DIFFERENTIAL EQUATIONS OF QUANTUM MECHANICS

I. M. SIGAL

Abstract. We review very briefly the main mathematical structures and results in some important areas of Quantum Mechanics involving PDEs and formulate open problems.

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1. Preface

This note follows closely the talk I gave at the ONEPAS and then repeated in a modified form at the MCQM seminar series. I inserted a few details and explanations in the text (often as footnotes), expanded the comments on the literature at the end of the main text along with three appendices giving some precise definitions omitted in the talk (and the main text). My goal was to describe the main mathematical structures and results of an important area of Quantum Mechanics involving PDEs and to formulate open problems.

Some of the open problems are closely related to the mainstream PDEs; others would draw blank for most of the PDE practitioners. The problems of the first type deal with quantum fluids such as superconductors, superfluids and Bose-Einstein

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1ONEPAS and MCQM stand for Online Northeast PDE and Analysis Seminar and Mathematical Challenges in Quantum Mechanics.
condensates which are natural to describe in terms of operators (density operators, etc), rather than functions, though passing to integral kernels one could produce the standard PDE description.

The problems of the second type concern particle systems interacting with quantized radiation, i.e. photons. The key goal here is to describe the processes of emission and absorption of radiation, say light, by systems of matter such as atoms and molecules. These are, obviously, not very fanciful problems and they deserve close attention.

Naturally, the material selected in this article adheres closely to my own research and is not comprehensive whatever interpretation of this word is used.

All references to the literature are collected in Section 9. I tried to be fair and acknowledge all recent contributions to the subjects covered. However, I am sure I missed many worthy works and I will appreciate any information about those.

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2. Schrödinger equation

Quantum systems of $n$ particles in the space $\mathbb{R}^3$ are described by the Schrödinger equation\footnote{The relation of solutions of the Schrödinger equation to quantum observable effects is a subject matter of Quantum Mechanics.}

$$i\partial_t \Psi_t = H_n \Psi_t,$$

where $\Psi_t = \Psi_t(x_1, \ldots, x_n)$, a family of Sobolev functions of the particle coordinates $x_1, \ldots, x_n$ in $\mathbb{R}^3$ and $H_n$ is an $n$–particle Schrödinger operator. For $n$ particles of masses $m_1, \ldots, m_n$ interacting via 2-body potentials $v_{ij}$ and with external potentials $V_i$, $H_n$ has the form

$$H_n := \sum_{i=1}^{n} h_{x_i} + \sum_{i<j} v_{ij}(x_i - x_j), \quad (2.1)$$

where $h_{x_i} = -\frac{1}{2m_i} \Delta x_i + V_i(x_i)$ is a one-particle Schrödinger operator with an external potential $V_i(x)$ acting on the $i$-th particle variable $x_i$. The function $\Psi_t$, called
the wave function, gives probability distributions at time $t$ for various physical observables.

One of the first results going back to J. von Neumann and elaborated by B. Simon can be formulated as

$$\text{global existence } \iff \text{self-adjointness of } H_n.$$  

By the Kato-Rellich theorem, the operator $H_n$ is self-adjoint for a fairly large class of potentials. Hence, the mathematical task, as suggested by the underlying physics, is to describe the space-time behaviour of solutions of (SE).

The main dichotomy here can be formulated as

- stability vs. collapse or disintegration.

By stability we mean the localization in space and periodicity in time. This can be further enlarged on and reduced to spectral properties of $H_n$:

- stability w. r. to collapse ($\inf H_n > -\infty$)
- stability w. r. to break-up ($\inf H$ is an eigenvalue)$^3$

Thus, the stability explains the existence of structures of matter such as atoms, molecules, ..., stars.

One can refine the first type of stability as the extensivity of the energy, i.e. $H_n \geq -cn$. The latter is known as the stability of matter.

We say a system undergoes decay, or, more precisely, local decay, if the probability ($\int_Q |\Psi_t|^2$) that it occupies any bounded domain ($Q \subset \mathbb{R}^3$) in the physical space vanishes with time. The description of all possible scenarios of such an evolution is provided by the scattering theory.

**Scattering.** The main mathematical problem of the scattering theory – the asymptotic completeness – states that

As time progresses, a quantum system settles in a superposition of states consisting of collections of stable freely moving fragments.

