is referred to [44–46, 67].

The extension of pair creation to settings with a trapping potential is nontrivial. We adopt the extension by Wu [68, 69], who applies the *ansatz*, or trial function,

$$\Psi_N^1(t,\vec{x})=C(t)\,e^{\mathcal{P}[K](t)}\Psi_N^0(t,\vec{x})\ , \tag{1.8}$$

where Ψ_N^0 is the tensor product (1.5), $C(t)$ is a normalization factor, and $\mathcal{P}[K](t)$ is an operator that spatially averages out the excitation of particles from the condensate Φ to other states with the effective kernel ("pair excitation function") K. This K is *not* a priori known (in contrast, e.g., to the case of the classical Boltzmann gas) but is determined by means consistent with the many-body dynamics, (1.4a). The formula for $\mathcal{P}$ is expressed conveniently in terms of many-body operators; see (3.7). In the periodic case, (1.8) formally reduces to the many-body wave function found in [44].

By (1.4) and (1.8), Wu derives a system of dispersive PDEs for Φ and K; see section 3.2 for an extension to a spatially varying scattering length. K and Φ are coupled non-locally; the coupling is controlled by the scattering length. Observable quantities, e.g., the condensate depletion, can be computed from K; see section 8.

The formalism of pair excitation appears generic for the many-body quantum dynamics. Classical concepts, and too restrictive assumptions about the form of the trap, are avoided. The consequences of pair excitation in a confining potential have been studied in a limited number of cases. The effect of a slowly varying trap has been studied via singular perturbations in time-independent [69] and time-dependent [48] settings. Here, in the same vein, we apply singular perturbation to the zeroth- and second-order homogenized equations for Φ and K. Other approaches that aim to transcend the NSE are outlined (albeit non-exhaustively) in section 3.

1.4. Periodic microstructure. Following [25], we set

$$g(x) = g_0[1 + A(x/\epsilon)] > 0 \,, \qquad 0 < \epsilon \ll 1 \,, \tag{1.9}$$

where $A(x)$ is smooth and periodic with zero average. For example, in one spatial dimension (1D) with unit period, impose $A(x+1) = A(x)$ and $\int_0^1 \mathrm{d}x\, A(x) = 0$.

1.5. Program. The heart of our analysis is perturbation theory at two levels.

The first level concerns the microscopic dynamics: perturbations are applied to the microscopic Hamiltonian H_N to single out the effect of pair excitation. We review Wu's method [68], which is a generalization of the periodic case [44]; and add an extension to include a spatially varying scattering length.

To serve these goals, we revisit the formalism of quantized fields, which underlies closely related works with a physics perspective [44, 68]. Most recently, Rodnianski and Schlein use quantized fields to derive estimates for the rate of convergence to the mean field limit [58]. An extension of this work in the spirit of Wu's approach is offered in [32]. By quantized fields, the N-body Hamiltonian is viewed as an operator on the Fock space, $\mathbb{F}$, the Hilbert space for states with arbitrary number of particles.

The next level of analysis focuses on solutions of the derived static macroscopic PDEs for Φ and K. If the coupling parameter g has the microstructure (1.9), the PDEs for the many-body bound state are amenable to classical periodic homogenization [2]. For the lowest bound state, we derive homogenized equations for Φ and K including a higher-order correction in ϵ. Solutions to these equations are determined for slowly varying traps, when the Boson system is *nearly* (but not exactly) translation invariant.

1.6. Limitations. The many-body perturbation scheme is general enough to include a wide class of external potentials, such as the periodic potentials of recent experimental setups [70]. However, periodic V_e's [38, 61] are not studied here.

The classical homogenization is carried out formally, restricted to up to two (nonzero) terms in each two-scale expansion (for Φ and K). The next higher-order terms and convergence of the expansions are not addressed in this article.

We focus on zero temperature, $T = 0$. For finite temperatures ($T > 0$), the condensate coexists with thermally excited states described by a set of (a priori unknown) wave functions, $\{\Phi_j\}$, which are taken orthogonal to Φ. This means that, for $T > 0$, the PDEs for Φ and K need to be complemented with PDEs for Φ_j. (For the mean field limit of this case see, e.g., [30, 37].) This task is left for future work.

1.7. Article outline. In section 2 we outline our conventions. In section 3, we review the main formalism: in section 3.1 we revisit the quantized fields; in section 3.2 we describe the perturbation method [68]; and in section 3.3 we delineate other approaches. In section 4, we summarize our main results. In section 5, we apply the many-body theory to a varying scattering length: in section 5.1 we uncover the mean field limit; in section 5.2 we develop macroscopic equations with pair creation; and in section 5.3 we outline corrections to the NSE. In section 6, we homogenize the derived PDEs: in section 6.2 we focus on the NSE; and in section 6.3 we describe the procedure for K. In section 7, we find approximate homogenized solutions for a slowly varying trap. In section 8, we compute the fraction of particles out of the condensate. In section 9, we discuss our results and some open problems.

2. Notation conventions. We adhere to the following conventions throughout.

- $\mathbb{C}$ is the complex plane and $\mathbb{N} = \{1, 2, \ldots\}$. The star (*) operation denotes Hermitian conjugation (applied to numbers, functions, and operators).
- d is the one-particle spatial coordinate. We take $d = 3$, unless we state otherwise; for example, in section 6 some results are stated for $d \geq 1$.
- $\mathfrak{B}(\gamma, \delta)$ is the δ-neighborhood of the hypersurface γ (embedded in $\mathbb{R}^d$).
- $\mathbb{T}^d$ denotes the d-dimensional unit torus (cell). Functions that satisfy $A(x + e_k) = A(x)$ for all $x = (x^1, \ldots, x^d) \in \mathbb{R}^d$ and $k = 1, \ldots d$, where e_k's are unit Cartesian vectors, are called 1-periodic. $\langle A \rangle$ is the average (or mean) of A.
- $(F, G)_2$ denotes the one-particle inner product $\int_{\mathfrak{D}} F(x)G(x)\,\mathrm{d}x$, $\mathfrak{D} \subseteq \mathbb{R}^d$, with induced norm $\|F\|_{L^2(\mathfrak{D})}$. An inner product in Fock space is denoted by $\langle \cdot, \cdot \rangle_{\mathbb{F}}$.
- $L^2_s(\mathbb{R}^{3n})$ is the space of symmetric L^2 functions on $\mathbb{R}^{3n}$, which are invariant under permutations of the particle spatial coordinates, $(x_1, \ldots, x_n)$.
- As usual, H^1 denotes the Sobolev space $W^{k,p}$ for $k = 1$ and $p = 2$, with dual space H^{-1}; and H^1_{av} is the space of H^1 1-periodic functions with zero average.
- The dual space $H^{-1}_{\mathrm{av}}(\mathbb{T}^d) = \{f \in H^{-1}(\mathbb{T}^d) \big| \langle f \rangle = 0\}$ is the Hilbert space equipped with $(f, h)_{H^{-1}_{\mathrm{av}}(\mathbb{T}^d)} = ((-\Delta)^{-1} f, h)_{L^2(\mathbb{T}^d)}$ [27, 51]. $\|A\|_{-1}$ denotes the H^{-1}_{av}-norm of the 1-periodic $A(x)$.
- The Fourier transform of $h \in L^2(\mathbb{R}^d)$ is defined by $\widehat{h}(\lambda) = \int_{\mathbb{R}^d} h(x) e^{-i\lambda \cdot x}\,\mathrm{d}x$.
- Suppose F is $L^2(\mathbb{T}^d)$, 1-periodic of zero mean. Define $\partial_x^{-\alpha} := \prod_{k=1}^d \partial_{x^k}^{-\alpha_k}$ by

$$\partial_x^{-\alpha} F(x) := \sum_{j \neq 0} \frac{\widehat{F}_j}{\prod_{k=1}^d (i2\pi j_k)^{\alpha_k}}\, e^{i2\pi j \cdot x}\ , \quad \alpha = (\alpha_1, \ldots, \alpha_d)\ ,$$

  $\alpha_k = 0, 1, \ldots$; $j = (j_1, \ldots, j_d) \in \mathbb{Z}^d := \{\ldots, -1, 0, 1, \ldots\}^d$, and $\sum_{j \neq 0} \widehat{F}_j\, e^{i2\pi j \cdot x}$ is the Fourier series for F. In this vein, we define $(-\Delta)^{-s}$ ($s > 0$) by $(-\Delta)^{-s} F(x) := \sum_{j \neq 0} [\widehat{F}_j / (4\pi^2 |j|^2)^s] e^{i2\pi j \cdot x}$; $\langle \partial^{-\alpha} F \rangle = 0 = \langle (-\Delta)^{-s} F \rangle$.
- Writing $f = \mathcal{O}(g)$ ($f = o(g)$) means that f/g is bounded (tends to zero) in some limit. The symbol $f \sim g$ is used to imply $f - g = o(g)$.

3. Background. In this section we review the Fock space formalism, and the many-body perturbation scheme introduced for 3D in [68, 69]. For further details on the quantized fields, the reader may consult, e.g., [3, 28, 29, 35, 58].

3.1. Fock space. The Fock space, $\mathbb{F}$, is defined as the Hilbert space $\mathbb{F} = \mathbb{C} \oplus \bigoplus_{n\geq 1} L^2_s(\mathbb{R}^{3n})$ (where $\bigoplus$ denotes the direct sum). $\mathbb{F}$ consists of vectors υ formed by sequences $\{\upsilon^{(n)}\}$ of n-particle symmetric wave functions, where $\upsilon^{(n)} \in L^2_s(\mathbb{R}^{3n})$ and $n \geq 0$. In this context, $|\mathrm{vac}\rangle := \{1, 0, \ldots\} = \upsilon^{(0)} \in \mathbb{F}$ denotes the "vacuum state", which has no particles at all. The N-particle state Ψ_N is represented in $\mathbb{F}$ by $\{\upsilon^{(n)}\}_{n\geq 0}$, where $\upsilon^{(n)} \equiv 0$ for $n \neq N$ and $\upsilon^{(N)} = \Psi_N$ [58].

The next step is to express the Hamiltonian as an operator on a sector of $\mathbb{F}$. For this purpose, consider the Boson field annihilation operator $\psi(x)$ and its adjoint, the creation operator $\psi^*(x)$, $x \in \mathbb{R}^3$. For a one-particle wave function $f \in L^2(\mathbb{R}^3)$, the creation and annihilation operators $a^*(f)$ and $a(f)$ on $\mathbb{F}$ are defined by

$$(a^*(f)\upsilon)^{(n)}(\vec{x}_n) = n^{-1/2} \sum_{j=1}^{n} f(x_j)\upsilon^{(n-1)}(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_n) \ , \tag{3.1}$$

$$(a(f)\upsilon)^{(n)}(\vec{x}_n) = \sqrt{n+1} \int_{\mathbb{R}^3} \mathrm{d}x \, f^*(x)\upsilon^{(n+1)}(x, \vec{x}_n) \ ; \quad \vec{x}_n := (x_1, \ldots, x_n) \ . \tag{3.2}$$

It follows that $a(f)$ and $a^*(g)$ satisfy the commutation relations $a(f)a^*(g) - a^*(g)a(f) =: [a(f), a^*(g)] = (f, g)_{L^2}$ and $[a(f), a(g)] = [a^*(f), a^*(g)] = 0$. Accordingly, the operator-valued distributions $\psi(x)$ and $\psi^*(x)$ are defined by[3]

$$a^*(f) = \int \mathrm{d}x \, f(x) \, \psi^*(x) \ , \qquad a(f) = \int \mathrm{d}x \, f^*(x) \, \psi(x) \ , \tag{3.3}$$

where $\psi(x)$, $\psi^*(x)$ are time-independent in the Schrödinger picture. Thus, $[\psi(x), \psi^*(y)] = \delta(x - y)$ and $[\psi^*(x), \psi^*(y)] = [\psi(x), \psi(y)] = 0$; evidently, $\psi(x)|\mathrm{vac}\rangle = 0$. The particle number operator, $\mathcal{N}$, on $\mathbb{F}$ satisfies $(\mathcal{N}\upsilon)^{(n)} = n\upsilon^{(n)}$ and is given by $\mathcal{N} = \int \mathrm{d}x \, \psi^*(x) \, \psi(x)$. Note that $\psi^*\psi$ corresponds to the particle density.

The Hamiltonian H_N on $\mathbb{F}$ corresponds to the operator $\mathcal{H}$ where $(\mathcal{H}\upsilon)^{(n)} = \mathcal{H}^{(n)}\upsilon^{(n)}$, $\mathcal{H}^{(n)} = H_n$. In view of (1.1), this $\mathcal{H}$ is written in the form

$$\mathcal{H} = \int \mathrm{d}x \ \psi^*(x)[-\Delta_x + V_{\mathrm{e}}(x)]\psi(x) + \frac{1}{2} \int \mathrm{d}x \, \mathrm{d}y \ \psi^*(x)\psi^*(y)\mathcal{V}(x, y)\psi(y)\psi(x) \ . \tag{3.4}$$

By restriction to the N-particle sector of $\mathbb{F}$, we will use the symbol H_N in place of $\mathcal{H}$.

3.2. Many-body perturbation theory. The perturbation scheme should express the intuitive physical picture that a small fraction of particles escape from the condensate to occupy other states. Accordingly, split $\psi(x)$ as [68, 69]

$$\psi(x) = \psi_0(t, x) + \psi_1(t, x) \ , \tag{3.5}$$

where ψ_0 is the Boson annihilation field operator for the condensate,

$$\psi_0(t, x) := N^{-1/2} a_0(t)\Phi(t, x) \ , \quad a_0(t) := N^{-1/2} \int \mathrm{d}x \, \Phi(x)\psi(x) \ , \tag{3.6}$$

Φ is the condensate wave function, $\|\Phi\|^2_{L^2(\mathbb{R}^3)} = N$, and the operator $a_0(t)$ obeys $[a_0(t), a_0^*(t)] = 1$ and $a_0(t)|\mathrm{vac}\rangle = 0$; ψ_1 is the Boson field annihilation operator in the space orthogonal to the condensate, i.e., $\int \mathrm{d}x \, \Phi(x)\psi_1(x) = 0$.[4]

[3] The domain of integration is implied by the variables and is often not shown.

[4] The t-dependence of ψ_1 will be suppressed, unless an explicit statement is made to the contrary.

The heart of the perturbation analysis lies in the treatment of ψ_1 as small in an appropriate sense. For a more precise statement, see Remark 3.1. This implies that the Hamiltonian (3.4) can be expanded in powers of ψ_1 and ψ_1^*, where different powers yield distinct approximations at the macroscopic level when combined with corresponding expressions for Ψ_N. A difficulty is to construct viable expressions for Ψ_N.

The standard mean field limit stems from the linearization of H_N in ψ_1^* and ψ_1 by use of the tensor product ansatz (1.5) [69]. Then, the NSE dynamics comes from enforcement of the N-body Schrödinger equation (1.4a), as shown in section 5.1.

The retainment of higher-than-linear ψ_1 and ψ_1^* terms in H_N warrants the inclusion of pair excitation [68]. For example, quadratic terms amount to pairs of opposite momenta for the periodic case. The expansion for H_N must be accompanied with the modification of the ansatz for Ψ_N according to (1.8); see section 5.2 for more details.

The operator $\mathcal{P}$ generating pairs from the condensate reads [68, 69]

$$\mathcal{P}(t) = [2N_0(t)]^{-1} \int\int \mathrm{d}x\, \mathrm{d}y\ \psi_1^*(t,x)\psi_1^*(t,y)\, K(t,x,y)\, a_0(t)^2\ , \tag{3.7}$$

where $N_0(t) = (\Psi_N, a_0^*(t)a_0(t)\Psi_N)_2$ is the number of particles at the condensate, $a_0^*(t)$ (a_0) is the creation (annihilation) operator for a particle at the state Φ, and K is the pair excitation function. In (3.7), a_0^2 annihilates two particles at the condensate, while $\psi_1^*(x)\psi_1^*(y)$ creates two particles at other states at positions x and y. Thus, (3.7) implies a particle-number-conserving scheme. For definiteness, we assume that

$$K(t,x,y) = K(t,y,x)\ , \qquad (\Phi(\cdot), K(\cdot,y))_2 = 0\ , \tag{3.8}$$

and $\|K(t,x,\cdot)\|_{L^2(\mathbb{R}^3)}, \|K(t,\cdot,\cdot)\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} < \infty$.

The ψ_1-expansion of the Hamiltonian is combined with the heuristic rule

$$N = a_0^*(t)a_0(t) + \int \mathrm{d}x\ \psi_1^*(t,x)\ \psi_1(t,x)\ , \tag{3.9}$$

which sets the particle number operator equal to the (fixed) number N. This replacement is made for later algebraic convenience. Equation (3.9) should be interpreted to mean that $\mathcal{N}\Psi_N = N\Psi_N$, by restriction to the N-sector of $\mathbb{F}$.

Remark 3.1. The number of particles out of the condensate equals

$$N_1 = \langle \Psi_N, \mathcal{N}_1\Psi_N\rangle_{\mathbb{F}}\ ; \qquad \mathcal{N}_1 := \int \psi_1^*(x)\psi_1(x)\,\mathrm{d}x\ . \tag{3.10}$$

The perturbation scheme relies on the assumption that N_1/N_0 be small, where $N_0 = \langle \Psi_N, a_0^*a_0\Psi_N\rangle_{\mathbb{F}}$ is the number of particles at the condensate; thus, $N_1/N \ll 1$.

Equation (3.9) introduces a bookkeeping procedure that respects conservation of the total number of particles. Accordingly, $a_0^*a_0$ in H_N will be replaced by $N - \int \mathrm{d}x\, \psi_1^*\psi_1$, so that N enters H_N explicitly; see section 5.

Remark 3.2. In this framework, the notion of quantum fluctuations describes the many-body dynamics that arise from the presence of quadratic and higher-order ψ_1 and ψ_1^* terms in the many-particle Hamiltonian, H_N. In this case, Ψ_N deviates significantly from the tensor product form (1.5).

