On Effective PDEs of Quantum Physics

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Abstract The Hartree-Fock equation is a key effective equation of quantum physics. We review the standard derivation of this equation and its properties and present some recent results on its natural extensions – the density functional, Bogolubov-de Gennes and Hartree-Fock-Bogolubov equations. This paper is based on a talk given at ISAAC2017.

1 Introduction

The Hartree-Fock equation (HFE) is a (if not the) key effective equation of quantum physics. It plays a role similar to that of the Boltzmann equation in classical physics. It gives a fairly accurate and yet sufficiently simple description of large (and not so large) systems of quantum particles. The trade-off here is the high dimension for nonlinearity: while the $n-$particle Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H_n \Psi \tag{1}$$

is a linear equation in $3n+1$ variables, the Hartree-Fock one is a nonlinear one in $3+1$ variables. Here $\hbar$ is the Planck constant divided by 2π and H_n is the Schrödinger operator or (quantum) Hamiltonian of the $n-$particle system, it is given in (14) below.

The HFE involves an orthonormal system of n functions, $\{\psi_i\}$, on $\mathbb{R}^3$, or the projection operator $\gamma := \sum_i |\psi_i\rangle\langle\psi_i|$ acting on $L^2(\mathbb{R}^3)$, and can be written in the latter case as

$$i\hbar \frac{\partial \gamma}{\partial t} = [h_\gamma, \gamma] \tag{2}$$

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where $h_\gamma := h + v * \rho_\gamma + ex(\gamma)$, with h a one-particle Schrödinger operator (say $h := -\frac{\hbar^2}{2m}\Delta + V(x)$, where $V(x)$ is an external potential), $\rho_\gamma(x,t) := \gamma(x,x,t) = \sum_i |\psi_i(x)|^2$ and $ex(\gamma)$ ("exchange term") is the operator with the integral kernel

$$ex(\gamma)(x,y) := -v(x-y)\gamma(x,y) \tag{3}$$

$$= -\sum_i \psi_i(x)v(x-y)\bar{\psi}_i(y). \tag{4}$$

(Here and in what follows, $A(x,y)$ stands for the integral kernel of an operator A.) Furthermore, to deal with quantum statistics (where the number of particles is not fixed but is a quantum observable), (2) is extended to arbitrary non-negative, trace class operator γ on $L^2(\mathbb{R}^3)$ satisfying $\gamma \le \mathbf{1}$ (expressing the Pauli exclusion principle). This describes fermions. For bosons, one drops the exchange term $ex(\gamma)$ and the condition $\gamma \le \mathbf{1}$.

Replacing $ex(\gamma)$ given above by a local function $\mathrm{xc}(\rho_\gamma)$ of the function $\rho_\gamma(x,t) := \gamma(x,x,t)$ leads to the Kohn-Sham equation underlying the density functional theory (DFT) which is exceptionally effective in the computations in Quantum Chemistry and in particular, of the electronic structure of matter.

It was discovered by Bardeen, Cooper and Schrieffer for fermions and by Bogolubov, for bosons, that for quantum fluids (superconductors and superfluids, respectively)

– the HFE falls short
– there are natural generalizations of the HFE describing these phenomena.

It turns out that this generalization is mathematically very natural and was overlooked in the mathematics literature, though the framework for it existed.

To explain how this generalization arises, we go back to the HFE and present its alternative derivation. We just indicate main steps; for details, see [3] and for background, [9, 36].

In abstract formulation, which applies also to statistical mechanics and quantum field theory, the states are defined as positive linear ('expectation') functionals on a C^* algebra, $\mathscr{A}$, elements of which are called observables, and the evolution of states is given by the von Neumann-Landau equation

$$i\hbar\partial_t\omega_t(A) = \omega_t([A,H]), \ \forall A \in \mathscr{A}, \tag{5}$$

where H is a quantum Hamiltonian which is affiliated with $\mathscr{A}$.

Technically, one takes for $\mathscr{A}$, an algebra of bounded operators (namely the Weyl algebra, $\mathfrak{W}$) on the fermionic/bosonic Fock space, which for spinless particles is written as

$$\mathscr{F} := \sum_0^\infty \circledast_1^n L^2(\mathbb{R}^d), \ d = 1,2,3, \tag{6}$$

where ⊕# stands either for the wedge product, $\wedge$, or symmetric product, Ⓢ. For a many-body system, the quantum Hamiltonian H on Fock space, $\mathscr{F}$ is given by $H := \oplus_0^\infty H_n$, with the $n-$particle Schrödinger operators H_n defined in (14) below. If one introduces annihilation and creation operators, $\psi(x)$ and $\psi^*(x)$ on $\mathscr{F}$, which map the n-particle sector in (6) into $(n-1)$- and $(n+1)$-sectors, respectively, then H is written in terms of these operators as

$$H = \int dx \; \psi^*(x) h \psi(x) + \frac{1}{2} \int dx dy \; v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y) , \tag{7}$$

with h a one-particle Schrödinger operator acting on the variable x and v a pair potential of the particle interaction (see (14) below).

We can think about the algebra of observables as generalized by (unbounded) operators $\psi(x)$ and $\psi^*(x)$. The Hartree-Fock approximation is obtained by restricting the evolution to the states, φ, determined by the expectation

$$\gamma(x, y) := \varphi[\psi^*(y) \, \psi(x)], \tag{8}$$

provided $\varphi[\psi(x)] = 0$, in the following way. Let $\psi^\#(x)$ stands for either $\psi(x)$ or $\psi^*(x)$. We require that $\varphi[\psi^\#(x_1) \, \dots \psi^\#(x_k)]$ to be zero if the number of ψ^*'s and ψ are not equal and is expressed in terms of sums of products of $\varphi[\psi^*(x_i) \, \psi(x_j)]$ according to the Wick theorem (see [9]), exactly as for the Gaussian processes in probability; such states are called the *quasifree states*.[1]

However, the property of being quasifree is not preserved by the dynamics (5) and the main question here is how to project the true quantum evolution onto the class of quasifree states. Following [3], we do this by restricting the evolution,

$$i\hbar \partial_t \varphi_t(A) = \varphi_t([A, H]) \tag{9}$$

to observables A, which are at most quadratic in the creation and annihilation operators. Then we arrive at a closed, self-consistent dynamics for φ_t. When expressed in terms of the operator γ with the integral kernel $\gamma(x, y)$, it gives exactly the Hartree-Fock equation, (2).

The point here is that states determined by the expectations (8) are not the most general quasifree states. The most general quasifree states φ determine and are determined by expectations of all possible pairs of $\hat{\psi}^\sharp(x) := \psi^\sharp(x) - \varphi(\psi(x))$:

$$\begin{cases} \gamma(x, y) := \varphi[\hat{\psi}^*(y) \, \hat{\psi}(x)], \\ \alpha(x, y) := \varphi[\hat{\psi}(x) \, \hat{\psi}(y)]. \end{cases} \tag{10}$$

[1] For application of the quasifree states in the classical kinetic theory see [46].

Mathematically, these are exactly the states discovered by Bardeen, Cooper and Schrieffer for fermions and by Bogolubov, for bosons, and for which the former received and the latter should have received the Nobel prize.

Now, let γ and α denote the operators with the integral kernels $\gamma(x, y)$ and $\alpha(x, y)$. After peeling off the spin components, definition (10) implies that

$$0 \leq \gamma = \gamma^* \quad (\leq \mathbf{1}) \quad \text{ and } \alpha^* = \bar{\alpha}, \tag{11}$$

where $\bar{\sigma} = C\sigma C$ with C being the complex conjugation and the condition $\gamma \leq \mathbf{1}$ applies only to fermions (as was mentioned above, it is an expression of the Pauli exclusion principle).

The operator γ can be considered as a one-particle density operator (matrix) of the system, so that $\rho_\gamma(x) := \gamma(x, x)$ is the particle density. The operator α gives the particle pair coherence ($\alpha(x, y)$ is a two-particle wave function). (For *confined* systems, γ and α are trace class and Hilbert-Schmidt operators, respectively, with $\mathrm{Tr}\gamma = \int \gamma(x, x)dx < \infty$ giving the particle number, while for *thermodynamic* systems, they are only locally so.)

Following [3], we define self-consistent approximation as the restriction of the many-body dynamics to quasifree states. More precisely, we map the solution ω_t of (5), with an initial state ω_0, into the family φ_t of quasifree states satisfying

$$i\hbar\partial_t\varphi_t(A) = \varphi_t([A, H]) \tag{12}$$

for all observables A, which are at most quadratic in the creation and annihilation operators. As the initial condition, φ_0, for (12) we take the 'quasifree projection' of ω_0. We call this map the *nonlinear quasifree approximation* of equation (5).

We expect φ_t to be a good approximation of ω_t, if ω_0 is close to the manifold of quasifree states.

The BdG equations give an equivalent formulation of the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity.

Evaluating (12) for monomials $A \in \{\psi(x), \psi^*(x)\psi(y), \psi(x)\psi(y)\}$, yields a system of coupled nonlinear PDE's for (ϕ, γ, α) where $\phi(x) := \varphi(\psi(x))$ and γ and α are defined in (10). For the standard many-body hamiltonian, (7), these give the (time-dependent) *Hartree-Fock-Bogolubov (HFB) or Bogolubov-de Gennes (BdG) equations*, depending on whether we deal with bosons or fermions (see (99), (100) and (101) or (108), (109) and (110) below). In the latter case, one takes $\phi(x, t) := \varphi_t(\psi(x)) = 0$. As was mentioned above, the HFB equaitons describes Bose-Einstein condensation and superfluidity while the BdG equations describes superconductivity, the remarkable quantum phenomena.

HFB and BdG equations provide a more faithful description of quantum systems going beyond the Gross-Pitaevski (i.e. the nonlinear Schrödinger) and Ginzburg-Landau equations, which can be derived from them in certain regimes. While the latter equations accumulated quite a substantial literature (see e.g. [16, 19, 54, 55] and [53] for recent books and a review), the research on the former ones is just beginning.

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There are many fundamental problems about the HFB and the BdG equations which are completely open. Generally, there are three types of questions one would like to ask about an evolution equation:

- Derivation;
- Well-posedness;
- Special solutions (say, stationary solutions or traveling waves) and their stability.

Some rigorous results on the derivation of the Hartree-Fock-Bogolubov (HFB) equations can be found in [34, 40, 48] (see also [6, 7, 30–32, 52] for earlier results and references). The well-posedness (or existence) for the time-dependent HFB equations for confined systems (see above) was proven in [4]. The well-posedness theory for the time-dependent Bogolubov-de Gennes (BdG) equations is developed in [5]. For thermodynamics systems (see above), it is open. Some important stationary solutions of the BdG and HFB equations were found in [22, 37] and [3, 49, 50], respectively.

In this contribution, we recall the standard derivation and properties of the HF (and H) equations and discuss recent work on the Kohn-Sham (KS), HF, BdG and HFB equations [3, 22, 23]. To fix ideas, we concentrate mostly on the BdG equations.

There is a considerable physics literature on the subject. As for rigorous works, the three fundamental contributions to the subject, [2, 33, 37], deal with foundational issues (relation to quasifree states and quadratic hamiltonians on the Fock space and the general variational problem), with the critical temperature and the superconducting solutions and with the derivation of the Ginzburg-Landau equations respectively. For more references, and discussion see some recent papers [3, 5, 22, 23] and reviews [38, 39]. The object of these and other works on the subject is the time-independent theory. The results we discuss are complementary to this work.

2 Hartree and Gross-Pitaevski Equations

2.1 *Origin and Properties*

In what follows we use the *units in which the (normalized) Planck constant* $\hbar$ *and the speed of light* c *are both equal to* 1 *and the typical particle mass is set to* $1/2$. With this agreement, the evolution of quantum n-particle system is given by the Schrödinger equation

$$i\frac{\partial \Psi}{\partial t} = H_n \Psi. \tag{13}$$

Here H_n is the Schrödinger operator or Hamiltonian of the physical system. For the system of n identical particles (say, electrons or atoms) of mass $1/2$, interacting with each other and moving in an external potential V the Hamiltonian is

$$H_n := \sum_{i=1}^{n} h_{x_i} + \frac{1}{2}\sum_{i\neq j} v(x_i - x_j), \tag{14}$$

where $h_x = -\Delta_x + V(x)$ and v is the interaction potential. For spinless fermions/bosons, it acts on the state space, which in the spinless case can be written as

$$\textcircled{\#}_1^n L^2(\mathbb{R}^d),\ d = 1, 2, 3.$$

The Schrödinger equation is an equation, (13), in $dn+1$ variables, $x_1, \dots, x_n$ and t. Even for a few particles it is prohibitively difficult to solve. Hence it is important to have manageable approximations.

One such an approximation, which has a nice unifying theme and connects to a large areas of physics and mathematics, is the self-consistent (or mean-field) one. In it one approximates solutions of n-particle Schrödinger equations by products of n one-particle functions (i.e. functions of $d+1$ variables) appropriately symmetrized. This results in a single nonlinear equation in $d+1$ variables, or several coupled such equations. The trade-off here is the number of dimensions for the nonlinearity. This method is especially effective when the number of particles, n, is sufficiently large.

We give a heuristic derivation of the self-consistent approximation for the Schrödinger equation above. (See [36] for details and references to rigorous results.) First, we observe

Proposition 1 *The Schrödinger equation is the Euler-Lagrange equation for stationary points of the action functional*

$$S(\Psi) := \int \big\{ - Im\langle \Psi, \partial_t \Psi\rangle - \langle \Psi, H_n \Psi\rangle \big\} dt, \tag{15}$$

Now, for bosons, we consider the the action functional (15) on the space (not linear!)

$$\{\Psi := \otimes_1^n \psi \,|\, \psi \in H^1(\mathbb{R}^3)\}, \tag{16}$$

where $(\otimes_1^n \psi)$ is the function of $3n+1$ variables defined by $(\otimes_1^n \psi)(x_1, \dots, x_n, t) := \psi(x_1, t) \dots \psi(x_n, t)$. For fermions, we take

$$\{\Psi := \wedge_1^n \psi_j : \psi_i \in H^1(\mathbb{R}^3)\ \forall i = 1, \dots, n\} \tag{17}$$

Here $(\wedge_1^n \psi_j)(x_1, \dots, x_n, t) := \det[\psi_i(x_j, t)]$ is the determinant of the $n \times n$ matrix $[\psi_i(x_j, t)]$, called the *Slater determinant*.

We begin with bosons. We have the following elementary result:

Proposition 2 *Let* $\|\psi\|^2 = n - 1 \approx n$ *and* $S_H(\psi) := \frac{n-1}{n} S(\otimes_1^n \psi)$ *('H' stands for the Hartree). Then we have*

$$S_H(\psi) = \int \int \{ -Im\langle \psi, \partial_t \psi\rangle - |\nabla \psi|^2 - V|\psi|^2 - \frac{1}{2}|\psi|^2 v * |\psi|^2 \} dx dt. \tag{18}$$

We see that the quadratic terms on the r.h.s. of (18) are of the order $O(n)$, while the quartic ones, are $O(vn^2)$ The regime in which these terms are of the same order, $O(n^2)$, i.e. for which, $v = O(1/n)$ is called the *mean-field* regime.

The Euler-Lagrange equation for stationary points of the action functional (18) considered on the first set of functions is

$$i\frac{\partial \psi}{\partial t} = (h + v * |\psi|^2)\psi, \tag{19}$$

with the normalization $\|\psi\|^2 = n - 1 \approx n$. This nonlinear evolution equation is called the *Hartree equation* (HE).