**Theorem 2.1** (Asymptotic completeness). *Suppose that the pair potentials $v_{ij}(x_i - x_j)$ entering $H_n$ satisfy $v_{ij}(y) = O(|y|^{-\mu})$, as $|x| \to \infty$, with $\mu > \sqrt{3} - 1$. Then the asymptotic completeness holds.*

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$^3$The condition $H_n \geq -C > -\infty$, which follows from a refined uncertainty relation, says that the particles are not sucked into attractive Coulomb singularities, contrary to the prediction of classical physics. The condition gap($\inf H$, rest) $> 0$ implies that, for initial conditions close to the ground state (eigenfunctions corresponding to the lowest energy $\inf H$), the solution to (SE) remains concentrated in a bounded set in the configuration space $\mathbb{R}^{3n}$ (with the motion of the centre of mass factored out) and that this property is stable w.r. to perturbations of the Hamiltonian.
Open problem: Prove the asymptotic completeness for $v_{ij}(y) = O(|y|^{-\mu})$, with $\mu \leq \sqrt{3} - 1$.

3. Including photons (Nonrelativistic QED)

To describe the real (or at least visible) world, we have to couple the particles to photons (i.e. to quantized electromagnetic field). The dynamics of the resulting system is described again by the Schrödinger equation:

\[ i\partial_t \Psi_t = H_\kappa \Psi_t, \quad (3.1) \]

but with the more complex Hamiltonian $H_\kappa$ acting on the state space $\mathcal{H} := \mathcal{H}_p \otimes \mathcal{H}_f$, which is the tensor product of the spaces of particles and photons. This Hamiltonian is given by

\[ H_\kappa = \sum_{j=1}^{n} \frac{1}{2m_j} \left( -i\nabla_{x_j} - \kappa A_\xi(x_j) \right)^2 + U(x) + H_f. \quad (3.2) \]

Here, $\kappa$ is the particle charge, $U(x)$, $x = (x_1, \ldots, x_n)$, is the total potential effecting the particles,

$A_\xi = \xi \ast A$ is the UV-regularized, quantized vector potential $A$ and

$H_f$ is the photon Hamiltonian.

The key phenomena one would like to describe are emission and absorption of the electromagnetic radiation. Physical description of these processes translates into the following mathematical problems:

- the existence of the ground state
- the instability of excited states
- the emergence of resonances.

The ground and excited states are eigenstates of $H_\kappa$ with the smallest and remaining eigenvalues (energies), respectively. The resonances are thought of physically as ‘metastable’ states, or ‘bound states with finite life-times’. Mathematically, they correspond to complex poles of an analytic continuation of the resolvent of $H_\kappa$ across the continuous spectrum to the second Riemann sheet.

Establishing the properties above and giving estimates of the renormalized energies and life-times are the main tasks of mathematical theory of radiation.

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4This Schrödinger equation was used by P.A. Dirac and E. Fermi already in the early days of Quantum Mechanics, see Fermi’s review [124].

5For the definitions of $A$ and $H_f$, see Appendix A.

6The instability of excited states means that $H_\kappa$ has no eigenvalues in a small neighbourhood of the excited eigenvalues of $H_\kappa=0$. As $\kappa$ is ‘turned on’, the real poles of the resolvent of $H_\kappa=0$ corresponding to the excited eigenvalues migrate to the second Riemann sheet.

To connect this instability to, say, the spontaneous emission of photons, one shows that the solution starting with the initial condition which is an excited eigenvector of $H_\kappa=0$, i.e. the tensor product of an excited eigenvector of the particle system and the photon vacuum, describes the particle system descending to the ground state, with the difference in energy carried out by a departing photon(s).
Theorem 3.1 (Problem of radiation). Assume $U(x)$ is a Kato-type potential and the Fermi Golden rule holds. Then for $\kappa > 0$ sufficiently small,

(a) $H_\kappa$ has a (unique) ground state exponentially localized in the particle coordinates,

(b) $H_\kappa$ has no excited states outside of a sufficiently small neighbourhood of the continuous spectrum, and

(c) $H_\kappa$ has resonances of the multiplicities equal to those of the vanished eigenvalues and which converge to the latter as $\kappa \to 0$.

The Fermi Golden rule expresses the effectiveness of the coupling of the particles to the electromagnetic field (that there is no accidental decoupling). The uniqueness of the ground state depends on symmetries present and could fail. Statements (b) and (c) express the instability of excited states and their turning to the resonances.

We discuss briefly difficulties arising in proving the theorem above. Since the photons are massless, they can be born out of the vacuum and absorbed back to the latter, as well as emitted and absorbed by the particle systems, in arbitrary large numbers and form dense fluctuating clouds around the particles. This leads to divergences in the formal perturbation series for various physical quantities (e.g. the energies of the ground states and resonances), the phenomenon known as the infrared problem.