3.3. On past works. Theoretical efforts to describe quantum fluctuations in BEC date back to the 1940s. Recent variants, e.g. [57,64], of Bogoliubov's approach [5] essentially invoke basis functions for particle excitations in correspondence to the

external potential, $V_e(x)$. In the translation-invariant case, V_e = const., the most convenient set of such basis functions of course represents states of fixed particle momenta, thus consisting of plane waves, $e^{ik\cdot x}$.

The scheme by Esry et al. [23, 24] is based on a combination of many-body techniques, namely, the Hartree-Fock, "random phase" and "configuration interaction" approximations. This scheme appears to be tailored to the shape of the trap; basis functions are chosen accordingly. Other theories offer corrections to the NSE from a mean field viewpoint for the interaction between the condensate and other states; see, e.g., Gardiner [26], Castin and Dum [8], and Kolomeisky et al. [43]. These schemes involve only the condensate wave function; hence, they seem not to be genuinely different from the limit where particle correlations are lumped to parameters of a macroscopic theory that involves one dependent variable (Φ). It should be mentioned that studies of the excitation spectrum based on what is known in physics as the "Bogoliubov-de Gennes equations" [56] retain mostly features of the NSE. We can hardly view these methods as an exact substitute for the pair excitation formalism of this article.

Static theories of BEC often focus on the low-density expansion for the ground state energy of the particle system; see, e.g., works by Lieb et al. [45–47]. For periodic boundary conditions (without a trap), the expansion parameter is known to be $\sqrt{\rho a^3}$ where ρ is the gas density [60, 67]. In the presence of a trap, the expansion for the ground state energy corresponds to having K act back to the NSE for Φ. (Thus, the NSE must acquire nontrivial corrections.) The issue of obtaining pair-excitation corrections to the mean-field energy of the Bose gas is not addressed here. Such corrections have been pursued via a hydrodynamic theory for superfluids in [50, 55, 56].

4. Overview of results. The main results of the remainder of this article concern: (i) the derivation of equations of motion for the condensate and pair excitation with a spatially varying scattering length; (ii) two-scale expansions for Φ and K when the scattering length has a periodic microstructure; (iii) solution of the effective (homogenized) equations for slowly varying traps; and (iv) description of an expansion for the fraction of particles out of the condensate.

4.1. Equations for Φ and K (sections 5.1 and 5.2). Starting from the Hamiltonian (1.1) with a spatially varying scattering length and the many-body wave function (1.8), we show that, for bound states, the condensate wave function $\Phi(x)$ and pair excitation kernel $K(x, y)$ satisfy

$$\mathcal{L}\Phi(x) := [-\Delta_x + V_e(x) + g(x)\Phi(x)^2 - \mu]\Phi(x) = 0 \,, \tag{4.1}$$

$$\begin{aligned}&[\mathcal{L}(x) + \mathcal{L}(y) + g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2]K(x,y) + g(x)\Phi(x)^2\delta(x-y)\\ &\quad = -\mathcal{C}[\Phi, K; A](x,y) + N^{-1}\aleph[\Phi, K; A](x,y) \,.\end{aligned} \tag{4.2}$$

In the above, $\mathcal{L}(x) = -\Delta_x + V_e(x) + g(x)\Phi(x)^2 - \mu$, and $\mathcal{C}[\Phi, K; A]$ and $\aleph[\Phi, K; A]$ are (in principle) nonlinear functionals of Φ and K; see (5.4) and (5.16).

4.2. Two-scale expansions (sections 6.2 and 6.3). If the interaction strength $g(x)$ has the periodic microstructure (1.9), then $\Phi = \Phi^\epsilon$ and $K = K^\epsilon$ admit expansions of the form

$$\Phi^\epsilon = \Phi_0(x) + \epsilon^2\Phi_2(x/\epsilon, x) + \dots \,, \quad K^\epsilon = K_0(x,y) + \epsilon^2 K_2(x/\epsilon, y/\epsilon, x, y) + \dots \,. \tag{4.3}$$

By classical homogenization, the zeroth-order terms Φ_0 and K_0 are found to essentially satisfy PDEs (4.1) and (4.2), with $g(x)$ replaced by g_0. The higher-order coefficients Φ_2 and K_2 carry information for the oscillations of the scattering length. The

corresponding equations are described in Proposition 6.8 (condensate wave function) and Proposition 6.11 (pair excitation kernel), along with Remarks 6.9 and 6.13. The energy per particle of the condensate is $e = e_0 + \epsilon^2 e_2 + \ldots$; see Remark 6.10.

4.3. Slowly varying trap (sections 7.1 and 7.2). For $V_{\rm e}(x) = U(\check{\epsilon}x)$, $\check{\epsilon} \ll 1$, we derive simplified formulas for the coefficients Φ_j and K_j ($j = 0, 2$) of two-scale expansions (4.3) by singular perturbation theory. A plausible boundary layer in the NSE stems from a neighborhood of the surface $\{x \in \mathbb{R}^3 \big| U(x) < \mu\}$.

The outer and inner solutions for Φ_0 are described by (7.6) and (7.9); see Remark 7.1. The solutions pertaining to Φ_2 are described in (7.11) and (7.14), along with Remark 7.3. Formulas for the energy e are provided in (7.8) and (7.13); the effect of oscillations in $g(x)$ is pointed out in Remark 7.2.

In regard to the coefficients K_j ($j = 0, 2$), we use center-of-mass coordinates and separate these into the fast $x - y$ and slow $\check{\epsilon}(x + y)/2$. Formulas (7.21) and (7.25) describe the outer and inner solutions for the Fourier transform of $K_0(x, y)$ in $x - y$ when $\check{\epsilon}(x+y)/2$ lies inside the trap. The corresponding outer solution for the Fourier transform of K_2 is provided by (7.32).

4.4. Description of condensate depletion (sections 8.1 and 8.2). The fraction $\xi^\epsilon_{\rm sc}$ of particles that occupy one-particle states other than the condensate is computed through two-scale expansions (4.3). First, on the basis of formal expression (8.1) for $\xi^\epsilon_{\rm sc}$ in terms of the trace of an operator depending on K, we derive a formal ϵ-expansion, $\xi^\epsilon_{\rm sc} \sim \xi_{{\rm sc},0} + \epsilon^2 \xi_{{\rm sc},2}$; see (8.3)–(8.5). Second, the coefficients of this expansion are computed explicitly for a macroscopic trap, $V_{\rm e}(x) = U(\check{\epsilon}x)$, by use of the formulas of section 7; see (8.11) and (8.13). The effects on $\xi_{\rm sc}$ of particle repulsions and trapping potential are commented in Remarks 8.2 and 8.3.

5. Equations of motion: Varying scattering length. In this section, we derive macroscopic equations from Hamiltonian (3.4). The starting point is to express H_N in terms of powers of ψ_1 and ψ_1^* via the simplified interaction (1.3). Thus, we write $H_N = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + H^{(4)}$ where $H^{(m)}$ denotes the constituent part of H_N where ψ_1 and ψ_1^* appear m times.

5.1. Mean field. Next, starting from the microscopic description we show by heuristics that $\Phi(t, x)$ obeys the NSE with a varying scattering length,

$$i\partial_t \Phi(t,x) = [-\Delta + V_{\rm e}(x) + g(x)|\Phi|^2 - (1/2)\zeta(t)]\Phi \ , \tag{5.1}$$

where

$$\zeta(t) := N^{-1} \int {\rm d}x \ g(x)\, |\Phi(t,x)|^4 \ . \tag{5.2}$$

For bound states, we set[5]

$$\Phi(t,x) = e^{-i(\mu - \zeta/2)t} \Phi(x) \ , \tag{5.3}$$

eliminating ζ from (5.1), where $\mu - \zeta/2$ is the energy per particle of the condensate. We consider the lowest μ and real Φ. Equation (5.1) yields

$$[-\Delta + V_{\rm e}(x) + g(x)\Phi^2]\Phi = \mu\Phi \ . \tag{5.4}$$

[5]For notational economy, we use the same symbol, Φ, for the time-independent wave function.

We proceed to show (5.1) by revisiting, and slightly modifying, Wu's approach [69]. The Hamiltonian (3.4) needs to be linearized in ψ_1 and ψ_1^*. Hence, we write

$$H_N \sim H^{(0)} + H^{(1)} \ , \tag{5.5}$$

where, by use of the operator identity $a_0^{*2}a_0^2 = a_0^* a_0(a_0^* a_0 - 1)$, we have

$$H^{(0)} = \int \mathrm{d}x \left\{ \Phi^*(t,x)[-\Delta + V_{\mathrm{e}}(x)]\Phi(t,x) + \frac{N-1}{2N}\, g(x)|\Phi(t,x)|^4 \right\} , \tag{5.6}$$

$$H^{(1)} = N^{-1/2} \int \mathrm{d}x \ \psi_1^* \Big\{ a_0(-\Delta + V_{\mathrm{e}})\Phi + N^{-1} a_0^* a_0^2\, g(x)\Phi|\Phi|^2 \Big\} + \ \text{c.c.} \ , \tag{5.7}$$

where "c.c." denotes the Hermitian conjugate of the first term in the right-hand side. Recall (3.9), by which $a_0^* a_0 \sim N$ to imply that

$$1 - \frac{1}{N}\langle \Psi_N, a_0^* a_0 \Psi_N \rangle_{\mathbb{F}} \ll 1 \ .$$

To this order, the N-body wave function is replaced by the tensor product (1.5):

$$\Psi_N^0 = \frac{{a_0^*}^N}{\sqrt{N!}} |\mathrm{vac}\rangle \ . \tag{5.8}$$

By Schrödinger equation (1.4a) with (5.5) and the Ψ_N given by (5.8), we obtain

$$(i\partial_t a_0^*)\widetilde{\Psi}_{N-1}(t) = [\widetilde{H}^{(0)} + \widetilde{H}^{(1)}]\widetilde{\Psi}_{N-1}(t) \ . \tag{5.9}$$

Here, we used the identity $a_0 {a_0^*}^n = {a_0^*}^n a_0 + n {a_0^*}^{n-1}$, and

$$\widetilde{\Psi}_{N-1}(t) := N \frac{{a_0^*}^{N-1}}{\sqrt{N!}} |\mathrm{vac}\rangle \ , \tag{5.10}$$

$$\widetilde{H}^{(0)} := N^{-1} a_0^*(t) \int \mathrm{d}x \left\{ \Phi^*(-\Delta + V_{\mathrm{e}})\Phi + \frac{N-1}{2N}\, g(x)\, |\Phi|^4 \right\} , \tag{5.11}$$

$$\widetilde{H}^{(1)} := N^{-1/2} \int \mathrm{d}x \ \psi_1^* \Big\{ (-\Delta + V_{\mathrm{e}})\Phi + \frac{N-1}{N} g(x)\, \Phi|\Phi|^2 \Big\} \ . \tag{5.12}$$

The next step is to write down an equation of motion for $a_0^*(t)$; (5.9) implies

$$i\partial_t a_0^* = \widetilde{H}^{(0)} + \widetilde{H}^{(1)} \ . \tag{5.13}$$

By $a_0 = N^{-1/2} \int \mathrm{d}x\, \Phi(x)\psi(x)$, (5.13) yields

$$\int \mathrm{d}y\, \psi^*(y)\, (i\partial_t \Phi) = \int \mathrm{d}y\, \psi^*(y) \Big\{ -\Delta_y + V_{\mathrm{e}} + \frac{N-1}{N} g(y)|\Phi|^2 - \frac{N-1}{2N}\zeta \Big\} \Phi(y) \ , \tag{5.14}$$

where $\zeta = \zeta(t)$ is defined by (5.2). The contraction of (5.14) with $\psi(x)$, where $[\psi(x),\, \psi^*(y)] = \delta(x-y)$, leads to (5.1).

5.2. Next higher order: Pair excitation. In the remainder of this article, we restrict attention to the lowest one-particle bound states. In this section, we derive an equation of motion for the pair excitation kernel K for varying scattering length. By (3.7), the stationary form of $K(t,x,y)$ consistent with (5.4) reads

$$K(t,x,y) = e^{-i(2\mu-\zeta)t}\, K(x,y)\ , \tag{5.15}$$

since, by (3.6), $a_0(t)$ depends on time via the factor $e^{i(\mu-\zeta/2)t}$. We show that the $K(x,y)$ entering the right-hand side of (5.15) satisfies the integro-differential equation

$$\begin{aligned} 0 = {} & (-\Delta_x - \Delta_y)K + g(x)\Phi(x)^2\delta(x-y) + \{-2\widetilde{\zeta} - 2\zeta - 2\zeta_{\rm e} + V_{\rm e}(x) + V_{\rm e}(y) \\ & + 2[g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2]\}K(x,y) + \int {\rm d}z\, g(z)\Phi^*(z)^2\, K(x,z)\, K(y,z) \\ & - N^{-1}\bigg\{\int {\rm d}z\, [\Phi(y)K(x,z) + \Phi(x)K(y,z)]g(z)|\Phi(z)|^2\Phi^*(z) \\ & + \Phi(x)\Phi(y)[g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2 - \zeta]\bigg\}\ , \end{aligned} \tag{5.16}$$

where Φ obeys (5.4), and $\widetilde{\zeta}$ and $\zeta_{\rm e}$ are constants defined in (5.21); cf. (4.9) of [69] with constant g. Assuming a unique solution of (5.16) in an appropriate space, we infer that if Φ is real, the corresponding $K(x,y)$ should be taken to be real.

We proceed to derive (5.16). By keeping quadratic in ψ_1 and ψ_1^* terms in H_N, and applying ansatz (1.8) with (3.7) and $N_0 = N$, we write the Hamiltonian as

$$H_N \sim H_{N,2} = H^{(0)} + H^{(1)} + H^{(2)}\ . \tag{5.17}$$

By (5.4) and the orthogonality of Φ with ψ_1, we assert that

$$H^{(0)} + H^{(1)} = N\big(\widetilde{\zeta} + \zeta_{\rm e} + \tfrac{1}{2}\zeta\big)\ , \tag{5.18}$$

$$H^{(2)} = \int {\rm d}x\ \psi_1^*[-\Delta + V_{\rm e} - \widetilde{\zeta} - \zeta_{\rm e} - \zeta + 2g(x)\Phi^2]\psi_1 \tag{5.19}$$

$$+ \frac{1}{2}N^{-1}{a_0}^2 \int {\rm d}x\ g(x)\, \Phi^*(x)^2\, {\psi_1^*}^2 + \ \text{c.c.}\ ; \tag{5.20}$$

$$\widetilde{\zeta} := N^{-1}\int {\rm d}x\, |\nabla\Phi|^2\ , \qquad \zeta_{\rm e} := N^{-1}\int {\rm d}x\, V_{\rm e}(x)|\Phi(x)|^2\ . \tag{5.21}$$

The next step is to apply the many-body (stationary) Schrödinger equation (1.4a) with H_N replaced by (5.17) and the Ψ_N given by (1.8) and (3.7); thus,

$$H_{N,2}\Psi_N^1 = E_N\Psi_N^1 \ \Rightarrow\ \big(e^{-\mathcal{P}}H_{N,2}e^{\mathcal{P}}\big)\Psi_N^0 = E_N\Psi_N^0\ . \tag{5.22}$$

Thus, the *non-Hermitian* operator $\widetilde{H} := e^{-\mathcal{P}}H_{N,2}e^{\mathcal{P}}$ should be isospectral with $H_{N,2}$ and have eigenfunction equal to the tensor product Ψ_N^0.

The transformed operator $\widetilde{H}$ can be computed via the Lie expansion (see, e.g., [66])

$$e^{-\mathcal{P}}\mathcal{A}e^{\mathcal{P}} = \sum_{n\geq 0}\frac{(-1)^n}{n!}\,[\mathcal{P},\mathcal{A}]_n\ , \tag{5.23}$$

where $[\mathcal{P},\mathcal{A}]_n$ is the iterated commutator defined by $[\mathcal{P},\mathcal{A}]_0 = \mathcal{A}$ and $[\mathcal{P},\mathcal{A}]_{n+1} = [\mathcal{P},[\mathcal{P},\mathcal{A}]_n]$. A crucial property is $[\mathcal{P},H_{N,2}]_n = 0$, $n \geq 3$. Following [69], we find

$$\widetilde{H} = e^{-\mathcal{P}} H_{N,2} e^{\mathcal{P}} = N\big(\widetilde{\zeta} + \zeta_{\mathrm{e}} + \tfrac{1}{2}\zeta\big) + \widetilde{H}_a + \widetilde{H}_a^c \ . \tag{5.24}$$

The terms $\widetilde{H}_a$ and $\widetilde{H}_a^c$ in (5.24) play distinct roles. First, $\widetilde{H}_a$ contains $\psi_1^*\psi_1$ and ψ_1^2 and, thus, is compatible with the Ψ_N^0 of (5.22):

$$\begin{aligned}\widetilde{H}_a = \int \mathrm{d}x \, \Big\{ & \psi_1^*(x)[-\Delta - \widetilde{\zeta} - \zeta_{\mathrm{e}} - \zeta + V_{\mathrm{e}} + 2g(x)|\Phi(x)|^2]\psi_1(x) \\ & + \tfrac{1}{2} g(x)\Phi^*(x)^2 \Big[K(x,x) + 2\int \mathrm{d}y \, K(x,y)\psi_1^*(y)\psi_1(x) \Big] \\ & + \tfrac{1}{2} N^{-1} g(x) {\Phi^*}^2 {a_0^*}^2 \psi_1(x)^2 \Big\} \ . \end{aligned} \tag{5.25}$$

By contrast, $\widetilde{H}_a^c$ contains $\psi_1^*\psi_1^*$, which is in principle incompatible with (5.22):

$$\begin{aligned}\widetilde{H}_a^c = N^{-1} \int \mathrm{d}x \, \Big\{ & \tfrac{1}{2} g(x)\Phi^2 {\psi_1^*}^2 - \int \mathrm{d}y \, (\Delta_x K)\psi_1^*(x)\psi_1^*(y) + (-\widetilde{\zeta} - \zeta_{\mathrm{e}} - \zeta + V_{\mathrm{e}}) \\ & \times \int \mathrm{d}y \, K(x,y) \, \psi_1^*(x)\psi_1^*(y) + 2g(x)|\Phi(x)|^2 \int \mathrm{d}y \, K(x,y) \, \psi_1^*(x)\psi_1^*(y) \\ & + \tfrac{1}{2} g(x)\Phi^*(x)^2 \int \mathrm{d}y \, \mathrm{d}z \ K(x,y)K(x,z)\psi_1^*(y)\psi_1^*(z) \Big\} a_0^2 \ . \end{aligned} \tag{5.26}$$

This $\widetilde{H}_a^c$ is written as

$$\widetilde{H}_a^c = (2N)^{-1} \int \mathrm{d}x \mathrm{d}y \ \psi_1^*(x)\psi_1^*(y) L(x,y) a_0^2 \ , \tag{5.27}$$

where the associated kernel is

$$\begin{aligned} L(x,y) = {} & g(x)\Phi(x)^2\delta(x-y) - (\Delta_x + \Delta_y)K + \{-2\widetilde{\zeta} - 2\zeta - 2\zeta_{\mathrm{e}} + V_{\mathrm{e}}(x) + V_{\mathrm{e}}(y) \\ & + 2[g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2]\} \, K(x,y) \\ & + \int \mathrm{d}z \ g(z)\Phi^*(z)^2 \, K(x,z) \, K(y,z) - \sigma(x)\Phi(y) - \sigma(y)\Phi(x) \ ; \end{aligned} \tag{5.28}$$

$\sigma(x)$ is to be determined. Note the appearance of the Dirac mass because of the (simplified) pseudopotential interaction.

