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

DIONISIOS MARGETIS†

Abstract. We study stationary quantum fluctuations around 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 inhomogeneous particle scattering processes. In the mean field limit, the wave function of the condensate (macroscopic quantum state) satisfies a defocusing cubic nonlinear Schrödinger-type equation, the Gross–Pitaevskii equation. We include consequences of *pair excitation*, i.e., the scattering of particles in pairs from the condensate to other states, proposed in [T. T. Wu, *J. Math. Phys.*, 2 (1961), pp. 105–123]. Our derivations rely on an uncontrolled yet physically motivated assumption for the many-body wave function. By relaxing mathematical rigor, from a particle Hamiltonian with a spatially varying interaction strength we derive via heuristics an integro–partial differential equation for the pair collision kernel, K, under a stationary condensate wave function, Φ. For a scattering length with periodic microstructure of subscale ϵ, we formally describe via classical homogenization the lowest many-body bound state in terms of Φ and K up to second order in ϵ. If the external potential is slowly varying, we solve the homogenized equations via boundary layer theory. As an application, 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

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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 noninteracting 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.

The modeling of dilute atomic gases involves at least three length scales: (i) the de Broglie wavelength, l_{dB}, associated with the wavelike motion of particles; (ii) the mean interparticle distance, l_d; and (iii) the scattering length, a, where $a \ll l_d \ll l_{dB}$. If ρ is the mean gas density, then $l_d = \rho^{-1/3}$ and $l_{dB} = (\rho a)^{-1/2}$, where $\rho a^3 \ll 1$ for a dilute gas. With a trapping potential, another length of interest 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) (the Gross–Pitaevskii equation) for the one-particle wave function, $\check{\Phi}(t, x)$, of the condensate [33, 34, 55, 69]. 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 [71].

In this article, we formally apply perturbation theory to study stationary effects beyond the NSE in the BEC of trapped atomic gases with a varying positive scattering

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†Department of Mathematics, Institute for Physical Science and Technology, and Center for Scientific Computation and Mathematical Modeling, University of Maryland, College Park, MD 20742-4015 (dio@math.umd.edu).

length at zero temperature. Our derivation of macroscopic equations relies on an uncontrolled but physically motivated *ansatz* for the many-body wave function; this ansatz accounts for the scattering of atoms in pairs, or *pair excitation*, from the condensate to other quantum states. We focus on the lowest many-particle bound state. A central variable is the pair collision kernel, $\check{K}(t, x, y)$, a function of two spatial variables. From a microscopic Hamiltonian with a confining potential, we (i) derive partial differential equations (PDEs) for the stationary $\check{\Phi}$ and $\check{K}$; (ii) homogenize these equations for atomic interactions with a periodic microstructure; and (iii) thereby describe the condensate depletion.

For nontranslation-invariant settings and constant scattering length, the formalism of pair excitation is due to Wu [69, 70] given previous work by Lee, Huang, and Yang for periodic systems [44]. 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 [69, 70] no explicit connection is made of an external potential or a varying scattering length to the fraction of particles out of the condensate. Here, we show by heuristics 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 a scattering length with periodic microstructure.

The physical motivation for our work is twofold. First, the consideration of inhomogeneous scattering processes, e.g., a periodically varying scattering length, aims to offer a simplified picture for realistic atomic collisions which may not be described by the usual model of pairwise, translation-invariant interactions; cf. (1.1). This element of inhomogeneity helps one to explore the possibility of controlling BEC through variations of particle interactions, e.g., near a Feshbach resonance [10, 12, 40, 63], or via an optical lattice [71]. Second, the need to transcend the NSE, and thus include $\check{K}$, stems from experimental efforts to relate properties of ultracold atomic gases to the superfluidity of liquid helium [11, 42, 71]. The helium system has high condensate depletion; i.e., a significant fraction of particles leave the condensate to occupy other states.

Our results concern deviations from the usual mean field description of the NSE, which are herein called *quantum fluctuations*, because of pair excitation in a setting of inhomogeneous scattering. Such quantum fluctuations (defined precisely in section 3) cannot be avoided in BEC; for example, these are responsible for phonon creation [44, 69]. We simplify the particle model by removing complications that are not absolutely essential for a fundamental treatment; e.g., the particles are taken to be spinless. We consider weakly and repulsively interacting atoms under nonperiodic trapping potentials, leaving periodic potentials for future work; see [38, 62] 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 $\check{K}$ with the condensate wave function, $\check{\Phi}$.

The mathematical context of our work 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 via heuristics. In regard to the macroscopic PDEs, periodic homogenization, in the spirit of Bensoussan, Lions, and Papanicolaou (see [2, 52]), is formally applied to nonlinear PDEs. By relaxing rigor, we seek classical, sufficiently regular solutions of the effective equations

via singular perturbations for traps that vary slowly in the spatial variables. The convergence and legitimacy of the related asymptotic expansions are 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 deem it necessary to review some related background (section 3). For broad reviews of BEC in trapped atomic gases, the reader may consult, e.g., [7, 11, 13, 42, 46, 54, 57].

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 BEC.[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 such that $\hbar = 2m = 1$ ($\hbar$: Planck's constant, m: atomic mass) and x_j are particle positions. $V_{\rm e} : \mathbb{R}^3 \to \mathbb{R}_+$ is a positive, smooth trapping potential with $V_{\rm e}(x) \to \infty$ as $|x| \to \infty$; and $\mathcal{V}$ can be thought of as a positive, symmetric, compactly supported interaction potential.

To simplify the analysis, we represent $\mathcal{V}$ by the Fermi pseudopotential for many-body problems, following Huang, Yang, and Luttinger [36], since in a dilute gas the mean interatomic distance is much larger than the support of $\mathcal{V}$. The Fermi pseudopotential for two-particle scattering amounts to an effective operator that reproduces the low-energy limit of the far field of the exact wave function [4]. So, we set[2]

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

where f is any two-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 definition of constant a can be found, e.g., in [22]. By omission of $(\partial/\partial x_{ij})x_{ij}$, we use [69, 70]

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

instead. An alternate approach would be to employ a regularized interaction potential, which would be scaled by N [20, 21, 22]: $V = N^{3b}g(x_i,x_j)\ V_1(N^b(x_i-x_j))$, where V_1 is compactly supported and smooth, and $b > 0$.

The N-particle wave function $\check{\Psi}_N(t,\vec{x})$, where $\vec{x} = (x_1, \ldots, x_N)$, generates all observable properties of the atomic gas. For bosons, this $\check{\Psi}_N$ is symmetric with respect to arbitrary permutations of the atom positions and satisfies

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

[1] A formal definition of BEC invokes the appropriate projection operator for the condensate; see Penrose and Onsager [53].

[2] Note that the scattering length, $a(x)$, enters our description as an ad hoc parameter. By contrast, in recent works by Elgart, Erdős, Schlein, and Yau (see [18, 20, 21, 22]) the (constant) scattering length emerges as an effective parameter from the mean field limit of the many-particle quantum dynamics.

For a wide variety of applications, it is reasonable to consider the initial data

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

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

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

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

where $\check{\Phi}(t,x)$ obeys a *linear* Schrödinger equation on $(0,\infty)\times\mathbb{R}^3$. A nonzero (and nonconstant) $\mathcal{V}$ in H_N (i) introduces *nonlinearities*, and (ii) may spoil 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. Known mean field limit. For large N, it is impractical to simulate particle model (1.1)–(1.4). 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, $\check{\Phi}$. More generally, it is desirable to formulate a macroscopic theory that encapsulates the major physics of 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) [69, 70]. Alternatively, consider the L^2-variation of the energy functional [13, 33, 34, 46, 55]

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

Hence, the condensate wave function, $\check{\Phi}$, satisfies

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

A rigorous derivation of (1.7) from the many-atom Hamiltonian dynamics is based on limits of the Bogoliubov–Born–Green–Kirkwood–Yvon (BBGKY) hierarchies for reduced particle density matrices [18, 20, 21, 22].

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, $\|\check{\Phi}\|_{L^2}^2$, are conserved. For one-particle bound states, one seeks solutions of the form $\check{\Phi}(t,x) = e^{-i\mu t}\Phi(x)$ of (1.7), 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].

1.3. Beyond mean field: Pair excitation. In the case with periodic boundary conditions and constant scattering length, the condensate is the state of zero momentum. This case is more transparent to physical interpretation since the system Hamiltonian is expressed conveniently in terms of the particle momenta.

Bogoliubov [5] addressed the problem of the particle energy spectrum for this setting by invoking a simplification of the Hamiltonian. His approach, discussed in [45, 46], makes use of a linear transformation for many-body operators that express creation and annihilation of particle momenta (in the Fourier space). The idea

of pair excitation was placed on a firm basis 10 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 stationary N-particle wave function, Ψ_N, that distinctly differs from the usual tensor product form: their formula expresses excitation of particles from zero momentum to *pairs of opposite momenta* [44]. For details, see, e.g., [44, 45, 46, 68].

The extension of pair creation to settings with an external potential and constant scattering length is nontrivial. We adopt Wu's approach [69, 70], which uses the ansatz

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

where $\check{\Psi}_N^0$ is the tensor product (1.5), $C(t)$ is a normalization factor, and $\mathcal{P}[\check{K}](t)$ is an operator that spatially averages out the excitation of particles from the condensate $\check{\Phi}$ to other states with the effective kernel $\check{K}$. This $\check{K}$ is *not* a priori known (in contrast, e.g., to the case of the classical Boltzmann gas) but is determined by enforcement of (1.4a) under a certain *approximation* for H_N [69], to be revisited and slightly modified in section 5.2. The formula for $\mathcal{P}$ is expressed in terms of many-body operators; see (3.7). In the periodic case, (1.8) reduces to the many-body wave function of [44].

Here, we extend this formalism to include a spatially varying scattering length; see section 5. A feature of the resulting description is that the (nonlocal) coupling of $\check{K}$ and $\check{\Phi}$ is partially controlled by the microstructure of the scattering length. Observable quantities, e.g., the condensate depletion, can be computed directly from $\check{K}$; see section 8.

Ansatz (1.8) is not strictly consistent with the exact many-body dynamics. An estimate for the error lies beyond our scope. In view of [32], we may expect that $\|\check{\Psi}_N - \check{\Psi}_N^1\|_{\mathcal{F}} = \mathcal{O}(C_1(t)N^{-1/2})$, where $\|\cdot\|_{\mathbb{F}}$ is the many-body Hilbert (Fock) space norm (defined in section 3.1) and $C_1(t)$ is bounded locally in time.