If the inter-particle interaction, v, is significant only at very short distances (one says that v is very short range, which technically can be quantified by assuming that the "particle scattering length" a is small), one replaces $v(x) \to 4\pi a\delta(x)$ and Equation (19) becomes

$$i\frac{\partial \psi}{\partial t} = h\psi + \kappa|\psi|^2\psi, \tag{20}$$

where $\kappa := 4\pi a$ (with the normalization $\|\psi\|^2 = n$). This equation is called the *Gross-Pitaevski equation* (GPE) or the *nonlinear Schrödinger equation*. It is derived using the Gross-Pitaevski approximation to the original quantum problem for a system of n bosons. The Gross-Pitaevski equation is widely used in the theory of superfluidity, and in the theory of Bose-Einstein condensation (see [36, 41] and references therein).

Proofs of the local and global existence for (19) and (20) can be found in [19, 21, 55].

2.1.1 Properties of the Hartree and Gross-Pitaevski Equations

We say that the map T on a space of solution is a *symmetry* of an equation iff the fact that ψ is a solution of the equation implies that $T\psi$ is also a solution. It is straightforward to prove the following

Proposition 3 *The Hartree and Gross-Pitaevski equations have the following symmetries*

1. *the time-translations,* $\psi(x,t) \to \psi(x,t+s),\ s \in \mathbb{R}$,
2. *the gauge transformations,*

$$\psi(x,t) \to e^{i\alpha}\psi(x,t),\ \alpha \in \mathbb{R},$$

3. *for* $V=0$, *the spatial translations,* $\psi(x,t) \to \psi(x+y,t),\ y \in \mathbb{R}^3$,
4. *for* $V=0$, *the Galilean transformations,* $v \in \mathbb{R}^3$,

$$\psi(x,t) \to e^{i(\frac{1}{2}v\cdot x - \frac{v^2 t}{4})}\psi(x-vt,t),$$

5. *for* V *spherically symmetric, the spatial rotations,* $\psi(x,t) \to \psi(Rx,t),\ R \in O(3)$,

As the result of the time-translational and the gauge symmetries, the energy and the number of particles functionals

$$E(\psi) := \int \left\{ |\nabla\psi|^2 + V|\psi|^2 + G(|\psi|^2) \right\} dx, \tag{21}$$

where $G(|\psi|^2) := \frac{1}{2}|\psi|^2 v * |\psi|^2$ for HE and $G(|\psi|^2) := \frac{1}{2}\kappa|\psi|^4$ for GPE, and

$$N(\psi) := \int |\psi|^2 dx,$$

are independent of time, t. Moreover, for $V=0$, the field momentum,

$$P(\psi) := \int \bar{\psi}(x,t)(-i\nabla_x)\psi(x,t)dx,$$

and, for V spherically symmetric, the field angular momentum,

$$L(\psi) := \int \bar{\psi}(x,t)(x \wedge (-i\nabla_x))\psi(x,t)dx,$$

are conserved. These conservation laws impose constraints on the dynamics leading to qualitative understanding of possible scenarios and are used in the proofs of the global existence, existence and stability of stationary solutions and traveling waves; for definitions and a review see [36].

We also note that HE and GPE are Hamiltonian systems (see Section 19.1 of [36]).

2.2 Particles Coupled to the Electromagnetic Field

We start with the action

$$S(\psi) = \int\int \{-\mathrm{Im}\langle\psi, \partial_t\psi\rangle \tag{22}$$

$$- |\nabla\psi|^2 - V|\psi|^2 - G(|\psi|^2)\} dxdt, \tag{23}$$

where $G(|\psi|^2)$ is given after (21), and use the principle of minimal coupling in which one replaces the usual derivatives ∂_t and ∇ by covariant ones, $\partial_{t\phi} = \partial_t + ie\phi$ and $\nabla_a = \nabla - iea$, where ϕ and a are the electric and magnetic potentials and e is the electric charge of ψ, and adds the action,

$$S_{\mathrm{EM}}(a, \phi) := \int\int \left\{|\partial_t a + \nabla\phi|^2 - |\operatorname{curl} a|^2\right\} dxdt,$$

of the the electro-magnetic field (for the latter, see e.g. [36], Sections 19.1.1 and 19.6). Then, assuming the external potential $V = 0$, the total action becomes

$$S(\psi, a, \phi) := \int\int \{ - \mathrm{Im}\langle\psi, \partial_{t\phi}\psi\rangle - |\nabla_a\psi|^2 - G(|\psi|^2)\} dxdt$$
$$+ S_{\mathrm{EM}}(a, \phi). \tag{24}$$

for a triple $(\psi, a, \phi) : \mathbb{R}^d \to \mathbb{C} \times \mathbb{R}^d \times \mathbb{R}$, of complex and real functions and a vector field. The Euler-Lagrange equations for this action are given by

$$i\frac{\partial\psi}{\partial t} = h_{a\phi}\psi + g(|\psi|^2)\psi, \tag{25a}$$

$$-\partial_t(\partial_t a + \nabla\phi) = \operatorname{curl}^* \operatorname{curl} a - \mathrm{Im}(\bar{\psi}\nabla_a\psi), \tag{25b}$$

$$-\operatorname{div}(\partial_t a + \nabla\phi) = e|\psi|^2, \tag{25c}$$

where $h_{a\phi} := -\Delta_a + e\phi + V$, with $\Delta_a = \nabla_a^2$, the covariant Laplacian, $g(s) = G'(s)$ and the vector quantity $J(x) := \mathrm{Im}(\bar{\psi}\nabla_a\psi)$ is the electric current, while $|\psi|^2$ is the charge density (remember we omit the charge of the particle), so that the second and third equations are Ampère's and Gauss law part of the Maxwell equations.

Moreover, curl^* is the L^2-adjoint of curl, so that for $d = 3$, we have $\operatorname{curl}^* = \operatorname{curl}$ and for $d = 2$, $\operatorname{curl} a := \partial_1 a_2 - \partial_2 a_1$ is a scalar, and for a scalar function, $f(x)$, $\operatorname{curl}^* f = (\partial_2 f, -\partial_1 f)$ is a vector.

It is straightforward to prove that (25) are the Euler-Lagrange equations for action (24). Now, in addition to translation and rotation invariance (if $V = 0$), equations (25) are invariant under the *local gauge transformations*: for any sufficiently regular function $\chi : \mathbb{R}^2 \times \mathbb{R} \to \mathbb{R}$,

$$T_\chi^{\text{gauge}} : (\psi(x,t), a(x,t), \phi(x,t)) \mapsto (e^{i\chi(x,t)}\psi(x,t), a(x,t) + \nabla_x \chi(x,t), \phi(x,t) - \partial_t \chi(x,t)). \tag{26}$$

Using this gauge invariance, we can choose χ so that a and/or ϕ satisfy certain additional conditions. This is called gauge fixing. For instance, we can choose χ so that $\operatorname{div} a = 0$ (the Coulomb gauge), or ϕ satisfies $\phi = 0$ (the temporal gauge). Both conditions break gauge invariance. The gauge fixing which preserves the gauge invariance is the Lorentz (or radiation) gauge

$$\operatorname{div} a + \partial_t \phi = 0.$$

Note that in the Coulomb gauge, $\operatorname{div} a = 0$, Eq. (27b) becomes the familiar Poisson equation, $-\Delta\phi = e|\psi|^2$.

Neglecting in (25) the magnetic field produced by changing charge distribution (and the electric field), we arrive at the Schrödinger-Poisson system

$$i\frac{\partial\psi}{\partial t} = h_\phi \psi + g(|\psi|^2)\psi, \tag{27a}$$

$$-\Delta\phi = e|\psi|^2, \tag{27b}$$

where $h_\phi := -\Delta + e\phi + V$

One can derive (25) from the many-body Schrödinger equation coupled to the quantized electromagnetic field.

3 The (Generalized) Hartree-Fock Equations

3.1 Formulation and Properties

The Euler-Lagrange equation for stationary points of the action functional (15) considered on the Hartree-Fock states, (17), is a system of nonlinear, coupled evolution equations

$$i\frac{\partial\psi_j}{\partial t} = (h + v * \sum_i |\psi_i|^2)\psi_j - \sum_i (v * \psi_i \bar{\psi}_j)\psi_i, \tag{28}$$

where, recall, $h := -\Delta + V$, for the unknowns $\psi_1, \dots, \psi_n$. This system plays the same role for fermions as the Hartree equation does for bosons. Equation (28) is called the *Hartree-Fock equations* (HFE).

Properties of HFE The Hartree-Fock equations are

1. invariant under the time-translations and gauge transformations, and, for $V = 0$, the spatial translations, $\psi_j(x) \to \psi_j(x+y)$, $y \in \mathbb{R}$, and the Galilean transformations, $v \in \mathbb{R}^3$, and, for V spherically symmetric, the rotations.
2. invariant under time and space independent unitary transformations of $\{\psi_1, \ldots, \psi_n\}$.
3. a Hamiltonian system (see Sections 24.6 and 24.7 of [36]).

Again, similarly to HE, as the result of the time-translational and the gauge symmetries, the energy and the number of particles functionals

$$E(\psi) := \int \Big\{ \sum_i (|\nabla\psi_i|^2 + V|\psi_i|^2) + \frac{1}{2}(\sum_i |\psi_i|^2) v * (\sum_i |\psi_i|^2) - \frac{1}{2}\int v(x-y)|\sum_i \psi_i(x)\psi_i(y)|^2 dy \Big\} dx, \tag{29}$$

$$N(\psi) := \sum_i \int_{\mathbb{R}^3} |\psi_i|^2 dx \tag{30}$$

are conserved, similarly, for linear and angular momenta. Moreover, HFE conserve the inner products, $\langle\psi_i, \psi_j\rangle$, $\forall i, j$. For a rigorous theory, see [8, 20, 42, 44, 45, 47].

The item (2) above shows that the natural unknown for HFE is the subspace spanned by $\{\psi_i\}$, or the corresponding projection $\gamma := \sum_i |\psi_i\rangle\langle\psi_i|$. HFE can be rewritten as an equation for γ:

$$i\frac{\partial\gamma}{\partial t} = [h_\gamma, \gamma] \tag{31}$$

where $h_\gamma := h + v * \rho_\gamma + ex(\gamma)$, with $\rho_\gamma(x) := \gamma(x,x) = \sum_i |\psi_i(x)|^2$ and $ex(\gamma)$ is the operator with the integral kernel

$$ex(\gamma)(x,y) := -v(x-y)\gamma(x,y) = -\sum_i \bar{\psi}_i(x) v(x-y)\psi_i(y). \tag{32}$$

Recall that $A(x,y)$ stands for the integral kernel of an operator A.

This can be extended to arbitrary non-negative density operators γ satisfying (for fermions) $\gamma \le 1$, and leads to a new class of nonlinear differential equations. (The properties $0 \le \gamma$ and $\gamma \le 1$ as well as all eigenvalues of γ as conserved under the evolution.)

Finally, note that the energy and the number of particles in the new formulation is given by

$$E(\gamma) := \mathrm{Tr}((h + \frac{1}{2}v * \rho_\gamma)\gamma) + Ex(\gamma), \tag{33}$$

$$N(\gamma) := \mathrm{Tr}\gamma = \int \rho_\gamma, \tag{34}$$

where, recall, $h := -\Delta + V$, $\rho_\gamma(x) := \gamma(x, x)$ and $Ex(\gamma) := -\frac{1}{2}\mathrm{Tr}(\gamma v\sharp\gamma)$, where $v\sharp\gamma$ is the operator with the integral kernel $v(x - y)\gamma(x, y)$. Note that

$$\mathrm{Tr}((v * \rho_\gamma)\gamma) = \int \rho_\gamma v * \rho_\gamma dx = \int\int \rho_\gamma(x)v(x - y)\rho_\gamma(y)dxdy,$$

$$\mathrm{Tr}(\gamma v\sharp\gamma) = \int\int v(x - y)|\gamma(x, y)|^2 dxdy.$$

It is straightforward to show that that equations (28), (29) and (30) can be rewritten as (31), (32), (33) and (34), respectively.

Note that the HE can be also formulated with γ being a rank one projection times n and extended to operators γ with no constraint on the size. In this case, the exchange terms $ex(\gamma)$ and $Ex(\gamma)$ should be omitted from the definition of h_γ and the energy.

γ is called the (one-particle) density operator and $\gamma(x, x)$ (or $\gamma(x, x, t)$) is interpreted as the one-particle density, so that $\mathrm{Tr}\gamma = \int \gamma(x, x)dx$ is the total number of particles. It should satisfy

$$0 \le \gamma = \gamma^* \ (\le 1) \tag{35}$$

where the second inequality is required only for fermions. The HF flow preserves these properties.

3.1.1 Exchange Energy Term

We extend Eq. (31) by allowing different exchange terms in the definition of h_γ, rather than just (32). Specifically, we let the exchange energy term, $ex(\gamma)$, to take the following forms:

- $ex(\gamma) := 0$ for the Hartree (or reduced Hartree-Fock, if $\gamma \le 1$) model,
- $ex(\gamma) := -v\sharp\,\gamma$ for the Hartree-Fock case and
- $ex(\gamma)$ is a local function, $ex(\gamma) = xc(\rho_\gamma)$, of the function $\rho_\gamma(x) := \gamma(x, x)$, say, coming from $Ex(\rho) = -c\int \rho^{4/3}$, in the density functional theory (DFT).

We call (31) with a general exchange energy term, $ex(\gamma)$, the *generalized Hartree-Fock equation* (gHFE).

3.2 Static gHF Equations

Clearly, γ, is a static solution to (31) iff γ solves the equation

$$[h_\gamma, \gamma] = 0. \tag{36}$$

For any reasonable function f and $\mu \in \mathbb{R}$, solutions of the equation

$$\gamma = f(\beta(h_\gamma - \mu)), \tag{37}$$

solves (36). Under certain conditions, the converse is also true. (The reason for introducing the parameters $\beta = 1/T$, $\mu > 0$ (the inverse temperature and chemical potential) will become clear later.)

Under certain conditions on f satisfied by our choice below, the chemical potential μ is determined by the condition that $\mathrm{Tr}\gamma = n$.

The physical function f is selected by either a thermodynamic limit (Gibbs states) or by a contact with a reservoir (or imposing the maximum entropy principle). For fermions, it is given by the Fermi-Dirac distribution

$$f(\lambda) = (e^\lambda + 1)^{-1}, \tag{38}$$

and for bosons, by the Bose-Einstein one

$$f(\lambda) = (e^\lambda - 1)^{-1}. \tag{39}$$

(One can also consider the Boltzmann distribution $f(\lambda) = e^{-2\lambda}$.) Inverting the function f and letting $f^{-1} =: s'$, we rewrite the stationary gHFE as

$$h_{\gamma,\mu} - \beta^{-1} s'(\gamma) = 0, \tag{40}$$

Here, recall, $h_{\gamma,\mu} := h_\gamma - \mu = -\Delta + V + ex(\gamma) - \mu$ and $0 < \beta \leq \infty$ (inverse temperature) and $\mu \geq 0$ (chemical potential). It follows from the equations $s' = f^{-1}$ and (38) that, up to a constant, the function s is given by

$$s(\lambda) = -(\lambda \ln \lambda + (1 - \lambda) \ln(1 - \lambda)), \tag{41}$$

for fermions, and by

$$s(\lambda) = -(\lambda \ln \lambda - (1 + \lambda) \ln(1 + \lambda)), \tag{42}$$

for bosons, so that for fermions, we have

$$s'(\lambda) = -\ln \frac{\lambda}{1 - \lambda}. \tag{43}$$

3.3 Coupling to the Electromagnetic Field

We couple the gHFE to the electromagnetic field. We assume that the particles are carry the unit charge density $e = -1$, so that the charge of density is $-\rho_\gamma$.