By (5.22) and (5.24), $K(x,y)$ is determined by the condition that $\widetilde{H}_a^c$ be zero [69]:

$$L(x,y) \equiv 0 \ . \tag{5.29}$$

To find $\sigma(x)$, use $\|\Phi\|^2_{L^2(\mathbb{R}^3)} = N$; thus, (5.28) leads to the integral equation

$$\begin{aligned} & \int \mathrm{d}y \, K(x,y)[-\Delta_y + V_{\mathrm{e}} + 2g(y)|\Phi(y)|^2]\Phi^*(y) + g(x)|\Phi(x)|^2\Phi(x) \\ & = N\sigma(x) + \Phi(x) \int \mathrm{d}y \, \sigma(y)\Phi^*(y) \ , \end{aligned} \tag{5.30}$$

which has the explicit solution

$$\sigma(x) = N^{-1}\Big\{ \int \mathrm{d}y \, K(x,y) g(y)|\Phi(y)|^2\Phi^*(y) + g(x)|\Phi(x)|^2\Phi(x) - \tfrac{1}{2}\zeta\Phi(x) \Big\} \ . \tag{5.31}$$

The substitution of this σ into (5.28) under (5.29) yields (5.16).

Equations (5.4) and (5.16) form the core of this article. Note that, to the present order of approximation, the NSE (5.1) is decoupled from K.

5.3. Extension. In this section we briefly discuss how the NSE is modified to include pair excitation with spatially varying scattering length, $g(x) = 8\pi a(x)$. We omit the derivation, since it is elaborate and lies outside the scope of this article, and refer the interested reader to [68] for constant g. An observation is that (5.16) is obtained from the constant-g PDE for K under simple replacements, e.g.,

$$g \int \mathrm{d}z\, \Phi^*(z)^2\, K(x,z)\, K(y,z) \Rightarrow \int \mathrm{d}z\, g(z)\Phi^*(z)^2\, K(x,z)\, K(y,z)\ . \tag{5.32}$$

Pair excitation can act back on (5.4), if terms cubic-in-ψ_1, ψ_1^* are included in the Hamiltonian H_N. By analogy with [68], the modified PDE for Φ reads

$$-B\Phi(x) + [-\Delta + g(x)\xi|\Phi|^2 + 2g(x)w(x,x)]\Phi + g(x)\widetilde{K}(x,x)\Phi^*(x) = \mu\Phi\ . \tag{5.33}$$

The parameter ξ is the condensate fraction ($0 < \xi < 1$), defined by [68]

$$\xi = \langle \Psi_N, N^{-1}(a_0^* a_0)\Psi_N\rangle_{\mathbb{F}} = 1 - N^{-1}\int w(x,x)\,\mathrm{d}x = 1 - N^{-1}\mathrm{tr}\mathcal{W}\ , \tag{5.34}$$

via operator notation. The operator $\mathcal{W}$ is written formally as

$$\mathcal{W} = \mathcal{W}_1\big(1-\mathcal{W}_1\big)^{-1}\ , \quad \mathcal{W}_1 = \mathcal{K}^*\mathcal{K}\ , \tag{5.35}$$

where $\mathcal{K}$ is the operator with kernel $K(x,y)$.[6] The kernel for $\mathcal{W}$ is

$$w(x,y) = \sum_{n\geq 1} w_n(x,y)\ ; \tag{5.36a}$$

$$w_1(x,y) = \int \mathrm{d}z\, K^*(x,z)K(z,y)\ ,\ w_n(x,y) = \int \mathrm{d}z\, w_1(x,z)w_{n-1}(z,y)\ , \tag{5.36b}$$

under the assumption that $\|K(x,\cdot)\|_{L^2(\mathbb{R}^d)} < \infty$. In the same vein, $\widetilde{K}(x,y)$ corresponds to the operator $\widetilde{\mathcal{K}} = \mathcal{K}(1-\mathcal{W}_1)^{-1}$. Formally, the respective kernels read [68]

$$\widetilde{K}(x,y) = \sum_{n\geq 0} \widetilde{K}_n(x,y)\ , \tag{5.37a}$$

$$\widetilde{K}_0(x,y) = K(x,y)\ ,\quad \widetilde{K}_n(x,y) = \int \mathrm{d}z\, K(x,z)\, w_n(z,y) \qquad n \geq 1\ . \tag{5.37b}$$

The constant B entering (5.33) is defined by [68]

$$\begin{aligned} B = {} & \tfrac{1}{2}\xi\zeta + \mu(\xi N)^{-1}\mathrm{Re}\int \mathrm{d}x\mathrm{d}y\, K(x,y)\widetilde{K}^*(y,x) \\ & + iN^{-1}\mathrm{Im}\int \mathrm{d}x\, g(x)\widetilde{K}(x,x)\Phi^*(x)^2 + (\xi N)^{-1}\int \mathrm{d}x\,[\Delta w(y,x)]\big|_{x=y}\ . \end{aligned} \tag{5.38}$$

The nonlinear eigenvalue problem corresponding to (5.33) is not further studied in this article.

[6] The operator $\mathcal{K} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is defined by $\mathcal{K}f(x) := \int K(x,y)f(y)\,\mathrm{d}y$ for $f \in L^2(\mathbb{R}^3)$. We anticipate that $\mathcal{W}_1$ is bounded with norm, $\|\mathcal{W}_1\|$, controlled by g_0; for sufficiently small g_0, $\|\mathcal{W}_1\|$ can be small enough to ensure invertibility of $1-\mathcal{W}_1$. In section 8, we sketch an argument that this statement holds for a slowly varying trap; see Remark 8.1. A rigorous proof that $(1-\mathcal{W}_1)^{-1}$ exists would require a priori estimates on the solution of (5.16), and lies beyond our present purposes.

6. Periodic homogenization. In this section, we study (5.4) and (5.16) with the periodic $g(x)$ of (1.9) for the lowest bound state. To demonstrate the computations with relative ease, we present the homogenization program mainly in 1D (sections 6.2 and 6.3). The homogenization results are then extended to 3D without further ado.

6.1. Preliminaries. In this subsection, we outline our main assumptions for one-particle spatial dimension $d = 1$, 2 or 3. The starting point consists of the two-scale expansions

$$\Phi^\epsilon = \Phi_0(\tilde{x}, x) + \sum_{n\geq 1} \epsilon^n \, \Phi_n(\tilde{x}, x) \ , \quad K^\epsilon = K_0(\tilde{x}_{(2)}, x_{(2)}) + \sum_{n\geq 1} \epsilon^n \, K_n(\tilde{x}_{(2)}, x_{(2)}) \ , \tag{6.1}$$

where $\tilde{x}_{(2)} := (\tilde{x}, \tilde{y}) = (x/\epsilon, y/\epsilon)$ is the fast variable and $x_{(2)} := (x, y)$ is the slow variable. The eigenvalue μ^ϵ for the condensate is real and expanded as

$$\mu^\epsilon = \sum_{n\geq 0} \epsilon^n \, \mu_n \ , \qquad \mu_n = \mathcal{O}(1) \quad \text{as } \epsilon \downarrow 0 \ . \tag{6.2}$$

The study of convergence of expansions (6.1) and (6.2) lies beyond our purposes. We restrict attention to the computation of the first *two nonzero* terms of these expansions, which we deem adequate for predictions regarding dilute atomic gases. The corresponding energy is discussed in section 7. The procedure presented here can be extended to higher orders, yet it becomes increasingly cumbersome in n.

Our main hypotheses are summarized in the following remarks.

Remark 6.1. We assume that the $A(\tilde{x})$ in (1.9) is 1-periodic and smooth; and $V_{\rm e}$ is a smooth, positive trapping potential, monotone in $|x|$ and growing algebraically at large distances, i.e., $V_{\rm e}(x) = \mathcal{O}(|x|^\varrho)$ as $|x| \to \infty$, $\varrho > 1$. In view of (1.9), we set

$$A(\tilde{x} + e_k) = A(\tilde{x}) \ , \quad \langle A \rangle = 0 \ , \tag{6.3}$$

for all $k = 1, \ldots, d$ where $\{e_k\}_{k=1}^d$ are unit Cartesian vectors.

Remark 6.2. We consider 1-periodic $\Phi_n(\cdot, x)$ and $K_n(\cdot, x_{(2)})$, and assume that $K_n(\tilde{x}_{(2)}, \cdot) \in W^{1,1}(\mathbb{R}^d \times \mathbb{R}^d)$ (see section 7). Further, we impose $\|\Phi_n(\tilde{x}, \cdot)\|_{H^1(\mathbb{R}^d)} < \infty$ and $\|K_n(\tilde{x}_{(2)}, \cdot)\|_{L^2} < \infty$. For later convenience, take $\Phi_n(\tilde{x}, x)$ to be bounded, sufficiently differentiable and decay rapidly for large x, as anticipated from properties of $V_{\rm e}(x)$ and $A(\tilde{x})$.

Remark 6.3. The physical domains of Φ^ϵ and K^ϵ are $\mathbb{R}^3$ and $\mathbb{R}^3 \times \mathbb{R}^3$ ($d = 3$). It will be explicitly shown that the kernel $K^\epsilon(x, y)$ is weakly singular on the diagonal ($x = y$), due to the presence of the forcing term proportional to the Dirac mass in (5.16); see Remark 7.4. In our homogenization program for the kernel $K(x, y)$ (section 6.3), we essentially restrict attention off the diagonal (for $x \neq y$).

In sections 6.2 and 6.3 we make use of a few results, which we state here in the form of lemmas for d spatial dimensions. The first lemma, given without proof, is a consequence of the Fredholm alternative (see also [51] and Lemma 4 in [25]).

LEMMA 6.4 (Solvability condition). *Equation $-\Delta u = S(\cdot, x)$, where $S(\cdot, x)$ is 1-periodic, admits a 1-periodic solution $u(\cdot, x)$ only if*

$$\langle S(\cdot, x) \rangle = \int_{\mathbb{T}^d} S(\tilde{x}, x) \, \mathrm{d}\tilde{x} = 0 \ . \tag{6.4}$$

If (6.4) is satisfied, the solution to $-\Delta_{\tilde{x}} u = S(\tilde{x}, x)$ reads (see Remark 5 in [25])

$$u(\tilde{x}, x) = -\Delta_{\tilde{x}}^{-1} S(\tilde{x}, x) + c(x) \ , \tag{6.5}$$

where $c(x)$ is reasonably arbitrary. Note that $\Delta_{\tilde{x}}^{-1} S$ is 1-periodic with zero mean. We refer to any solution of form (6.5) with $\langle S \rangle = 0$ as "admissible".

The next lemma concerns oscillatory integrals; for similar results, see, e.g., [19].

LEMMA 6.5 (Oscillatory integrals I). *Consider the function $h : \mathbb{R}^d \to \mathbb{R}$ and the 1-periodic $P : \mathbb{R}^d \to \mathbb{R}$ with $\langle P \rangle = 0$. Suppose P is bounded ($P \in L^\infty(\mathbb{R}^d)$) and h has m summable derivatives for some $m \in \mathbb{N}$, with $\partial_x^\beta h := \partial_{x_1}^{\beta_1} \cdots \partial_{x_d}^{\beta_d} h \to 0$ as $|x| \to \infty$, where $\sum_{k=1}^d \beta_k \leq m-1$, $\beta_k \geq 0$, $\beta = (\beta_1, \ldots, \beta_d)$; then,*

$$\int_{\mathbb{R}^d} P\left(\frac{x}{\epsilon}\right) h(x)\, \mathrm{d}x = \mathcal{O}(\epsilon^m) \qquad \text{as } \epsilon \downarrow 0 \ . \tag{6.6}$$

Proof. Define the 1-periodic $P^{(-\alpha)}(\tilde{x}) := \partial_{\tilde{x}}^{-\alpha} P(\tilde{x})$ where $|\alpha| := \sum_{k=1}^d \alpha_k = m$.

$$\begin{aligned} I(\epsilon) &:= \epsilon^d \int_{\mathbb{R}^d} P(\tilde{x})\, h(\epsilon\tilde{x})\, \mathrm{d}\tilde{x} = \epsilon^d \int \mathrm{d}\tilde{x}\, [\partial_{\tilde{x}}^\alpha P^{(-\alpha)}(\tilde{x})]\, h(\epsilon\tilde{x}) \\ &= (-1)^{|\alpha|} \epsilon^{|\alpha|+d} \int \mathrm{d}\tilde{x}\, P^{(-\alpha)}(\tilde{x})\, h^{(\alpha)}(\epsilon\tilde{x}) \ , \quad h^{(\alpha)}(x) := \partial_x^\alpha h \ , \end{aligned} \tag{6.7}$$

where we applied integration by parts with vanishing boundary terms. Consequently,

$$|I(\epsilon)| \leq \epsilon^m \|P^{(-\alpha)}\|_{L^\infty} \int_{\mathbb{R}^d} |h^{(\alpha)}(x)|\, \mathrm{d}x \leq C\epsilon^m, \tag{6.8}$$

which is the desired estimate. □

Another result for oscillatory integrals invokes the Fourier transform.

LEMMA 6.6 (Oscillatory integrals II). *Consider $h : \mathbb{R}^d \to \mathbb{C}$ and the 1-periodic $P : \mathbb{R}^d \to \mathbb{C}$ where $h \in L^2(\mathbb{R}^d)$, $P \in L^2(\mathbb{T}^d)$ and $\langle P \rangle = 0$. Suppose that the Fourier transform of $h(x)$ satisfies $e^{i\lambda\cdot x_0}\widehat{h}(\lambda) = c_1\, \lambda^{-2s} + o(|\lambda|^{-2s})$ as $|\lambda| \to \infty$, $\lambda \in \mathbb{R}^d$, for some $s > d/4$, $x_0 \neq 0$ and constant $c_1 \in \mathbb{C}$. Then, we have the asymptotic formula*

$$\int_{\mathbb{R}^d} P\left(\frac{x}{\epsilon}\right) h(x)\, \mathrm{d}x = c_1\, \epsilon^{2s}\, (-\Delta)^{-s} P\left(\frac{x_0}{\epsilon}\right) + o(\epsilon^{2s}) \quad \text{as } \epsilon \downarrow 0 \ . \tag{6.9}$$

Note that the condition $4s > d$ is consistent with $h \in L^2(\mathbb{R}^d)$.