If we think of $H_\kappa$ as a perturbation of the Hamiltonian $H_{\kappa=0}$ of the decoupled system in which the particles and photons do not interact, then we run into another, related, manifestation of the infrared problem: the bound state energies of the Hamiltonian $H_{\kappa=0}$ are not isolated.

The standard perturbation theory fails in treating such eigenvalues and one needs a new theory. The spectral renormalization-group theory developed to prove Theorem 3.1 is exactly the theory which deals with this problem.

The next problem is to show that, as we experience in everyday life, most of the photons born out by a particle system escape it at some characteristic time and travel freely unless they encounter with another particle system. The mathematical formulation of this property leads to the problem of asymptotic completeness which we have already met in the previous section.

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7The photon clouds lead to renormalizations of various physical quantities (such as the mass of electron and energies of the ground state and resonances), which would diverge if the ultra-violet cut-off (UV) is removed.

8Indeed, the bound state energies of $H_{\kappa=0}$ are exactly the bound state energies, $E_{\text{part}}^{(k)}$, of the particle Hamiltonian

$$H_{\text{part}} = \sum_{j=1}^{n} \frac{1}{2m_j} (-i\Delta_{x_j}) + U(x).$$

However, the values $E_{\text{part}}^{(k)} + \lambda$, where $\lambda \in \sigma(H_T)$ is an arbitrary photon energy, also belong to the spectrum of $H_{\kappa=0}$. Since the photon energies fill in the semi-axis $[0, \infty)$, for each bound state energy $E_{\text{part}}^{(k)}$, there is a continuous spectrum branch $[E_{\text{part}}^{(k)}, \infty)$ of $H_{\kappa=0}$.
To formulate the result here, let \( N_{\text{ph}} \) be the quantum observable (self-adjoint operator) of the number of photons, \( \Sigma := \inf_{\sigma_{\text{ess}}(H_{\text{part}})} \), the ionization threshold, and \( \Psi_t \), a solution to (3.1). Then, we have

**Theorem 3.2** (Rayleigh scattering). Assume that initially the energy is localized below the ionization threshold, \( \Sigma \), of the particle system and that \( \sup_t \langle \Psi_t, N_{\text{ph}} \Psi_t \rangle < \infty \) (satisfied in special cases). Then the asymptotic completeness holds.

*Open problem:* Prove that \( \sup_t \langle \Psi_t, N_{\text{ph}} \Psi_t \rangle < \infty \) for general particle systems (like atoms).

### 4. Effective Equations

To describe systems of a large number of particles, say from 10 to \( 10^{20} \), it is necessary to design effective approaches giving some aggregate, or 'collective', information. Often, such approaches provide information which is practically impossible to extract from solving the original equations even if this was feasible. In the quantum many-body problem, the key effective approach is the Hartree-Fock approximation, trading the number of particles for the nonlinearity. This approximation, its natural extension and the effective equations it leads to are described below.

**Hartree and Hartree-Fock equations and their extensions.** Consider a system of \( n \) identical *bosons* or *fermions* whose evolution is described by the Schrödinger equation

\[
 i \partial_t \Psi_t = H_n \Psi_t, \tag{SE}
\]

where \( H_n \) is the Schrödinger operator given in (2.1), with \( m_i = m \), \( v_{ij} = v \) and \( V_j = V \). To obtain an effective, one-particle approximation for large \( n \), we restrict (SE) to the Hartree and Hartree-Fock states given by symmetric and anti-symmetric products of one-particle wave functions:

\[
 \otimes_1^n \psi \quad \text{and} \quad \wedge_1^n \psi,
\]

This leads to equations for \( \psi \) and \( \psi_1, \ldots, \psi_n \) - the *Hartree* (H) and *Hartree-Fock* (HF) equations, widely used in physics and chemistry.

However, these equations fail to account for quantum fluids i.e. quantum gases exhibiting some quantum behaviour at the macroscopic scale such as superconductivity, superfluidity and Bose-Einstein (BE) condensation. For this, one needs another conceptual step.
Non-Abelian random Gaussian fields and Wick states. In rigorous quantum statistical mechanics, the states are described by linear, positive (normalized) functionals, $\omega$, on a $C^*$-algebra of observables, $\mathcal{A}$ and their evolution is given by the von Neumann-Landau equation

$$\partial_t \omega_t(A) = -\omega_t(i[H, A]), \quad \forall A \in \mathcal{A},$$

(4.2)

where $\omega_t$ is the state at time $t$.