As before, we use the principle of minimal coupling assuming the inter-particle potentials and external potentials are of the electromagnetic nature. This gives the system of self-consistent equations for γ and the vector and scalar potentials a and ϕ:

$$i\partial_t\gamma = [h_{\phi,a,\gamma}, \gamma], \tag{44}$$

$$-\operatorname{div}(\partial_t a + \nabla\phi) = 4\pi(\kappa - \rho_\gamma), \tag{45}$$

$$-\partial_t(\partial_t a + \nabla\phi) = \operatorname{curl}^* \operatorname{curl} a - j(\gamma, a), \tag{46}$$

where $\kappa(x)$ is an external (positive) charge distribution, $j(\gamma, a)$ is the current given by $j(\gamma, a)(x) := -4\pi[-i\nabla_a, \gamma]_+(x, x)$, with $[A, B]_+ := AB + BA$,

$$h_{\phi,a,\gamma} = -\Delta_a - \phi + ex(\gamma). \tag{47}$$

Since $e = -1$, we have that $\nabla_a = \nabla + ia$ and $\Delta_a = \nabla_a^2$. We call (44), (45), (46) and (47) the *gHFem equations*.

We will discuss symmetries of this system in a more general context later on. Here we only note briefly that, in addition to the rigid motion symmetries, it has the gauge symmetry which did not make its appearance so far and which plays a central role in quantum physics.

As above, the energy and the number of particles are conserved and are given by

$$E(\gamma, a, \phi) := \operatorname{Tr}(h_a\gamma) + Ex(\gamma) + E_{\text{em}}(a, \phi), \tag{48}$$

$$N(\gamma) := \operatorname{Tr}\gamma = \int \rho_\gamma, \tag{49}$$

where $h_a := -\Delta_a$ and $E_{\text{em}}(a, \phi)$ is the energy of the the electro-magnetic field, given by

$$E_{\text{em}}(a, \phi) := \frac{1}{8\pi}\int \left\{|\partial_t a + \nabla\phi|^2 + |\operatorname{curl} a|^2\right\} dx. \tag{50}$$

The conservation of N is obvious. To prove the conservation of E, we use the definition $j := -4\pi d_a \operatorname{Tr}\big((-\Delta_a)\gamma\big)$ and the relation $dEx = ex$, to compute

$$\partial_t(\operatorname{Tr}(h_a\gamma) + Ex(\gamma)) = \operatorname{Tr}(h_{a,\gamma}\dot\gamma) - \frac{1}{4\pi}\int j\dot a \tag{51}$$

where $h_{a,\gamma} = -\Delta_a + ex(\gamma)$. By (44) and $h_{a,\gamma} = h_{\phi,a,\gamma} + \phi$, we have $\mathrm{Tr}(h_{a,\gamma}\dot{\gamma}) = \mathrm{Tr}(\phi\dot{\gamma}) = \int \phi\dot{\rho}_\gamma$, this gives

$$\partial_t(\mathrm{Tr}(h_a\gamma) + Ex(\gamma)) = \int \phi\dot{\rho}_\gamma - \frac{1}{4\pi}\int j\dot{a}. \tag{52}$$

Next, using that $E = -\dot{a} - \nabla\phi$, we compute

$$\partial_t E_{\mathrm{em}}(a,\phi) = \frac{1}{4\pi}\int \big[-(\dot{a} + \nabla\phi)\cdot\dot{E} + \mathrm{curl}^*\,\mathrm{curl}\,a\cdot\dot{a}\big]dx. \tag{53}$$

Combining the last two relations and and integrating by parts gives

$$\begin{aligned}\partial_t E(\gamma,a,\phi) =& \frac{1}{4\pi}\int \big(\phi(4\pi\dot{\rho}_\gamma + \mathrm{div}\,\dot{E}) \\ &- (\dot{E} + j - \mathrm{curl}^*\,\mathrm{curl}\,a)\dot{a}\big).\end{aligned} \tag{54}$$

Now, using (45) and (46) ($\mathrm{div}\,E = 4\pi(\kappa - \rho_\gamma)$, and $\dot{E} = \mathrm{curl}^*\,\mathrm{curl}\,a - j(\gamma,a)$) yields $\partial_t E(\gamma,a,\phi) = 0$. $\square$

Above, we assumed the external magnetic field is zero.

To describe crystals we take κ to be either periodic (crystals) or uniform (jellium).

If κ and ρ_γ are $\mathscr{L}$-periodic, then integrating (45) over a fundamental cell, Ω, of the lattice $\mathscr{L}$, we arrive at the solvability condition (the charge conservation law)

$$\int_\Omega \rho_\gamma = \int_\Omega \kappa. \tag{55}$$

3.4 Static gHFem Equations

It is easy to see that (γ,a,ϕ) is a static solution to (44), (45) and (46) if and generically only if (γ,a,ϕ) solves the equations

$$\gamma = f(\beta(h_{\phi,a,\gamma} - \mu)), \tag{56}$$

$$\Delta\phi = 4\pi(\kappa - \rho_\gamma), \tag{57}$$

$$\mathrm{curl}^*\,\mathrm{curl}\,a = j(\gamma,a), \tag{58}$$

where, recall, $h_{\phi,a,\gamma} := -\Delta_a - \phi + ex(\gamma)$ and f is a sufficiently regular function f. Physically relevant f are given by either (38) or (39), depending on whether the particles in question are fermions or bosons. (Remember that the unit charge of γ is $e = -1$.)

To this we add the solvability condition (55), which determines the chemical potential μ.

3.4.1 Free Energy

The static gHF equations (56), (57) and (58) arise as the Euler-Lagrange equations for the free energy functional

$$F_\beta(\gamma, a) := E(\gamma, a) - \beta^{-1} S(\gamma) - \mu N(\gamma), \tag{59}$$

where $S(\gamma) = -\mathrm{Tr}(\gamma \ln \gamma + (1-\gamma)\ln(1-\gamma))$ is the entropy, $N(\gamma) := \mathrm{Tr}\gamma$ is the number of particles and $E(\gamma, a)$ is the static part of energy (48), with ϕ expressed in terms of ρ_γ by solving the Poisson equation (57) for ϕ,

$$E(\gamma, a) = \mathrm{Tr}\big((-\Delta_a)\gamma\big) + \frac{1}{2}\int (\kappa - \rho_\gamma) 4\pi(-\Delta)^{-1}(\kappa - \rho_\gamma) dx$$
$$+ \frac{1}{8\pi}\int dx |\operatorname{curl} a(x)|^2 + Ex(\gamma). \tag{60}$$

This, not quite trivial, fact is proven in [22]. (For a formal statement in a more general situation see Theorem 4 below.)

We demonstrate informally that (56), (57) and (58) are the Euler-Lagrange equations for (59). By the definitions of $E(\gamma, a)$, $Ex(\gamma)$ and $S(\gamma)$, we have

$$d_\gamma E(\gamma, a)\xi = \mathrm{Tr}(h_\gamma \xi) \tag{61}$$

and

$$d_\gamma S(\gamma) = \mathrm{Tr}(s(\gamma)\xi), \tag{62}$$

which implies (56) with ϕ given by (57). Next, using the definition $j_a := -4\pi d_a \mathrm{Tr}\big((-\Delta_a)\gamma\big)$, we find

$$d_a E(\gamma, a)\alpha = \frac{1}{4\pi}\int \big(j_a - \operatorname{curl}^* \operatorname{curl} a\big)\alpha, \tag{63}$$

which yields (58).

3.4.2 Electrostatics

We describe the important case of electrostatics here, i.e. the time-independent case with $a = 0$. In this case, Eqs. (56), (57) and (58) become

$$\gamma = f(\beta(h_{\phi,\gamma} - \mu)), \tag{64}$$

$$\Delta\phi = 4\pi(\kappa - \rho_\gamma), \tag{65}$$

where $h_{\phi,\gamma} := -\Delta - \phi + ex(\gamma)$, which after solving Eq. (57) for ϕ, gives

$$\gamma = f(\beta(h_\gamma - \mu)), \tag{66}$$

where $h_\gamma := -\Delta - \phi_{\rho_\gamma} + ex(\gamma)$, with $\phi_\rho = \Delta^{-1} 4\pi(\kappa - \rho)$. To this we add the solvability condition (55), which determines the chemical potential μ. Moreover, we associate with the charge density, $\kappa - \rho$, the potential

$$\phi_\rho = 4\pi(-\Delta)^{-1}(\kappa - \rho), \tag{67}$$

satisfying the Poisson equation (65).

The energy and free energy for (66) are given by

$$E(\gamma) := \mathrm{Tr}((-\Delta)\gamma) \tag{68}$$

$$+ \frac{1}{2}\int (\kappa - \rho_\gamma)(x) 4\pi(-\Delta)^{-1}(\kappa - \rho_\gamma)(x) dx + Ex(\gamma), \tag{69}$$

$$F_\beta(\gamma) := E(\gamma) - \beta^{-1} S(\gamma) - \mu N(\gamma). \tag{70}$$

4 Density Functional Theory

The starting point of the (time-dependent) density functional theory (DFT) are the equations (44), (45) and (46) but with the exchange term $ex(\gamma)$ is taken to be of the form $\mathrm{xc}(\rho_\gamma)$, where $\mathrm{xc}(\lambda)$ is a local function combining contributions of the exchange and correlation energy. For the former one usually take the expression $-c\rho^{4/3}$, going back to Dirac, and the latter is found empirically. This simple but profound modification opens an incredible computational potential of the theory.

We concentrate on the simplest case of electrostatics. In this case Eq. (66) becomes

$$\gamma = f(\beta(h_{\rho_\gamma} - \mu)), \tag{71}$$

where f is given by (38) and, with $\phi_\rho = (-\Delta)^{-1} 4\pi(\kappa - \rho) =: v * (\kappa - \rho)$,

$$h_\rho := -\Delta - \phi_\rho + \mathrm{xc}(\rho). \tag{72}$$

Equation (71) is an extension of the key equation of the DFT – the Kohn-Shan equation – to positive temperature $T = 1/\beta > 0$. The energy and free energy for (71) are given by

$$E(\gamma) := \mathrm{Tr}((-\Delta)\gamma) + \frac{1}{2}\int (\rho_\gamma - \kappa) v * (\rho_\gamma - \kappa) + \mathrm{Xc}(\rho_\gamma), \tag{73}$$

$$F_\beta(\gamma) := E(\gamma) - \beta^{-1}S(\gamma) - \mu N(\gamma). \tag{74}$$

Let den be the map from operators, A, into functions $\rho_A(x) = \text{den}[A](x) := A(x,x)$ with $A(x,y)$ being generalized kernel of A ('den' stands for 'density'). Taking the diagonal of (71), we arrive at the following equation for ρ

$$\rho = \text{den}[f(\beta(h_\rho - \mu))]. \tag{75}$$

Equation (75) gives an equivalent formulation of the Kohn-Sham equation (71). For κ (and ρ) $\mathscr{L}$-periodic, we add to equation (75) the charge conservation law (cf. (55)), which determines the chemical potential μ,

$$\int_\Omega \rho = \int_\Omega \kappa, \tag{76}$$

where Ω is a fundamental cell of the lattice $\mathscr{L}$.

Conversely, starting from (75) and (76), we define the potential $\phi = (-\Delta)^{-1}4\pi(\kappa - \rho)$ produced by the charge distribution $\kappa - \rho$. Then ϕ satisfies

$$-\Delta\phi = 4\pi(\kappa - \rho). \tag{77}$$

Note that because of the minimal coupling, there is *no (pure) DFT theory* when the system in question is coupled to the magnetic field.

4.1 Crystals

Here one deals with the electrostatics, (64), or, in the DFT context, (71) (or (75)). for an ideal crystal, one assumes that $\kappa = \kappa_{\text{per}}$ is periodic w.r. to some lattice $\mathscr{L}$, representing an $\mathscr{L}$ periodic charge distribution of crystal ions. An example of such an κ_{per} is

$$\kappa_{\text{per}}(x) = \sum_{l \in \mathscr{L}} \kappa_a(x - l)\,. \tag{78}$$

where κ_a denotes an ionic ('atomic') potential.

The simplest special case of periodic κ is κ constant. Such a system is called the *jellium*. For $\kappa = \kappa_{\text{jel}}$ constant, (75) has the solution $(\rho_{\text{jel}} = \kappa_{\text{jel}}, \mu_{\text{jel}})$. Indeed, (76) reduces to $\rho_{\text{jel}} = \kappa_{\text{jel}}$ and (75) to one equation for μ, which has a unique solution for μ near μ_{jel} [23].

The existence (without uniqueness) of a certain periodic, trace class solution to equation (71) (or (75)) with certain class of density terms xc is obtained in [1] via variation techniques. (See [17, 18] for earlier results for the Hartree and Hartree-Fock equations. We present a somewhat different proof of the latter result in Sect. 7.) The next result proven in [23], establishes, under more restrictive conditions, uniqueness and quantitative bounds needed for the next result.

Let Ω be a fundamental cell of the lattice $\mathscr{L}$ and $|\Omega|$ denote its area. Denote by $H^s_{\rm per}(\mathbb{R}^d)$ the locally Sobolev space of $\mathscr{L}$-periodic functions with the inner product given by that of $H^s(\Omega)$. We have:

Theorem 1 (Ideal crystal) *Let $T > 0$, $d = 2$ or 3, $\beta = 1/T$ be sufficiently large and $|\Omega|$ be sufficiently small. We assume that*

1. *$\kappa_{\rm per}$ is the $\mathscr{L}$−periodic background charge distribution s.t.*
   (a) *$\kappa_{\rm per} \in H^s_{\rm per}$ for $s \geq 2$ and $||\kappa_{\rm per}||_{H^s}$ is sufficiently small;*
   (b) *$\kappa_{\rm jel} = \frac{1}{|\Omega|}\int_\Omega \kappa_{\rm per}$ and $\kappa'_{\rm per} = \kappa_{\rm per} - \kappa_{\rm jel}$ satisfy $|xc(\kappa_{\rm jel})| < \frac{\kappa^2_{\rm jel}}{w^2_{d-1}}$ and $\kappa'_{\rm per} \in H^s_{\rm per}$ for $s \geq 2$, where w_d is the volume of the d-sphere;*
2. *$xc \in W^{s,\infty}$ for $s \geq 2$ and $\|xc\|_{W^{s,\infty}}$ is sufficiently small.*

Then the Kohn-Sham equation (75) has a unique solution $(\rho_{\rm per}, \mu_{\rm per}) \in H^s_{\rm per}(\mathbb{R}^d) \times \mathbb{R}_+$ satisfying

$$\|\rho_{\rm per} - \kappa_{\rm per}\|_{H^s} \lesssim \|\kappa'_{\rm per}\|_{H^s_{\rm per}}, \tag{79}$$

$$|\mu_{\rm per} - \mu_{\rm jel}| \lesssim \|\kappa'_{\rm per}\|_{H^s_{\rm per}}. \tag{80}$$

where $(\rho_{\rm jel} = \kappa_{\rm jel}, \mu_{\rm jel})$ is a solution to (75) with $\kappa = \kappa_{\rm jel}$.