Proof. By $P(x) = \sum_{j\neq 0} \widehat{P}(j)\, e^{i2\pi j\cdot x}$ and $\widehat{h}(\lambda) = \int_{\mathbb{R}^d} e^{-i\lambda\cdot x}\, h(x)\, \mathrm{d}x$,

$$\begin{aligned} \int_{\mathbb{R}^d} P\left(\frac{x}{\epsilon}\right) h(x)\, \mathrm{d}x &= \sum_{j\neq 0} \widehat{P}(j) \int e^{i(2\pi j/\epsilon)\cdot x} h(x)\, \mathrm{d}x = \sum_{j\neq 0} \widehat{P}(j)\, \widehat{h}\left(-\frac{2\pi j}{\epsilon}\right) \\ &= \sum_{j\neq 0} \widehat{P}(j) \left[\frac{c_1 e^{i2\pi j\cdot(x_0/\epsilon)}}{(-2\pi j/\epsilon)^{2s}} + o(\epsilon^{2s}|j|^{-2s})\right] \qquad \text{as } \epsilon \downarrow 0 \ , \end{aligned} \tag{6.10}$$

which leads to the desired result, in view of the Fourier series for $(-\Delta)^{-s} P(x_0/\epsilon)$. □

A few comments on the relevance of Lemmas 6.5 and 6.6 are in order. We apply both lemmas to integrals with $P(\tilde{x}) \equiv \partial_{\tilde{x}}^{-\alpha} A(\tilde{x})$. Lemma 6.5 is invoked for integrals where h involves: (i) products of Φ_n, supplied with sufficient regularity, i.e., high enough m; or (ii) products of K_n, for which $m = 1$ by hypothesis. Lemma 6.6 is used to refine information about integrals containing products of K_n, in anticipation of a

singularity on the diagonal for each factor. For example, in section 6.3 we encounter an integral of the form

$$\int_{\mathbb{R}^d} \mathrm{d}z\ P\left(\frac{z}{\epsilon}\right) f(z)\,\kappa_0(x,z)\,\kappa_0(z,y) = \sum_{j\neq 0} \widehat{P}(j) \int \mathrm{d}z\ e^{i(2\pi j/\epsilon)\cdot z} f(z)\,\kappa_0(x,z)\,\kappa_0(z,y)\ ,$$

where, by inspection of PDE (5.16) and from section 7 for $K_0 = \kappa_0$, $\kappa_0(x,z)$ is weakly singular at $z = x$. As $\epsilon \downarrow 0$, the major contribution to integration comes from balls of radii $\mathcal{O}(\epsilon)$ centered at $z = x$ and $z = y$. By assuming $|x-y| > \mathcal{O}(\epsilon)$, we can isolate these two contributions; thus, we compute

$$\begin{aligned}\int \mathrm{d}z\ e^{i(2\pi j/\epsilon)\cdot z} f(z)\,\kappa_0(x,z)\,\kappa_0(z,y) \sim f(x)\kappa_0(x,y) \int \mathrm{d}z\ e^{i(2\pi j/\epsilon)\cdot z}\,\kappa_0(x,z) \\ + f(y)\kappa_0(x,y) \int \mathrm{d}z\ e^{i(2\pi j/\epsilon)\cdot z}\,\kappa_0(z,y)\ . \end{aligned} \tag{6.11}$$

The emerging integrals can be estimated by recourse to Lemma 6.6 if sufficient information is provided for the Fourier transform of $\kappa_0(\cdot, z)$. In the case where V_{e} tends to become a constant (in some appropriate sense), the system becomes translation invariant and $K_n(\tilde{x}_{(2)}, x_{(2)})$ depends only on $x - y$. For a slowly varying V_{e}, an additional, *slow* variable is proportional to $x + y$ and can be treated as a parameter; thus, $K_n(\tilde{x}_{(2)}, x, y)$ depends primarily on $x - y$ (see section 7 for details).

Remark 6.7. We assume that the Fourier transform of $K_0(\tilde{x}_{(2)}, x, \cdot)$, with fixed $\tilde{x}_{(2)}$ and x, satisfies the hypothesis of Lemma 6.6 with $x_0 \approx x$ and $s \geq 1$. In fact, the value $s = 1$ is extracted by heuristics in section 7 via the center-of-mass coordinates and singular perturbations for macroscopic traps.

6.2. Effective equations for condensate. For $d = 1$, (5.4) for the condensate wave function becomes

$$\{-\partial_x^2 + V_{\mathrm{e}}(x) + g_0[1 + A(x/\epsilon)](\Phi^\epsilon)^2\}\Phi^\epsilon(x) = \mu^\epsilon \Phi^\epsilon\ . \tag{6.12}$$

In this section, we focus on (6.12) under (6.1) and (6.2). We will show that, as in the case of the focusing NSE [25], we have $\Phi_1 \equiv 0$.

Proposition 6.8 (Consistency of two-scale expansion with NSE). *The formal two-scale expansion for $\Phi^\epsilon(x)$, $x \in \mathbb{R}$, up to $\mathcal{O}(\epsilon^2)$, reads*

$$\Phi^\epsilon(x) = f_0(x) + \epsilon^2 \left\{g_0 f_0(x)^3 \left[\partial_{\tilde{x}}^{-2} A(\tilde{x})\right] + f_2(x)\right\} + \ \ldots\ , \tag{6.13}$$

where f_0, $f_2 \in H^1(\mathbb{R})$, $N^{-1}\|f_0\|^2_{L^2(\mathbb{R})} = 1$, $(f_0, f_2)_2 = 0$, and

$$\mathcal{L}_0 f_0 := [-\partial_x^2 + V_{\mathrm{e}}(x) + g_0 f_0(x)^2 - \mu_0] f_0 = 0\ , \tag{6.14}$$

$$\mathcal{L}_2 f_2 := [-\partial_x^2 + V_{\mathrm{e}}(x) + 3g_0\, f_0(x)^2 - \mu_0] f_2(x) = 3g_0^2 f_0^5\ \|A\|^2_{-1} + \mu_2 f_0\ ; \tag{6.15}$$

$\mathcal{L}_2 := \mathcal{L}_0 + 2g_0 f_0^2$. The lowest eigenvalue μ^ϵ is given by expansion (6.2) *with*

$$\mu_0 = \zeta_0 + \widetilde{\zeta_0} + \zeta_{\mathrm{e}0}\ , \tag{6.16}$$

$$\mu_1 = 0\ , \tag{6.17}$$

$$\mu_2 = -3g_0^2\,\|A\|_{-1}^2\,\frac{(f_0,\mathcal{L}_2^{-1}f_0^5)_2}{(f_0,\mathcal{L}_2^{-1}f_0)_2}\ , \tag{6.18}$$

and

$$\zeta_0 := g_0N^{-1}\|f_0^2\|_{L^2}^2\ ,\quad \widetilde{\zeta}_0 := N^{-1}\|\partial_x f_0\|_{L^2}^2\ ,\quad \zeta_{\mathrm{e}0} := N^{-1}(f_0,V_{\mathrm{e}}f_0)_2\ . \tag{6.19}$$

In the proof of Proposition 6.8 we invoke the 1D versions of Lemmas 6.4 and 6.5. We do not address the existence of solution to (6.14), assuming that a finite-energy solution, f_0, exists. For a rigorous variational treatment of bound states of NSE, see, e.g., [59, 63] (and [31] for nodal solutions).[7] Given a nontrivial f_0, the existence of a reasonably unique finite-energy f_2 should stem from the invertibility of $\mathcal{L}_2$ (as outlined in the proof below).

Proof. The substitution of (6.1) and (6.2) into (6.12) along with the replacement of ∂_x by $\partial_x+\epsilon^{-1}\partial_{\tilde{x}}$ yield the following cascade of equations for Φ_n:

$$\mathcal{O}(\epsilon^0):\ -\partial_{\tilde{x}}^2\Phi_0 = 0 =: S_0\ , \tag{6.20}$$

$$\mathcal{O}(\epsilon^1):\ -\partial_{\tilde{x}}^2\Phi_1 = 2\partial_x\partial_{\tilde{x}}\Phi_0 =: S_1\ , \tag{6.21}$$

$$\mathcal{O}(\epsilon^2):\ -\partial_{\tilde{x}}^2\Phi_2 = 2\partial_{\tilde{x}}\partial_x\Phi_1 - \{-\partial_x^2+V_{\mathrm{e}}(x)+g_0[1+A(\tilde{x})]\Phi_0^2-\mu_0\}\Phi_0 =: S_2\ , \tag{6.22}$$

$$\mathcal{O}(\epsilon^3):\ -\partial_{\tilde{x}}^2\Phi_3 = 2\partial_{\tilde{x}}\partial_x\Phi_2 - \{-\partial_x^2+V_{\mathrm{e}}(x)+3g_0[1+A(\tilde{x})]\Phi_0^2-\mu_0\}\Phi_1 + \mu_1\Phi_0 =: S_3\ , \tag{6.23}$$

$$\mathcal{O}(\epsilon^4):\ -\partial_{\tilde{x}}^2\Phi_4 = 2\partial_{\tilde{x}}\partial_x\Phi_3 - \{-\partial_x^2+V_{\mathrm{e}}+3g_0[1+A(\tilde{x})]\Phi_0^2-\mu_0\}\Phi_2 - 3g_0[1+A(\tilde{x})]\Phi_0\Phi_1^2+\mu_1\Phi_1+\mu_2\Phi_0 =: S_4\ . \tag{6.24}$$

Note the appearance of V_{e} only in the equations for $n\geq 2$. Equations (6.20)–(6.24) suffice for our purpose of determining Φ_0 along with the corrections Φ_1 and Φ_2.

To determine μ_n for $n\geq 1$, we need to consider the normalization condition $\|\Phi^\epsilon\|_{L^2}^2 = N$ (which affects the prefactor in the nonlinear term of the NSE for Φ^ϵ). The two-scale expansion (6.1) for Φ^ϵ yields the conditions

$$\|\Phi_0\|_{L^2}^2 = N\ ,\quad (\Phi_0,\Phi_1)_2 = 0\ ,\quad \|\Phi_1\|_{L^2}^2 + 2(\Phi_0,\Phi_2)_2 = 0\ , \tag{6.25}$$

where N is a treated as an $O(1)$ parameter.

PDEs (6.20)–(6.24) for Φ_n are recast conveniently to

$$-\partial_{\tilde{x}}^2\Phi_n = S_n(\tilde{x},x)\ ;\qquad S_n(\tilde{x}+1,x) = S_n(\tilde{x},x)\ . \tag{6.26}$$

Equation (6.26) is solved via Lemma 6.4 for $d=1$.

By (6.5), (6.20) and (6.21), the admissble Φ_0 and Φ_1 are $\tilde{x}$-independent:

$$\Phi_0(\tilde{x},x) = f_0(x)\ ,\qquad \Phi_1(\tilde{x},x) = f_1(x)\ . \tag{6.27}$$

By contrast, the remaining terms of expansion (6.1) are strictly $(\tilde{x},x)$-dependent.

To derive an equation for $f_0(x)$ we resort to (6.22). By applying Lemma 6.4 to $S_2(\tilde{x},x)$ we obtain (6.14). Formula (6.16) for μ_0 is obtained by taking the L^2-inner product of (6.14) with f_0 and using the first one of relations (6.25), $\|f_0\|_{L^2}^2 = N$. The enforcement of (6.14) in (6.22) leads to

$$\partial_{\tilde{x}}^2\Phi_2 = g_0A(\tilde{x})f_0(x)^3\ \Rightarrow\ \Phi_2(\tilde{x},x) = g_0f_0(x)^3\,[\partial_{\tilde{x}}^{-2}A(\tilde{x})] + f_2(x)\ . \tag{6.28}$$

[7] In [31, 59] the authors primarily address the focusing NSE. We deem their variational approach as applicable to the defocusing case with a trapping potential.

We address the $f_2(x)$ introduced above at a later stage of this proof.

Next, $\Phi_1(x) = f_1(x)$ is determined with recourse to (6.23). Application of solvability condition (6.4) to the right-hand side of (6.23) entails

$$[-\partial_x^2 + V_{\rm e}(x) + 3g_0 f_0(x)^2 - \mu_0] f_1(x) = \mu_1 f_0(x) \qquad (g_0 > 0) \ . \tag{6.29}$$

We now show that (6.29) admits only the trivial solution,

$$\mu_1 = 0 \ , \quad f_1 = 0 \ \text{(a.e.)} \ . \tag{6.30}$$

Consider the following argument for given μ_0 and (nontrivial) f_0. Equation (6.29) has the form $\mathcal{L}_2 f_1 = \mu_1 f_0$, where the operator $\mathcal{L}_2[f_0] = \mathcal{L}_0[f_0] + 2g_0 f_0^2$ is symmetric. By (6.14) we have that $\mathcal{L}_0$ is positive, i.e., $(f, \mathcal{L}_0 f)_2 \geq 0$ for any $f \in H^1(\mathbb{R})$. In view of the second condition in (6.25), the (L^2-) inner product of (6.29) with f_1 furnishes $(f_1, \mathcal{L}_2 f_1)_2 = \mu_1 (f_1, f_0)_2 = 0$. On the other hand, for any $f_1 \in H^1(\mathbb{R})$, $(f_1, \mathcal{L}_2 f_1)_2 = (f_1, \mathcal{L}_0 f_1)_2 + 2g_0 (f_1, f_0^2 f_1)_2 > 0$ only if $\|f_1\|_{L^2} \neq 0$; thus, $\mathcal{L}_2$ is positive definite. Notice that 0 does not belong to the point spectrum of $\mathcal{L}_2$. We infer that $f_1 = 0$ (a.e.). Thus, (6.29) yields $\mu_1 = 0$. By (6.29), $\Phi_3(\tilde{x}, x)$ is given by

$$\Phi_3(\tilde{x}, x) = -2g_0 (\partial_x f_0^3)[\partial_{\tilde{x}}^{-3} A(\tilde{x})] + 3g_0 f_0(x)^2 f_1(x) \, [\partial_{\tilde{x}}^{-2} A(\tilde{x})] + f_3(x) \ . \tag{6.31}$$

We turn our attention to $f_2(x)$ entering (6.28). By (6.24), we obtain

$$\begin{aligned} S_4(\tilde{x}, x) = {} & \partial_x^2 f_2 - V_{\rm e}(x) \, f_2(x) - 3g_0 f_0 [1 + A(\tilde{x})] \{ f_0(x) [g_0 f_0(x)^3 (\partial_{\tilde{x}}^{-2} A) + f_2] + f_1^2 \} \\ & + \mu_0 \, f_2(x) + \mu_1 f_1(x) + \mu_2 f_0(x) - g_0 [3(\partial_x^2 f_0^3) + (V_{\rm e} - \mu_0) f_0(x)^3] (\partial_{\tilde{x}}^{-2} A) \\ & + 6g_0 \, \partial_x (f_0^2 f_1) (\partial_{\tilde{x}}^{-1} A) \ . \end{aligned} \tag{6.32}$$

Hence, solvability condition (6.4) applied on S_4 readily provides (6.15) by use of (6.30). To derive (6.15) from (6.32), we invoke the relations

$$\langle A \, (\partial_{\tilde{x}}^{-2} A) \rangle = (A, \partial_{\tilde{x}}^{-2} A)_2 = -\|A\|_{-1}^2 \ . \tag{6.33}$$

It remains to assert (6.18) for μ_2. Equation (6.15) is recast to the form $\mathcal{L}_2 f_2 = b(x)$, where $b(x) := 3g_0^2 f_0^5 \, \|A\|_{-1}^2 + \mu_2 f_0$ and the operator $\mathcal{L}_2 = \mathcal{L}_0 + 2g_0 f_0^2$ is invertible, as is concluded in the course of deriving (6.30); thus, $f_2 = \mathcal{L}_2^{-1} b(x)$:

$$f_2(x) = 3g_0^2 \|A\|_{-1}^2 \, \mathcal{L}_2^{-1} f_0^5 + \mu_2 \, \mathcal{L}_2^{-1} f_0 \ . \tag{6.34}$$

The term μ_2 can now be determined with recourse to the third one of conditions (6.25), which reduces to $(\Phi_0, \Phi_2)_2 = 0$. By (6.28), we have

$$\mu_2 (f_0, \mathcal{L}_2^{-1} f_0)_2 = -3g_0^2 \|A\|_{-1}^2 (f_0, \mathcal{L}_2^{-1} f_0^5)_2 - g_0 (f_0, (\partial_{\tilde{x}}^{-2} A) f_0^3)_2 \ . \tag{6.35}$$

This relation yields (6.18). We applied Lemma 6.5 to the integral for $(f_0, (\partial_{\tilde{x}}^{-2} A) f_0^3)_2$ with $P(\tilde{x}) \equiv \partial_{\tilde{x}}^{-2} A(\tilde{x})$; note that $\langle \partial_{\tilde{x}}^{-2} A \rangle = 0$ and f_0 is sufficiently regular. By (6.34),

$$f_2(x) = 3g_0^2 \|A\|_{-1}^2 \left[\mathcal{L}_2^{-1} f_0^5 - \frac{(f_0, \mathcal{L}_2^{-1} f_0^5)_2}{(f_0, \mathcal{L}_2^{-1} f_0)_2} \, \mathcal{L}_2^{-1} f_0 \right] , \tag{6.36}$$

which indeed satisfies $(f_0, f_2)_2 = 0$. This observation concludes our proof. □

Remark 6.9. Proposition 6.8 can be directly extended to d spatial dimensions, $d \geq 2$. The two-scale expansion for Φ^ϵ reads

$$\Phi^\epsilon(x) = f_0(x) + \epsilon^2 \, \{ g_0 f_0(x)^3 \, [\Delta_{\tilde{x}}^{-1} A(\tilde{x})] + f_2(x) \} + \ \dots \ , \tag{6.37}$$

where $f_0(x)$ and $f_2(x)$ satisfy

$$[-\Delta_x + V_{\rm e}(x) + g_0 f_0(x)^2 - \mu_0] f_0 = 0 \ , \tag{6.38}$$

$$[-\Delta_x + V_{\rm e}(x) + 3g_0\, f_0(x)^2 - \mu_0] f_2(x) = 3g_0^2 f_0^5 \ \|A\|_{-1}^2 + \mu_2 f_0 \ ; \tag{6.39}$$

$\|A\|_{-1} = \|A\|_{H^{-1}_{\rm av}(\mathbb{T}^d)}$.

Remark 6.10. Proposition 6.8 provides an expansion for μ. A corresponding expansion for the energy, e, per particle of the condensate follows from the relation $e = \mu - \zeta/2$ via Lemma 6.5: $e = e_0 + \epsilon^2 e_2 + \dots$, where

$$e_0 = \mu_0 - \frac{g_0}{2} N^{-1} \int f_0(x)^4 \, {\rm d}x \ , \quad e_2 = \mu_2 - 2g_0 N^{-1} \int f_0(x)^3 \, f_1(x) \, {\rm d}x \ . \tag{6.40}$$

6.3. Effective equations for pair excitation. In this section, we focus on (5.16) by neglecting terms proportional to N^{-1}.[8] For $d = 1$, the equation of interest reads

$$\begin{aligned} 0 = {} & (-\partial_x^2 - \partial_y^2) K^\epsilon + g_0 [1 + A(x/\epsilon)] \Phi^\epsilon(x)^2 \delta(x-y) + \{ -2\widetilde{\zeta}^\epsilon - 2\zeta^\epsilon - 2\zeta_{\rm e}^\epsilon \\ & + V_{\rm e}(x) + V_{\rm e}(y) + 2g_0 ([1 + A(x/\epsilon)] |\Phi^\epsilon(x)|^2 + [1 + A(y/\epsilon)] |\Phi^\epsilon(y)|^2) \} K^\epsilon(x,y) \\ & + g_0 \int {\rm d}z \, [1 + A(z/\epsilon)] \Phi^\epsilon(z)^2 \, K^\epsilon(x,z) \, K^\epsilon(y,z) \ , \end{aligned} \tag{6.41}$$

where

$$\begin{aligned} & \zeta^\epsilon := g_0 N^{-1} \int {\rm d}x \, [1 + A(x/\epsilon)] \Phi^\epsilon(x)^4 \ , \quad \widetilde{\zeta}^\epsilon := N^{-1} \int {\rm d}x \ (\partial_x \Phi^\epsilon)^2 \ , \\ & \zeta_{\rm e}^\epsilon := N^{-1} \int {\rm d}x \, V_{\rm e}(x) \, \Phi^\epsilon(x)^2 \ . \end{aligned} \tag{6.42}$$

By substituting expansion (6.1) for $K^\epsilon(x,y)$ into PDE (6.41), we derive effective equations for the coefficients K_n. The nonlocal term will be treated with recourse to Lemma 6.5 with $m = 1$ and Lemma 6.6 for $s = 1$ (see Remark 6.7). In the following, we treat Φ_n as known.