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 [70] and time-dependent [48, 49] settings. Here, we formally homogenize the equations of motion for stationary $\check{\Phi}$ and $\check{K}$ under a periodic scattering length *and* a macroscopic trap; and we apply singular perturbations for a slowly varying trap to extract explicit solutions to homogenized equations. Other past works that aim to transcend the NSE are outlined (nonexhaustively) in section 3.3.

1.4. Periodic microstructure of scattering length. 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 many-body microscopic dynamics; perturbations are formally applied to the microscopic Hamiltonian H_N to single out the effect of pair excitation. We review Wu's method [69], which is a generalization of the periodic case [44], and add an extension to include a spatially varying scattering length.

For this purpose, we revisit the formalism of quantized fields, which underlies closely related works with a physics perspective [44, 69]. In this context, the N-body

Hamiltonian is viewed as an operator on the Fock space, $\mathbb{F}$, i.e., the Hilbert space for quantum states with an arbitrary number of particles.

The next level of our analysis concerns approximate, classical solutions of the derived PDEs for bound states of $\check{\Phi}$ and $\check{K}$. 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 via heuristics homogenized equations for $\check{\Phi}$ and $\check{K}$. Solutions to these equations are then determined for slowly varying traps, when the boson system is *nearly* (but not exactly) translation invariant.

1.6. Main assumptions. There are two main sets of assumptions. One set is physics-motivated and invokes a scale separation needed for approximations. If l_c is the correlation length of bosons [69], l_d is the mean interparticle distance, l_{sc} is the length over which the scattering length varies, and l_e is the typical size of the trap, then

$$l_{sc} \ll a \ll l_d \ll l_c \ll l_e \ . \tag{1.10}$$

We set $\epsilon := l_{sc}/l_c$ and $\check{\epsilon} := l_c/l_e$; ϵ expresses the microstructure of the scattering length, while $\check{\epsilon}$ is used to describe the slow spatial variation of the external potential. In addition, we assume that $\check{\epsilon} \ll \epsilon$ so that corrections from the $\check{\epsilon}$-based asymptotics for the slowly varying trap are small compared to $\mathcal{O}(\epsilon^2)$ terms of the homogenization expansion. The condition $a \ll l_d \ll l_c$ ensures that the atomic gas is sufficiently dilute.

Another set of assumptions concerns the regularity of the stationary $\check{\Phi}$ and $\check{K}$. By relaxing mathematical rigor, we hypothesize that these functions are sufficiently regular and decay rapidly enough with the spatial variables (section 6.1). In particular, regarding $\check{K}(t,x,y)$ we anticipate a weak (Coulombic) singularity on its diagonal $(x=y)$ for $(x,y) \in \mathbb{R}^6$; this type of singularity is shown formally for a slowly varying trap (section 7.2).

1.7. 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 [71]. However, periodic $V_{\rm e}$'s [38, 62] are not studied here.

The origin and nature of the (seemingly empirical) ansatz (1.8) are not further investigated. By the result in [32] for coherent states without a trap, one may expect that the resulting error (in some appropriate metric) scales as $N^{-1/2}$ for large N and fixed time t.

The classical homogenization is carried out formally up to the first two (nonzero) orders in each two-scale expansion (for stationary $\check{\Phi}$ and $\check{K}$). The next higher-order terms and convergence of the expansions are not touched upon.

We focus on zero temperature, $T=0$. For finite, small temperatures $(T>0)$, the condensate coexists with thermally excited states described by a set of (a priori unknown) wave functions, $\{\check{\Phi}_j\}_{j=1}^{\infty}$, which are taken orthogonal to $\check{\Phi}$. This means that, for $T>0$, the PDEs for $\check{\Phi}$ and $\check{K}$ need to be complemented with PDEs for $\check{\Phi}_j$. (For a mean field limit of this case, see, e.g., [30, 37].) This task is left for future work.

1.8. 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 [69]; and in section 3.3 we delineate past works. 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; and in section 5.2 we develop a macroscopic PDE for pair creation. In section 6, we homogenize the derived PDEs: in section 6.1 we discuss some technical preliminaries and assumptions; in section 6.2 we focus on the NSE; and in section 6.3 we describe the procedure for the stationary $\check{K}$. 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 outline some open problems.

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

- $\mathbb{C}$ is the complex plane, $\mathbb{Z}$ is the set of all integers, and $\mathbb{N} = \{1, 2, \ldots\}$. The star (*) operation denotes Hermitian conjugation.
- 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 $d = 1$.
- $\mathfrak{B}(\gamma, \delta)$ 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 $\|F\|_{L^2(\mathfrak{D})}$. The scalar product in the Fock space, $\mathbb{F}$, is denoted by $\langle \cdot, \cdot \rangle_{\mathbb{F}}$ (to be defined precisely in section 3.1); the induced norm is $\| \cdot \|_{\mathbb{F}}$.
- $L^2_s(\mathbb{R}^{3n})$ 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, 52]. $\|A\|_{-1}$ 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 $\widehat{h}(\lambda) = \int_{\mathbb{R}^d} h(x) e^{-i\lambda \cdot x}\,\mathrm{d}x$.
- Let (the 1-periodic) F be in $L^2(\mathbb{T}^d)$. If F has zero mean, define $\partial_x^{-\alpha}$ by

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

  where $\alpha_k = 0, 1, \ldots$, $j = (j_1, \ldots, j_d) \in \mathbb{Z}^d$, 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 $(-\Delta)^{-s} F(x) := \sum_{j \neq 0} [\widehat{F}_j / (4\pi^2 |j|^2)^s] e^{i2\pi j \cdot x}$; note that $\langle \partial^{-\alpha} F \rangle = 0 = \langle (-\Delta)^{-s} F \rangle$.
- 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 $f - g = o(g)$ in some limit.

3. Background. In this section, we review the Fock space formalism and the many-body perturbation scheme introduced for three spatial dimensions (3D) in [69, 70]. For further details on the quantized fields, the reader may consult, e.g., [3, 28, 29, 35, 59].

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 $\check{\Psi}_N$ is represented in $\mathbb{F}$ by $\{\upsilon^{(n)}\}_{n\geq 0}$, where $\upsilon^{(n)} \equiv 0$ for $n \neq N$ and $\upsilon^{(N)} = \check{\Psi}_N$ [59]. The scalar product on $\mathbb{F}$ is defined by $\langle \upsilon_1, \upsilon_2\rangle_{\mathbb{F}} = \sum_{n\geq 0}\langle \upsilon_1^{(n)}, \upsilon_2^{(n)}\rangle_{L^2(\mathbb{R}^{3n})}$; and $\|\cdot\|_{\mathbb{F}}$ denotes the induced norm.

The next step is to express the Hamiltonian as an operator on a physically appropriate sector of $\mathbb{F}$. For a one-particle wave function $f \in L^2(\mathbb{R}^3)$, the creation and annihilation operators $\mathrm{a}^*(f)$ and $\mathrm{a}(f)$ on $\mathbb{F}$ are defined by

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

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

It follows that $\mathrm{a}(f)$ and $\mathrm{a}^*(g)$ satisfy the commutation relations $\mathrm{a}(f)\mathrm{a}^*(g) - \mathrm{a}^*(g)\mathrm{a}(f) =: [\mathrm{a}(f),\mathrm{a}^*(g)] = (f,g)_2$ and $[\mathrm{a}(f),\mathrm{a}(g)] = [\mathrm{a}^*(f),\mathrm{a}^*(g)] = 0$. Accordingly, the operator-valued distributions $\psi(x)$ and $\psi^*(x)$, called, respectively, the boson field annihilation and creation operators, are defined by[3]

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

where $\psi(x)$ and $\psi^*(x)$ 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 corresponds to the operator $\mathcal{H}$ on $\mathbb{F}$, 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 (abusing notation) the symbol H_N in place of $\mathcal{H}$. Further, we will write $\check{\Psi}_N$ to denote the N-particle state as a vector in $\mathbb{F}$.

3.2. Many-body perturbation theory. For weakly interacting atoms (dilute gas), the perturbation scheme should express the physical picture that only a small fraction of particles escape from the condensate to occupy other states; i.e., the depletion of the condensate is relatively small. Accordingly, split $\psi(x)$ as [69, 70]

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

where ψ_0 is the boson field annihilation operator for the condensate. If $a_0(t) := N^{-1/2}\mathrm{a}(\check{\Phi})$ is the operator annihilating one particle at state $\check{\Phi}$, we have the relations

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

where $N^{-1}\|\check{\Phi}\|^2_{L^2(\mathbb{R}^3)} = 1$, $[a_0(t),a_0^*(t)] = 1$, $a_0(t)|\mathrm{vac}\rangle = 0$, ψ_1 is the boson field annihilation operator in the space orthogonal to the condensate, and $\int \mathrm{d}x\,\check{\Phi}^*(t,x)\psi_1(t,x) = 0$.[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.

Remark 3.1. The heart of the perturbation analysis lies in the treatment of ψ_1 as small in an appropriate sense; see Remark 3.2. This amounts to expanding the Hamiltonian (3.4) in powers of ψ_1 and ψ_1^*, where different powers yield distinct approximations at large scales when combined with corresponding expressions for $\check{\Psi}_N$.

The usual mean field limit stems formally from linearization of H_N in ψ_1^* and ψ_1 by use of the tensor product ansatz (1.5) [70]. Then, the NSE dynamics come 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 amounts to pair excitation [69]. The expansion for H_N must be accompanied with the modification of the ansatz for $\check{\Psi}_N$ according to (1.8); see section 5.2 for details.

In view of (1.8), the operator $\mathcal{P}$ generating pairs from the condensate reads as [69, 70]

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

where $N_0(t) = (\check{\Psi}_N^1, a_0^*(t)a_0(t)\check{\Psi}_N^1)_2$ is the number of particles at the condensate, and $\check{K}$ 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 x and y in other states. For definiteness, assume that

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

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

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, $\mathcal{N}$, equal to the (fixed) number N. This replacement is made for later algebraic convenience. Equation (3.9) should be interpreted in the sense that $\mathcal{N}\check{\Psi}_N^1 = N\check{\Psi}_N^1$, by restriction to the N-sector of $\mathbb{F}$.