Proof (Idea of proof of Theorem 1) We write (75) as a fixed point problem

$$\rho = \Phi(\rho, \mu), \ \ \Phi(\rho, \mu) := \mathrm{den}[f(\beta(h_\rho - \mu))]. \tag{81}$$

To this we add the charge conservation law (76) with Ω a fundamental cell of $\mathscr{L}$.

To handle the constraint (76), we let P denote the projection onto constants, $Pf := \frac{1}{|\Omega|}\int_\Omega f$, and let $\bar{P} = 1 - P$ and split (81) into two equations

$$\rho' = P\Phi(\rho' + \rho'', \mu), \tag{82}$$

$$\rho'' = \bar{P}\Phi(\rho' + \rho'', \mu). \tag{83}$$

where $\rho' := P\rho = \frac{1}{|\Omega|}\int_\Omega \rho$ and $\rho'' := \bar{P}\rho = \rho - \rho'$. By the constraint (76), we have $\rho' = \frac{1}{|\Omega|}\int_\Omega \kappa$. Hence (82) and (83) are equations for μ and ρ''. We first solve (83) for ρ'' by a fixed point theorem and then (82) for μ, by an implicit function argument.

A *central* open problem here is to determine whether the (locally) free energy minimizing solution *breaks spontaneously symmetry* or not. The spontaneous symmetry breaking means that ρ_γ has lower (coarser) symmetry than κ ('spontaneous symmetry breaking').

4.2 Macroscopic Perturbations

A key problem in solid state physics is derivation of an effective, macroscopic equations for crystals from microscopic ones. In the full generality this problem is far from our reach. However one can reasonably hope to derive such equations starting from the DFT microscopic theory.

We consider macroscopic perturbations (say, local deformations) of ideal crystals and the dielectric response to them. At the first step, one would like to prove existence of solutions under local deformation of crystals. The appropriate spaces for our analysis are the homogenous Sobolev spaces:

$$\dot{H}^s(\mathbb{R}^3) = \left\{ f : \|f\|^2_{\dot{H}^s} := \int |p|^{2s} |\hat{f}|^2(p) < \infty \right\}. \tag{84}$$

We note that $\dot{H}^s$ and $\dot{H}^{-s}$ are dual spaces under the usual $L^2(\mathbb{R}^3)$ pairing $\langle \cdot, \cdot \rangle$ and that $\dot{H}^s$, unlike H^s, contains only s-order derivative in its norm.

We state some of the assumptions used below. To begin with we assume $d = 3$.

[A1] (regularity of κ)

$\kappa = \kappa_{\text{per}} + \kappa'$, where

κ_{per} is $\mathscr{L}$-periodic and satisfies

$\kappa_{\text{per}} \in H^2_{\text{per}}(\mathbb{R})^3$

and $\kappa' \in (H^2 \cap H^{-2})(\mathbb{R}^3)$,

[A2] (regularity of xc**)**

xc $\in C^4(\mathbb{R}_+)$ together with its derivatives

is bounded near the origin as

$|\text{xc}(\lambda)| < \epsilon\lambda$ for ϵ small.

Since κ' is not periodic, constraint (76) does not apply here. Let $(\rho_{\text{per}}, \mu_{\text{per}})$ be the periodic solution to the Kohn-Sham equation (75), with the $\mathscr{L}-$periodic background charge density κ_{per} given in Theorem 1. The next result shows that the periodic solutions of Theorem 1 are stable under local perturbations.

Theorem 2 (Stability under local perturbations) *Let $d = 3$ and the constraints of Theorem 1 be obeyed and assume [A1] and [A2]. In addition, let $\|\kappa\|_{H^2 \cap H^{-2}} \ll 1$*

and $\|\kappa'\|_{H^2} \ll 1$. *Then the Kohn-Sham equation* (75)*, with* $\kappa = \kappa_{\text{per}} + \kappa'$ *and* $\mu = \mu_{\text{per}}$*, has a unique solution* ρ *satisfying*

$$\rho = \rho_{\text{per}} + \rho' \;\; \textit{with} \;\; \rho' \in (H^2 \cap H^{-2})(\mathbb{R}^3) \;\textit{and} \tag{85}$$

$$\|\rho'\|_{H^2 \cap H^{-2}} \lesssim \|\kappa'\|_{H^2 \cap H^{-2}}. \tag{86}$$

Theorem 2 is proven in [23]. Similar results for $T = 1/\beta = 0$ were proven in [1, 11, 12, 15, 17] (see [14, 39] for very nice reviews).

Dielectric response We consider Eq. (75) in the macroscopic variables at $1 << \beta < \infty$. Let $\mathscr{L}_\delta := \delta\mathscr{L}$ be a microscopic crystalline lattice (on the microscopic scale 1) with a fundamental domain Ω_δ centered at the origin. Let $\kappa_{\text{per}}^\delta$ be $\mathscr{L}_\delta-$periodic microscopic charge distribution of the form

$$\kappa_{\text{per}}^\delta(x) = \delta^{-d}\kappa_{\text{per}}(\delta^{-1}x) \tag{87}$$

where κ_{per} is a $\mathscr{L}-$periodic function on $\mathbb{R}^d$. Note that under this scaling, the L^1-norm is preserved.

We consider a macroscopically perturbed background charge distribution (written in the macroscopic coordinate x)

$$\kappa_\delta(x) = \kappa_{\text{per}}^\delta(x) + \kappa'(x), \tag{88}$$

where $\kappa'(x) \in L^2(\mathbb{R}^d)$ is a small local perturbation living on the macroscopic scale (1), producing macroscopically deformed crystal. To study the macroscopic behavior, we rescale the Kohn-Sham equations (75) to obtain

$$\rho_\delta = \text{den}[f_{FD}(\beta(h_{\phi_\delta} - \mu)], \tag{89}$$

where $h_{\phi_\delta} = -\delta^2\Delta - \delta\phi_\delta(x)$ with the potential ϕ_δ given by

$$\phi_\delta := (-\Delta)^{-1}4\pi(\kappa_\delta - \rho_\delta)\,. \tag{90}$$

Given $\kappa_{\text{per}}^\delta$, Theorem 8 implies that (89) has a $\mathscr{L}_\delta$-periodic solution $\rho_{\text{per}}^\delta = \delta^{-3}\rho_{\text{per}}(\delta^{-1}x)$, with associated potential $\phi_{\text{per}}^\delta = \delta^{-1}\phi_{\text{per}}(\delta^{-1}x)$. We list additional assumptions needed for the next and key result.

Let $h_{\text{per}} = -\Delta - \phi_{\text{per}}$. Let $\xi(\mathbb{R}^3)$ denote the size of the spectral gap of h_{per} at μ on $L^2(\mathbb{R}^3)$ and $\xi(\Omega)$ denote the size of the spectral gap of h_{per} at μ on $L^2(\Omega)$ with periodic boundary condition.

[A3] (spectral gap condition)

$$\xi := \xi(\mathbb{R}^3) - \frac{5}{6}\xi(\Omega) > 0.$$

[A4] (scaling condition)

$\delta \ll 1$ and $\beta \geq C\xi^{-1}\ln(1/\delta)$ for C large.

We now present the main result of [23] on the derivation of the effective Poisson equation:

Theorem 3 *Suppose that $d = 3$ and fix a solution ρ_{per} as above. Let assumptions [A1]–[A4] hold. Then the rescaled Kohn-Sham equation (89), with background charge distribution defined in (88) and $\mu = \mu_{\text{per}}$, has a unique solution ρ_δ in $L^2_{\text{per}} + \dot{H}^{-1} + \dot{H}^{-2}$ with associated potential ϕ_δ of the form*

$$\phi_\delta = \phi^\delta_{\text{per}} + \phi_0 + \phi_{\text{rem},1} + \phi_{\text{rem},2}, \tag{91}$$

where ϕ^δ_{per} is the potential associated to the periodic solution ρ^δ_{per}, $\phi_{\text{rem},i}$, $i = 1, 2$, obey the estimates

$$\|\phi_{\text{rem},1}\|_{\dot{H}^1(\mathbb{R}^3)} \lesssim \delta^{1/2} \text{ and } \|\phi_{\text{rem},2}\|_{L^2(\mathbb{R}^3)} \lesssim \delta \tag{92}$$

and ϕ_0 satisfies the equation

$$-\operatorname{div} \epsilon_0 \nabla \phi_0 = \kappa' \tag{93}$$

with a real positive 3×3 matrix, ϵ_0, given in (94), (95), (96) and (97) below.

A similar result for $T = 1/\beta = 0$ was proven in [13, 14] (see also [27–29]).

Remark 1

1. We note that in general $\xi(\mathbb{R}^3) \leq \xi(\Omega)$. One sees this by passing to Bloch-Floquet decomposition of h_{per} and noting that $\xi(\mathbb{R}^3)$ is the inf of all spectral gaps of the fiber decomposed operators on $L^2(\Omega)$.
2. The number $\frac{5}{6}$ comes from Hardy's inequality. In dimension $d = 3$, Hardy's inequality is $\|f\|_{L^6(\mathbb{R}^3)} \lesssim \|\nabla f\|_{L^2(\mathbb{R}^3)}$. We note that if $p = 6$, then its conjugate is $q = \frac{6}{5}$.
3. The constant C appearing in [A4] can be taken to be any number $C > 100$.
4. The 3×3 matrix ϵ_0 in (93) is of the form

$$\epsilon_0 = \mathbf{1}_{3\times 3} + \epsilon_0', \tag{94}$$

$$\epsilon_0' = \frac{1}{|\Omega|} \operatorname{Tr}_{L^2(\Omega)} \oint r^2_{\text{per}}(z)(-i\nabla) r_{\text{per}}(z)(-i\nabla) r_{\text{per}}(z) \tag{95}$$

$$- \frac{1}{|\Omega|} \|\rho_1\|^2_{\dot{H}^{-1}(\Omega;\mathbb{C}^3)}, \tag{96}$$

where $r_{\text{per}}(z) = (z - h_{\text{per}})^{-1}$, $h_{\text{per}} = -\Delta - \phi_{\text{per}} + \text{xc}(\rho_{\text{per}})$, and

$$\rho_1 = 2\chi_{\mathbb{R}^3\setminus\Omega^*}(-i\nabla)\,\text{den}\oint r_{\text{per}}^2(z)(-i\nabla)r_{\text{per}}(z)\,. \tag{97}$$

Here χ_Q denotes a characteristic function of the set Q and Ω^* stands for a fundamental cell of the reciprocal lattice.

5 Hartree-Fock-Bogoliubov Equations

For appropriate spaces, it is shown in [3] that, for the Hamiltonian H given in Eq. (7), φ_t satisfies (12) if and only if the triple (ϕ, γ, α) of 1^{st}- and 2^{nd}-order truncated expectations of φ_t, defined by (cf. (10))

$$\begin{cases} \phi(x,t) := \varphi_t(\psi(x)), \\ \gamma(x,y,t) := \varphi_t[\psi^*(y)\,\psi(x)] - \varphi_t[\psi^*(y)]\,\varphi[\psi(x)], \\ \alpha(x,y,t) := \varphi_t[\psi(x)\,\psi(y)] - \varphi[\psi(x)]\,\varphi_t[\psi(y)]\,, \end{cases} \tag{98}$$

satisfies the time-dependent Hartree-Fock-Bogoliubov equations

$$i\partial_t\phi = h(\gamma)\phi + |\phi|^2\phi + k(\alpha)\bar{\phi}\,, \tag{99}$$

$$i\partial_t\gamma = [h(\gamma^\phi), \gamma]_- + [k(\alpha^\phi), \alpha]_-\,, \tag{100}$$

$$i\partial_t\alpha = [h(\gamma^\phi), \alpha]_+ + [k(\alpha^\phi), \gamma]_+ + k(\alpha^\phi), \tag{101}$$

where the subindex t is not displayed, $[A_1, A_2]_\pm = A_1A_2^{T/*} \pm A_2A_1^{T/*}$, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\alpha^\phi := \alpha + |\phi\rangle\langle\bar{\phi}|$, and

$$h(\gamma) = h + v * d(\gamma) + v \sharp \gamma\,, \tag{102}$$

$$k(\alpha) = v \sharp \alpha\,, \quad d(\alpha)(x) := \alpha(x,x). \tag{103}$$

In these equations, $v \sharp \alpha$ is the operator with the integral kernel $v \sharp \alpha\,(x;y) := v(x-y)\alpha(x;y)$.

Here, ϕ describes the Bose-Einstein condensed atoms, γ, thermal atomic cloud and σ, the superfluid component of the atomic gas.

For the pair potential $v(x-y) = g\delta(x-y)$, the HFB equations in a somewhat different form have first appeared in the physics literature; see [26, 35, 51] and, for further discussion, [3, 4].

Note that if we drop the third terms in (99) and (100), then we arrive at, essentially, the Gross-Pitaevski and Hartree equations, respectively. If we drop the last term on the r.h.s. of (101), then equations (99), (100) and (101) have solutions of the form $(\phi, 0, 0)$ and $(0, \gamma, 0)$, where ϕ and γ solve the Gross-Pitaevski and Hartree equations, $i\partial_t\phi_t = h\phi_t + |\phi_t|^2\phi_t$ and $i\partial_t\gamma_t = [h(\gamma_t), \gamma_t]_-$, respectively. The last term on the r.h.s. of (101) prevents the 100% condensation.

Equations (99), (100) and (101), with the last term on the r.h.s. of (101) dropped, form the no quantum depletion model. Equations (99) and (100), with $\alpha = 0$, are called the two-gas model.

Given appropriate spaces, here are some key properties of (99), (100) and (101) at a glance [3, 4]:

(A) *Conservation of the total particle number*: If φ_t solves Eq. (12) then the number of particles,

$$\mathcal{N}(\phi_t, \gamma_t, \sigma_t) := \varphi_t(N), \tag{104}$$

where N is the particle-number operator, is conserved.

(B) *Existence and conservation of the energy*: If φ_t solves (12) then the energy

$$\mathcal{E}(\mu(\varphi_t)) := \varphi_t(H) \tag{105}$$

is conserved. Moreover, $\mathcal{E}$ is given explicitly by the expression

$$\mathcal{E}(\phi, \gamma, \alpha) = \mathrm{Tr}[h(\gamma^\phi) + b[|\phi\rangle\langle\phi|]\gamma + \frac{1}{2}b[\gamma]\gamma] + \frac{1}{2}\int v(x-y)|\alpha^\phi(x,y)|^2 dxdy\,. \tag{106}$$

(C) *Positivity preservation property*: If $\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar\alpha & 1+\bar\gamma \end{pmatrix} \geq 0$ at $t = 0$, then this holds for all times.

(D) *Global well-posedness of the HFB equations*: If the pair potential v is in the Sobolev space $W^{p,1}$, with $p > d$, and satisfies $v(x) = v(-x)$ and the initial condition $(\phi_0, \gamma_0, \alpha_0)$ is in a certain mixed functional – operator space and satisfies $\begin{pmatrix} \gamma_0 & \alpha_0 \\ \bar\alpha_0 & 1+\bar\gamma_0 \end{pmatrix} \geq 0$, then the HBF equations (99), (100) and (101) have a unique global solution in the same space.

6 Bogoliubov-de Gennes Equations

6.1 Formulation

We assume for simplicity that the external potential is zero, $V = 0$. Since the Bogoliubov-de Gennes (BdG) equations describe the phenomenon of superconductivity, they are naturally coupled to the electromagnetic field. We describe the latter by the vector and scalar potentials a and ϕ.