PROPOSITION 6.11. *The two-scale expansion for the pair excitation function $K^\epsilon(x,y)$, $(x,y) \in \mathbb{R}^2$, reads*

$$\begin{aligned} K^\epsilon(x,y) = {} & \kappa_0(x,y) + \epsilon^2 \{ g_0 (\partial_{\tilde{x}}^{-2} A(\tilde{x})) f_0(x)^2 \, \delta(x-y) + 2g_0 [(\partial_{\tilde{x}}^{-2} A(\tilde{x})) f_0(x)^2 \\ & + (\partial_{\tilde{y}}^{-2} A(\tilde{y})) f_0(y)^2] \kappa_0(x,y) + \kappa_2(x,y) \} + \dots \ , \end{aligned} \tag{6.43}$$

where $\kappa_0(x,y)$ and $\kappa_2(x,y)$ satisfy

$$\begin{aligned} \mathcal{L}_{(xy)} \kappa_0 := {} & \{ -\Delta_{xy} + V_{\rm e}(x) + V_{\rm e}(y) + 2g_0 [f_0(x)^2 + f_0(y)^2] - 2\mu_0 \} \kappa_0 \\ = {} & -\mathcal{C}[f_0^2, \kappa_0] \kappa_0(x,y) + B_0(x,y) \ , \qquad \Delta_{xy} := \partial_x^2 + \partial_y^2 \ , \end{aligned} \tag{6.44}$$

$$\mathcal{L}_{(xy)} \kappa_2 = -2\mathcal{C}[f_0^2, \kappa_0] \kappa_2(x,y) + B_2(x,y) \ , \tag{6.45}$$

[8] Because of this simplification, the orthogonality of K^ϵ and Φ^ϵ is strictly abandoned. This loss is not expected to distort the essential physics (with $d = 3$) for large N [69].

with $\mathcal{L}_{(xy)} = \mathcal{L}_0(x) + \mathcal{L}_0(y) + g_0[f_0(x)^2 + f_0(y)^2]$. *Recall that* $\mathcal{L}_0(x) = -\partial_x^2 + V_{\rm e}(x) + g_0 f_0(x)^2 - \mu_0$. *The operator* $\mathcal{C}[f,F]$ *and forcing terms* $B_0(x,y)$, $B_2(x,y)$ *are*

$$\mathcal{C}[f,F]K(x,y) := g_0 \int \mathrm{d}z\, f(z)\ \mathrm{Sym}\{F,K\}(z;x,y)\ , \tag{6.46}$$

$$\mathrm{Sym}\{F,K\}(z;x,y) := \tfrac{1}{2}[F(x,z)K(y,z) + K(x,z)F(y,z)]\ , \tag{6.47}$$

$$B_0(x,y) := -g_0\, f_0(x)^2\, \delta(x-y)\ , \tag{6.48}$$

$$\begin{aligned} B_2(x,y) :=\ & 2g_0\big[3g_0\|A\|_{-1}^2 f_0(x)^4 - f_0(x)f_2(x)\big]\,\delta(x-y) + \{2Z_2 \\ & +9g_0^2\|A\|_{-1}^2[f_0(x)^4 + f_0(y)^4] - 4g_0[f_0(x)f_2(x) + f_0(y)f_2(y)]\}\kappa_0 \\ & -2\mathcal{C}[f_0f_2,\kappa_0]\kappa_0 + 6g_0\,\|A\|_{-1}^2\,\mathcal{C}[f_0^4,\kappa_0]\kappa_0\ ; \end{aligned} \tag{6.49}$$

$$Z_2 := N^{-1}g_0\big[2(f_0^3,f_2)_2 - 3g_0\,\|A\|_{-1}^2\,\|f_0^3\|_{L^2}^2\big]\ . \tag{6.50}$$

In the above, $f_0(x)$ and $f_2(x)$ are supposed to satisfy (6.14) and (6.15). We do not address the existence and uniqueness of solutions to (6.44) and (6.45).[9] Given an f_0, the K_0 is assumed to exist uniquely. We show that $K_1 = 0$, in correspondence to Φ_1 (see Proposition 6.8); our argument makes use of small enough g_0.

We first state a property pertaining to the nonlocal term $\mathcal{C}[f_0^2,\kappa_0]u$.

LEMMA 6.12. *For given* $\kappa \in L^2(\mathbb{R}^d\times\mathbb{R}^d)$, *the linear operator* $\tilde{\mathcal{C}}[f,\kappa]$ *defined by*

$$\tilde{\mathcal{C}}[f,\kappa]u(x,y) := g_0 \int_{\mathbb{R}^d} f(z)\,\kappa(x,z)\,u(z,y)\,\mathrm{d}z\ , \qquad u\in L^2(\mathbb{R}^d\times\mathbb{R}^d)\ , \tag{6.51}$$

is bounded in $L^2(\mathbb{R}^d\times\mathbb{R}^d)$.

We omit the proof of this lemma, since this relies on standard estimates. We are now in position to delineate the proof of Proposition 6.11.

Proof. The starting point consists of expansions (6.1) for Φ^ϵ and K^ϵ, which we substitute in PDE (6.41) by use of the replacement

$$\Delta_{xy} \ \Rightarrow\ \epsilon^{-2}\,\{(\partial_{\tilde{x}} + \epsilon\partial_x)^2 + (\partial_{\tilde{y}} + \epsilon\partial_y)^2\}\ . \tag{6.52}$$

By dominant balance, we find a cascade of equations for K_n. These have the form

$$-\Delta_{\tilde{x}\tilde{y}}K_n(\tilde{x}_{(2)},x_{(2)}) = S_n^{\rm sc}(\tilde{x}_{(2)},x_{(2)})\ , \tag{6.53}$$

where the source terms $S_n^{\rm sc}$ are described below. To ensure the solvability of (6.53) for 1-periodic functions $K_n(\cdot,x_{(2)})$, we apply condition (6.4). By (6.5), the admissible solution to (6.53) reads

$$K_n(\tilde{x}_{(2)},x_{(2)}) = -\Delta_{\tilde{x}\tilde{y}}^{-1}S_n^{\rm sc}(\tilde{x}_{(2)},x_{(2)}) + \kappa_n(x,y)\ . \tag{6.54}$$

To obtain the source terms $S_n^{\rm sc}$, we note the expansions

$$\zeta^\epsilon \sim \zeta_0 + \epsilon^2\zeta_2\ ,\ \zeta_0 = g_0N^{-1}\|f_0\|_2^2\ ,\ \zeta_2 = 4g_0N^{-1}\left[(f_0^3,f_2)_2 - g_0\|A\|_{-1}^2\|f_0^3\|_2^2\right]\ , \tag{6.55}$$

[9] A complication is the delta function on the right-hand sides of these equations, which destroys the L^2 structure of their forcing terms. The appropriate weak formulation lies beyond our scope.

$$\tilde{\zeta}^\epsilon \sim \tilde{\zeta}_0 + \epsilon^2 \tilde{\zeta}_2 \ , \quad \tilde{\zeta}_0 = N^{-1}\|\partial_x f_0\|_2^2 \ ,$$
$$\tilde{\zeta}_2 = N^{-1}\Big[g_0^2 \|A\|_{-1}^2 \|f_0^3\|_2^2 + 2(\partial_x f_0, \partial_x f_2)_2\Big] \ , \tag{6.56}$$

$$\zeta_{\rm e}^\epsilon \sim \zeta_{\rm e0} + \epsilon^2 \zeta_{\rm e2} \ , \quad \zeta_{\rm e0} = N^{-1}(f_0, V_{\rm e} f_0)_2 \ , \ \zeta_{\rm e2} = 2N^{-1}(f_2, V_{\rm e} f_0)_2 \ . \tag{6.57}$$

Regarding (6.55), we have simplified the integrals containing A. Specifically, we write $A\partial_{\tilde{x}}^{-2} A = \langle A(\partial_{\tilde{x}}^{-2} A)\rangle + Q_{\rm os}$ where $\langle Q_{\rm os}\rangle = 0$ and $\langle A(\partial_{\tilde{x}}^{-2} A)\rangle = -\|A\|_{-1}^2$; and drop the integral that involves $Q_{\rm os}$ by virtue of Lemma 6.5.

Accordingly, the first two equations of the cascade do not involve $V_{\rm e}$ explicitly:

$$\mathcal{O}(\epsilon^0): \qquad -\Delta_{\tilde{x}\tilde{y}} K_0 = 0 =: S_0^{\rm sc} \ , \tag{6.58}$$
$$\mathcal{O}(\epsilon^1): \qquad -\Delta_{\tilde{x}\tilde{y}} K_1 = 2(\partial_x \partial_{\tilde{x}} + \partial_y \partial_{\tilde{y}}) K_0 =: S_1^{\rm sc} \ . \tag{6.59}$$

In view of (6.54), we obtain

$$K_0(\tilde{x}, \tilde{y}, x, y) = \kappa_0(x, y) \ , \qquad K_1(\tilde{x}, \tilde{y}, x, y) = \kappa_1(x, y) \ . \tag{6.60}$$

In order to find equations for κ_0 and κ_1, we have to consider the next two higher-order terms K_n ($n = 2, 3$).

Proceeding to the next higher order, $\mathcal{O}(\epsilon^2)$, we find

$$S_2^{\rm sc}(\tilde{x}_{(2)}, x_{(2)}) = -\mathcal{L}_{(xy)}\kappa_0 - \mathcal{C}[f_0^2, \kappa_0]\kappa_0 + B_0(x, y)$$
$$- g_0 A(\tilde{x}) f_0^2 \delta(x - y) - 2g_0\{A(\tilde{x}) f_0(x)^2 + A(\tilde{y}) f_0(y)^2\}\kappa_0 \ . \tag{6.61}$$

Lemma 6.5 has been invoked for removal, to this order, of the oscillatory term $A(z/\epsilon)$ from the kernel of the nonlocal term in PDE (6.41); the lemma dictates that this contribution should appear at least to $\mathcal{O}(\epsilon^3)$ in the perturbation scheme. The application of solvability condition (6.4) to (6.61) yields PDE (6.44) via $\langle S_2^{\rm sc}\rangle = 0$.

Since μ_0 is the lowest point of the spectrum for the condensate, 0 is not an eigenvalue of $\mathcal{L}_{(xy)}$. In particular, $\mathcal{L}_{(xy)}$ is positive definite, i.e., $(f, \mathcal{L}_{(xy)} f)_2 > 0$ for every nonzero $f \in H^1(\mathbb{R}^2)$. It follows that $\mathcal{L}_{xy}^{-1}$ exists. We will invoke the invertibility of $\mathcal{L}_{xy}$ below in order to determine κ_1.

By virtue of (6.44), K_2 satisfies

$$-\Delta_{\tilde{x}\tilde{y}} K_2 = -g_0 A(\tilde{x}) f_0^2 \delta(x - y) - 2g_0[A(\tilde{x}) f_0(x)^2 + A(\tilde{y}) f_0(y)^2]\kappa_0 \ , \tag{6.62}$$

by which

$$K_2 = g_0(\partial_{\tilde{x}}^{-2} A) f_0^2 \delta(x-y) + 2g_0\{(\partial_{\tilde{x}}^{-2} A) f_0(x)^2 + (\partial_{\tilde{y}}^{-2} A) f_0(y)^2\}\kappa_0 + \kappa_2(x, y) \ , \tag{6.63}$$

where $\kappa_2(x, y)$ must be consistent with the solvability condition on $S_3^{\rm sc}$.

Next, we address K_3, bearing in mind $\Phi_1 = 0$ and Lemma 6.6 (for $s = 1$). Thus, we derive (6.53) with

$$S_3^{\rm sc} = -\big\{\mathcal{L}_{(xy)} + \mathcal{C}[f_0^2, \kappa_0]\big\}\kappa_1 + 2g_0(\partial_{\tilde{x}}^{-1} A)\partial_x\big[f_0(x)^2 \delta(x - y)\big]$$
$$+ 4g_0\{(\partial_{\tilde{x}}^{-1} A)\, \partial_x[f_0(x)^2 \kappa_0] + (\partial_{\tilde{y}}^{-1} A)\, \partial_y[f_0(y)^2 \kappa_0]\}$$
$$- 2g_0[A(\tilde{x}) f_0(x)^2 + A(\tilde{y}) f_0(y)^2] \ . \tag{6.64}$$

The solvability condition (6.4), $\langle S_3^{\rm sc}\rangle = 0$, yields the homogeneous PDE

$$\big\{\mathcal{L}_{(xy)} + \mathcal{C}[f_0^2, \kappa_0]\big\}\kappa_1 = 0 \ . \tag{6.65}$$

By the invertibility of $\mathcal{L}_{(xy)}$ and Lemma 6.12, we conclude that the operator $\mathcal{L}_{(xy)} + \mathcal{C}[f_0^2, \kappa_0]$ is invertible if g_0 is sufficiently small [41]. Thus, the solution to (6.65) is

$$\kappa_1(x,y) = 0 \quad \text{(a.e.)} \ . \tag{6.66}$$

Hence, the equation for K_3 becomes

$$\begin{aligned} -\Delta_{\tilde{x}\tilde{y}} K_3 &= 2g_0(\partial_{\tilde{x}}^{-1}A)\partial_x\big[f_0^2\delta(x-y)\big] + 4g_0[(\partial_{\tilde{x}}^{-1}A)\partial_x(f_0(x)^2\kappa_0) \\ &\quad + (\partial_{\tilde{y}}^{-1}A)\partial_y(f_0(y)^2\kappa_0)] - 2g_0[A(\tilde{x})f_0(x)^2 + A(\tilde{y})f_0(\tilde{y})^2]\kappa_1 \\ \Rightarrow K_3 &= -2g_0(\partial_{\tilde{x}}^{-3}A)\partial_x\big[f_0^2\delta(x-y)\big] - 4g_0[(\partial_{\tilde{x}}^{-3}A)\partial_x(f_0^2\kappa_0) + (\partial_{\tilde{y}}^{-3}A)\partial_y(f_0^2\kappa_0)] \\ &\quad + 2g_0\big[\big(\partial_{\tilde{x}}^{-2}A(\tilde{x})\big)f_0(x)^2 + \big(\partial_{\tilde{y}}^{-2}A(\tilde{y})\big)f_0(y)^2\big]\kappa_1 + \kappa_3(x,y) \ . \end{aligned} \tag{6.67}$$

Next, we consider the equation for K_4, $-\Delta_{\tilde{x}\tilde{y}}K_4 = S_4^{\mathrm{sc}}(\tilde{x}_{(2)}, x_{(2)})$, and find

$$\begin{aligned} S_4^{\mathrm{sc}} &= -\mathcal{L}_{(xy)}K_2 - 2g_0\big[1 + A(\tilde{x})\big]f_0(x)\big[g_0(\partial_{\tilde{x}}^{-2}A)f_0^3 + f_2]\delta(x-y) \\ &\quad - 2g_0\big[A(\tilde{x})f_0(x)^2 + A(\tilde{y})f_0(y)^2\big]K_2 - 4g_0\big\{[1 + A(\tilde{x})]f_0(x)\Phi_2(\tilde{x},x) \\ &\quad + [1 + A(\tilde{y})]f_0(y)\Phi_2(\tilde{y},y)\big\}\kappa_0 + 2(\partial_{\bar{x}}\partial_x + \partial_{\bar{y}}\partial_y)K_3(\tilde{x}_{(2)}, x_{(2)}) \\ &\quad - g_0 \lim_{\epsilon\to 0}\int \mathrm{d}z\ \big[1 + A\big(\tfrac{z}{\epsilon}\big)\big]\big\{f_0(z)^2\big[K_2\big(\tilde{x}, \tfrac{z}{\epsilon}, x, z\big)\kappa_0(y,z) \\ &\qquad + \kappa_0(x,z)K_2\big(\tilde{y}, \tfrac{z}{\epsilon}, y, z\big)\big] + 2f_0(z)\big[g_0(\partial_{\tilde{z}}^{-2}A)f_0(z)^3 + f_2(z)\big] \\ &\qquad \times \kappa_0(x,z)\kappa_0(y,z)\big\} + 2(\tilde{\zeta}_2 + \zeta_2 + \zeta_{e2})\kappa_0(x,y) + \mathrm{OS} \ , \end{aligned} \tag{6.68}$$

where "OS" stands for terms oscillatory in $(x/\epsilon, y/\epsilon)$, which stem from $\mathcal{C}[Af_0^2, \kappa_0]\kappa_0$ by virtue of Lemma 6.6; such terms do not contribute to $\langle S_4^{\mathrm{sc}}\rangle$. Recall (6.28) in regard to Φ_2. Equation (6.45) results via evaluation of the requisite limit as $\epsilon \downarrow 0$ with recourse to (6.63) and Lemma 6.5, and enforcement of $\langle S_4^{\mathrm{sc}}\rangle = 0$. Note that the limit of the nonlocal term in the right-hand side of (6.68) yields the expression

$$\begin{aligned} &-2\mathcal{C}[f_0^2, \kappa_0]\kappa_2 - 2\mathcal{C}[f_0 f_2, \kappa_0]\kappa_0 + 6g_0\|A\|_{-1}^2\mathcal{C}[f_0^4, \kappa_0]\kappa_0 \\ &\quad + g_0^2\|A\|_{-1}^2\big[f_0(x)^4 + f_0(y)^4\big]\kappa_0(x,y) \ . \end{aligned}$$

This observation concludes our proof. □

Remark 6.13. Proposition 6.11 can be extended to d spatial dimensions, where $d = 2$, 3. The two-scale expansion for K^ϵ reads

$$\begin{aligned} K^\epsilon(x,y) &= \kappa_0(x,y) + \epsilon^2\{g_0(\Delta_{\tilde{x}}^{-1}A(\tilde{x}))f_0(x)^2\,\delta(x-y) + 2g_0[(\Delta_{\tilde{x}}^{-1}A(\tilde{x}))f_0(x)^2 \\ &\quad + (\Delta_{\tilde{y}}^{-1}A(\tilde{y}))f_0(y)^2]\kappa_0 + \kappa_2(x,y)\} + \ \ldots \ , \end{aligned} \tag{6.69}$$

where $\kappa_0(x,y)$ and $\kappa_2(x,y)$ satisfy (6.44) and (6.45) with $\Delta_{xy} = \Delta_x + \Delta_y$ and $\mathcal{L}_0(x) = -\Delta_x + V_{\mathrm{e}}(x) + g_0 f_0(x)^2 - \mu_0$. The definitions of $\mathcal{C}$, B_0, B_2 and Z_2 can be written down from (6.47)–(6.50).