Remark 3.2. The number of particles out of the condensate equals

$$N_1 = \langle\check{\Psi}_N, \mathcal{N}_1\check{\Psi}_N\rangle_{\mathbb{F}} \sim \langle\check{\Psi}_N^1, \mathcal{N}_1\check{\Psi}_N^1\rangle_{\mathbb{F}}\ , \qquad \mathcal{N}_1 := \int \psi_1^*(x)\psi_1(x)\,\mathrm{d}x\ . \tag{3.10}$$

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

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

Definition 3.3. Quantum fluctuations *describe the many-body dynamics that arise from quadratic and higher-order ψ_1 and ψ_1^* terms in the many-particle Hamiltonian, H_N. In this case, $\check{\Psi}_N$ deviates 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., [58, 65], of Bogoliubov's approach [5] essentially invoke basis functions for particle excitations in correspondence to the shape of the external potential, $V_{\mathrm{e}}(x)$. In the translation-invariant case, $V_{\mathrm{e}} = \mathrm{const.}$, with periodic boundary conditions, the most convenient set of such basis functions of course represents states of definite particle momenta, thus consisting of plane waves.

The scheme by Esry [23] and Esry et al. [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 ($\check{\Phi}$). It should be mentioned that studies of the excitation spectrum based on what is known as the "Bogoliubov–de Gennes equations" [57] seem to mostly retain 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 [45], Lieb et al. [46], and Lieb and Yngvanson [47]. For periodic boundary conditions (without a trap), the expansion parameter is known to be $\sqrt{\rho a^3}$, where ρ is the (uniform) gas density [61, 68]. In the presence of a trap, the expansion for the ground state energy corresponds to having $\check{K}$ act back to the NSE for $\check{\Phi}$. (Thus, the NSE must acquire nontrivial corrections.) The issue of obtaining 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, e.g., [51, 56, 57].

4. Overview of our results. The main results of this article concern (i) the derivation of equations of motion for the condensate and pair excitation under a spatially varying scattering length; (ii) two-scale expansions for stationary $\check{\Phi}$ and $\check{K}$ when the scattering length has a periodic microstructure; (iii) solution of the effective (homogenized) equations for slowly varying traps, $V_e(x) = U(\check{\epsilon}x)$; and (iv) description of the fraction of particles out of the condensate.

4.1. Macroscopic equations of motion (sections 5.1 and 5.2). Starting from the Hamiltonian (1.1) with (1.2) and the many-body wave function (1.8), we show that, for the lowest bound state, the time-independent condensate wave function $\Phi(x) = e^{ie_c t}\check{\Phi}(t,x)$ (where e_c is the energy per particle of the condensate) and corresponding pair excitation kernel $K(x,y)$ satisfy equations of the form

$$\mathcal{L}[\Phi]\Phi(x) = 0\ , \tag{4.1}$$

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

In the above, $\mathcal{L}[\Phi(x)] := -\Delta_x + V_{\rm e}(x) + g(x)\Phi(x)^2 - \mu := \mathcal{L}(x)$, $\mu = e_c + \zeta/2$, where ζ is defined via (5.2), and $\mathcal{C}[\Phi, K; A]$ and $\aleph[\Phi, K; A]$ are (in principle) nonlinear functionals of Φ and K; see (5.4) and (5.17).

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

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

By classical homogenization, we show why the $\mathcal{O}(\epsilon)$ terms should vanish. The zeroth-order terms, Φ_0 and K_0, are found to be ϵ-independent and subject to PDEs (4.1) and

(4.2) with $g(x)$ replaced by g_0. The coefficient Φ_2 partly contains the slowly varying parts $\Phi_0(x) = f_0(x)$ and $f_2(x)$; and K_2 contains $K_0(x,y) = \kappa_0(x,y)$ and $\kappa_2(x,y)$. Both Φ_2 and K_2 also carry information for the oscillations of the scattering length; see Proposition 6.9 (condensate wave function) and Proposition 6.12 (pair-excitation kernel) for $d = 1$, along with Remarks 6.10 and 6.14 for $d = 3$. The ensuing energy per particle of the condensate reads as

$$e_c = e_{c,0} + \epsilon^2 e_{c,2} + \cdots \ ; \tag{4.4}$$

see Remark 6.11 for formulas pertaining to $e_{c,0}$ and $e_{c,2}$.

4.3. Slowly varying trap (sections 7.1 and 7.2). For $V_{\rm e}(x) = U(\breve{\epsilon}x)$, $\breve{\epsilon} \ll 1$, 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. We point out that a plausible boundary layer in the NSE stems from a vicinity 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) under the change of variables $\phi_0(x) := f_0(x/\breve{\epsilon})$; see also Remark 7.1. The solutions pertaining to Φ_2 are described in (7.11) and (7.14), along with Remark 7.3, under $\phi_2(x) := f_2(x/\breve{\epsilon})$. Formulas for the energy e_c are provided in (7.8) and (7.13); and the effect of the periodic microstructure of $g(x)$ 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 $\bar{x} = x - y$ and the slow $X = \breve{\epsilon}(x + y)/2$. Formulas (7.22) and (7.26) describe the outer and inner solutions for the Fourier transform of $K_0(x,y)$ with respect to $\bar{x}$ when X lies inside the trap, with the change of variables $ß_0(\bar{x}, X) := \kappa_0(X/\breve{\epsilon} + \bar{x}/2, X/\breve{\epsilon} - \bar{x}/2)$. The corresponding outer solution for the Fourier transform in $\bar{x}$ of K_2 is provided by (7.33) with $ß_2(\bar{x}, X) := \kappa_2(X/\breve{\epsilon} + \bar{x}/2, X/\breve{\epsilon} - \bar{x}/2)$.

4.4. Description of condensate depletion (sections 8.1 and 8.2). The fraction, $\xi_{\rm dp}$, of particles that occupy states out of the condensate is computed through two-scale expansions (4.3). First, on the basis of formal expression (8.1) for $\xi_{\rm dp}$ in terms of the trace of an operator depending on K, we derive the ϵ-expansion

$$\xi_{\rm dp} = \xi_{\rm dp,0} + \epsilon^2 \xi_{\rm dp,2} + \cdots \ ; \tag{4.5}$$

see (8.4)–(8.6). Second, the coefficients of this expansion are computed explicitly for a macroscopic trap, $V_{\rm e}(x) = U(\breve{\epsilon}x)$, by use of formulas from section 7; see (8.12) and (8.14). The combined effect on $\xi_{\rm dp}$ of the oscillatory particle repulsions and the trapping potential is discussed in Remark 8.2.

5. Equations of motion: Varying scattering length. In this section, we derive macroscopic equations from Hamiltonian (3.4) with interaction (1.3). Our starting point is to express H_N in terms of powers of ψ_1 and ψ_1^* via the simplified point interaction (1.3). Thus, we write $H_N = H^{(0)} + H^{(1)} + H^{(2)} + H^{(3)} + H^{(4)}$, where $H^{(m)}$ denotes the constituent of H_N where each of ψ_1 and ψ_1^* appears m times [69].

5.1. Mean field. Starting from the microscopic description we now show formally that $\check{\Phi}(t,x)$ obeys the NSE with a varying scattering length, namely,

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

where

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

For bound states, we set

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

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

$$[-\Delta + V_{\rm e}(x) + g(x)\Phi^2]\Phi = \mu\Phi \ , \qquad \mu = \zeta_\Delta + \zeta_e + \zeta \ , \tag{5.4}$$

$$\zeta_\Delta := N^{-1}\int {\rm d}x\, |\nabla\Phi|^2 \ , \qquad \zeta_{\rm e} := N^{-1}\int {\rm d}x\, V_{\rm e}(x)|\Phi(x)|^2 \ . \tag{5.5}$$

We proceed to show (5.1) by revisiting, and slightly modifying, Wu's approach [70]. The Hamiltonian (3.4) needs to be linearized in ψ_1 and ψ_1^*. Hence, we write

$$H_N \approx H^{(0)} + H^{(1)} \ , \tag{5.6}$$

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

$$H^{(0)} = \int {\rm d}x\, \left\{\check{\Phi}^*(t,x)[-\Delta + V_{\rm e}(x)]\check{\Phi}(t,x) + \frac{N-1}{2N}\, g(x)|\check{\Phi}(t,x)|^4\right\} \ , \tag{5.7}$$

$$H^{(1)} = N^{-1/2}\int {\rm d}x\ \psi_1^*\left\{a_0(-\Delta + V_{\rm e})\check{\Phi} + N^{-1}a_0^* a_0^2\, g(x)\check{\Phi}|\check{\Phi}|^2\right\} + \ {\rm c.c.} \ , \tag{5.8}$$

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

$$1 - \langle\check{\Psi}_N, (a_0^* a_0/N)\check{\Psi}_N\rangle_{\mathbb{F}} \ll 1 \ .$$

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

$$\check{\Psi}_N^0(t) = \frac{a_0^*(t)^N}{\sqrt{N!}}|{\rm vac}\rangle \ , \tag{5.9}$$

which means that N particles are created at the state $\check{\Phi}$. By Schrödinger equation (1.4a) with (5.6) and (5.9), we obtain

$$(i\partial_t a_0^*)\widetilde{\Psi}_{N-1}(t) = [\widetilde{H}^{(0)} + \widetilde{H}^{(1)}]\widetilde{\Psi}_{N-1}(t) \ ; \tag{5.10}$$

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

$$\widetilde{\Psi}_{N-1}(t) := N\frac{{a_0^*}^{N-1}}{\sqrt{N!}}|{\rm vac}\rangle \ , \tag{5.11}$$

$$\widetilde{H}^{(0)} := N^{-1}a_0^*(t)\int {\rm d}x\, \left\{\check{\Phi}^*(-\Delta + V_{\rm e})\check{\Phi} + \frac{N-1}{2N}\, g(x)\, |\check{\Phi}|^4\right\} \ , \tag{5.12}$$

$$\widetilde{H}^{(1)} := N^{-1/2}\int {\rm d}x\ \psi_1^*\left\{(-\Delta + V_{\rm e})\check{\Phi} + \frac{N-1}{N}g(x)\, \check{\Phi}|\check{\Phi}|^2\right\} \ . \tag{5.13}$$

The next step is to write an equation of motion for $a_0^*(t)$; (5.10) implies

$$i\partial_t a_0^* = \widetilde{H}^{(0)} + \widetilde{H}^{(1)} \ . \tag{5.14}$$

By $a_0^*(t) = N^{-1/2}\int {\rm d}x\, \check{\Phi}(t,x)\psi^*(x)$, (5.14) yields

$$\int {\rm d}y\ \psi^*(y)\, (i\partial_t\check{\Phi}) = \int {\rm d}y\ \psi^*(y)\left\{-\Delta_y + V_{\rm e} + \frac{N-1}{N}g(y)|\check{\Phi}|^2 - \frac{N-1}{2N}\zeta\right\}\check{\Phi}(t,y) \ , \tag{5.15}$$

where $\zeta = \zeta(t)$ is defined by (5.2). The contraction of (5.15) with $\psi(x)$ by use of $[\psi(x),\, \psi^*(y)] = \delta(x-y)$ leads to (5.1).