It is convenient to organize the operators γ and α (see (10)) into the self-adjoint matrix-operator

$$\eta := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & \mathbf{1} - \bar{\gamma} \end{pmatrix}. \tag{107}$$

Assuming γ carries electric charge in units of -1 (i.e. the charge density is $-\rho_\gamma$, the time-dependent BdG equations can be written as (see e.g. [22, 24, 25])

$$i\partial_t \eta = [\Lambda(\eta, a), \eta], \tag{108}$$

with $\Lambda(\eta, a) = \left(\begin{smallmatrix} h_{\gamma a} & v\sharp\alpha \\ v\sharp\bar{\alpha} & -\overline{h_{\gamma a}} \end{smallmatrix}\right)$, where $v(x)$ is a pair potential, the operator $v \sharp \alpha$ is defined through the integral kernels as $v \sharp \alpha\, (x; y) := v(x - y)\alpha(x; y)$, and

$$h_{\gamma a} := h_a + v * \rho_\gamma - v \sharp \gamma\ ,\ \ \rho_\gamma(x) := \gamma(x; x). \tag{109}$$

Above $h_a = -\Delta_a$ and the terms $v * \rho_\gamma$ and $-v \sharp \gamma$ describe the self-interaction and exchange energies. Equation (108) is coupled to the Ampère's law part of the Maxwell equations

$$-\partial_t(\partial_t a + \nabla\phi) = \operatorname{curl}^* \operatorname{curl} a - j(\gamma, a), \tag{110}$$

where ϕ is the scalar potential and $j(\gamma, a)$ is the superconducting current, given by

$$j(\gamma, a)(x) := [-i\nabla_a, \gamma]_+(x, x).$$

Here, recall, $[A, B]_+ := AB + BA$.

Finally, recall that γ and α satisfy (11). In fact, one has the stronger property

$$0 \leq \eta = \eta^* \leq 1. \tag{111}$$

Remarks

(1) In general, h_a might contain also an external potential $V(x)$, due to the impurities.
(2) For $\alpha = 0$, Eq. (108) becomes the time-dependent Hartree-Fock equation (44) for γ. Thus the HFE is the special diagonal case of the BdG equations.
(3) We may assume that the physical space is either $\mathbb{R}^d$ or a finite box in $\mathbb{R}^d$ and γ and α are gauge periodic operators trace-class and Hilbert-Schmidt operators w.r. to trace per volume. For a detailed discussion of spaces see [22].
(4) One should be able to derive (108) and (110) from hamiltonian (7) coupled to the quantized electro-magnetic filed.

Connection with the BCS theory Equation (108) can be reformulated as an equation on the Fock space involving an effective quadratic hamiltonian (see [3] for the bosonic version). These are the effective BCS equations and the effective BCS hamiltonian (see [24, 25, 38]).

6.2 Symmetries

The equations (108), (109) and (110) are invariant under the *gauge* transformations and, if the external potential V is zero, also under *translations* and *rotations*, defined as

$$T_\chi^{\text{gauge}} : (\gamma, \alpha, a, \phi) \mapsto (e^{i\chi}\gamma e^{-i\chi}, e^{i\chi}\alpha e^{i\chi}, a + \nabla\chi, \phi - \partial_t\chi), \tag{112}$$

for any sufficiently regular function $\chi : \mathbb{R}^d \to \mathbb{R}$, and

$$T_h^{\text{trans}} : (\gamma, \alpha, a, \phi) \mapsto (U_h\gamma U_h^{-1}, U_h\alpha U_h^{-1}, U_h a, U_h\phi), \tag{113}$$

for any $h \in \mathbb{R}^d$,

$$T_\rho^{\text{rot}} : (\gamma, \alpha, a, \phi) \mapsto (U_\rho\gamma U_\rho^{-1}, U_\rho\alpha U_\rho^{-1}, \rho U_\rho a, U_\rho\phi), \tag{114}$$

for any $\rho \in O(d)$. Here U_h and U_ρ are the standard translation and rotation transforms $U_h : f(x) \mapsto f(x+h)$ and $U_\rho : f(x) \mapsto f(\rho^{-1}x)$. In terms of η, say the gauge transformation, T_χ^{gauge}, could be written as

$$\eta \to \hat{T}_\chi^{\text{gauge}}\eta(\hat{T}_\chi^{\text{gauge}})^{-1}, \quad \text{where } \hat{T}_\chi^{\text{gauge}} = \begin{pmatrix} e^{i\chi} & 0 \\ 0 & e^{-i\chi} \end{pmatrix}. \tag{115}$$

Notice the difference in action of this transformation on the diagonal and off-diagonal elements of η.

The invariance under the gauge transformations can be proven by using the relation

$$\hat{T}_\chi^{\text{gauge}} g'(\eta)(\hat{T}_\chi^{\text{gauge}})^{-1} = g'(\hat{T}_\chi^{\text{gauge}}\eta(\hat{T}_\chi^{\text{gauge}})^{-1}),$$

proven by expanding $g'(\eta)$ (or $g^\#(\beta H_{\eta a})$), and the gauge covariance of $\Lambda(\eta, a)$:

$$(\hat{T}_\chi^{\text{gauge}})^{-1}(\Lambda(\hat{T}_\chi^{\text{gauge}}\eta, a)) = \Lambda(\eta, a). \tag{116}$$

The gauge symmetry is not a physical one, but rather an invariance of the solution space (or the covariance of the equations) under 'reparametrizations'. Therefore the natural objects are gauge-equivalent classes of solutions. This leads to the notion of gauge or *magnetic translations* (mt, below) and gauge or magnetic rotations. The former are given by the transformations

$$T_{bs} : (\eta, a) \to (T^{\text{gauge}}_{\chi_s})^{-1} T^{\text{trans}}_s (\eta, a), \tag{117}$$

for any $s \in \mathbb{R}^d$, where $\chi_s(x) := x \cdot a_b(s)$, where $a_b(x)$ is the vector potential with the constant magnetic field, $\operatorname{curl} a_b = b$. The invariance under these transformations will be called the *magnetic translation* (mt) symmetry. The latter is given by the transformations

$$T_{b\rho} : (\eta, a) \to (T^{\text{gauge}}_{\chi_\rho})^{-1} T^{\text{rot}}_\rho (\eta, a), \tag{118}$$

for $\rho \in O(d)$. We remark that in general T_{bs} and $T_{b\rho}$ are only projective representations of $\mathscr{L}$ and $O(d)$, respectively.

Finally, the equations (108), (109) and (110) are invariant under the transformations (see [2])

$$\eta \to \mathbf{1} - \eta \ \text{ and } \ \eta \to -\overline{J^* \eta J} \ \text{ (the particle-hole symmetry).}$$

Here $J := \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}$. The second relation follows from (the particle-hole symmetry)

$$J^* \Lambda J = -\bar{\Lambda}. \tag{119}$$

The form (107) of the matrix operator η is characterized by the relation

$$J^* \eta J = \mathbf{1} - \bar{\eta}. \tag{120}$$

By the above, the evolution preserves this relation, i.e. if an initial condition has this property, then so does the solution.

6.3 Conservation Laws

The Bogolubov-de Gennes equations (108), (109) and (110) form a hamiltonian system with the conserved energy functional

$$E(\eta, a) = \operatorname{Tr}_\Omega\big(h_a \gamma\big) + \frac{1}{2}\operatorname{Tr}_\Omega\big((v * \rho_\gamma)\gamma\big) - \frac{1}{2}\operatorname{Tr}_\Omega\big((v\sharp\gamma)\gamma\big) \tag{121}$$

$$+ \frac{1}{2}\operatorname{Tr}_\Omega\big(\alpha^*(v\sharp\alpha)\big) + \frac{1}{2}\int_\Omega dx |\operatorname{curl} a(x)|^2. \tag{122}$$

where Ω is either $\mathbb{R}^d$ or a fundamental cell of a macroscopic lattice in $\mathbb{R}^d$ (see Sect. 6.6).

The energy $E(\eta, a)$ can be derived from the total quantum hamiltonian, H_{tot}, of the many body system coupled to the quantum electromagnetic field, through quasifree reduction as $E(\eta, a) := \varphi(H_{\text{tot}})$, where φ is a quasifree state in question (see (10) and [3] or [38]). Its conservation law is related to the conservation of the total energy $\varphi(H_{\text{tot}})$. (The combinatorial coefficients of each term result from restriction to $SU(2)$ invariant states and peeling of spin variables (cf. [38]).)

Conservation of (121)–(122) can be also proven directly similarly to the proof of the conservation law of (48).

6.4 Stationary Bogoliubov-de Gennes Equations

We consider stationary, rather than static, solutions to (108) of the form

$$\eta_t := \hat{T}^{\text{gauge}}_{\chi}\eta, \tag{123}$$

with η and $\dot{\chi} \equiv \mu$ independent of t and a independent of t and $\phi = 0$. We have

Proposition 4 *Equation* (123)*, with* η *and* $\dot{\chi} \equiv \mu$ *independent of* t*, is a solution to* (108) *iff* η *solves the equation*

$$[\Lambda_{\eta a}, \eta] = 0, \tag{124}$$

where $\Lambda_{\eta a} \equiv \Lambda_{\eta a \mu} := \Lambda(\eta, a) - \mu S$*, with* $S := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$*, and is given explicitly*

$$\Lambda_{\eta a} := \begin{pmatrix} h_{\gamma a} - \mu & v\sharp\alpha \\ v\sharp\alpha^* & -\bar{h}_{\gamma a} + \mu \end{pmatrix}, \tag{125}$$

with $h_{\gamma a} := -\Delta_a + v * \rho_\gamma - v\sharp\gamma$ *and, recall,* $v\sharp\alpha$ *is an operator with the integral kernel* $v(x-y)\alpha(x, y)$.

Proof Plugging (123) into (108) and using that for χ independent of x,

$$\partial_t \eta_t = i\dot{\chi}\hat{T}^{\text{gauge}}_{\chi}[S, \eta]$$

and (116), we obtain

$$-\dot{\chi}[S, \eta] = [\Lambda(\eta, a), \eta]. \tag{126}$$

Since $\dot{\chi} \equiv \mu$, the latter equation can be rewritten as (124).

For any reasonable function f, solutions of the equation

$$\eta = f(\beta\Lambda_{\eta a}), \tag{127}$$

solve (124) and therefore give stationary solutions of (108). Under certain conditions, the converse is also true.

The physical function f is selected by either a thermodynamic limit (Gibbs states) or by a contact with a reservoir, or imposing the maximum entropy principle. It is given by the Fermi-Dirac distribution (38), i.e.

$$f(h) = (1 + e^h)^{-1}. \tag{128}$$

Inverting the function f, one can rewrite (127) as $\beta \Lambda_{\eta a} = f^{-1}(\eta)$. Let $f^{-1} =: s'$. Then the static Bogoliubov-de Gennes equations can be written as

$$\Lambda_{\eta a} - \beta^{-1} s'(\eta) = 0, \tag{129}$$

$$\text{curl}^* \, \text{curl}\, a - j(\gamma, a) = 0. \tag{130}$$

Here $0 < \beta \leq \infty$ (inverse temperature) and $s(\eta) := -(\eta \ln \eta + (1-\eta)\ln(1-\eta))$ (see (41)).

Remarks

(1) One can express these equations in terms of eigenfunctions of the operator $\Lambda_{\eta a}$, which is the form appearing in physics literature (see [2, 3]).

(2) If we drop the direct $v * \rho_\gamma$ and exchange self-interaction $-v\sharp\gamma$, then the operator $h_{\gamma a \mu}$ and therefore $\Lambda_{\eta a}$ are independent of γ and consequently Eq. (127) defines γ in terms of α and a:

$$\eta_{\beta a} = f(\beta \Lambda_{\alpha a}), \quad \text{where} \quad \Lambda_{\alpha a} := \Lambda_{\eta a}\big|_{\gamma=0}. \tag{131}$$

(3) For (127) to give η of the form (107), the function $f(h)$ should satisfy the conditions

$$f(\bar{h}) = \overline{f(h)} \text{ and } f(-h) = \mathbf{1} - f(h). \tag{132}$$

The function $f(h)$ given in (128) satisfies these conditions. From now on, *we assume $f(h)$ has explicit form* (128).

6.5 Free Energy

The stationary Bogoliubov-de Gennes equations (129) and (130) arise as the Euler-Lagrange equations for the free energy functional

$$F_\beta(\eta, a) := E(\eta, a) - \beta^{-1} S_1(\eta) - \mu N(\eta), \tag{133}$$

where $S(\eta) = \text{Tr}\, s(\eta)$ is the entropy, $N(\eta) := \text{Tr}\gamma$ is the number of particles, and $E(\eta, a)$ is the energy functional given in (121)–(122) with η and a time-independent.

It is shown in [22] that on carefully chosen spaces

(a) The free energy functional F_β is well defined;
(b) F_β is continuously (Gâteaux) differentiable;
(c) If $0 < \eta < 1$ and (η, a) is even in the sense of [22], Eq. (1.17), then critical points of F_β satisfy the BdG stationary equations (129) and (130);
(d) Minimizers of F_β are its critical points.

Now, we define the partial gradients $\partial_\eta F_\beta(\eta, a)$ and $\partial_a F_\beta(\eta, a)$ by $d_\eta F_\beta(\eta, a)\eta' = \mathrm{Tr}(\eta' \partial_\eta F_\beta(\eta, a))$ and $d_a F_\beta(\eta, a)a' = \int a' \cdot \partial_a F_\beta(\eta, a)$, respectively. (Though the expression for $F_\beta(\eta, a)$ is often formal, $\partial_\eta F_\beta(\eta, a)$ and $\partial_a F_\beta(\eta, a)$ could be well-defined on appropriate spaces.)

Theorem 4 *Minimizers of the free energy $F_\beta(\eta, a)$ are critical points of $F_\beta(\eta, a)$, i.e. they satisfy the Euler-Lagrange equations*

$$\partial_\eta F_\beta(\eta, a) = 0 \text{ and } \partial_a F_\beta(\eta, a) = 0, \tag{134}$$

for some β and μ (the latter are determined by fixing $S(\eta)$ and $\mathrm{Tr}(\gamma)$). The Gâteaux derivatives, $\partial_\eta F_\beta(\eta, a)$ and $\partial_a F_\beta(\eta, a)$, are given by

$$\partial_\eta F_\beta(\eta, a) = \Lambda_{\eta a} - \beta^{-1} g'(\eta), \tag{135}$$

and

$$\partial_a F_\beta(\eta, a) := \mathrm{curl}^* \mathrm{curl}\, a - j(\gamma, a), \tag{136}$$

where, recall, $j(\gamma, a)(x) := [-i\nabla_a, \gamma]_+(x, x)$, with $[A, B]_+ := AB + BA$. Consequently, the equations (134) can be rewritten as (129) and (130).

For the translation invariant case, the corresponding result is proven in [37]. In general case, but with $a = 0$ (which is immaterial here), the fact that BdG is the Euler-Lagrange equation of BCS was used in [33], but seems with no proof provided.

By (134), (135) and (136), we can write the equations (129) and (130) as

$$F'_\beta(\eta, a) = 0, \tag{137}$$

where $F'_\beta(\eta, a) = (\partial_\eta F_\beta(\eta, a), \partial_a F_\beta(\eta, a))$.