7. Slowly varying trap. For $d = 3$, we now focus on expansions (6.37) and (6.69), and discuss via heuristics approximate solutions for the homogenized coefficients with $V_{\mathrm{e}}(x) = U(\breve{\epsilon}x)$, $0 < \breve{\epsilon} \ll 1$, $x \in \mathbb{R}^3$; $\breve{\epsilon} \ll \epsilon$. Our analysis is local, in the spirit of [14,69]. As $\breve{\epsilon} \downarrow 0$, the system is expected to become *nearly* translation invariant. This suggests that, order-by-order in ϵ, we separate the spatial variables into slow and fast ones in terms of $\breve{\epsilon}$. This scale separation is carried out via singular perturbations (since $\breve{\epsilon}$ multiplies the highest-order derivatives in the governing PDEs) [9]. For each homogenized coefficient, we consider only the leading-order contribution in $\breve{\epsilon}$.

Our approximations serve the need of computing observables such as the energy per particle of the condensate and the fraction of particles out of the condensate. These observables involve integrals on $\mathbb{R}^3$ or $\mathbb{R}^6$. To leading order in $\check{\epsilon}$, the contribution to integration comes, in a sense described below, from the region $\{x \,|\, U(x) < \mu_0\}$ which (loosely) defines the interior of the trap. Outside this region, $\Phi^\epsilon(\tilde{x}, \cdot)$ is expected to decay rapidly; for all practical purposes, its values will be taken to be zero outside the trap. A respective consideration holds for $K^\epsilon(\tilde{x}_{(2)}, \cdot)$.

7.1. Condensate wave function. Next, we focus on two-scale expansion (6.37) for Φ^ϵ (see Remark 6.9). By changing variable according to $x \mapsto \check{x} = \check{\epsilon}\, x$, the PDE for $\phi_0^{\check{\epsilon}}(\check{x}) := f_0(\check{x}/\check{\epsilon})$ becomes

$$[-\check{\epsilon}^2 \Delta_{\check{x}}^2 + U(\check{x}) + g_0(\phi_0^{\check{\epsilon}})^2 - \mu_0^{\check{\epsilon}}]\phi_0^{\check{\epsilon}} = 0 \ , \tag{7.1}$$

along with the normalization condition

$$\int \phi_0^{\check{\epsilon}}(x)^2 \, \mathrm{d}x = \check{\epsilon}^3 N \ . \tag{7.2}$$

Treating $\phi_0^{\check{\epsilon}}(x)$ as $\mathcal{O}(1)$, we choose to set

$$\check{\epsilon}^3 N = 1 \ . \tag{7.3}$$

In the same vein, the PDE for $\phi_2^{\check{\epsilon}}(\check{x}) := f_2(\check{x}/\check{\epsilon})$ reads

$$[-\check{\epsilon}^2 \Delta_{\check{x}}^2 + U(\check{x}) + 3g_0\,(\phi_0^{\check{\epsilon}})^2 - \mu_0^{\check{\epsilon}}]\phi_2^{\check{\epsilon}} = 3g_0^2(\phi_0^{\check{\epsilon}})^5 \ \|A\|_{-1}^2 + \mu_2^{\check{\epsilon}}\phi_0^{\check{\epsilon}} \ , \tag{7.4}$$

supplemented with the condition $(\phi_2^{\check{\epsilon}}, \phi_0^{\check{\epsilon}})_2 = 0$ by Proposition 6.8.

7.1.1. Zeroth-order homogenized solution. We briefly discuss an approximate solution to (7.1) by use of boundary layer theory [69].[10]

Outer solution. This is associated with the 'Thomas-Fermi approximation' [13]. By allowing $\check{\epsilon} = 0$, we reduce (7.1) to

$$[U(\check{x}) + \phi_0^0(\check{x})^2 - \mu_0^0]\phi_0^0 = 0 \ , \tag{7.5}$$

which in turn yields an approximate formula for $\phi_0^{\check{\epsilon}}$:

$$\phi_0^0(\check{x}) = \begin{cases} g_0^{-1/2}\sqrt{\mu_0^0 - U(\check{x})} & \check{x} \in \mathfrak{R}_0^\delta \ , \\ 0 & \check{x} \in \mathfrak{R}_0^{\mathrm{c},\delta} \ . \end{cases} \tag{7.6}$$

Here, $\mathfrak{R}_0^\delta$ is the region that results from exclusion of a δ-neighborhood (to be specified below) of the boundary of $\mathfrak{R}_0 := \{x \in \mathbb{R}^3 \,|\, U(x) < \mu_0^0\}$ for small enough δ: $\mathfrak{R}_0^\delta = \mathfrak{R}_0 - \mathfrak{B}(\partial\mathfrak{R}_0, \delta)$. This $\mathfrak{R}_0$ is bounded with boundary $\partial\mathfrak{R}_0 = \{U(x) = \mu_0^0\}$, comprising classical turning points for the potential $U(x)$. Similarly, $\mathfrak{R}_0^{\mathrm{c},\delta}$ stems from excluding from the complement of $\mathfrak{R}_0$, $\mathfrak{R}_0^{\mathrm{c}} = \mathbb{R}^3 \setminus \mathfrak{R}_0$, a δ-neighborhood of $\partial\mathfrak{R}_0$. Evidently, the extension of ϕ_0^0 across $\partial\mathfrak{R}_0$ is continuous, while $\nabla\phi_0^0(\check{x}) = -g_0^{-1/2}[\mu_0^0 - U(\check{x})]^{-1/2}\nabla U$ in $\mathfrak{R}_0^\delta$. The vanishing of ϕ_0^0 in $\mathfrak{R}_0^{\mathrm{c},\delta}$, which implies that ϕ_0 decays rapidly outside the trap, can be refined by use of the Wentzel-Kramers-Brillouin (WKB) formula [9], e.g., for a spherically symmetric V_{e} [14, 49].

[10] The 'outer solution' pertains to a leading-order approximation of the respective PDE by regular perturbation (with $\check{\epsilon} = 0$) away from boundary layers, inside *and* outside the trap.

The value of the constant μ_0^0 can be evaluated with recourse to (7.2) under (7.3):

$$\mu_0 \sim \mu_0^0 = |\mathfrak{R}_0|^{-1} g_0 + \langle U \rangle_{\mathfrak{R}_0} \ ; \qquad \langle U \rangle_{\mathfrak{R}_0} := |\mathfrak{R}_0|^{-1} \int\limits_{\mathfrak{R}_0} U(x)\, \mathrm{d}x \ , \tag{7.7}$$

where $|\mathfrak{R}_0|$ is the (g_0-dependent) volume of $\mathfrak{R}_0$, $|\mathfrak{R}_0| := \int_{\mathfrak{R}_0} \mathrm{d}x$. Result (7.7) yields an approximate energy per particle of the condensate (see Remark 6.10):

$$e_0^0 = \mu_0^0 - \frac{g_0}{2} \int\limits_{\mathfrak{R}_0} \phi_0^0(x)^4 \, \mathrm{d}x = \frac{1}{2} |\mathfrak{R}_0|^{-1} g_0 + \langle U \rangle_{\mathfrak{R}_0} - \frac{1}{2g_0} \int\limits_{\mathfrak{R}_0} \big[U(x) - \langle U \rangle_{\mathfrak{R}_0} \big]^2 \, \mathrm{d}x \ . \tag{7.8}$$

By definition of $\mathfrak{R}_0$, $(2g_0)^{-1} \int_{\mathfrak{R}_0} (U(x) - \langle U \rangle_{\mathfrak{R}_0})^2 dx < |\mathfrak{R}_0|^{-1} g_0/2 + \langle U \rangle$; thus, $e_0^0 > 0$, as it should.

Inner solution. We seek a (local) description of $\phi_0(x)$ inside possible boundary layers, noticing that the extension of ϕ_0^0 by (7.6) breaks down near $\partial\mathfrak{R}_0$. In particular, the extension of $\nabla\phi_0^0$ is not $L^2_{loc}(\mathbb{R}^3)$ by integration on any region that contains a measurable part of $\partial\mathfrak{R}_0$, in contrast to the anticipated behavior of $\nabla\phi_0^{\breve{\epsilon}}$.

To remedy this pathology, consider the variation of $\phi_0^{\breve{\epsilon}}$ along the local normal to $\partial\mathfrak{R}_0$ (for C^1 boundary $\partial\mathfrak{R}_0$) [69]. For fixed $x_{bd} \in \partial\mathfrak{R}_0$ (where $U(x_{bd}) = \mu_0^0$), define $\nu(x_{bd}) := \nabla U(x_{bd})/|\nabla U(x_{bd})|$. By the expansion $U(x) = U(x_{bd}) + U_o\, \nu \cdot (x - x_{bd}) + o(|x - x_{bd}|)$ with $U_o = |\nabla U(x_{bd})| > 0$ and a flat boundary approximation, we locally reduce (7.1) to the 1D equation

$$[-\partial_\eta^2 + \eta + (\phi_0^{in})^2]\phi_0^{in} = 0 \ ; \quad \eta := \left(\frac{U_o}{\breve{\epsilon}^2} \right)^{1/3} \nu \cdot (\breve{x} - x_{bd}) \ , \ \phi_0^{in} := \frac{g_0^{1/2}}{(\breve{\epsilon} U_o)^{1/3}} \phi_0^{\breve{\epsilon}} \ , \tag{7.9a}$$

In (7.9a), $\breve{x}$ lies in the local normal to $\partial\mathfrak{R}_0$ near x_{bd}, viz., $\breve{x} - x_{bd} = b\, \nu(x_{bd})$ for $|b| \leq \mathcal{O}(\epsilon^{2/3})$, so that $\eta = \mathcal{O}(1)$; and tangential derivatives of $\breve{\phi}_0$ have been neglected. Thus, the boundary layer width near $\partial\mathfrak{R}_0$ is estimated to be $\mathcal{O}(\breve{\epsilon}^{2/3})$; thus, $\delta = \mathcal{O}(\breve{\epsilon}^{2/3})$. The boundary conditions for (7.9) via asymptotic matching with (7.6) are

$$\phi_0^{in} \to 0 \quad \text{as } \eta \to \infty \ , \quad \phi_0^{in} \sim \sqrt{-\eta} \quad \text{as } \eta \to -\infty \ . \tag{7.9b}$$

Remark 7.1. It is known that (7.9) is solved by a 2nd Painlevé transcendent [39, 69]. It has been shown that $\phi_0^{in}(\eta) \sim \sqrt{2}\, \mathrm{Ai}(\eta)$ as $\eta \to +\infty$ where Ai is the Airy function; see, e.g., [49] and references therein. Let $P_{II}(\eta)$ denote this particular 2nd Painlevé transcendent.

Equations (7.6) and (7.9) combined should yield a composite approximation for $\phi_0^{\breve{\epsilon}}$ that is sufficiently regular across $\partial\mathfrak{R}_0$.

7.1.2. Higher-order homogenized solution. In the spirit of 7.1.1, we now focus on (7.4), which takes the form

$$(-\breve{\epsilon}^2\Delta + U_{\text{eff}})\phi_2^{\breve{\epsilon}} = F_2 \ ; \ U_{\text{eff}} := U + 3g_0(\phi_0^{\breve{\epsilon}})^2 - \mu_0^{\breve{\epsilon}} \ , \ F_2 := 3g_0^2(\phi_0^{\breve{\epsilon}})^5 \|A\|_{-1}^2 + \mu_2^{\breve{\epsilon}}\phi_0^{\breve{\epsilon}} \ . \tag{7.10}$$

By (7.6), we find $U_{\text{eff}}(\breve{x}) \sim 2[\mu_0^0 - U(\breve{x})] > 0$ for $\breve{x} \in \mathfrak{R}_0^\delta$ (inside the trap); and $U_{\text{eff}}(\breve{x}) \sim U(\breve{x}) - \mu_0^0 > 0$ outside the trap. Thus, $\phi_2^{\breve{\epsilon}}$ should decay rapidly outside $\mathfrak{R}_0$. (This behavior can be captured more precisely by the WKB approximation, which we do not pursue here.) We proceed in the same vein as in section 7.1.1.

Outer solution. By setting $\check{\epsilon} = 0$ in (7.10), we find that $\phi_2^{\check{\epsilon}}(\check{x})$ is approximated by

(7.11)
$$\phi_2^0(\check{x}) = \begin{cases} g_0^{-1/2}\{\frac{3}{2}[\mu_0^0 - U(\check{x})]^{3/2}\|A\|_{-1}^2 + \frac{1}{2}\mu_2^0[\mu_0^0 - U(\check{x})]^{-1/2}\} & \check{x} \in \mathfrak{R}_0^{\delta} \ , \\ 0 & \check{x} \in \mathfrak{R}_0^{c,\delta} \ . \end{cases}$$

Note that the extension of this $\phi_2^0(\check{x})$ across $\partial\mathfrak{R}_0$ is not L^2_{loc}. This observation calls for using boundary layer theory in the vicinity of $\partial\mathfrak{R}_0$ (as discussed below). The value of μ_2^0 comes from the condition $(f_0, f_2)_2 = 0$ (by Proposition 6.8), which yields

$$\mu_2^{\check{\epsilon}} \sim \mu_2^0 = -3\|A\|_{-1}^2|\mathfrak{R}_0|^{-1} \int\limits_{\mathfrak{R}_0} [\mu_0^0 - U(x)]^2 \, \mathrm{d}x \ ; \tag{7.12}$$

μ_0^0 is described by (7.7). By Remark 6.10, the respective contribution to the energy per particle of the condensate is

$$e_2^0 = -3g_0^{-1}\|A\|_{-1}^2 \int\limits_{\mathfrak{R}_0} [\mu_0^0 - U(x)]^3 \, \mathrm{d}x < 0 \ . \tag{7.13}$$

Remark 7.2. The perturbations of this section indicate that the oscillations of the scattering length cause a decrease in the energy per particle of the condensate. The magnitude of this decrease is found to be proportional to $\|A\|_{-1}^2$.

Inner solution. Consider (7.10) along the local normal to $\partial\mathfrak{R}_0$, inside the boundary layer conjectured in section 7.1.1. By the definitions of (7.9a), taking $\eta = \mathcal{O}(1)$ we assert that $U_{\mathrm{eff}}(\check{x}) \sim (U_o\check{\epsilon})^{2/3}[\eta + 3P_{II}(\eta)^2]$ and $F_2(\check{x}) \sim \mu_2^0 g_0^{-1/2}(U_o\check{\epsilon})^{1/3}P_{II}(\eta)$, in view of Remark 7.1. Thus, we obtain the equation

$$\partial_{\eta\eta}\phi_2^{in} - [\eta + 3P_{II}(\eta)^2]\phi_2^{in} = P_{II}(\eta) \ ; \quad \phi_2^{in} := -(\mu_2^0)^{-1}g_0^{1/2}(U_o\check{\epsilon})^{1/3}\phi_2^{\check{\epsilon}} \ . \tag{7.14a}$$

By matching with the outer solution (7.11) for $\mathcal{O}(\epsilon^{2/3}) < |\check{x} - x_{bd}| \ll 1$, we require that $\phi_2^{in}(\eta)$ satisfies

$$\phi_2^{in}(\eta) \to 0 \quad \text{as } \eta \to \infty \ , \qquad \phi_2^{in}(\eta) \sim -\frac{1}{2}(-\eta)^{-1/2} \quad \text{as } \eta \to -\infty \ . \tag{7.14b}$$

Remark 7.3. It follows that $\phi_2^{in}(\eta) = P_{II}'(\eta)$, the derivative of the 2nd Painlevé transcendent of section 7.1.1 [39]; in particular, $\phi_2^{in}(\eta) \sim \sqrt{2}\,\mathrm{Ai}'(\eta)$ as $\eta \to \infty$.

7.2. Pair excitation kernel. Next, we turn our attention to expansion (6.69) for spatial dimension $d = 3$ (see Remark 6.13). This expansion can be invoked for the depletion of the condensate (section 8). Again, the underlying idea is that, for a slowly varying trap, the Boson system is nearly translation invariant. Accordingly, $K^{\epsilon}(x, y)$ is expected to depend predominantly on $x - y$ [68, 69]. Here, we follow the technique invoked in [69] where $x - y$ is treated as a fast variable (in $\check{\epsilon}$).