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

$$\check{K}(t,x,y) = e^{-i(2\mu-\zeta)t}\, K(x,y)\ . \tag{5.16}$$

The exponential on the right-hand side is a consequence of ansatz (1.8) and the fact that we look for stationary solutions of (1.4a). We show that $K(x,y)$ satisfies

$$\begin{aligned} 0 = {} & (-\Delta_x - \Delta_y)K + g(x)\Phi(x)^2\delta(x-y) + \{-2\zeta_\Delta - 2\zeta - 2\zeta_{\rm e} + V_{\rm e}(x) + V_{\rm e}(y) \\ & + 2[g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2]\}K(x,y) + \int {\rm d}z\, g(z)\Phi^*(z)^2\, K(x,z)\, K(y,z) \\ & - N^{-1}\Big\{\int {\rm d}z\, [\Phi(y)K(x,z) + \Phi(x)K(y,z)]g(z)|\Phi(z)|^2\Phi^*(z) \\ & + \Phi(x)\Phi(y)[g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2 - \zeta]\Big\}\ , \end{aligned} \tag{5.17}$$

where Φ obeys (5.4), and ζ, ζ_Δ, and $\zeta_{\rm e}$ are defined in (5.2) and (5.5); cf. (4.9) of [70] with constant g. Assuming a unique solution of (5.17) (in some appropriate space), we infer that if Φ is real, the corresponding $K(x,y)$ should be taken to be real.

We proceed to derive (5.17). By keeping quadratic 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

$$H_N \approx H_{N,2} = H^{(0)} + H^{(1)} + H^{(2)}\ . \tag{5.18}$$

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

$$H^{(0)} + H^{(1)} = N\big(\zeta_\Delta + \zeta_{\rm e} + \tfrac{1}{2}\zeta\big)\ , \tag{5.19}$$

$$H^{(2)} = \int {\rm d}x\ \psi_1^*[-\Delta + V_{\rm e} - \zeta_\Delta - \zeta_{\rm e} - \zeta + 2g(x)\Phi^2]\psi_1 \tag{5.20}$$

$$+\ \tfrac{1}{2}N^{-1}{a_0}^2 \int {\rm d}x\ g(x)\,\Phi^*(x)^2\,{\psi_1^*}^2 + \ \text{c.c.}\ . \tag{5.21}$$

The next step is to apply the many-body (stationary) Schrödinger equation (1.4a) with H_N replaced by (5.18) and the $\check{\Psi}_N$ given by $\check{\Psi}_N(t) = e^{-iE_Nt}\Psi_N$ under (1.8) and (3.7); thus, the pair-excitation approximation Ψ_N^1 for Ψ_N obeys

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

Note that the non-Hermitian operator $e^{-\mathcal{P}}H_{N,2}e^{\mathcal{P}}$ is required to have an eigenstate equal to the tensor product Ψ_N^0.

The operator $e^{-\mathcal{P}}H_{N,2}e^{\mathcal{P}}$ can be computed via the Lie expansion [67]

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

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 $[\mathcal{P},H_{N,2}]_n = 0$, $n \ge 3$. Following [70], we find

$$e^{-\mathcal{P}}H_{N,2}e^{\mathcal{P}} = N\big(\zeta_\Delta + \zeta_{\rm e} + \tfrac{1}{2}\zeta\big) + H_a + H_a^c\ . \tag{5.24}$$

The terms H_a and H_a^c in (5.24) have distinct roles. First, H_a contains $\psi_1^*\psi_1$ and ψ_1^2 and is thus manifestly compatible with (5.22):

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

By contrast, H_a^c contains $\psi_1^*\psi_1^*$, which in principle is *not* compatible with (5.22):

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

This H_a^c is written as

$$H_a^c = (2N)^{-1} \int \mathrm{d}x \mathrm{d}y \; \psi_1^*(x)\psi_1^*(y) L(x,y) a_0^2 \, , \tag{5.25}$$

where the associated kernel is

$$\begin{aligned} L(x,y) = {} & g(x)\Phi(x)^2\delta(x-y) - (\Delta_x + \Delta_y)K + \{-2\zeta_\Delta - 2\zeta - 2\zeta_\mathrm{e} + V_\mathrm{e}(x) + V_\mathrm{e}(y) \\ & + 2[g(x)|\Phi(x)|^2 + g(y)|\Phi(y)|^2]\} \, K(x,y) \\ & + \int \mathrm{d}z \; g(z)\Phi^*(z)^2 \, K(x,z) \, K(y,z) - \sigma(x)\Phi(y) - \sigma(y)\Phi(x) \; ; \end{aligned} \tag{5.26}$$

$\sigma(x)$ is to be determined. Note that the appearance of the Dirac mass in (5.26) is due to the (simplified) interaction (1.3).

By (5.22) and (5.24), $K(x,y)$ is determined by the condition that H_a^c be zero [70]:

$$L(x,y) \equiv 0 \, . \tag{5.27}$$

To find $\sigma(x)$, use $\|\Phi\|^2_{L^2(\mathbb{R}^3)} = N$; thus, (5.26) leads to the integral equation

$$\begin{aligned} & \int \mathrm{d}y \, K(x,y)[-\Delta_y + V_\mathrm{e} + 2g(y)|\Phi(y)|^2]\Phi^*(y) + g(x)|\Phi(x)|^2\Phi(x) \\ & = N\sigma(x) + \Phi(x) \int \mathrm{d}y \, \sigma(y)\Phi^*(y) \, , \end{aligned} \tag{5.28}$$

which has the explicit solution

$$\sigma(x) = N^{-1} \Big\{ \int \mathrm{d}y \, K(x,y) g(y)|\Phi(y)|^2\Phi^*(y) + g(x)|\Phi(x)|^2\Phi(x) - \tfrac{1}{2}\zeta\Phi(x) \Big\} \, . \tag{5.29}$$

The substitution of this σ into (5.26) under (5.27) yields (5.17).

Equations (5.4) and (5.17) form the core of this article. Note that, to the present order of many-body perturbation, the NSE (5.1) is decoupled from K.

6. Periodic homogenization. In this section, we formally study (5.4) and (5.17) with the periodic $g(x)$ of (1.9) for the lowest bound state. To demonstrate the computations with relative ease, we first present the homogenization program in 1D (sections 6.2 and 6.3). We then extend the homogenization results to 3D.

6.1. Preliminaries. In this subsection, we outline a few technical assumptions and preliminary results. The starting point consists of the two-scale expansions

$$\Phi^\epsilon(x) = \Phi(x) = \Phi_0(\tilde{x}, x) + \sum_{n\geq 1} \epsilon^n \, \Phi_n(\tilde{x}, x) \ ,$$

$$K(x,y) = K_0(\tilde{x}, \tilde{y}, x, y) + \sum_{n\geq 1} \epsilon^n \, K_n(\tilde{x}, \tilde{y}, x, y) \ , \quad \tilde{x} = x/\epsilon \ , \ \tilde{y} = y/\epsilon \ , \tag{6.1}$$

where $\tilde{x}$ and $\tilde{y}$ are fast variables and the superscript ϵ is dropped for ease of notation. The real eigenvalue, μ, for the condensate is

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

The study of convergence of expansions (6.1) and (6.2) lies beyond our purposes. We restrict our 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 with n.

Our main hypotheses are summarized in the following remarks.

Remark 6.1. We assume that the $A(x)$ in (1.9) is 1-periodic and smooth; and $V_{\rm e}(x)$ is smooth, positive, and 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

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

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

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

Remark 6.3. The physical domains of Φ and K are $\mathbb{R}^3$ and $\mathbb{R}^3 \times \mathbb{R}^3$ ($d = 3$), respectively. It will be explicitly shown via heuristics that the kernel $K(x, y)$ is weakly singular on the diagonal ($x = y$), due to the presence of the Dirac mass in (5.17); see Remark 7.4. In our classical homogenization program for the kernel $K(x, y)$ (section 6.3), we essentially restrict our attention off the diagonal ($x \neq y$).

In sections 6.2 and 6.3, we make use of a few results which we need to 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 [52] 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 as (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 $P : \mathbb{R}^d \to \mathbb{C}$ 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 $\sum_{k=1}^d \beta_k \le m-1$, $\beta_k \ge 0$, $\beta = (\beta_1, \ldots, \beta_d)$; 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 $|\alpha| := \sum_{k=1}^d \alpha_k = m$:

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

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

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

which provides 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 $s > d/4$, $x_0 \ne 0$, and constant $c_1 \in \mathbb{C}$. Then,*

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

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

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

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

which leads to (6.9) in view of the Fourier series for $(-\Delta_x)^{-s} P(x/\epsilon)$ at $x = x_0$. ∎

Remark 6.7. A few comments on the relevance of Lemmas 6.5 and 6.6 are in order. We apply both lemmas to integrals with $P(x) \equiv \partial_x^{-\alpha} A(x)$. Lemma 6.5 is invoked for integrals where h involves (i) products of Φ_n, supplied with sufficient regularity (large 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 of these products. For example, in section 6.3 we encounter an integral of the form

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

where, by inspection of PDE (5.17) and from section 7 for $K_0 = \kappa_0$, $\kappa_0(x,z)$ is weakly singular at $z = x$; see Remark 7.4. 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 claim that these contributions are nonoverlapping and can be separated; thus, we compute

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

The emerging integrals are then estimated with 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} becomes a constant, the system becomes translation invariant and K_n depends only on $x-y$. For a slowly varying V_{e}, each term K_n depends primarily on the *fast* variable $x-y$; an additional, *slow* variable is proportional to $x+y$ and can be treated as a parameter (see section 7).