Remarks

(1) Due to the symmetry (120), $S(\eta) = \mathrm{Tr} s(\eta) = -Tr \eta \ln \eta$, with $s(\lambda)$ given in (41).
(2) $F_\beta(\eta, a)$ is a Helmholtz free energy. This energy depends on the temperature and the average magnetic field, $b = \frac{1}{|Q|} \int_Q \mathrm{curl}\, a$ (for a sample occupying a finite domain Q), in the sample, as thermodynamic parameters. Alternatively,

one can consider the free energy depending on the temperature and an applied magnetic field, h. For a sample occupying a finite domain Q, this leads (through the Legendre transform) to the Gibbs free energy

$$G_{\beta Q}(\eta, a) := F_{\beta Q}(\eta, a) - \Phi_Q h,$$

where $\Phi_Q = b|Q| = \int_Q \operatorname{curl} a$ is the total magnetic flux through the sample. The parameters b or h do not enter the equations (129) and (130) explicitly.

6.6 Ground/Gibbs States

We are looking for stationary states which minimize the free energy per unit volume. More precisely, with some license, we say that (η_*, a_*) is a ground/Gibbs state (depending on whether $\beta = \infty$ or $\beta < 0$), if there is a macroscopic lattice $\mathscr{L}^{\text{macro}}$, s.t. (η_*, a_*) satisfies

- $T_s^{\text{trans}}(\eta, a) = \hat{T}_{\chi_s}^{\text{gauge}}(\eta, a)$, $\forall\, s \in \mathscr{L}^{\text{macro}}$ and for some function $\chi_\cdot : \mathscr{L}^{\text{macro}} \times \mathbb{R}^d \to \mathbb{R}$,

for some lattice $\mathscr{L}^{\text{macro}} \subset \mathbb{R}^d$ with macroscopic fundamental cell Ω^{macro}, and (η_*, a_*) minimizes $F_{\beta\Omega^{\text{macro}}}(\eta, a)$ among states having the above property. This is equivalent to considering the equations on a large twisted torus.

In what follows, we will deal with $\beta < \infty$, i.e. with the Gibbs states only.

In general, equations (129) and (130) have the following stationary solutions which are candidates for the Gibbs state:

1. Normal state: $(\eta_*, 0)$, with $\alpha_* = 0$.
2. Superconducting state: $(\eta_*, 0)$, with $\alpha_* \neq 0$.
3. Mixed state: (η_*, a_*), with $\alpha_* \neq 0$ and $a_* \neq 0$.

One expects that the Gibbs state has the maximal possible symmetry. If the external fields are zero, then the equations are magnetically translationally invariant. Thus, one expects that the Gibbs state is magnetically translational invariant.

We have the following general result

Proposition 5 ([22]) *If η is mt-invariant, then $\alpha = 0$ (i.e. the state (η, a) is normal).*

In the opposite direction we have

Conjecture 5 *For $\beta < \infty$ sufficiently small, a Gibbs, normal state is mt-invariant and therefore unique.*

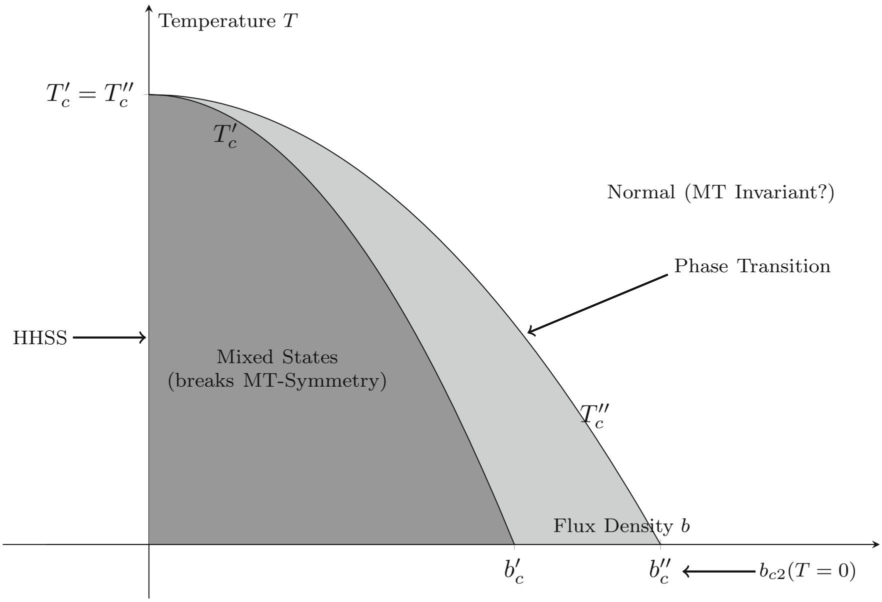
A stronger form of this conjecture is

Conjecture 6 *A Gibbs, normal state is mt-invariant and therefore unique.*

6.7 Symmetry Breaking

Theorem 7 ([22]) *Let $d = 2$. Suppose that $b > 0$ and assume that the interaction potential $v \leq -C|x|^{-\kappa}$, $\kappa < 2$. Then $\exists 0 < \beta_c''(b) \leq \beta_c'(b) < \infty$ s.t.*

- *If $\beta < \beta_c''(b)$, then any Gibbs state is normal;*
- *If $\beta > \beta_c'(b)$, then the ground/Gibbs state is a mixed state.*



In view of Proposition 5 and Conjecture 5 above, this result suggests that under the stated conditions and as the temperature is lowered, the symmetry of the Gibbs state is broken spontaneously.

The corresponding result for $b = 0$ was proved in [37]. In this case, there are no mixed states and the 'mixed state' in the statement should be replaced by the 'superconducting state'. Consequently, there are no symmetry breaking in this case.

6.8 Stability

To formulate the next result, we need some definitions. Recall that $F_\beta'(\eta, a)$ is the *gradient* of $F_\beta(\eta, a)$ in the metric

$$\langle(\eta', a'), (\xi', c')\rangle := \mathrm{Tr}((\eta')^* \xi') + \int a' \cdot c'.$$

Consequently, the Gâteaux derivative $dF'_\beta(\eta, a)$ is the Hessian of $F_\beta(\eta, a)$ at (η, a) and therefore is formally symmetric. It can be shown that it is self-adjoint.

Let $u = (\eta, a)$. We say that a solution u_* to (137) is (linearly or energetically) *stable* iff the linearization $dF'_\beta(u_*)$ of the map $F'_T(u)$ (i.e. the *hessian*, $F''_T(u_*)$, of the functional $F_T(u)$) at u_* is non-negative, i.e.

$$dF'_\beta(u_*) \geq 0,$$

and *unstable* otherwise.

Note that the stability implies the energy minimization property locally in space (i.e. on a sufficiently large twisted torus).

We also consider a weaker notion of stability – the stability w.r. to generation of the superconducting α-component, which we call the α-*stability*.

Proposition 6 ([22]) *Let $b > 0$. The mt invariant (normal) state is α-stable for $\beta < \beta''_c(b)$ and, if $v(r) < -|r|^{-\kappa}$ with $\kappa < 2$, unstable for $\beta > \beta'_c(b)$.*

6.8.1 Normal States

For $b = 0$ we can choose $a = 0$ and the magnetic translation invariance becomes the usual translation invariance. In this case, if we drop the direct and exchange self-interactions from $h_{\gamma a \mu}$, then, as was mentioned above, the normal state is given by (131), with $a = 0$. If the direct and exchange self-interactions are present, then the existence of the normal states is established in [10].

These are normal translationally invariant states. For $b \neq 0$, the simplest normal states are the magnetically translation (mt-) invariant ones. The existence of the mt-invariant normal states for $b \neq 0$ is proven in [22]. They are of the form ($\eta = \eta_{\beta,b},\ a = a_b$), where $a_b(x)$ is the magnetic potential with the constant magnetic field b ($\text{curl}\, a_b = b$) and (cf. (131))

$$\eta_{\beta b} := \begin{pmatrix} \gamma_{\beta b} & 0 \\ 0 & \mathbf{1} - \bar{\gamma}_{\beta b} \end{pmatrix}, \tag{138}$$

with $\gamma_{\beta b}$ a solution to the equation

$$\gamma = s^\sharp(\beta h_{\gamma, a_b}),$$

with $s^\sharp := (s')^{-1}$. (For $s(x) = -(x \ln x + (1 - x) \ln(1 - x))$, we have $s^\sharp(h) = \left(e^h + 1\right)^{-1}$ and therefore $\gamma_{\beta b}$ solves the equation $\gamma = \left(e^{\beta h_{\gamma, a_b}} + 1\right)^{-1}$.)

6.8.2 Superconducting States

The existence of superconducting, translationally invariant solutions is proven in [37] (see this paper and [38] for the references to earlier results and [22], for a somewhat different approach).

6.8.3 Mixed States

For the mixed states, in the cylinder geometry, which means effectively $d = 2$, there is the following specific possibility:

- Vortex lattices: For a mesoscopic lattice $\mathscr{L}$ (i.e. much finer that $\mathscr{L}^{\text{macro}}$), the state (η, a) satisfies $T_s^{\text{trans}}(\eta, a) = \hat{T}_{\chi_s}^{\text{gauge}}(\eta, a)$, for every $s \in \mathscr{L}^{\text{meso}}$ and for some maps $\chi_s : \mathscr{L} \times \mathbb{R}^2 \to \mathbb{R}$.

  The map $\chi_s : \mathscr{L} \times \mathbb{R}^2 \to \mathbb{R}$ satisfies the co-cycle conditions,

$$\chi_{s+t}(x) - \chi_s(x+t) - \chi_t(x) \in 2\pi\mathbb{Z}, \ \forall s, t \in \mathscr{L}, \tag{139}$$

and are called the *summands of automorphy* (see [53] for a relevant discussion). (The map $e^{i\chi} : \mathscr{L} \times \mathbb{R}^2 \to U(1)$, where $\chi(x, s) \equiv \chi_s(x)$ is called the *factor of automorphy*.)

Excitations of the ground state are given by magnetic vortices, which are defined by the condition

- $T_\rho^{\text{rot}}(\eta, a) = \hat{T}_{g_\rho}^{\text{gauge}}(\eta, a)$ for every $\rho \in O(2)$ and some functions $g_\rho : O(2) \times \mathbb{R}^2 \to \mathbb{R}$.

The existence of vortex lattices is proven in [22]). One might be able to prove the existence of vortices by making lattices coarser (or $b \to 0$) in the vortex lattice solutions.

6.8.4 Magnetic Flux Quantization

Denote by $\Omega_{\mathscr{L}}$ a fundamental cell of $\mathscr{L}$. One has the following results

(a) Magnetic vortices: $\frac{1}{2\pi}\int_{\mathbb{R}^2} \operatorname{curl} a = \deg g \in \mathbb{Z}$;
(b) Vortex lattices: $\frac{1}{2\pi}\int_{\Omega_{\mathscr{L}}} \operatorname{curl} a = c_1(\chi) \in \mathbb{Z}$.

Here $\deg g$ is the degree (winding number) of the map $e^{ig} : O(2) \to U(1)$ (which is map of a circle into itself, here we assume that $g(\rho) \equiv g_\rho$ is independent of x) and $c_1(\chi)$ is the first Chern number associated to the summand of automorphy $\chi : \mathscr{L} \times \mathbb{R}^2 \to \mathbb{R}$ (see [53]).

7 Existence of Periodic Solutions by the Variational Technique

Let $d = 2$ or 3. An operator A on $L^2(\mathbb{R}^d)$ is said to be ($\mathscr{L}-$) periodic iff $U_s A U_s^* = A, \forall s \in \mathscr{L}$, where U_s is the translation operator by $s \in \mathbb{R}^d$. In what follows for any periodic operator A, the trace is understood as the trace per volume

$$\mathrm{Tr} A := \mathrm{Tr}_{L^2(\mathbb{R}^3)} \chi_\Omega A \chi_\Omega \tag{140}$$

where χ_Ω is the indicator function on a fundamental domain Ω of $\mathscr{L}$. Let $L^2_{\mathrm{per}}(\mathbb{R}^d)$ denote the local L^2 space of $\mathscr{L}$-periodic functions with the inner product of $L^2(\Omega)$. We define the spaces

$$I^{s,p} = \{\gamma \in \mathscr{B}(L^2_{\mathrm{per}}(\mathbb{R}^d)) : \|\gamma\|_{s,p} := \|M^s \gamma M^s\|_p < \infty\}, \tag{141}$$

where $M = \sqrt{-\Delta}$ and $\|\cdot\|_p$ is the usual Schatten tracial p-norm. Set

$$\begin{aligned} I_0^{s,p} = & I^{s,p} \cap \{\mathrm{Tr}\, \gamma = Z\} \cap \{0 \le \gamma = \gamma^* \le 1\} \\ & \cap \{\|(-\Delta)^{-1/2}(\rho_\gamma - \kappa)\|_{L^2(\Omega)} < \infty\} \end{aligned} \tag{142}$$

In this section we use the variational approach and the fact that (71) (or (75)) is the Euler-Lagrange equations for free energy (74) to prove the following (see [22])

Theorem 8 *Let $\beta < \infty$. Let $\kappa = \kappa_{\mathrm{per}}$ is $\mathscr{L}-$periodic (an ideal crystal) and Xc assume is smooth bounded below, and C^1 on with Xc' bounded. Then there exists $\mu \in \mathbb{R}$ such that the KS equation (71) on $I_0^{1,1}$ have an $\mathscr{L}-$periodic, energy minimizing solution γ satisfying $\int_\Omega \gamma(x,x) = \int_\Omega \kappa$.*

Since we minimize the free energy for $\mathrm{Tr}\gamma$ constant, we drop the term $-\mu\mathrm{Tr}\gamma$ from (74) to arrive at the free energy functional to be minimized

$$\begin{aligned} \mathscr{F}_\beta(\gamma) = & \mathrm{Tr}((-\Delta)\gamma) + \frac{1}{2}\langle(\rho_\gamma - \kappa), (-\Delta)^{-1}(\rho_\gamma - \kappa)\rangle_{L^2(\Omega)} \\ & + \int_\Omega \mathrm{Xc}(\rho_\gamma) - \beta^{-1} S(\gamma)\,. \end{aligned} \tag{143}$$

Moreover, recall $\rho_\gamma(x) = \gamma(x,x)$ and $\mathrm{Xc}'(s) = \mathrm{xc}(s)$ and

$$S(\gamma) = \mathrm{Tr}\, s(\gamma), \quad s(x) = -(x\ln(x) + (1-x)\ln(1-x))\,. \tag{144}$$

We set $\mathscr{F}_\beta(\gamma) = \infty$ if any of the terms is not defined.

Theorem 9 (Main Result) *Under the conditions of Theorem 8, $\mathscr{F}_\beta(\gamma)$ has a minimizer on the set $I_0^{1,1}$. Moreover, this minimizer satisfies KS equation (71).*

We prove this theorem in a series of steps. We will use standard minimization techniques to prove that $\mathscr{F}_\beta(\gamma)$ is coercive and weakly lower semi-continuous, and $I_0^{1,1}$ weakly closed.

Part 1: coercivity

Lemma 1 *Assume that* $\operatorname{Tr}\gamma = Z$. *We have the lower bound*

$$\mathscr{F}_\beta(\gamma) \geq \frac{1}{2}\operatorname{Tr}((-\Delta\gamma) + \frac{1}{2}\langle(\rho-\kappa), (-\Delta)^{-1}(\rho-\kappa)\rangle - C\,. \tag{145}$$

for some constant C.