The simplest and in a sense a single most important class of (fixed-time) states, $\chi$, consists of quantum (non-Abelian) generalization of random Gaussian fields, i.e. states uniquely determined by the two-point correlations:

$$\chi(\psi^*(y) \psi(x)),$$

(4.3)

where $\psi(x)$ and $\psi^*(x)$ are quantum fields adjoint to each other (the annihilation and creation operators). These are exactly the HF states: If $\chi_t$ is an evolving HF state, then the operator $\gamma$ with the integral kernel $\chi_t(\psi^*(y) \psi(x))$ satisfies the HF equation

$$i\partial_t \gamma = [h\gamma, \gamma],$$

(4.4)

where $h_\gamma$ is the $\gamma$-dependent, one-particle Schrödinger operator,

$$h_\gamma = -\Delta + V + v * \rho_\gamma - v^\sharp \gamma,$$

(4.5)

with $\rho_\gamma(x, t) := \gamma(x, x, t)$ (charge density) and $v^\sharp \gamma$ the operator with the integral kernel $(v^\sharp \gamma)(x, y) = v(x-y)\gamma(x; y)$. The terms $v * \rho_\gamma$ and $v^\sharp \gamma$ are the direct ('electrostatic') and exchange (HF) self-interaction energies.

However, the above states are not the most general ‘quadratic’ (or quantum Gaussian) states. The most general ones are defined by all one- and two-point correlations:

$$\chi_t(\psi(x)), \quad \chi_t(\psi^*(y) \psi(x)) \quad \text{and} \quad \chi_t(\psi(x) \psi(y)).$$

(4.6)

This type of states were introduced by Bardeen-Cooper-Schrieffer for fermions and by Bogolubov, for bosons. For such states all correlations are either 0 or are sums of products of one- and two-point ones. This is the Wick property from quantum field theory (QFT) and consequently, we call such states the Wick states. (In mathematical literature, they are called the quasifree states.) They give the most general effective one-body description to the $n$–body dynamics.

Remark. If we replace the exchange energy operator, $ex(\gamma) := v^\sharp \gamma$ in the operator entering the Hartree-Fock equation by a multiplication operator by a local function $xc(\rho_\gamma)$ of $\rho_\gamma$ which models exchange and correlation energies, we arrive at the time-dependent Kohn-Sham equation, a key equation of the density functional theory (DFT).

\footnote{For a moment, we ignore the expectation $\chi(\psi(x))$.}

\footnote{For more details see [33] and Appendix E of [74].}
Dynamics. Restricting the von Neumann-Landau evolution (4.2) to Wick states yields a system of coupled nonlinear PDE’s for the functions

\[
\begin{align*}
\phi(x,t) &:= \chi_t(\psi(x)), \\
\gamma(x,y,t) &:= \chi_t(\psi^*(y) \psi(x)), \\
\alpha(x,y,t) &:= \chi_t(\psi(x) \psi(y)).
\end{align*}
\]

These are the (time-dependent) Bogolubov-de Gennes (fermions) and Hartree-Fock-Bogolubov (bosons) equations.\(^{11}\)

For the Bose-Einstein condensation, \(\phi\) is the wave function of the BE condensate and \(\gamma(x,y,t)\) and \(\alpha(x,y,t)\) yield the density matrix of the non-condensed atoms and the ‘pair wave function’ for the superfluid component.

For fermions, \(\phi(x,t) := \chi_t(\psi(x)) = 0\) and \(\gamma(x,y,t)\) describes the normal electrons, while \(\alpha(x,y,t)\) superconducting ones (more precisely, Cooper pairs of electrons).

In what follows, we associate with the functions \(\gamma(x,y,t)\) and \(\alpha(x,y,t)\), the operators \(\gamma\) and \(\alpha\), whose integral kernels these functions are.

As usual for evolution equations, the first mathematical problem here is

The well-posedness of the initial value problem.

Physically, the first problem one would like to address is existence of a ground/Gibbs state and its symmetry.

**Ground/Gibbs state and symmetry breaking.** It is easy to show that the energy, \(E(\chi_t) := \chi_t(H)\), if it exists, is conserved. For systems with non-compact symmetries, like translations, the energy is infinite. In this case, one considers ‘local’ or ‘renormalized’ energy.

The notion of energy allows us to define the key state - the ground state: a static solution minimizing the (local/renormalized) energy.

**Key problems:** Existence and symmetry of the ground state, the excitation spectrum and the dynamics nearby.

The most important symmetry is the translational one which holds in the absence of external interactions (potentials). Nothing is known about breaking of this symmetry in the ground states for both equations.