Remark 6.8. We assume that the Fourier transform of $K_0(\tilde{x},\tilde{y},x,\cdot)$, with fixed $(\tilde{x},\tilde{y})$ 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 slowly varying traps; cf. (7.21).

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

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

In this section, we start with (6.12) and apply (6.1) and (6.2).

PROPOSITION 6.9 (consistency of two-scale expansion with NSE). *The formal two-scale expansion for $\Phi(x)$, $x \in \mathbb{R}$, up to $\mathcal{O}(\epsilon^2)$ reads as*

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

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 is given by expansion (6.2) *with*

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

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

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

and

$$\zeta_0 := g_0 N^{-1}\|f_0^2\|^2_{L^2}\;,\quad \zeta_{\Delta 0} := N^{-1}\|\partial_x f_0\|^2_{L^2}\;,\quad \zeta_{\mathrm{e}0} := N^{-1}(f_0, V_{\mathrm{e}} f_0)_2\;. \tag{6.19}$$

In the proof of Proposition 6.9 we invoke the one-dimensional 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., [60, 64] (and [31] for nodal solutions).[5] Given an acceptable solution f_0, the existence of a 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 $\partial_x + \epsilon^{-1}\partial_{\tilde{x}}$ yields the following cascade of equations for Φ_n:

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

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

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

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

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

Note the appearance of $V_{\rm e}$ 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 $\|\Phi\|_{L^2}^2 = N$ (which affects the prefactor in the nonlinear term of the NSE for Φ). The two-scale expansion (6.1) for Φ thus yields the relations

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

where N is 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 admissible 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

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

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

$$[-\partial_x^2 + V_{\rm e}(x) + 3g_0f_0(x)^2 - \mu_0]f_1(x) = \mu_1 f_0(x) \qquad (g_0 > 0) \ . \tag{6.29}$$

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

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

[5] In [31, 60] the authors primarily address the focusing NSE. Their variational approach should also be applicable to the defocusing case with a trapping potential.

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 $\|f_1\|_{L^2} > 0$; 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

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

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

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

Next, we 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 we conclude in the course of deriving (6.30); thus, $f_2 = \mathcal{L}_2^{-1} b(x)$, yielding

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

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 obtain

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

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 $P(\tilde{x}) \equiv \partial_{\tilde{x}}^{-2} A(\tilde{x})$, where $\langle \partial_{\tilde{x}}^{-2} A \rangle = 0$ 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 satisfies $(f_0, f_2)_2 = 0$. This observation concludes our proof. ∎

Remark 6.10. Proposition 6.9 can be directly extended to d spatial dimensions, $d \geq 2$. The two-scale expansion for Φ reads as

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

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

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

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

Remark 6.11. Proposition 6.9 provides an expansion for μ. A corresponding expansion for the energy, e_c, per particle of the condensate follows from the relation $e_c = \mu - \zeta/2$ via Lemma 6.5: $e_c = e_{c,0} + \epsilon^2 e_{c,2} + \cdots$, where

$$e_{c,0} = \mu_0 - \frac{g_0}{2} N^{-1} \int f_0(x)^4\, \mathrm{d}x \ , \qquad e_{c,2} = \mu_2 - 2g_0 N^{-1} \int f_0(x)^3\, f_2(x)\, \mathrm{d}x \ . \tag{6.40}$$

6.3. Effective equations for kernel K. In this section, we focus on (5.17) by neglecting terms proportional to N^{-1}.[6] For $d = 1$, the equation of motion reads as

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

where

$$\zeta = g_0 N^{-1} \int {\rm d}x\, [1 + A(x/\epsilon)]\Phi(x)^4\ , \qquad \zeta_\Delta = N^{-1} \int {\rm d}x\ (\partial_x \Phi)^2\ ,$$

$$\zeta_{\rm e} = N^{-1} \int {\rm d}x\, V_{\rm e}(x)\, \Phi(x)^2\ . \tag{6.42}$$

By substituting expansion (6.1) for $K(x,y)$ 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 6.8). In the following, we treat Φ_n as known.

PROPOSITION 6.12. *The two-scale expansion for the pair-excitation kernel $K(x,y)$, $(x,y) \in \mathbb{R}^2$, reads as*

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

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

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

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

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 $B_0(x,y)$ and $B_2(x,y)$ are

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

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

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

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

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

[6] Because of this simplification, the orthogonality of K and Φ is strictly abandoned. This is not expected to distort the essential physics of the problem (with $d = 3$) [70].

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).[7] Given a solution f_0, the respective K_0 is assumed to exist uniquely. We show that $K_1 = 0$, in correspondence to Φ_1 (see Proposition 6.9); our argument makes use of a small g_0.

We first state a property pertaining to term $\mathcal{C}[f_0^2, \kappa_0]u$ of (6.44) and (6.45).

LEMMA 6.13. *For given $\kappa \in L^2(\mathbb{R}^d \times \mathbb{R}^d)$ and bounded f, 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 on $L^2(\mathbb{R}^d \times \mathbb{R}^d)$.

The proof of this lemma relies on standard estimates and is omitted. We are now in position to delineate the proof of Proposition 6.12.

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

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

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

$$-\Delta_{\tilde{x}\tilde{y}} K_n(\tilde{x},\tilde{y},x,y) = S_n^{\mathrm{sc}}(\tilde{x},\tilde{y},x,y)\ , \tag{6.53}$$

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

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

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

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

$$\begin{aligned} \zeta_\Delta &\sim \zeta_{\Delta 0} + \epsilon^2\zeta_{\Delta 2}\ , \quad \zeta_{\Delta 0} = N^{-1}\|\partial_x f_0\|_{L^2}^2\ , \\ \zeta_{\Delta 2} &= N^{-1}\left[g_0^2\|A\|_{-1}^2\|f_0^3\|_{L^2}^2 + 2(\partial_x f_0, \partial_x f_2)_2\right]\ ; \end{aligned} \tag{6.56}$$

$$\zeta_{\mathrm{e}} \sim \zeta_{\mathrm{e}0} + \epsilon^2\zeta_{\mathrm{e}2}\ , \quad \zeta_{\mathrm{e}0} = N^{-1}(f_0, V_{\mathrm{e}} f_0)_2\ ,\ \zeta_{\mathrm{e}2} = 2N^{-1}(f_2, V_{\mathrm{e}} f_0)_2\ . \tag{6.57}$$

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

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

$$\mathcal{O}(\epsilon^0): \qquad -\Delta_{\tilde{x}\tilde{y}} K_0 = 0 =: S_0^{\mathrm{sc}}\ , \tag{6.58}$$

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

[7] A difficulty is the presence of the Dirac mass in these equations, which destroys the L^2 structure of the forcing. The weak formulations of the respective boundary value problems lie beyond our scope.

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 (for $n=2,\,3$).

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

$$\begin{aligned} S_2^{\rm sc}(\tilde{x},\tilde{y},x,y)&=-\mathcal{L}_{(xy)}\kappa_0-\mathcal{C}[f_0^2,\kappa_0]\kappa_0+B_0(x,y)\\ &\quad-g_0A(\tilde{x})f_0^2\delta(x-y)-2g_0\{A(\tilde{x})f_0(x)^2+A(\tilde{y})f_0(y)^2\}\kappa_0\ . \end{aligned} \tag{6.61}$$

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

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 $\mathcal{L}_{(xy)}$ in order to determine κ_1.

By virtue of (6.44), K_2 satisfies

$$-\Delta_{\tilde{x}\tilde{y}}K_2=-g_0A(\tilde{x})f_0^2\delta(x-y)-2g_0[A(\tilde{x})f_0(x)^2+A(\tilde{y})f_0(y)^2]\kappa_0\ , \tag{6.62}$$

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 that $\Phi_1=0$ and invoking Lemma 6.6 (for $s=1$). Thus, we derive (6.53) with

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

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 6.13, 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

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

Next, we consider the equation for K_4, $-\Delta_{\tilde{x}\tilde{y}}K_4 = S_4^{\rm sc}$ and find

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

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

$$\begin{aligned} &-2\mathcal{C}[f_0^2,\kappa_0]\kappa_2 - 2\mathcal{C}[f_0f_2,\kappa_0]\kappa_0 + 6g_0\|A\|_{-1}^2\mathcal{C}[f_0^4,\kappa_0]\kappa_0 \\ &\quad + g_0^2\|A\|_{-1}^2\big[f_0(x)^4 + f_0(y)^4\big]\kappa_0(x,y)\ . \end{aligned}$$

This observation concludes our proof. ∎

Remark 6.14. Proposition 6.12 can be extended to d spatial dimensions, where $d = 2$, 3. The two-scale expansion for K reads as

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

where $\kappa_0(x,y)$ and $\kappa_2(x,y)$ satisfy (6.44) and (6.45) with $\Delta_{xy} = \Delta_x + \Delta_y$ and $\mathcal{L}_0(x) = -\Delta_x + V_{\rm e}(x) + g_0f_0(x)^2 - \mu_0$. The definitions of $\mathcal{C}$, B_0, B_2, and Z_2 follow from (6.47)–(6.50).

7. Slowly varying trap. By taking $d = 3$, we now focus on expansions (6.37) and (6.69) and discuss via heuristics approximate solutions for the homogenized coefficients with $V_{\rm e}(x) = U(\check{\epsilon}x)$, $0 < \check{\epsilon} \ll 1$, $x \in \mathbb{R}^3$. As $\check{\epsilon} \downarrow 0$, 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 $\check{\epsilon}$. This scale separation is carried out via singular perturbations (since $\check{\epsilon}$ multiplies the highest-order derivatives in the governing PDEs) [9]. For each homogenized coefficient, we consider only the leading-order contribution in $\check{\epsilon}$.

As stated in section 1.6, the approximations of this section hold in the asymptotic regime $a \ll l_d \ll l_c \ll l_e$, where l_d is the mean interparticle distance, l_c is the system correlation length (over which Φ changes appreciably), l_e is the typical size of the trap, and $\check{\epsilon} = l_c/l_e$. We consider $\check{\epsilon} \ll \epsilon = l_{sc}/l_c$ (l_{sc}: period of scattering length).