Proof Recall that $f_{FD}(\lambda) = \left(e^\lambda + 1\right)^{-1}$. First observe that $\frac{1}{2}\operatorname{Tr}(-\Delta\gamma) - \beta^{-1}S(\gamma)$ with $\operatorname{Tr}\gamma = Z$ has minimizer

$$\gamma = f(\beta(-\frac{1}{2}\Delta - \mu)) \tag{146}$$

for a suitable Lagrangian multiplier, μ, from $\operatorname{Tr}\gamma = Z$. Evaluating $\frac{1}{2}\operatorname{Tr}(-\Delta\gamma) - \beta^{-1}S(\gamma)$ at this minimizer gives some constant, say, C_1.

Recalling definition (143) and using that Ex is bounded below, say by C_2, gives (145).

Part 2: Convergence We follow the ideas of [18]. By Part 1, we note that each term on the r.h.s. of (145) is either positive or constant. Thus, $\mathscr{F}_\beta$ is bounded below. Let γ_n be a minimizing sequence of $\mathscr{F}_\beta(\gamma)$. Then we see that $\|\gamma_n\|_{I^{1,1}} = \operatorname{Tr}(-\Delta)\gamma_n$ and $\|\nabla^{-1}\rho_{\gamma_n}\|_{L^2(\Omega)}$ are uniformly bounded. We look for a limit of the sequence (γ_n). The non-abelian Hölder inequality show that

$$\|\gamma_n\|_{I^{0,2}} \leq \|\gamma_n\|_\infty \|\gamma_n\|_{I^{0,1}} \leq Z < \infty \tag{147}$$

is bounded. Hence, upto a subsequence, the kernels $\gamma_n(x, y)$ are in $L^2_{per}(\mathbb{R}\times\mathbb{R})$ (the space of $\mathscr{L}$-periodic under the action $(x, y) \to (x+s, y+s)$, $s \in \mathscr{L}$), locally L^2 functions on $(\mathbb{R}^2 \times \mathbb{R}^2)$ and converges weakly to some $\gamma_0'(x, y) \in L^2_{per}(\mathbb{R}^2 \times \mathbb{R}^2)$. We extend $\gamma_0'(x, y)$ to all of $\mathbb{R}^2 \times \mathbb{R}^2$ by periodicity. Let γ_0' denote the operator whose kernel is $\gamma_0'(x, y)$. Clearly, $\gamma_n \rightharpoonup \gamma_0'$ weakly in $I^{0,2}$.

Now, we show that $\gamma_0' \in I_0^{1,1}$. That is, $\gamma_0' \in I^{1,1}$ and $\operatorname{Tr}(\gamma_0') = Z$, $(\gamma_0')^* = \gamma_0'$, and $0 \leq \gamma_0' \leq 1$. Using the Bloch-Floquet decomposition, we see that

$$\int_{\Omega^*} d\hat{\xi}\, \operatorname{Tr}_{L^2(\Omega)}[(1-\Delta_\xi)^{1/2}(\gamma_n)_\xi(1-\Delta_\xi)^{1/2}] \tag{148}$$

$$= \int_{\Omega^*} d\hat{\xi}\, \operatorname{Tr}_{L^2(\Omega)}[(1-\Delta_\xi)\gamma_n] \tag{149}$$

$$= \operatorname{Tr}(1-\Delta)\gamma_n < \infty\,. \tag{150}$$

where the second line follows by expanding the traces on $L^2(\Omega)$ in an orthonormal basis of eigenfunctions of $-\Delta_\xi$ and the fact $0 \leq (\gamma_n)_\xi$. This shows that $(1-\Delta_\xi)^{1/2}(\gamma_n)_\xi(1-\Delta_\xi)^{1/2}$ is trace class (hence HS) for almost every $\xi \in \Omega^*$. It follows that the full operator $(1-\Delta)^{1/2}\gamma_n(1-\Delta)^{1/2}$ is HS in trace per volume norm and whose trace is equal to (150). Hence a weak limit exists and necessarily is $(1-\Delta)^{1/2}\gamma_0'(1-\Delta)^{1/2}$. We see that

$$Z = \lim_{n\to\infty} \mathrm{Tr}(\gamma_n) \tag{151}$$

$$= \lim_{n\to\infty} \mathrm{Tr}((1-\Delta)^{1/2}\gamma_n(1-\Delta)^{1/2}(1-\Delta)^{-1}) = \mathrm{Tr}(\gamma_0') \tag{152}$$

since $1-\Delta$ is HS (in trace-per-volume norm) for $d = 2, 3$. The fact $\gamma_0' \in I_0^{1,1}$ is proved by using a compactness argument pointwise in the fiber decomposition through a Bloch-Floquet argument similar to one used in (148), (149) and (150). Note that the fact $\gamma_0' = \gamma_0'^*$ and the bound $0 \leq \gamma_0' \leq 1$ is preserved by weak HS (per volume) convergence.

Finally, we show that $\sqrt{\rho_n} \in H^1(\Omega)$ and converges to some $\rho_0'' \in H^1(\Omega)$ weakly. Let $\varphi_\lambda(\xi, x)$ denote the eigenvectors of γ_ξ with eigenvalue λ in its Bloch-Floquet-Zack decomposition. Since the map $f \mapsto \int_\Omega |\nabla\sqrt{f}|^2$ is convex, we see that

$$\int_\Omega |\nabla\sqrt{\rho(x)}|^2 dx = \int_\Omega \left|\nabla\left(\int_{\Omega^*} d\xi \sum \lambda_\xi |\varphi_\xi(x)|^2\right)^{1/2}\right|^2 dx \tag{153}$$

$$\lesssim \int_\Omega\int_{\Omega^*} dx d\hat{\xi} \sum \lambda_\xi |\nabla|\varphi_{\lambda_\xi}(\xi, x)||^2 \tag{154}$$

$$\lesssim \int_\Omega\int_{\Omega^*} dx d\hat{\xi} \sum \lambda_\xi |\nabla\varphi_{\lambda_\xi}(\xi, x)|^2 \tag{155}$$

$$= \mathrm{Tr}(-\Delta\gamma) \tag{156}$$

This shows that $\sqrt{\rho_n}$ are bounded in $H^1(\Omega)$ and thus converges weakly, in H^1 to $\sqrt{\rho_0''} \in H^1(\Omega)$. Compactness of $H^1(\Omega)$ in $L^2(\Omega)$ shows that $\sqrt{\rho_n}$ converges to $\sqrt{\rho_0''}$ in L^2, hence $\rho_n \to \rho_0''$ in $L^1(\Omega)$. It follows that for any smooth bounded periodic function f

$$\langle\rho_0'', f\rangle = \lim_{n\to\infty}\langle\rho_n, f\rangle = \lim_{n\to\infty} \mathrm{Tr}\gamma_n f \tag{157}$$

$$= \lim_{n\to\infty} \mathrm{Tr}(\gamma_0' f) \tag{158}$$

$$= \langle\rho_0', f\rangle \tag{159}$$

Thus, we denote the common limit as $\gamma_0 := \rho_0' = \rho_0''$ and $\rho_0 := \mathrm{den}[\gamma_0]$. We summarize the types of convergences here:

$$(1-\Delta)^{1/2}\gamma_n(1-\Delta)^{1/2} \rightharpoonup (1-\Delta)^{1/2}\gamma_0(1-\Delta)^{1/2} \text{ weakly in } I^{0,2} \tag{160}$$

$$\sqrt{\rho_n} \rightharpoonup \sqrt{\rho_0} \text{ in } H^1(\Omega) \tag{161}$$

$$\rho_n - \kappa \to \rho_0 - \kappa \text{ in } H^{-1}(\Omega) \tag{162}$$

for some $\gamma_0 \in I_0^{1,1}$ and $\rho_0 := \mathrm{den}[\gamma_0]$. The last line follows by compact embedding theorem on Ω.

Part 3: Weak lower semi-continuity

Lemma 2 *The functional $\mathscr{F}_\beta$ is weakly lower semi-continuous with respect to convergence* (160), (161) *and* (162).

Proof We study the functional $\mathscr{F}_\beta(\gamma)$ term by term. For the first term on the r.h.s. of (143), it satisfies $\mathrm{Tr}(h\gamma) = \|\gamma\|_{I^{1,1}}$ and is linear, it is $\|\cdot\|_{I^{1,1}}$-weakly lower semi-continuous. The Coulumb term $\langle(\kappa-\rho_\gamma), (-\Delta)^{-1}(\kappa-\rho_\gamma)\rangle$ is quadratic and easily seen to be $\dot{H}^{-1}(\Omega)$-weakly lower semi-continuous. The exchange-correlation term is weakly lower semi-continuous by (161) (which implies that $Xc(\rho_n) \to Xc(\rho_0)$ a.e.) and Fatou's lemma.

Thus, we study the term $-\beta^{-1}S(\gamma)$. We use an idea from [43] which allows to reduce the problem to a finite-dimensional one. To the latter end, we recall that $S(\gamma) = \mathrm{Tr}(s(\gamma))$ for $s(x) = -x\ln x$. In Bloch-Floquet decomposition, this term is

$$-S(\gamma_n) = -\int_{\Omega^*} d\hat{\xi}\, S((\gamma_n)_\xi) = -\int_{\Omega^*} d\hat{\xi}\, \mathrm{Tr}(s((\gamma_n)_\xi)) \tag{163}$$

where $s(x) = \frac{1}{2}(-x\ln(x) - (1-x)\ln(1-x))$. We define the relative entrop of A and B to be

$$S(A|B) := \mathrm{Tr}(s(A|B)), \quad s(A|B) := A(\ln(A) - \ln(B))\,. \tag{164}$$

Then we see that

$$S(A) = S(B) - S(A|B) - \mathrm{Tr}[(A-B)\ln(B)]\,. \tag{165}$$

Using this formula, writing $A = (\gamma_n)_\xi$ and $B = (\gamma_*)_\xi = \left(\frac{C}{1+e^{\beta\sqrt{-\Delta}}}\right)_\xi$ where C is chosen so that $\mathrm{Tr}(g_*) = Z$,

$$-S(\gamma_n) = \int_{\Omega^*} d\hat{\xi}\, (-1)S((\gamma_*)_\xi) + \mathrm{Tr}((\gamma_n)_\xi - (\gamma_*)_\xi \ln(\gamma_*)_\xi) \tag{166}$$

$$+ S((\gamma_n)_\xi|(\gamma_*)_\xi) \tag{167}$$

We note that $\ln((\gamma_*)_\xi) \lesssim 1 + \sqrt{-\beta\Delta_\xi}$ and $|S(\gamma_*)| < \infty$. By (160) and linearity (hence convexity), (166) converges in the limit to $-S(\gamma_*) + \mathrm{Tr}((\gamma_0 - \gamma_*)\ln(\gamma_*)$. So it suffices that we control the last term (167). We improve convergence for a.e. ξ. By considering $\sqrt{(\gamma_n)_\xi}$ and dropping to a subsequence, (148) shows that $(1 - \Delta_\xi)^{1/2}\sqrt{(\gamma_n)_\xi}$ converges weakly in HS norm for almost every $\xi \in \Omega^*$. Similarly,

$$\int_{\Omega^*} d\hat{\xi}\, \mathrm{Tr}_{L^2(\Omega)}[\sqrt{(\gamma_n)_\xi}(1 - \Delta_\xi)\sqrt{(\gamma_n)_\xi}] \tag{168}$$

$$= \int_{\Omega^*} d\hat{\xi}\, \mathrm{Tr}_{L^2(\Omega)}[(1 - \Delta_\xi)\gamma_n] \tag{169}$$

$$= \mathrm{Tr}(1 - \Delta)\gamma_n < \infty \tag{170}$$

by expanding the trace using an orthonormal basis of $(\gamma_n)_\xi$. Thus, weak convergence is also obtained for $\sqrt{(\gamma_n)_\xi}(1 - \Delta_\xi)^{1/2}$. Regarding $\sqrt{(\gamma_n)_\xi}$ as an kernel in $L^2(\Omega \times \Omega)$, and since Ω is compact, we may assume that $(\gamma_n)_\xi \to (\gamma_0)_\xi$ in HS norm for almost every $\xi \in \Omega^*$. Now, by [43], we can write

$$S((\gamma_n)_\xi|(\gamma_*)_\xi) + \mathrm{Tr}((\gamma_*)_\xi - (\gamma_n)_\xi) = \sup_{\lambda \in (0,1)} \mathrm{Tr}(s_\lambda((\gamma_n)_\xi|(\gamma_*)_\xi)) \tag{171}$$

where $s_\lambda(x)(A|B) = \lambda^{-1}(s(\lambda A + (1 - x)B) - \lambda s(A) - (1 - \lambda)s(B))$. Moreover, $s_\lambda(A|B) \geq 0$ for any A, B since the entropy function s is concave. Hence, we may write

$$S((\gamma_n)_\xi|(\gamma_*)_\xi) + \mathrm{Tr}((\gamma_*)_\xi - (\gamma_n)_\xi) = \sup_{\lambda \in (0,1)} \sup_P \mathrm{Tr}(P s_\lambda((\gamma_n)_\xi|(\gamma_*)_\xi)) \tag{172}$$

where the $\sup_P$ is taken over all finite rank projections P. It follows that for any λ sufficiently small and any finite rank projection P,

$$S((\gamma_n)_\xi|(\gamma_*)_\xi) + \mathrm{Tr}((\gamma_*)_\xi - (\gamma_n)_\xi) \geq \mathrm{Tr}(P s_\lambda((\gamma_n)_\xi|(\gamma_*)_\xi)) \tag{173}$$

Taking $n \to \infty$, since P is finite rank and $(\gamma_n)_\xi \to (\gamma_0)_\xi$ in HS norm (hence operator norm) for almost every $\xi \in \Omega^*$,

$$\liminf_{n\to\infty} S((\gamma_n)_\xi|(\gamma_*)_\xi) + \mathrm{Tr}((\gamma_*)_\xi - (\gamma_0)_\xi) \geq \mathrm{Tr}(P s_\lambda((\gamma_0)_\xi|(\gamma_*)_\xi)) \tag{174}$$

Now taking $\limsup_{\lambda\to 0^+}$ and $\sup_P$, we see that

$$\liminf_{n\to\infty} S((\gamma_n)_\xi|(\gamma_*)_\xi)+\mathrm{Tr}((\gamma_*)_\xi-(\gamma_0)_\xi) \geq \mathrm{Tr}(s((\gamma_0)_\xi|(\gamma_*)_\xi)) . \tag{175}$$

The proof is complete by Fatou's Lemma applied to the integral $\int_{\Omega^*} d\hat{\xi}$ and the fact

$$\int d\hat{\xi}\mathrm{Tr}((\gamma_*)_\xi-(\gamma_0)_\xi)=\mathrm{Tr}(\gamma_*)-\mathrm{Tr}(\gamma_0)=0 . \tag{176}$$

Proof of Theorem 9: Existence of Minimizer. With the results above, the proof is standard. Let $(\gamma_n)\in I_0^{1,1}$ be a minimizing sequence for $\mathscr{F}$. Lemma 1 shows that $\mathscr{F}_\beta$ is coercive. Hence $\|\gamma_n\|_{(1)}$ is bounded uniformly in n. By Sobolev-type embedding theorems, (γ_n) converges strongly in $I_0^{s,1}$ for any $s<1$. Moreover, together with the Banach-Alaoglu theorem, the latter implies that (γ_n) converges weakly in $I_0^{1,1}$. Hence, denoting the limit by γ_0, we see that, by Lemma 2, $\mathscr{F}_\beta$ is lower semi-continuous:

$$\liminf_{n\to\infty}\mathscr{F}_\beta(\gamma_n)\geq\mathscr{F}_\beta(\gamma_0). \tag{177}$$

Hence, γ_0 is indeed a minimizer. To show that minimizer satisfies the gHF equation, we start with some lemmas.