The transformation to the center-of-mass coordinates reads

$$(x, y) \mapsto (x_{\#}, X) = \left(x - y, \frac{x + y}{2}\right) \ . \tag{7.15}$$

This change of variables is motivated by the observation that $\kappa_j(x, y)$ $(j = 0, 2)$ are controlled primarily by forcings proportional to the Dirac mass, $\delta(x - y)$, when the external potential is sufficiently slowly varying.

7.2.1. Zeroth-order kernel. The $3D$ analog of (6.44) reads

$$
\begin{aligned}
0 = \big(& -\tfrac{\check\epsilon^2}{2}\Delta_{\check X} - 2\Delta_{x_\#}\big)\mathfrak{B}_0^{\check\epsilon} + \big\{U(\check X + \tfrac{\check\epsilon}{2}x_\#) + U(\check X - \tfrac{\check\epsilon}{2}x_\#) \\
& + 2g_0\big[\phi_0^{\check\epsilon}(\check X + \tfrac{\check\epsilon}{2}x_\#)^2 + \phi_0^{\check\epsilon}(\check X - \tfrac{\check\epsilon}{2}x_\#)^2\big] - 2\mu_0^{\check\epsilon}\big\}\mathfrak{B}_0^{\check\epsilon} + g_0\phi_0^{\check\epsilon}(\check X)^2\,\delta(x_\#) \\
& + g_0\int_{\mathbb{R}^3} \mathrm{d}z\ \phi_0^{\check\epsilon}(\check X - \tfrac{\check\epsilon}{2}x_\# + \check\epsilon z)^2\,\mathfrak{B}_0^{\check\epsilon}(x_\# - z, \check X + \tfrac{\check\epsilon}{2}z)\,\mathfrak{B}_0^{\check\epsilon}(z, \check X - \tfrac{\check\epsilon}{2}x_\# + \tfrac{\check\epsilon}{2}z)\ ,
\end{aligned}
\tag{7.16}
$$

where, in the spirit of section 7.1, we define

$$
\check X := \check\epsilon X > \mathcal{O}(\check\epsilon)\ ,\ x_\# = \mathcal{O}(1)\ ,\ \mathfrak{B}_0^{\check\epsilon}(x_\#, \check X) := \kappa_0(\check X/\check\epsilon + x_\#/2, \check X/\check\epsilon - x_\#/2)\ .
\tag{7.17}
$$

Thus, variations of κ_0 with respect to X are slow and variations with respect to $x_\#$ are fast. This view is consistent with the (anticipated) nearly translation invariant character of the Boson system. Apply the approximations [69]

$$
U(\check\epsilon X + \tfrac{\check\epsilon}{2}x_\#) + U(\check\epsilon X - \tfrac{\check\epsilon}{2}x_\#) \sim 2U(\check X)\ ,
$$

$$
\phi_0^{\check\epsilon}(\check\epsilon X + \tfrac{\check\epsilon}{2}x_\#)^2 + \phi_0^{\check\epsilon}(\check\epsilon X - \tfrac{\check\epsilon}{2}x_\#)^2 \sim 2\phi_0^{\check\epsilon}(\check X)^2\ ,
$$

$$
\begin{aligned}
\int \mathrm{d}z\ & \phi_0^{\check\epsilon}(\check X - \tfrac{\check\epsilon}{2}x_\# + \check\epsilon z)^2\,\mathfrak{B}_0^{\check\epsilon}(x_\# - z, \check X + \tfrac{\check\epsilon}{2}z)\,\mathfrak{B}_0^{\check\epsilon}(z, \check X - \tfrac{\check\epsilon}{2}x_\# + \tfrac{\check\epsilon}{2}z) \\
& \sim \phi_0^{\check\epsilon}(\check X)^2 \int \mathrm{d}z\,\mathfrak{B}_0^{\check\epsilon}(x_\# - z, \check X)\,\mathfrak{B}_0^{\check\epsilon}(z, \check X)\ ,
\end{aligned}
$$

since the major contribution to integration is expected to come from $z = \mathcal{O}(1)$. Hence, the nonlocal term in (7.16) is reduced to a convolution integral.

Accordingly, we solve (7.16) approximately via the Fourier transform of $\mathfrak{B}_0^{\check\epsilon}(\cdot, \check X)$, treating $\check X$ as a parameter. The Fourier transform $\widehat{\mathfrak{B}}_0^{\check\epsilon}(\lambda, \check X)$ satisfies

$$
\big(-\tfrac{\check\epsilon^2}{2}\Delta_{\check X} + 2\lambda^2\big)\widehat{\mathfrak{B}}_0^{\check\epsilon} + 2[U(\check X) + 2g_0\phi_0^{\check\epsilon}(\check X)^2]\widehat{\mathfrak{B}}_0^{\check\epsilon} + g_0\phi_0^{\check\epsilon}(\check X)^2 + g_0\phi_0^{\check\epsilon}(\check X)^2(\widehat{\mathfrak{B}}_0^{\check\epsilon})^2 \approx 0\ .
\tag{7.18}
$$

We solve this equation by singular perturbations for $\check\epsilon \ll 1$.

Outer solution. By setting $\check\epsilon = 0$ in (7.18), we uncover the approximation $\widehat{\mathfrak{B}}_0^0$ where

$$
\tfrac{1}{2}g_0\phi_0^0(\check X)^2(\widehat{\mathfrak{B}}_0^0)^2 + [U(\check X) + 2g_0\phi_0^0(\check X)^2 + \lambda^2 - \mu_0^0]\widehat{\mathfrak{B}}_0^0 + \tfrac{1}{2}g_0\phi_0^0(\check X)^2 = 0\ ;
\tag{7.19}
$$

$\lambda_0(\check X)^2 := U(\check X) + 2g_0\phi_0^0(\check X)^2 - \mu_0^0$, and $\check X \in \mathbb{R}^3 \setminus \mathfrak{B}(\partial\mathfrak{R}_0, \mathcal{O}(\epsilon^{2/3}))$ (see section 7.1). Equation (7.19) has the solution

$$
\widehat{\mathfrak{B}}_0^0(\lambda, \check X) = \frac{-\lambda^2 - \lambda_0(\check X)^2 + \sqrt{[\lambda^2 + \lambda_0(\check X)^2]^2 - g_0^2\phi_0^0(\check X)^4}}{g_0\phi_0^0(\check X)^2}\ ,
\tag{7.20}
$$

with $\widehat{\mathfrak{B}}_0^0(\cdot, \check X) \in L^2(\mathbb{R}^3)$. In particular, if $g_0(\phi_0^0)^2 \ll \lambda^2 + \lambda_0^2$ we have

$$
\widehat{\mathfrak{B}}_0^0(\lambda, \check X) \sim -\frac{1}{2}\frac{g_0\phi_0^0(\check X)^2}{\lambda^2 + \lambda_0(\check X)^2}\ ,
$$

which is consistent with the hypotheses of Lemma 6.6 for $s = 1$.

A further simplification of (7.20) ensues from (7.6) [69]:

$$\widehat{\mathfrak{B}}_0^0(\lambda,\breve{X}) = \frac{-\lambda^2 - g_0\phi_0^0(\breve{X})^2 + |\lambda|\sqrt{\lambda^2 + 2g_0\phi_0^0(\breve{X})^2}}{g_0\phi_0^0(\breve{X})^2} \qquad \text{if } \breve{X}\in\mathfrak{R}_0^\delta \ . \tag{7.21}$$

On the other hand, if $\breve{X}\in\mathfrak{R}_0^{c,\delta}$ we obtain $\widehat{\mathfrak{B}}_0^0(\lambda,\breve{X})=0$, which can be refined via the WKB method in $\breve{X}$ (for fixed λ). Equation (7.21) is inverted to give the pair-excitation kernel (for $\breve{X}\in\mathfrak{R}_0^\delta$) [69]

$$\mathfrak{B}_0^0(x_\#,\breve{X}) = \pi^{-2}\left(\frac{g_0}{2}\right)^{3/2}\phi_0^0(\breve{X})^3\vartheta(x_\#,\breve{X})^{-1}\mathrm{Im}[S_{00}(i\vartheta)-S_{04}(i\vartheta)] \ , \tag{7.22}$$

where $\vartheta(x_\#,\breve{X}) = (2g_0)^{1/2}\phi_0^0(\breve{X})|x_\#|$ and $S_{\alpha\beta}$ is Lommel's function [65].

Remark 7.4. In the limit $x_\# = x-y\to 0$ with $\breve{X}\in\mathfrak{R}_0^\delta$ (inside the trap),

$$\mathfrak{B}_0^0(x_\#,\breve{X}) \sim -\left(\frac{g_0}{8\pi}\right)\frac{\phi_0^0(\breve{X})^2}{|x_\#|} \ . \tag{7.23}$$

Boundary layer. We now consider the pair excitation kernel when the slow center-of-mass coordinate $\breve{\epsilon}(x+y)/2$ lies inside the boundary layer for $\phi_0^{\breve{\epsilon}}$, near $\partial\mathfrak{R}_0$ (see section 7.1.1). We (locally) define $\mathfrak{B}_0^{in}(\chi_\#,\eta) := (U_o\breve{\epsilon})^{-1}\kappa_0(x,y)$ with $\chi_\# := (U_o\breve{\epsilon})^{1/3}x_\# = (U_o\breve{\epsilon})^{1/3}(x-y)$; here, $\eta(\breve{X}) = (U_o/\breve{\epsilon}^2)^{1/3}\nu(x_{bd})\cdot(\breve{X}-x_{bd})$ and $x_{bd}\in\partial\mathfrak{R}_0$. Accordingly, by a flat boundary approximation, (7.16) is reduced to

$$\begin{aligned} 0 = {} & \big[-\tfrac{1}{2}\partial_\eta^2 - 2\Delta_{\chi_\#} + 2\eta + 4(\phi_0^{in})^2\big]\mathfrak{B}_0^{in} + (\phi_0^{in})^2\,\delta(\chi_\#) \\ & + (\phi_0^{in})^2\int \mathrm{d}z\ \mathfrak{B}_0^{in}(\chi_\#-z,\eta)\,\mathfrak{B}_0^{in}(z,\eta) \ , \qquad \breve{X}\in\mathfrak{B}(\partial\mathfrak{R}_0,\mathcal{O}(\breve{\epsilon}^{2/3})) \ . \end{aligned} \tag{7.24}$$

By assuming $\mathfrak{B}_0^{in}(\cdot,\eta)\in L^2(\mathbb{R}^3)$, we obtain an ordinary differential equation for its Fourier transform, $\widehat{\mathfrak{B}}_0^{in}(\lambda,\eta)$:

$$-\tfrac{1}{2}\partial_\eta^2\widehat{\mathfrak{B}}_0^{in} + 2\big[\lambda^2+\eta+2(\phi_0^{in})^2\big]\widehat{\mathfrak{B}}_0^{in} + (\phi_0^{in})^2(\widehat{\mathfrak{B}}_0^{in})^2 + (\phi_0^{in})^2 = 0 \ ; \tag{7.25a}$$

recall $-\partial_\eta^2\phi_0^{in}+\eta\phi_0^{in}+(\phi_0^{in})^3=0$. Consider λ as fixed. Boundary conditions for (7.25a) stem from asymptotic matching with the outer solution, $\widehat{\mathfrak{B}}_0^0$, of (7.20) as $\eta\to\pm\infty$:[11]

$$\widehat{\mathfrak{B}}_0^{in}(\lambda,\eta) \sim -1+|\lambda|\sqrt{-\frac{2}{\eta}} \quad \text{as } \eta\to-\infty \ , \quad \widehat{\mathfrak{B}}_0^{in}(\lambda,\eta)\to 0 \quad \text{as } \eta\to\infty \ . \tag{7.25b}$$

Equations (7.25) form a canonical boundary value problem for the zeroth-order homogenized pair excitation kernel in the center-of-mass boundary layer close to $\partial\mathfrak{R}_0$. The solution of (7.25) and subsequent Fourier inversion to obtain $\mathfrak{B}_0^{in}$ are not further pursued in this article.

[11] Note that $|\lambda|$ is not allowed to become arbitrarily large in (7.25b). If η is kept fixed and $|\lambda|\to\infty$, a different asymptotic limit ensues: $\widehat{\mathfrak{B}}_0^{in}=\mathcal{O}(\lambda^{-2})$, consistent with $\mathfrak{B}_0^{in}(\cdot,\eta)\in L^2(\mathbb{R}^3)$.

7.2.2. Higher-order kernel, κ_2. The heuristics of the preceding subsection can be extended to $\mathfrak{ß}_2^{\check\epsilon}(x_\#, \check X) := \kappa_0(\check X/\epsilon + x_\#/2, \check X/\epsilon - x_\#/2)$. We outline the procedure for the outer solution below.

The function $\mathfrak{ß}_2^{\check\epsilon}(x_\#, \check X)$ obeys

$$\begin{aligned} 4\Lambda(x_\#, \check X) \approx\ & [-\check\epsilon^2\Delta_{\check X} - 4\Delta_{x_\#} + 4W(\check X)]\mathfrak{ß}_2^{\check\epsilon}(x_\#, \check X) \\ & + 4g_0\phi_0^{\check\epsilon}(\check X)^2 \int \mathrm{d}z\ \mathfrak{ß}_0^{\check\epsilon}(x_\# - z, \check X)\mathfrak{ß}_2^{\check\epsilon}(z, \check X)\ , \end{aligned} \tag{7.26}$$

for given $\phi_0^{\check\epsilon}(\check X)$, $\phi_2^{\check\epsilon}(\check X)$ and $\mathfrak{ß}_0^{\check\epsilon}(x_\#, \check X)$, where

$$W(x) = U(x) + 2g_0\phi_0^{\check\epsilon}(x)^2 - \mu_0^{\check\epsilon}\ , \tag{7.27}$$

$$\begin{aligned} \Lambda(x,y) = & -g_0\{\phi_0^{\check\epsilon}(y)\phi_2^{\check\epsilon}(y) - 3g_0\|A\|_{-1}^2\phi_0^{\check\epsilon}(y)^4\}\delta(x) \\ & + \{Z_2 + 9g_0^2\|A\|_{-1}^2\phi_0^{\check\epsilon}(y)^4 - 4g_0\phi_0^{\check\epsilon}(y)\phi_2^{\check\epsilon}(y)\}\mathfrak{ß}_0^{\check\epsilon}(x,y) \\ & - g_0[\phi_0^{\check\epsilon}(y)\phi_2^{\check\epsilon}(y) - 3g_0\|A\|_{-1}^2\phi_0^{\check\epsilon}(y)^4]\int \mathrm{d}z\, \mathfrak{ß}_0^{\check\epsilon}(x-z,y)\mathfrak{ß}_0^{\check\epsilon}(z,y)\ , \end{aligned} \tag{7.28}$$

and Z_2 is a constant defined by (6.50).

Equation (7.26) is Fourier-transformed in $x_\#$, by treatment of $\check X$ as a parameter. The transformed outer solution which approximates $\widehat{\mathfrak{ß}}_2^{\check\epsilon}(\lambda, \check X)$ is

$$\widehat{\mathfrak{ß}}_2^0(\lambda, \check X) = \frac{\widehat\Lambda_0(\lambda, \check X)}{\lambda^2 + W_0(\check X) + g_0\phi_0^0(\check X)^2\,\widehat{\mathfrak{ß}}_0^0(\lambda, \check X)}\ , \qquad \check X \in \mathbb{R}^3 \setminus \mathfrak{B}(\partial\mathfrak{R}_0, \delta)\ , \tag{7.29}$$

where $\delta = \mathcal{O}(\epsilon^{2/3})$; $\widehat\Lambda_0(\lambda, \check X)$ and $W_0(\check X)$ result from the replacement of $\phi_0^{\check\epsilon}(\check X)$, $\phi_2^{\check\epsilon}(\check X)$ and $\widehat{\mathfrak{ß}}_0^{\check\epsilon}(\lambda, \check X)$ in $\widehat\Lambda(\lambda, \check X)$ and $W(\check X)$ by the outer solutions $\phi_0^0(\check X)$, $\phi_2^0(\check X)$ and $\widehat{\mathfrak{ß}}_0^0(\lambda, \check X)$, respectively. The extension of this $\widehat{\mathfrak{ß}}_2^0(\lambda, \cdot)$ across $\partial\mathfrak{R}_0$ is not continuous because $\phi_0^0\phi_2^0$ is not. By virtue of (7.6) and (7.11), we have the simplified formulas

$$\widehat\Lambda_0(\lambda, \check X) = \frac{3}{2}g_0^2\|A\|_{-1}^2[\phi_0^0(\check X)^4 + |\mathfrak{R}_0|^{-1}\|(\phi_0^0)^2\|_{L^2}^2]\,[1 + \widehat{\mathfrak{ß}}_0^0(\lambda, \check X)]^2\ , \tag{7.30}$$

$$W_0(\check X) = g_0\phi_0^0(\check X)^2\ , \quad \check X \in \mathfrak{R}_0^\delta\ ; \tag{7.31}$$

accordingly,

$$\begin{aligned} \widehat{\mathfrak{ß}}_2^0(\lambda, \check X) = & \frac{3}{2}g_0^2\|A\|_{-1}^2[\phi_0^0(\check X)^4 + |\mathfrak{R}_0|^{-1}\|(\phi_0^0)^2\|_{L^2}^2] \\ & \times \frac{[1 + \widehat{\mathfrak{ß}}_0^0(\lambda, \check X)]^2}{\lambda^2 + g_0\phi_0^0(\check X)^2[1 + \widehat{\mathfrak{ß}}_0^0(\lambda, \check X)]}\ , \qquad \check X \in \mathfrak{R}_0^\delta\ . \end{aligned} \tag{7.32}$$

Notice that this $\widehat{\mathfrak{ß}}_2^0$ has a zero at $\lambda = 0$ for fixed $\check X$. On the other hand, if $\check X \in \mathfrak{R}_0^{\mathrm{c},\delta}$ we obtain $\widehat{\mathfrak{ß}}_2^0(\lambda, \check X) = 0$.