Our approximations serve the need to compute physical 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 from the region $\{x \in \mathbb{R}^3 \,\big|\, U(x) < \mu_0\}$ which (loosely) defines the interior of the trap (as explained below). Outside this region, $\Phi(\tilde{x},\cdot)$ is expected to decay rapidly and, for all practical purposes, will be set to zero. A similar consideration holds for $K(\tilde{x},\tilde{y},\cdot)$ via center-of-mass coordinates.

7.1. Condensate wave function. Next, we focus on two-scale expansion (6.37) for Φ (see Remark 6.10). Change the variable by $x \mapsto \breve{x} = \breve{\epsilon}\, x$, set $\phi_0(\breve{x}) := f_0(\breve{x}/\breve{\epsilon})$, and drop the $\breve{}$ symbol on top of $\breve{x}$ (for ease of notation). The PDE for $\phi_0(x)$ reads as

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

along with the normalization condition

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

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

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

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

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

supplemented with the condition $(\phi_2, \phi_0)_2 = 0$ via Proposition 6.9.

7.1.1. Zeroth-order homogenized solution. We now briefly discuss an approximate solution to (7.1) by use of classical boundary layer theory [70].[8]

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

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

which in turn yields an approximate formula for ϕ_0:

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

Here, $\mathfrak{R}_0^\delta$ is the region that results from exclusion of a δ-neighborhood (to be specified below) of the boundary of $\mathfrak{R}_0 := \{x \in \mathbb{R}^3 \,\big|\, U(x) < \mu_0^0\}$ for small enough δ; $\mathfrak{R}_0^\delta = \mathfrak{R}_0 \setminus \mathfrak{B}(\partial\mathfrak{R}_0, \delta)$. This $\mathfrak{R}_0$ is open, bounded with boundary $\partial\mathfrak{R}_0 = \{U(x) = \mu_0^0\}$ consisting of 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 $\nabla\phi_0^0(x) = -g_0^{-1/2}[\mu_0^0 - U(x)]^{-1/2}\nabla U$ 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, 50].

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

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

where $|\mathfrak{R}_0|$ is the (g_0-dependent) volume of $\mathfrak{R}_0$, $|\mathfrak{R}_0| := \int_{\mathfrak{R}_0}\mathrm{d}x$. By Remark 6.11, result (7.7) yields an approximate energy, $e_c \sim e_{c,0}^0$, per particle of the condensate:

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

[8] In the following, the term "outer solution" pertains to a leading-order approximation of some PDE by regular perturbation (with $\breve{\epsilon} = 0$) away from boundary layers, inside *and* outside the trap.

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

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 in $L^2_{loc}(\mathbb{R}^3)$ by integration on any region that contains a measurable part of $\partial\mathfrak{R}_0$, in contrast to the anticipated behavior of $\nabla\phi_0$.

To remedy this pathology (which is due to naively setting $\breve{\epsilon}=0$ for the outer solution) consider the variation of ϕ_0 along the local normal to $\partial\mathfrak{R}_0$ (for C^1 boundary $\partial\mathfrak{R}_0$) [70]. 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 one-dimensional equation

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

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

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

Remark 7.1. It is known that (7.9) is solved by a second Painlevé transcendent [39, 70]. 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., [50] and the references therein. Let $P_{II}(\eta)$ denote this particular second Painlevé transcendent: $\phi_0^{in}=P_{II}$.

Equations (7.6) and (7.9) combined should yield a composite approximation for ϕ_0 that is sufficiently regular across $\partial\mathfrak{R}_0$.

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

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

By (7.6), we find $U_{\text{eff}}(x)\sim 2[\mu_0^0-U(x)]>0$ for $x\in\mathfrak{R}_0^\delta$ (inside the trap); and $U_{\text{eff}}(x)\sim U(x)-\mu_0^0>0$ outside the trap. Thus, ϕ_2 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 $\breve{\epsilon}=0$ in (7.10), we find that $\phi_2(x)$ is approximated by

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

The value of μ_2^0 comes from the condition $(f_0,f_2)_2=0$ (by Proposition 6.9):

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

μ_0^0 is described by (7.7). By Remark 6.11, the respective contribution to the energy per particle of the condensate is

$$(7.13)\qquad e_{c,2}\sim e^0_{c,2}=-3g_0^{-1}\|A\|^2_{-1}\int_{\mathfrak{R}_0}[\mu_0^0-U(x)]^3\,\mathrm{d}x<0\ .$$

Note that the extension of $\phi_2^0(x)$ across $\partial\mathfrak{R}_0$ is not in $L^2_{loc}(\mathbb{R}^3)$. This observation calls for using boundary layer theory in the vicinity of $\partial\mathfrak{R}_0$ (as discussed below).

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 $\|A\|^2_{-1}$.

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 $U_{\rm eff}(x) \sim (U_o\check{\epsilon})^{2/3}[\eta + 3P_{II}(\eta)^2]$ and $F_2(x) \sim \mu_2^0 g_0^{-1/2}(U_o\check{\epsilon})^{1/3}P_{II}(\eta)$, in view of Remark 7.1. Thus, we obtain the equation

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

By matching the inner and outer solutions for $\mathcal{O}(\check{\epsilon}^{2/3}) < |x - x_{bd}| \ll 1$, 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 second 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 6.14). 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, $K(x, y)$ is expected to depend primarily on $x - y$ [69, 70]. Here, we follow the technique invoked in [70], where $x - y$ is treated as a fast variable (in $\check{\epsilon}$).

The related transformation to the center-of-mass coordinates reads as

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

This change of variables is motivated by the observation that $\kappa_j(x, y)$ $(j = 0, 2)$ are controlled by forcing terms proportional to the Dirac mass, $\delta(x - y)$.

7.2.1. Zeroth-order kernel. The analogue of (6.44) in 3D reads as

$$\begin{aligned} 0 = {} & \big(-\tfrac{\check{\epsilon}^2}{2}\Delta_X - 2\Delta_{\bar{x}}\big)ß_0 + \big\{U(X + \tfrac{\check{\epsilon}}{2}\bar{x}) + U(X - \tfrac{\check{\epsilon}}{2}\bar{x}) \\ & + 2g_0\big[\phi_0(X + \tfrac{\check{\epsilon}}{2}\bar{x})^2 + \phi_0(X - \tfrac{\check{\epsilon}}{2}\bar{x})^2\big] - 2\mu_0\big\}ß_0 + g_0\phi_0(X)^2\,\delta(\bar{x}) \\ & + g_0\int_{\mathbb{R}^3} \mathrm{d}z\ \phi_0(X - \tfrac{\check{\epsilon}}{2}\bar{x} + \check{\epsilon}z)^2\, ß_0(\bar{x} - z, X + \tfrac{\check{\epsilon}}{2}z)\, ß_0(z, X - \tfrac{\check{\epsilon}}{2}\bar{x} + \tfrac{\check{\epsilon}}{2}z)\ , \end{aligned} \tag{7.16}$$

where we defined the slow variable $X := \check{\epsilon}(x + y)/2 > \mathcal{O}(\check{\epsilon})$, and

$$\bar{x} = x - y = \mathcal{O}(1)\ , \qquad ß_0(\bar{x}, X) := \kappa_0(X/\check{\epsilon} + \bar{x}/2, X/\check{\epsilon} - \bar{x}/2)\ . \tag{7.17}$$

Thus, variations of κ_0 with respect to $\bar{x}$ are considered fast. This view is consistent with the anticipated nearly translation-invariant character of the boson system. Now apply the approximations [70]

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

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

$$\int \mathrm{d}z\ \phi_0(X-\tfrac{\check\epsilon}{2}\bar x+\check\epsilon z)^2\,ß_0(\bar x-z,X+\tfrac{\check\epsilon}{2}z)\,ß_0(z,X-\tfrac{\check\epsilon}{2}\bar x+\tfrac{\check\epsilon}{2}z)$$
$$\sim \phi_0(X)^2\int \mathrm{d}z\,ß_0(\bar x-z,X)\,ß_0(z,X)\ ,$$

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 in $\bar x$, treating X as a parameter. The Fourier transform, $\widehat{ß}_0(\lambda,X)$, of $ß_0(\cdot,X)$ satisfies

$$(7.18)\quad \big(-\tfrac{\check\epsilon^2}{2}\Delta_X+2\lambda^2\big)\widehat{ß}_0+2[U(X)+2g_0\phi_0(X)^2]\widehat{ß}_0+g_0\phi_0(X)^2+g_0\phi_0(X)^2(\widehat{ß}_0)^2\approx 0\ .$$

We now solve the last equation by singular perturbations.

Outer solution. By setting $\check\epsilon=0$ in (7.18) and $\widehat{ß}_0\sim\widehat{ß}_0^0$, we obtain

$$(7.19)\qquad \tfrac12 g_0\phi_0^0(X)^2(\widehat{ß}_0^0)^2+[U(X)+2g_0\phi_0^0(X)^2+\lambda^2-\mu_0^0]\widehat{ß}_0^0+\tfrac12 g_0\phi_0^0(X)^2=0\ ,$$

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

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

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

$$(7.21)\qquad \widehat{ß}_0^0(\lambda,X)\sim-\frac12\frac{g_0\phi_0^0(X)^2}{\lambda^2+\lambda_0(X)^2}\ ,$$

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

A further simplification of (7.20) ensues from (7.6) [70]:

$$(7.22)\qquad \widehat{ß}_0^0(\lambda,X)=\frac{-\lambda^2-g_0\phi_0^0(X)^2+|\lambda|\sqrt{\lambda^2+2g_0\phi_0^0(X)^2}}{g_0\phi_0^0(X)^2}\qquad \text{if } X\in\mathfrak{R}_0^\delta\ .$$

On the other hand, if $X\in\mathfrak{R}_0^{\mathrm{c},\delta}$, we obtain $\widehat{ß}_0^0(\lambda,X)=0$, which can be refined via the WKB method in X (for fixed λ); we do not pursue the WKB solution here. Equation (7.22) is inverted to give the pair-excitation kernel (for $X\in\mathfrak{R}_0^\delta$) [70]

$$(7.23)\qquad ß_0^0(\bar x,X)=\pi^{-2}\left(\frac{g_0}{2}\right)^{3/2}\phi_0^0(X)^3\vartheta(\bar x,X)^{-1}\mathrm{Im}[S_{00}(i\vartheta)-S_{04}(i\vartheta)]\ ,$$

where $\vartheta=\vartheta(\bar x,X)=(2g_0)^{1/2}\phi_0^0(X)|\bar x|$ and $S_{\alpha\beta}$ is Lommel's function [66].