Lemma 3 *Let $\gamma\in I_0^{1,1}$ be such that $s(\gamma):=-(\gamma\ln\gamma+(1-\gamma)\ln(1-\gamma))$ is trace class and γ' satisfy*

$$\mathrm{Tr}\gamma'=0 \text{ and } (\gamma')^2\lesssim(\gamma(1-\gamma))^2 . \tag{178}$$

Then, $\mathscr{F}_\beta(\gamma)$ is Gâteaux differentiable at γ with respect to variations γ' and

$$d_\gamma\mathscr{F}_\beta(\gamma)g'=d_\gamma F_\beta(\gamma)\gamma'=\mathrm{Tr}[(h_\phi-\beta^{-1}s'(\gamma))\gamma'] . \tag{179}$$

Proof We consider first the variation in $I_0^{1,1}$ of the form $\gamma+\epsilon\gamma'$ for $\epsilon>0$ small. Note that if γ' satisfies (178), then for ϵ small enough, $\gamma+\epsilon\gamma'\in I_0^{1,1}$. Let $d_\gamma F_\beta(\gamma,a)\gamma':=\partial_\epsilon F_\beta(\gamma+\epsilon\gamma',a)\mid_{\epsilon=0}$, if the r.h.s. exists. From (133) and (121) and the assumption that Xc' is bounded, we see that

$$d_\gamma F_\beta(\gamma,a)\gamma'=\mathrm{Tr}(h_\phi\gamma')-\beta^{-1}dS(\gamma)\gamma', \tag{180}$$

where $-\Delta\phi=4\pi(\kappa-\rho)$ provided $dS(\gamma)\gamma':=\partial_\epsilon S(\gamma+\epsilon\gamma')\mid_{\epsilon=0}$ exists. Differentiability of S is proved in the next lemma.

Lemma 4 *Let $\gamma\in I_0^{1,1}$ be such that $s(\gamma):=-(\gamma\ln\gamma+(1-\gamma)\ln(1-\gamma))$ is trace class and γ' satisfy the second condition in* (178)*. Then S is Gâteaux differentiable* *and its derivative is given by*

$$dS(\gamma)\gamma' = \mathrm{Tr}(s'(\gamma)\gamma'). \tag{181}$$

Proof For simplicity, we will only consider the case $s(\lambda) = -\lambda \ln(\lambda)$ as the full case is similar. Denote $\gamma'' := \gamma + \epsilon\gamma'$. We write

$$\begin{aligned} S(\gamma'') - S(\gamma) &= -\mathrm{Tr}(\gamma(\ln\gamma'' - \ln\gamma) \\ &\quad + \epsilon\gamma'(\ln\gamma'' - \ln\gamma) + \epsilon\gamma'\ln\gamma) && (182) \\ &=: A + B - \epsilon\mathrm{Tr}(\gamma'\ln\gamma). && (183) \end{aligned}$$

Using the formula $\ln a - \ln b = \int_0^\infty [(b+t)^{-1} - (a+t)^{-1}]dt$ and the second resolvent equation, we compute

$$\begin{aligned} A :=& -\mathrm{Tr}(\gamma(\gamma'' - \ln\gamma)) = -\mathrm{Tr}\int_0^\infty \{\gamma[(\gamma+t)^{-1} - (\gamma''+t)^{-1}]\}dt \\ =& -\mathrm{Tr}\int_0^\infty \{\gamma(\gamma+t)^{-1}\epsilon\gamma'(\gamma''+t)^{-1}\}dt \\ =& -\mathrm{Tr}\left(\int_0^\infty \{\gamma(\gamma+t)^{-1}\epsilon\gamma'(\gamma+t)^{-1}\}dt\right. \\ & \left. - \int_0^\infty \{\gamma(\gamma+t)^{-1}\epsilon\gamma'(\gamma+t)^{-1}\epsilon\gamma'(\gamma''+t)^{-1}\}dt\right). \end{aligned} \tag{184}$$

Similarly, we have

$$\begin{aligned} B :=& -\mathrm{Tr}(\epsilon\gamma'(\ln\gamma'' - \ln\gamma)) && (185) \\ =& -\mathrm{Tr}\int_0^\infty \{\epsilon\gamma'[(\gamma+t)^{-1} - (\gamma''+t)^{-1}]\}dt \\ =& -\mathrm{Tr}\int_0^\infty \{\epsilon\gamma'(\gamma+t)^{-1}\epsilon\gamma'(\gamma''+t)^{-1}\}dt. && (186) \end{aligned}$$

Combining the last two relations with (183), we find

$$S(\gamma + \epsilon\gamma') - S(\gamma) = \epsilon S_1 + \epsilon^2 R_2 \tag{187}$$

$$S_1 := -\mathrm{Tr}\gamma'\ln\gamma - \mathrm{Tr}\int_0^\infty \{\gamma(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\}dt \tag{188}$$

$$\begin{aligned} R_2 := -\mathrm{Tr}\int_0^\infty &\{\gamma(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\gamma'(\gamma''+t)^{-1} \\ &- \gamma'(\gamma+t)^{-1}\gamma'(\gamma''+t)^{-1}\}dt \end{aligned} \tag{189}$$

The estimates below show that the integrals on the r.h.s. converge. We can compute the integral

$$\mathrm{Tr}\int_0^\infty \{\gamma(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\}dt \tag{190}$$

$$=\mathrm{Tr}\int_0^\infty \{\gamma(\gamma+t)^{-2}\gamma'\}dt = \mathrm{Tr}\gamma' \tag{191}$$

in the expression for S_1. Moreover, using $\gamma(\gamma+t)^{-1}-1=-t(\gamma+t)^{-1}$, we can rewrite the expression for R_2. Together, we obtain

$$S_1 :=\mathrm{Tr}\{\gamma'\ln\gamma+\gamma'\}, \tag{192}$$

$$R_2 :=\mathrm{Tr}\int_0^\infty \{t(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\gamma'(\gamma''+t)^{-1}\}dt. \tag{193}$$

Using $(\gamma')^2 \lesssim (\gamma(1-\gamma))^2$ and γ is trace class, we see that (192) is well defined and finte. To demonstrate the convergence in (193), we estimate the integrand on the r.h.s. of (193). we can formally write

$$(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\gamma'(\gamma''+t)^{-1} \tag{194}$$

$$=(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\sum_{n\geq 0}\epsilon^n[-\gamma'(\gamma+t)^{-1}]^n\,. \tag{195}$$

Since γ' and γ are bounded. We see that

$$t\|(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\epsilon^n[-\gamma'(\gamma+t)^{-1}]^n\|_{I^{0,1}} \tag{196}$$

$$\leq\epsilon^n t\|(\gamma+t)^{-1}\|_\infty\|\gamma'(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\|_{I^{0,1}}\|\gamma'(\gamma+t)^{-1}\|_\infty^n \tag{197}$$

$$\leq\epsilon^n\|\gamma'(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\|_{I^{0,1}}\|\gamma'(\gamma+t)^{-1}\|_\infty^n \tag{198}$$

Thus, if $\epsilon < \frac{1}{2}\|\gamma'(\gamma+t)^{-1}\|_\infty^{-1}$ for all $t\in[0,\infty)$ and $\int_0^\infty\|\gamma'(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\|_{I^{0,1}}dt < \infty$, then we have convergence. By the condition in (178) on γ', we have

$$\|\gamma'(\gamma+t)^{-1}\|_\infty \leq \|\gamma(\mathbf{1}-\gamma)(\gamma+t)^{-1}\|_\infty \leq \|\eta(\eta+t)^{-1}\|_\infty$$

where $\eta\gamma(\mathbf{1}-\gamma)$. Since $0\leq\gamma\leq 1$, so does η. Hence

$$\|\gamma'(\gamma+t)^{-1}\|_\infty \leq 1$$

Next,

$$\begin{aligned}&\|\gamma'(\gamma+t)^{-1}\gamma'(\gamma+t)^{-1}\|_{I^{0,1}}\\&\leq\|\gamma'(\gamma+t)^{-1}\|_{I^2}\|\gamma'(\gamma+t)^{-1}\|_{I^{0,2}}\end{aligned}\tag{199}$$

Now, we show that (199) is $L^2(dt)$. By the condition in (178) on γ', we have

$$\|\gamma'(\gamma+t)^{-1}\|_{I^2}\leq\|\gamma(\mathbf{1}-\gamma)(\gamma+t)^{-1}\|_{I^2}\leq\|\eta(\eta+t)^{-1}\|_{I^2},$$

where $\eta:=\gamma(\mathbf{1}-\gamma)$. Thus,

$$\|\gamma'(\gamma+t)^{-1}\|_{I^2}\lesssim\mathrm{Tr}(\eta^2(t+\eta)^{-2})=\int_{\Omega^*}d\hat{\eta}\,\mathrm{Tr}(\eta_\xi^2(t+\eta_\xi)^{-2})$$

Let $\mu_{\xi,n}$ be the eigenvalues of the operator $\eta_\xi:=\gamma_\xi(\mathbf{1}-\gamma_\xi)$. Then we have

$$\|\eta_\xi(\eta_\xi+t)^{-1}\|_{I^2}^2=\sum_n\mu_{\xi,n}^2(\mu_{\xi,n}+t)^{-2},\tag{200}$$

and therefore

$$\begin{aligned}\int_0^\infty\|\eta_\xi(\eta_\xi+t)^{-1}\|_{I^2}^2dt&=\int_0^\infty\sum_n\mu_{\xi,n}^2(\mu_{\xi,n}+t)^{-2}dt\\&=\sum_n\mu_{\xi,n}=\mathrm{Tr}\eta_\xi.\end{aligned}\tag{201}$$

Since $\gamma(\mathbf{1}-\gamma)$ is a trace class operator, this proves the claim and, with it, the convergence of the integral in (193).

To sum up, we proved the expansion (187) with S_1 given by (192), which is the same as (181), and R_2 bounded. In particular, this implies that S is C^1 and its derivative is given by (181).

And finally, we have the following:

Lemma 5 *Suppose that* γ *is a minimizer of* $\mathscr{F}_\beta$ *on* $I_0^{1,1}$, *then* $0<\gamma<1$.

Proof We prove that γ cannot have eigenvalues 0 and 1 simultaneously. The case where only 0 or only 1 is an eigenvalue is treated similarly. If not, decomposing into Bloch-Floquet decomposition γ_ξ, we see that γ_ξ has a kernel for a subset, $S_0\subset\Omega^*$, and eigenspace of 1 on $S_1\subset\Omega^*$, both of positive measure. For $\lambda=0,1$, let $P_{\lambda,\xi}$ denote the projection onto the λ-eigenvector for each $\xi\in S$ in a way such that $P_{\lambda,\xi}$ is measurable in ξ. Let

$$P=\int_{\Omega^*}d\hat{\xi}\,f(\xi)(P_{0,\xi}-P_{1,\xi})\,.\tag{202}$$

where $f(\xi) \geq 0$ is chosen so that $\mathrm{Tr}P = 0$. Since $0 \leq \gamma \leq 1$, it is not hard to sees that P satisfies (178). Following the proof of Lemmas 3 and 4, we compute

$$\mathscr{F}_\beta(\gamma + \epsilon P) - \mathscr{F}_\beta(\gamma) \tag{203}$$

$$= \beta^{-1} \int_{\Omega^*} d\hat{\xi} (\epsilon f(\xi)) \ln(\epsilon f(\xi)) P_{0,\xi} \tag{204}$$

$$+ (1 - \epsilon f(\xi)) \ln(1 - \epsilon f(\xi)) P_{1,\xi}) + O(\epsilon) \tag{205}$$

By choosing $f(x) = \frac{|S_1|}{|S_0|}\chi_{S_0} + \frac{|S_0|}{|S_1|}\chi_{S_1}$, for example, we note that the first term is of order $O(\epsilon \ln \epsilon) \gg O(\epsilon)$ and negative. This contradicts minimality of γ.

Proof (Proof of Theorem 9: Solution to KS equation (71)) By the minimizer existence part of Theorem 9, let $\gamma_0 \in I_0^{1,1}$ denote the minimizer of the free energy $\mathscr{F}_\beta$. For notational convenience let $A := d_\gamma \mathscr{F}(\gamma_0)$. We show that A is multiple of the identity. Let

$$v_0 := \gamma_0(1 - \gamma_0) \int_{\Omega^*} d\hat{\xi}\, 1, \tag{206}$$

and let

$$v := \gamma_0(1 - \gamma_0) \int_{\Omega^*} d\hat{\xi} u_\xi \tag{207}$$

where $u_\xi \in L^2_\xi(\Omega)$ is an arbitrary elements of the fiber space in the Bloch-Floquet decomposition and $\|u_\xi\|_2$ is uniformly bounded upto a null set in Ω^* and v is orthogonal to v_0. By Lemma 5, we see that $0 < \gamma_0 < 1$. This shows that $\gamma(1 - \gamma)$ is a (possibly unbounded) bijection. Hence the linear space spanned by all such v's is dense in $L^2(R^3)$. Let

$$\gamma' = P_v - \frac{\|v\|_2^2}{\|v_0\|_2^2} P_{v_0}\,. \tag{208}$$

where P_x is the orthogonal projection onto x. Then we note that γ' satisfies the condition (178). Hence, by minimality of γ_0, Lemma 3 shows that

$$\mathrm{Tr}(A\gamma') \geq 0\,. \tag{209}$$

We note that if γ' satisfies condition (178), so does $-\gamma'$. It follows that

$$\mathrm{Tr}(A\gamma') = 0\,. \tag{210}$$

It follows that

$$0 = \int_{\Omega^*} d\hat{\xi}\, \mathrm{Tr}(A_\xi g'_\xi) \tag{211}$$

$$= \int_{\Omega^*} d\hat{\xi}\, \mathrm{Tr}(A_\xi (P_v)_\xi) - \frac{\|v\|_2^2}{\|v_0\|_2^2} \mathrm{Tr}(A_\xi (P_0)_\xi) \tag{212}$$

$$= \langle v, Av\rangle - \frac{\|v\|_2^2}{\|v_0\|_2^2} \langle v_0, Av_0\rangle\,. \tag{213}$$

Let $\hat{x} = x/\|x\|$, then we see that

$$\langle \hat{v}, A\hat{v}\rangle = \langle \hat{v}_0, A\hat{v}_0\rangle \tag{214}$$

for all v orthogonal to v_0 of the form (207). Since the space of v_0 and all such v's are dense, we conclude that A is a multiple of the identity, which we denote by μ. This shows that

$$0 = A - \mu = d_\gamma \mathscr{F}(\gamma_0) - \mu \mathbf{1} = h_{A,\mu,\phi} - \beta^{-1} s'(\gamma_0)\,. \tag{215}$$

The case for $d_a \mathscr{F}_\beta(\gamma_0) = 0$ is much easier. Its proof is standard and can be found, for example, in [22].

Finally, to see that $\mu \in \mathbb{R}$, we simply note that $\mu\mathbf{1} = h_\phi - \beta^{-1} s'(\gamma_0)$ is symmetric.

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