Approximation (7.29) breaks down if $\check X \in \mathfrak{B}(\partial\mathfrak{R}_0, \mathcal{O}(\epsilon^{2/3}))$. A remedy is to use the local coordinate η and the inner solutions for ϕ_0, ϕ_2 and $\mathfrak{ß}_0$; and proceed as in section 7.2.1, invoking boundary layer theory and asymptotic matching. By construction, the ensuing approximation should be continuous across $\partial\mathfrak{R}_0$. We leave details of this computation to the interested reader.

8. Application: Condensate depletion. In this section, we describe the partial depletion of the condensate, as particles scatter from it in pairs, to the first two orders of the homogenization program for the lowest bound state. To leading order, the condensate is partially depleted because of the repulsive particle interactions with strength g_0 ($g_0 > 0$). To the next higher order, the depletion is influenced by the oscillatory character of the scattering length, i.e., the function $A(x/\epsilon)$. In the case with a slowly varying trap, we explicitly compute the fraction of particles out of the condensate. We show how this fraction is controlled by an appropriate norm of $A(x/\epsilon)$. Recall that $\Phi^\epsilon(x)$ and $K^\epsilon(x,y)$ are considered real; and $K^\epsilon(x,y) = K^\epsilon(y,x)$.

8.1. Homogenization-based expansion. We seek a formal ϵ-expansion for the condensate depletion on the basis of our homogenization. By (5.34), the fraction of particles that occupy states out of the condensate, or *depletion fraction*, is [68]

$$\xi^\epsilon_{\rm sc} := 1 - \xi^\epsilon = N^{-1}\langle \Psi^\epsilon_N, (\psi_1^*\psi_1)\Psi^\epsilon_N\rangle_{\mathbb{F}} = N^{-1}\int w^\epsilon(x,x)\,{\rm d}x = N^{-1}{\rm tr}\mathcal{W}^\epsilon\ , \tag{8.1}$$

where the operator $\mathcal{W}^\epsilon$ has kernel $w^\epsilon(x,y)$ defined by (5.36); $0 < \xi^\epsilon_{\rm sc} < 1$. For ease of notation, we provide an expansion for $\xi^\epsilon_{\rm sc}$ in terms of a formal expansion for $\mathcal{W}^\epsilon$. In view of Remark 3.1, we assume that $\xi^\epsilon_{\rm sc}$ is small enough that the many-body perturbation scheme leading to the PDEs for Φ^ϵ and K^ϵ makes sense,

$$\xi^\epsilon_{\rm sc} \ll 1\ . \tag{8.2}$$

Specifically, we show that, in correspondence to Proposition 6.11 (with Remark 6.13), the depletion fraction can be expanded as

$$\xi^\epsilon_{\rm sc} = \xi_{{\rm sc},0} + \epsilon^2\xi_{{\rm sc},2} + \ldots = {\rm tr}\mathcal{W}_{(0)} + \epsilon^2\,{\rm tr}\mathcal{W}_{(2)} + \ldots\ , \tag{8.3}$$

where

$$\mathcal{W}_{(0)} = \sum_{n\geq 1}\mathcal{K}_{(0)}^{2n} = \mathcal{K}_{(0)}^2(1-\mathcal{K}_{(0)}^2)^{-1}\ , \tag{8.4a}$$

$$\begin{aligned}\mathcal{W}_{(2)} = &\sum_{\substack{n:{\rm even}\\ n\geq 2}}\sum_{m=0}^{\frac{n-2}{2}}\mathcal{K}_{(0)}^{2m}\{\{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\},\mathcal{K}_{(0)}^{2n-2-4m}\}\mathcal{K}_{(0)}^{2m}\\ &+\sum_{\substack{n:{\rm odd}\\ n\geq 1}}\left[\sum_{m=0}^{\frac{n-3}{2}}\mathcal{K}_{(0)}^{2m}\{\{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\},\mathcal{K}_{(0)}^{2n-2-4m}\}\mathcal{K}_{(0)}^{2m} + \mathcal{K}_{(0)}^{n-1}\{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\}\mathcal{K}_{(0)}^{n-1}\right]\ ;\end{aligned} \tag{8.4b}$$

$\mathcal{K}_{(l)}$ ($l = 0, 2$) is the operator with kernel $\kappa_l(x,y)$; and the anticommutator $\{\cdot,\cdot\}$ is $\{\mathcal{A},\mathcal{B}\} := \mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A}$, as usual. Note that $\mathcal{K}_{(0)}$ and $\mathcal{K}_{(2)}$ may not commute in general. In the special case where $\mathcal{K}_{(0)}$ and $\mathcal{K}_{(2)}$ commute, we can write

$$\mathcal{W}_{(2)} = 2\sum_{n\geq 1} n\mathcal{K}_{(0)}^{2n-1}\mathcal{K}_{(2)} = 2\mathcal{K}_{(0)}\mathcal{K}_{(2)}(1-\mathcal{K}_{(0)}^2)^{-2}\ . \tag{8.5}$$

For sufficiently small g_0, the operator $\mathcal{K}_{(0)}$ is expected to be appropriately bounded so that $(1-\mathcal{K}_{(0)}^2)^{-k}$ exists for $k = 1, 2$; see section 8.2 (Remark 8.1).

We proceed to sketch a derivation of (8.3) and (8.4), by resorting to an extension of the binomial expansion for non-commuting operators. Noting the formal relations $\mathcal{W}^\epsilon = \sum_{n\geq 1} \mathcal{W}_n^\epsilon$, $\mathcal{W}_n^\epsilon = (W_1^\epsilon)^n$ and $\mathcal{W}_1^\epsilon = (\mathcal{K}^\epsilon)^2$, where $\mathcal{K}^\epsilon$ has kernel $K^\epsilon(x,y)$, we seek a two-scale expansion for the kernel $w_1^\epsilon(x,y)$ of $\mathcal{W}_1^\epsilon$ up to $\mathcal{O}(\epsilon^2)$. By (6.43) with Remark 6.13, we find

$$w_1^\epsilon(x,y) = \int \mathrm{d}z\, \kappa_0(x,z)\kappa_0(z,y) + \epsilon^2 \Bigg\{ g_0\big[(\Delta_{\tilde{x}}^{-1}A)f_0(x)^2 + (\Delta_{\tilde{y}}^{-1}A)f_0(y)^2\big] \\ \times \bigg[\kappa_0(x,y) + 2\int \mathrm{d}z\, \kappa_0(x,z)\kappa_0(z,y)\bigg] + 2\int \mathrm{d}z\, \mathrm{Sym}[\kappa_0,\kappa_2](z;x,y)\Bigg\} + \dots \ , \tag{8.6}$$

where Sym[·] is defined by (6.47). Equation (8.6) suggests the operator form

$$\mathcal{W}_1^\epsilon = \mathcal{K}_{(0)}^2 + \epsilon^2\big[\varpi\mathcal{K}_{(0)}(1+2\mathcal{K}_{(0)}) + \{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\}\big] + \dots \ , \tag{8.7}$$

where $\varpi(\cdot,\cdot,x,y)$ is 1-periodic in $\mathbb{R}^3\times\mathbb{R}^3$ with $\langle\varpi\rangle = 0$. Now raise $\mathcal{W}_1^\epsilon$ to the power n $(n = 1,2,\dots)$, sum up the terms $(\mathcal{W}_1^\epsilon)^n$, and take the total trace of the resulting $\mathcal{W}^\epsilon$ up to order $\mathcal{O}(\epsilon^2)$ (by integration on the diagonal, for $x = y$ and $\tilde{x} = \tilde{y}$) in order to compute $\xi_{\mathrm{sc}}^\epsilon$ by (8.1). The contribution of ϖ can be eliminated by virtue of Lemma 6.5. Thus, $\xi_{\mathrm{sc}}^\epsilon$ is effectively determined up to $\mathcal{O}(\epsilon^2)$ from the sum of traces of

$$\big[\mathcal{K}_{(0)}^2 + \epsilon^2\,\{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\}\big]^n \ , \quad n = 1,\,2,\,\dots \ ,$$

where in principle $\mathcal{K}_{(0)}$ and $\{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\}$ do not commute. Equations (8.3) and (8.4) result by direct multiplication, induction, and summation in n.

8.2. Slowly varying potential. Consider the external potential $V_{\mathrm{e}}(x) = U(\breve{\epsilon}x)$. By use of the center-of-mass coordinates and a slow variable in $\breve{\epsilon}$, as in section 7, the operators $\mathcal{K}_{(0)}$ and $\mathcal{K}_{(2)}$ are found to commute approximately. Indeed, let $x_\# = x - y$ and $\breve{X} = \breve{\epsilon}(x+y)/2$, along with $\kappa_0(x,y) = ß_0(x_\#,\breve{X})$ and $\kappa_2(x,y) = ß_2(x_\#,\breve{X})$, and apply the approximation

$$\int \kappa_0(x,z)\kappa_2(z,y)\,\mathrm{d}z = \int ß_0\bigg(z',\breve{X} + \frac{\epsilon x_\#}{2} - \frac{\epsilon z'}{2}\bigg)\, ß_2\bigg(x_\# - z',\breve{X} - \frac{\epsilon z'}{2}\bigg)\,\mathrm{d}z' \\ \sim \int ß_0(z',\breve{X})\, ß_2(x_\# - z',\breve{X})\,\mathrm{d}z' = \int ß_2(z',\breve{X})\, ß_0(x_\# - z',\breve{X}) \ , \tag{8.8}$$

to leading order in $\breve{\epsilon}$, as $\breve{\epsilon}\downarrow 0$. Symbolically, we write

$$\mathcal{K}_{(0)}\mathcal{K}_{(2)} \sim \mathcal{K}_{(2)}\mathcal{K}_{(0)} \ \Rightarrow\ \{\mathcal{K}_{(0)},\mathcal{K}_{(2)}\} \sim 2\mathcal{K}_{(0)}\mathcal{K}_{(2)} \ ,$$

to imply (8.8). Alternatively, replace each operator by the Fourier transform of the above approximation for $ß_l(\cdot,\breve{X})$, treating $\breve{X}$ as a $\mathcal{O}(1)$ parameter.

A few comments on the operator $\mathcal{K}_{(0)}$ are in order. The appropriate norm of $\mathcal{K}_{(0)} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is written as

$$\|\mathcal{K}_{(0)}\|^2 = N^{-1}\|\kappa_0\|^2_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = N^{-1}\iint |\kappa_0(X + x_\#/2, X - x_\#/2)|^2\,\mathrm{d}x_\#\mathrm{d}X \\ = (N\breve{\epsilon}^3)^{-1}\iint |ß_0(x_\#,\breve{X})|^2\,\mathrm{d}x_\#\mathrm{d}\breve{X} \sim \frac{N^{-1}}{(2\pi)^3}\int\limits_{\mathfrak{R}_0}\mathrm{d}\breve{X}\int\limits_{\mathbb{R}^3}\mathrm{d}\lambda\,|\widehat{ß}_0^0(\lambda,\breve{X})|^2 \ ; \tag{8.9}$$

cf. section 7.2.1. By formula (7.21) for $\widehat{\mathfrak{K}}_0^0$, use of spherical coordinates for λ, and the change of variable $|\lambda| \mapsto \tau$ with $|\lambda| = \sqrt{2g_0(\phi_0^0)^2}\,\sinh\tau$ inside $\mathfrak{R}_0^\delta$, we find $\widehat{\mathfrak{K}}_0^0 = -e^{-2\tau}$ and directly obtain

$$\|\mathcal{K}_{(0)}\|^2 \sim \frac{2^{7/2}}{105\pi^2}\int\limits_{\mathfrak{R}_0} \mathrm{d}x\,[\mu_0^0 - U(x)]^{3/2}\ . \tag{8.10}$$

In addition, we notice that, since $\mu_0 \to 0$ as $g \downarrow 0$, the volume $|\mathfrak{R}_0|$ should become arbitrarily small in this limit; thus, $\|\mathcal{K}_{(0)}\| \to 0$ as $g_0 \downarrow 0$.

Remark 8.1. The above sketchy argument suggests that if g_0 is nonzero but small enough, then $(1-\mathcal{K}_0^2)^{-1}$ is meaningful [41].

8.2.1. Zeroth-order depletion. By (8.3) and (8.4a) along with the use of the Fourier representation for $\mathcal{K}_{(0)}$ and spherical coordinates, we wind up with the integral

$$\begin{aligned}
\xi_{\mathrm{sc}}^\epsilon \sim \xi_{\mathrm{sc},0} &= \frac{1}{(2\pi)^3}\sum_{n\geq 1}\int\limits_{\mathfrak{R}_0}\mathrm{d}x\int \mathrm{d}\lambda\ |\widehat{\mathfrak{K}}_0^0(\lambda,x)|^{2n} \\
&= \frac{1}{2\pi^2}\sum_{n\geq 1}\int\limits_{\mathfrak{R}_0}\mathrm{d}x\int_0^\infty \mathrm{d}|\lambda|\ |\lambda|^2\,|\widehat{\mathfrak{K}}_0^0(\lambda,x)|^{2n} \\
&= \frac{1}{2\pi^2}\sum_{n\geq 1}\frac{8n}{(16n^2-1)(16n^2-9)}\int\limits_{\mathfrak{R}_0}\mathrm{d}x\,[2g_0\phi_0^0(x)^2]^{3/2} \\
&= \frac{\sqrt{2}}{12\pi^2}\int\limits_{\mathfrak{R}_0}\mathrm{d}x\ [\mu_0^0 - U(x)]^{3/2}\ . \qquad (8.11)
\end{aligned}$$

Remark 8.2. The approximate depletion fraction $\xi_{\mathrm{sc},0}$ scales with g_0 in a fashion depending upon the shape of the trapping potential, $U(x)$. For example, if $U(x) = |x|^\varrho$, we find $\xi_{\mathrm{sc},0} \sim c\,g_0^{\frac{3}{2}\frac{\varrho+2}{\varrho+3}}$.

8.2.2. Higher-order depletion. Next, we indicate how the oscillatory part, $A(x/\epsilon)$, of the scattering length can cause a decrease of the depletion fraction. In (8.3), the coefficient $\xi_{\mathrm{sc},2}$ contains information about $A(x/\epsilon)$. By using the series of (8.5), along with the hypothesis of a slowly varying trap, we compute

$$\xi_{\mathrm{sc},2} \sim \frac{1}{(2\pi)^3}\sum_{n\geq 0}2(n+1)\int\limits_{\mathfrak{R}_0}\mathrm{d}x\int \mathrm{d}\lambda\ \widehat{\mathfrak{K}}_0^0(\lambda,x)^{2n+1}\widehat{\mathfrak{K}}_2^0(\lambda,x)\ . \tag{8.12}$$

By formulas (7.29)–(7.31), we have

$$\begin{aligned}
\xi_{\mathrm{sc},2} \sim -\frac{3\sqrt{2}}{8\pi^2}\|A\|_{-1}^2\int\limits_{\mathfrak{R}_0}\big\{&g_0^2\phi_0^0(x)^4 \\
&+ |\mathfrak{R}_0|^{-1}\|g_0(\phi_0^0)^2\|_{L^2}^2\big\}[g_0\phi_0^0(x)^2]^{1/2}\,\mathrm{d}x\ , \qquad (8.13)
\end{aligned}$$

where $\phi_0^0(x)$ is introduced in (7.6). Notice

Remark 8.3. The periodic oscillations of the scattering length cause a relative decrease of the depletion fraction by an amount proportional to $\|A\|_{-1}^2$, in contrast to the effect of repulsive interactions to zeroth order.

9. Conclusion. We studied the Bose-Einstein condensation of dilute atomic gases with repulsive particle interactions at zero temperature. Our goal with this work was to explore a many-particle scenario for transcending the mean field formalism of the NSE when the scattering length has a periodic microstructure. The main effect beyond mean field is pair excitation, by which particles are scattered in pairs from the condensate to other states at different positions; a macroscopic-like function that describes this process is the pair excitation kernel, $K(x, y)$. Our focus was the lowest many-body bound state, which depends on both the condensate wave function, $\Phi(x)$, and the kernel $K(x, y)$.

We applied perturbation theory at the microscopic and macroscopic levels. First, by revisiting Wu's formulation [68], we demonstrated how the integro-PDE for K can emerge from the particle Hamiltonian when the scattering length has a periodic microstructure. This stage involves manipulation of operators in the Fock space. Second, by classical homogenization theory, we derived effective equations for Φ and K up to the second order in the subscale ϵ of the scattering length. Third, in order to obtain some insight into solutions of these effective equations, we considered a slowly varying trap, $U(\check{\epsilon}x)$, and applied singular perturbation theory to leading order in $\check{\epsilon}$. Lastly, we indicated what predictions can possibly be made for the fraction, $\xi_{\rm sc}$, of particles out of the condensate.

A noteworthy result is an expansion for $\xi_{\rm sc}$, which reveals the dependence of this fraction on the physical parameters, including the size and shape of the trap, the strength of the repulsive interactions, particularly the oscillatory part of the scattering length. According to our formula for $\xi_{\rm sc}$, the oscillations of the scattering length favor a relative decrease of the depletion fraction. This finding suggests that the spatial manipulation of the scattering length may cause an effect opposite to raising the (positive) interaction strength in the unperturbed (lacking periodic microstructure) system.

Our work has not addressed several pending issues. For example, although we indicated that K acts back on Φ and thus modifies the NSE, we have not studied the correction to the condensate energy that stems from the coupling of the PDE for Φ with K. Another issue concerns settings with a spatially periodic and time-dependent scattering length and trapping potential. Our analysis was restricted to zero temperature, in the absence of thermally excited states. The extension of pair excitation to finite but small temperatures (well below the phase transition point) is a task worthy of attention. An issue is to derive (from the microscopic Hamiltonian) equations of motion for Φ, K and, in addition, the wave functions of thermally excited states. Furthermore, the homogenization of such macroscopic equations would be the next step. The modeling and analysis of the finite-temperature Boson gas beyond mean field in a trap is left for near-future work.

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