Remark 7.4. By (7.23), in the limit $\bar x=x-y\to 0$ with $X\in\mathfrak{R}_0^\delta$ (inside the trap), we have

$$(7.24)\qquad \kappa_0(x,y)\sim ß_0^0(\bar x,X)\sim-\frac{g_0}{8\pi}\,\frac{\phi_0^0(X)^2}{|\bar x|}\ .$$

Boundary layer. We now consider the pair-excitation kernel when the slow center-of-mass coordinate $\check\epsilon(x+y)/2$ lies inside the boundary layer for ϕ_0, near $\partial\mathfrak{R}_0$ (see section 7.1.1). We (locally) define $ß_0^{in}(\chi,\eta):=(U_o\check\epsilon)^{-1}\kappa_0(x,y)$ with $\chi:=(U_o\check\epsilon)^{1/3}\bar x=$

$(U_o\check{\epsilon})^{1/3}(x-y)$ and $\eta(X)=(U_o/\check{\epsilon}^2)^{1/3}\nu(x_{bd})\cdot(X-x_{bd})$, where $x_{bd}\in\partial\mathfrak{R}_0$. Accordingly, by a flat boundary approximation, (7.16) is reduced to

$$\begin{aligned}0\approx{}&\big[-\tfrac{1}{2}\partial_\eta^2-2\Delta_\chi+2\eta+4(\phi_0^{in})^2\big]ß_0^{in}(\chi,\eta)+(\phi_0^{in})^2\,\delta(\chi)\\&+(\phi_0^{in})^2\int \mathrm{d}z\; ß_0^{in}(\chi-z,\eta)\,ß_0^{in}(z,\eta)\;,\quad X\in\mathfrak{B}(\partial\mathfrak{R}_0,\delta)\;,\;\eta=\eta(X)\;,\end{aligned}\tag{7.25}$$

where $\delta=\mathcal{O}(\check{\epsilon}^{2/3})$.

By assuming $ß_0^{in}(\cdot,\eta)\in L^2(\mathbb{R}^3)$, we obtain an ordinary differential equation for its Fourier transform, $\widehat{ß}_0^{in}(\lambda,\eta)$:

$$-\tfrac{1}{2}\partial_\eta^2\widehat{ß}_0^{in}+2\big[\lambda^2+\eta+2(\phi_0^{in})^2\big]\widehat{ß}_0^{in}+(\phi_0^{in})^2(\widehat{ß}_0^{in})^2+(\phi_0^{in})^2\approx 0\;;\tag{7.26a}$$

recall that $-\partial_\eta^2\phi_0^{in}+\eta\phi_0^{in}+(\phi_0^{in})^3=0$. Consider λ fixed. Boundary conditions for (7.26a) stem from asymptotic matching with the outer solution, $\widehat{ß}_0^0$, of (7.20) as $\eta\to\pm\infty$:[9]

$$\widehat{ß}_0^{in}(\lambda,\eta)\sim -1+|\lambda|\sqrt{-\frac{2}{\eta}}\quad\text{as }\eta\to-\infty\;,\qquad \widehat{ß}_0^{in}(\lambda,\eta)\to 0\quad\text{as }\eta\to\infty\;.\tag{7.26b}$$

Equations (7.26) form a 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 (7.26) and subsequent Fourier inversion to obtain $ß_0^{in}$ are not further pursued in this article.

7.2.2. Higher-order kernel, $\boldsymbol{\kappa_2}$. The heuristics of the preceding subsection can be extended to $ß_2(\bar{x},X):=\kappa_2(X/\epsilon+\bar{x}/2,X/\epsilon-\bar{x}/2)$. We outline the procedure for the outer solution below.

The function $ß_2(\bar{x},X)$ obeys

$$\begin{aligned}4\Lambda(\bar{x},X)\approx{}&[-\check{\epsilon}^2\Delta_X-4\Delta_{\bar{x}}+4W(X)]ß_2(\bar{x},X)\\&+4g_0\phi_0(X)^2\int \mathrm{d}z\; ß_0(\bar{x}-z,X)ß_2(z,X)\;,\end{aligned}\tag{7.27}$$

for given $\phi_0(X)$, $\phi_2(X)$, and $ß_0(\bar{x},X)$, where

$$W(x):=U(x)+2g_0\phi_0(x)^2-\mu_0\;,\tag{7.28}$$

$$\begin{aligned}\Lambda(x,y):={}&-g_0\{\phi_0(y)\phi_2(y)-3g_0\|A\|_{-1}^2\phi_0(y)^4\}\delta(x)\\&+\{Z_2+9g_0^2\|A\|_{-1}^2\phi_0(y)^4-4g_0\phi_0(y)\phi_2(y)\}ß_0(x,y)\\&-g_0[\phi_0(y)\phi_2(y)-3g_0\|A\|_{-1}^2\phi_0(y)^4]\int \mathrm{d}z\, ß_0(x-z,y)ß_0(z,y)\;,\end{aligned}\tag{7.29}$$

and Z_2 is a constant defined by (6.50).

Equation (7.27) can be Fourier-transformed in $\bar{x}$, by treatment of X as a parameter. The transformed outer solution, which approximates $\widehat{ß}_2(\lambda,X)$, is

$$\widehat{ß}_2^0(\lambda,X)=\frac{\widehat{\Lambda}_0(\lambda,X)}{\lambda^2+W_0(X)+g_0\phi_0^0(X)^2\,\widehat{ß}_0^0(\lambda,X)}\;,\qquad X\in\mathbb{R}^3\setminus\mathfrak{B}(\partial\mathfrak{R}_0,\delta)\;,\tag{7.30}$$

[9]Note that (7.26b) holds provided $|\lambda|(-\eta)^{-1/2}\ll 1$. If instead η is kept fixed and $|\lambda|\to\infty$, a different asymptotic limit ensues in which $\widehat{ß}_0^{in}=\mathcal{O}(\lambda^{-2})$, consistent with $ß_0^{in}(\cdot,\eta)\in L^2(\mathbb{R}^3)$.

where $\delta = \mathcal{O}(\epsilon^{2/3})$, and $\widehat{\Lambda}_0(\lambda, X)$ and $W_0(X)$ result from the replacement of $\phi_0(X)$, $\phi_2(X)$, and $\widehat{ß}_0(\lambda, X)$ in $\widehat{\Lambda}(\lambda, X)$ and $W(X)$ by the outer solutions $\phi_0^0(X)$, $\phi_2^0(X)$, and $\widehat{ß}_0^0(\lambda, X)$, respectively. The extension of this $\widehat{ß}_2^0(\lambda, \cdot)$ 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

$$\widehat{\Lambda}_0(\lambda, X) = \frac{3}{2} g_0^2 \|A\|_{-1}^2 [\phi_0^0(X)^4 + |\mathfrak{R}_0|^{-1} \|(\phi_0^0)^2\|_{L^2}^2] \, [1 + \widehat{ß}_0^0(\lambda, X)]^2 \ , \tag{7.31}$$

$$W_0(X) = g_0 \phi_0^0(X)^2 \ , \qquad X \in \mathfrak{R}_0^\delta \ . \tag{7.32}$$

Accordingly, we obtain

$$\begin{aligned} \widehat{ß}_2^0(\lambda, X) = {} & \frac{3}{2} g_0^2 \|A\|_{-1}^2 [\phi_0^0(X)^4 + |\mathfrak{R}_0|^{-1} \|(\phi_0^0)^2\|_{L^2}^2] \\ & \times \frac{[1 + \widehat{ß}_0^0(\lambda, X)]^2}{\lambda^2 + g_0 \phi_0^0(X)^2 [1 + \widehat{ß}_0^0(\lambda, X)]} \ , \qquad X \in \mathfrak{R}_0^\delta \ . \end{aligned} \tag{7.33}$$

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

Approximation (7.30) breaks down if $X \in \mathfrak{B}(\partial\mathfrak{R}_0, \mathcal{O}(\epsilon^{2/3}))$, near classical turning points. A remedy is to use the local coordinate η and the inner solutions for ϕ_0, ϕ_2, and $ß_0$, and to proceed as in section 7.2.1, by invoking boundary layer theory and asymptotic matching. 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 nonzero orders in ϵ for the lowest bound state. In the 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. In the case with a slowly varying trap, we explicitly compute the fraction of particles out of the condensate. We show that this fraction is controlled by the $H_{\rm av}^{-1}$-norm of (the periodic) $A(x)$. Recall that $\Phi(x)$ and $K(x, y)$ are considered real; and K is taken symmetric, $K(x, y) = K(y, x)$. Our resulting, simple formulas for the condensate depletion are valid under assumptions (1.10).

8.1. Homogenization-based expansion. We seek a formal ϵ-expansion for the condensate depletion on the basis of our homogenization program. The fraction of particles that occupy states out of the condensate, or *depletion fraction*, is [69]

$$\xi_{\rm dp} = \langle \Psi_N, (\psi_1^* \psi_1 / N) \Psi_N \rangle_{\mathbb{F}} = N^{-1} \int w(x, x) \, {\rm d}x = N^{-1} {\rm tr} \mathcal{W} \ , \tag{8.1}$$

where $0 < \xi_{\rm dp} < 1$ and the operator $\mathcal{W}$ has representation $w(x, y)$ defined by

$$w(x, y) = \sum_{n \geq 1} w_n(x, y) \ , \tag{8.2a}$$

$$w_1(x, y) = \int {\rm d}z \, K^*(x, z) K(z, y) \ , \qquad w_n(x, y) = \int {\rm d}z \, w_1(x, z) w_{n-1}(z, y) \ . \tag{8.2b}$$

Next, we provide an expansion for $\xi_{\rm dp}$ in terms of a formal expansion for $\mathcal{W}$. In view of Remark 3.2, we assume that $\xi_{\rm dp}$ is small enough so that the many-body perturbation scheme leading to the PDEs for Φ and K makes sense, namely,

$$\xi_{\rm dp} \ll 1 \ ; \tag{8.3}$$

cf. Remark 3.2. Specifically, we show that, in correspondence to Proposition 6.12 (with Remark 6.14), the depletion fraction can be formally expanded as

$$\xi_{\rm dp} = \xi_{{\rm dp},0} + \epsilon^2 \xi_{{\rm dp},2} + \cdots = {\rm tr}\mathcal{W}_{(0)} + \epsilon^2\, {\rm tr}\mathcal{W}_{(2)} + \cdots \ , \tag{8.4}$$

where

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

$$\begin{aligned} \mathcal{W}_{(2)} = & \sum_{\substack{n:{\rm even}\\ n\geq 2}} \sum_{m=0}^{\frac{n-2}{2}} \mathcal{K}_{(0)}^{2m} \{\{\mathcal{K}_{(0)}, \mathcal{K}_{(2)}\}, \mathcal{K}_{(0)}^{2n-2-4m}\} \mathcal{K}_{(0)}^{2m} \\ & + \sum_{\substack{n:{\rm odd}\\ (n\geq 1)}} \left[\sum_{m=0}^{\frac{n-3}{2}} \mathcal{K}_{(0)}^{2m} \{\{\mathcal{K}_{(0)}, \mathcal{K}_{(2)}\}, \mathcal{K}_{(0)}^{2n-2-4m}\} \mathcal{K}_{(0)}^{2m} + \mathcal{K}_{(0)}^{n-1} \{\mathcal{K}_{(0)}, \mathcal{K}_{(2)}\} \mathcal{K}_{(0)}^{n-1} \right] \ . \end{aligned} \tag{8.5b}$$

In the above, $\mathcal{K}_{(l)}$ ($l = 0, 2$) is the operator with representation $\kappa_l(x,y)$; and the anticommutator $\{\cdot,\cdot\}$ is $\{\mathcal{A},\mathcal{B}\} := \mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A}$. Note that $\mathcal{K}_{(0)}$ and $\mathcal{K}_{(2)}$ may not commute in general. If $\mathcal{K}_{(0)}$ and $\mathcal{K}_{(2)}$ commuted, we would write

$$\mathcal{W}_{(2)} = 2\sum_{n\geq 1} n \mathcal{K}_{(0)}^{2n-1} \mathcal{K}_{(2)} = 2\mathcal{K}_{(0)}\mathcal{K}_{(2)} (1-\mathcal{K}_{(0)}^2)^{-2} \ . \tag{8.6}$$

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

We proceed to sketch a derivation of (8.4) and (8.5), by resorting to an extension of the binomial expansion for noncommuting operators. Noting the formal relations $\mathcal{W} = \sum_{n\geq 1} \mathcal{W}_n$, $\mathcal{W}_n = (W_1)^n$, and $\mathcal{W}_1 = (\mathcal{K})^2$, where $\mathcal{K}$ has representation $K(x,y)$, we seek a two-scale expansion for the representation $w_1(x,y)$ of $\mathcal{W}_1$ up to $\mathcal{O}(\epsilon^2)$. By (6.43) with Remark 6.14, we find

$$\begin{aligned} w_1(x,y) = & \int {\rm d}z\, \kappa_0(x,z)\kappa_0(z,y) + \epsilon^2 \Bigg\{ g_0 \big[(\Delta_{\tilde{x}}^{-1} A) f_0(x)^2 + (\Delta_{\tilde{y}}^{-1} A) f_0(y)^2 \big] \\ & \times \left[\kappa_0(x,y) + 2\int {\rm d}z\, \kappa_0(x,z)\kappa_0(z,y) \right] + 2\int {\rm d}z\, {\rm Sym}[\kappa_0,\kappa_2](z;x,y) \Bigg\} + \cdots \ , \end{aligned} \tag{8.7}$$

where ${\rm Sym}[\cdot]$ is defined by (6.47). Equation (8.7) suggests the operator form

$$\mathcal{W}_1 = \mathcal{K}_{(0)}^2 + \epsilon^2 \big[\varpi \mathcal{K}_{(0)} (1 + 2\mathcal{K}_{(0)}) + \{\mathcal{K}_{(0)}, \mathcal{K}_{(2)}\} \big] + \cdots \ , \tag{8.8}$$

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

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

where in principle $\mathcal{K}_{(0)}$ and $\{\mathcal{K}_{(0)}, \mathcal{K}_{(2)}\}$ do not commute. Equations (8.4) and (8.5) result by direct multiplication, induction, and summation in n.

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

$$\begin{aligned}\int \kappa_0(x,z)\kappa_2(z,y)\,\mathrm{d}z &= \int ß_0\left(z', X + \frac{\epsilon\bar{x}}{2} - \frac{\epsilon z'}{2}\right) ß_2\left(\bar{x} - z', X - \frac{\epsilon z'}{2}\right)\mathrm{d}z' \\ &\sim \int ß_0(z', X)\, ß_2(\bar{x} - z', X)\,\mathrm{d}z' = \int ß_2(z', X)\, ß_0(\bar{x} - z', X)\,\mathrm{d}z' \ , \end{aligned} \tag{8.9}$$

formally, 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 (8.9). Alternatively, replace each operator by the Fourier transform of the above approximation for $ß_l(\cdot, X)$, treating X as an $\mathcal{O}(1)$ 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 formally as

$$\begin{aligned}\|\mathcal{K}_{(0)}\|^2 &= N^{-1}\|\kappa_0\|^2_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = (N\breve{\epsilon}^3)^{-1}\iint |ß_0(\bar{x}, X)|^2\,\mathrm{d}\bar{x}\mathrm{d}\,X \\ &\sim \frac{N^{-1}}{(2\pi)^3}\int_{\mathfrak{R}_0}\mathrm{d}X\int_{\mathbb{R}^3}\mathrm{d}\lambda\,|\widehat{ß}^0_0(\lambda, X)|^2 \ ; \end{aligned} \tag{8.10}$$

cf. section 7.2.1. By formula (7.22) for $\widehat{ß}^0_0$, use of spherical coordinates for λ ($\lambda \in \mathbb{R}^3$), and the change of variables $|\lambda| \mapsto \tau$ with $|\lambda| = \sqrt{2g_0(\phi^0_0)^2}\,\sinh\tau$ inside $\mathfrak{R}^\delta_0$, we find $\widehat{ß}^0_0 = -e^{-2\tau}$ and directly obtain

$$\|\mathcal{K}_{(0)}\|^2 \sim \frac{2^{7/2}}{105\pi^2}\int_{\mathfrak{R}_0}\mathrm{d}x\,[\mu^0_0 - U(x)]^{3/2} \ . \tag{8.11}$$

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 reasonably defined [41].

8.2.1. Zeroth-order depletion. By (8.4) and (8.5a) along with the use of the Fourier representation for $\mathcal{K}_{(0)}$ and spherical coordinates, we wind up with

$$\begin{aligned}\xi_{\rm dp} \sim \xi_{\rm dp,0} &= \frac{1}{(2\pi)^3}\sum_{n\geq 1}\int_{\mathfrak{R}_0}\mathrm{d}x\int\mathrm{d}\lambda\ |\widehat{ß}^0_0(\lambda, x)|^{2n} \\ &= \frac{1}{2\pi^2}\sum_{n\geq 1}\int_{\mathfrak{R}_0}\mathrm{d}x\int_0^\infty \mathrm{d}|\lambda|\ |\lambda|^2\,|\widehat{ß}^0_0(\lambda, x)|^{2n} \\ &= \frac{1}{2\pi^2}\sum_{n\geq 1}\frac{8n}{(16n^2-1)(16n^2-9)}\int_{\mathfrak{R}_0}\mathrm{d}x\,[2g_0\phi^0_0(x)^2]^{3/2} \\ &= \frac{\sqrt{2}}{12\pi^2}\int_{\mathfrak{R}_0}\mathrm{d}x\ [\mu^0_0 - U(x)]^{3/2} \ . \end{aligned} \tag{8.12}$$

8.2.2. Next higher-order depletion. Next, we indicate how the oscillatory part, $A(x/\epsilon)$, of the scattering length can affect the depletion fraction. In (8.4), the coefficient $\xi_{\mathrm{dp},2}$ contains information about $A(x/\epsilon)$. By using series (8.6), along with the hypothesis of a slowly varying trap, we compute

$$\xi_{\mathrm{dp},2} \sim \frac{1}{(2\pi)^3} \sum_{n\geq 0} 2(n+1) \int_{\mathfrak{R}_0} \mathrm{d}x \int \mathrm{d}\lambda \, \widehat{\mathfrak{b}}_0^0(\lambda, x)^{2n+1} \widehat{\mathfrak{b}}_2^0(\lambda, x) \ . \tag{8.13}$$

By formulas (7.30)–(7.32), we have

$$\xi_{\mathrm{dp},2} \sim -\frac{3\sqrt{2}}{8\pi^2} \|A\|_{-1}^2 \int_{\mathfrak{R}_0} \left\{ g_0^2 \phi_0^0(x)^4 + |\mathfrak{R}_0|^{-1} \|g_0 (\phi_0^0)^2\|_{L^2}^2 \right\} [g_0 \phi_0^0(x)^2]^{1/2} \, \mathrm{d}x \ , \tag{8.14}$$

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

Remark 8.2. The periodic oscillations of the scattering length are found to 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 in ϵ.

9. Conclusion. We studied BEC of dilute atomic gases with repulsive particle interactions at zero temperature. Our goal was to transcend the mean field formalism of the NSE when the scattering length has a periodic microstructure. The main stationary effect beyond mean field considered here was pair excitation, by which particles are scattered in pairs from the condensate to other states at different positions, x and y; a 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 both the many-particle microscopic and macroscopic levels. First, by revisiting Wu's formulation [69], we demonstrated how the integro-PDE for K can emerge from the particle Hamiltonian when the scattering length has a periodic microstructure. This stage involved formal 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 $\check{\epsilon}$. Last, we indicated what predictions can possibly be made for the fraction, ξ_{dp}, of particles out of the condensate.

A noteworthy result is an expansion for ξ_{dp}, which reveals the dependence of this fraction on the size and shape of the trap, and the form and strength of the repulsive particle interactions, particularly the oscillatory part of the scattering length. According to our formula for ξ_{dp}, 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 competing with the increase of the (positive) interaction strength in the unperturbed (lacking periodic microstructure) system.

Our work has not addressed several issues. For example, 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 *time-dependent* settings, with a spatially periodic or time-dependent scattering length and trapping potential. Our analysis was restricted to zero temperature, in the absence of thermally excited states. 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 for finite but small temperatures. 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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