Whenever systems are considered for positive temperatures, the energy and the ground state are replaced by the free energy and the Gibbs equilibrium state.

5. Hartree-Fock-Bogolubov system

We describe the full Hartree-Fock-Bogolubov (HFB) system in Appendix B. Here, we consider the reduced HFB system (2−gas model) resulting from neglecting the

\(^{11}\)For more details see Appendix B.
α-component:
\[ i\partial_t \phi = h\phi + v \ast (|\phi|^2 + 2\rho_\gamma)\phi, \]  
\[ i\partial_t \gamma = [h_{\gamma,\phi}, \gamma], \]  
where \( h = -\Delta + V \) is a one-particle Schrödinger operator, \( \rho_\gamma(x,t) := \gamma(x;x,t) \), the one-particle density and
\[ h_{\gamma,\phi} := h + v \ast (\rho_\gamma + |\phi|^2). \]
These are coupled Gross-Pitaevskii and Hartree equations. The term \( v \ast (\rho_\gamma + |\phi|^2) \) is the direct (‘electrostatic’) self-interaction produced by the combined charge density \( \rho_\gamma + |\phi|^2 \) of non-condensed and condensed particles (atoms).

In addition to the general problems formulated in the previous section, the following problems are of a special interest for the HFB system:
- Bose-Einstein condensation,
- Collapse oscillations for \( \lambda < 0 \) (correction to the Papanicolaou-Sulem-Sulem collapse law?).

Physically there are two important set-ups here:
External (attractive or confined) potentials \( V \) vs translational invariance (\( V = 0 \)).

6. Bogolubov-de Gennes system

For fermions, \( \phi(x,t) := \chi_t(\psi(x)) = 0 \) and, since the Wick states describe superconductors, \( (\gamma,\alpha) \) are coupled to the electromagnetic field. With the latter described by the magnetic potential \( a \) and the electrostatic potential, \( \varphi \), and, with the former taken in the Coulomb gauge (\( \text{div} \ a = 0 \)) and the latter absorbed in the inter-particle (pair) interaction potential, the equations for \( \gamma,\alpha \) and \( a \) read

\[ i\partial_t \gamma = [h_{a,\gamma}, \gamma]_+ + [v^s\alpha, \alpha]_-, \]  
\[ i\partial_t \alpha = [h_{a,\gamma}, \alpha]_+ - [v^s\alpha, \gamma]_+ + v^s\alpha, \]  
\[ -\partial_t^2 a = \text{curl}^* \text{curl} a + j(\gamma,\alpha), \]
where \( [A,B]_- = AB^* - BA^*, [A,B]_+ = AB^* + BA^*, \) with \( A := CAC \), with \( C \) being the complex conjugation, \( v(x-y) \) is a pair potential, \( v^s \alpha \) is, recall, the operator with the integral kernel \( (v^s\alpha)(x,y) = v(x-y)\alpha(x,y), j(\gamma,\alpha)(x) := [-i\nabla_a, \gamma]_+(x,x) \) is the current density, and, finally (cf. Eq. (4.5)),
\[ h_{a,\gamma} := -\Delta_a + v \ast \rho_\gamma - v^s\gamma, \]
with \( \Delta_a := (\nabla + ia)^2 \). Here we have assumed, for simplicity, that the external potential is zero, \( V = 0 \), and have chosen the unit electric charge to be \( e = -1 \).

These are the celebrated Bogolubov-de Gennes (BdG) system. They give the ‘mean-field’ (BCS) theory of superconductivity. Eq. (6.1) is essentially the HF

\footnote{For a discussion of gauges, the origin of the BdG equations (in particular, an elimination of the electric potential) and properties of \( \gamma \) and \( \alpha \) see Appendix C.}
equation coupled to the other two equations and Eq. (6.3) comes from two Maxwell equations (Ampère’s and Faraday’s laws).

As was pointed out in Section 4, the key problem here is the existence and symmetry of the ground state and the description of the nearby dynamics.

Experiments show that at the lowest energy (locally), states of quantum matter typically enjoy the maximal available symmetry. With this in mind, we begin with describing the symmetry group of the BdG system.

**Gauge (magnetic) translational invariance.** Arguably, the simplest and most important symmetry is the translational one. In the magnetic fields this symmetry is broken. However, for constant magnetic fields, there is a non-abelian symmetry replacing it.

The BdG equations are invariant under the $t$-independent gauge transform

$$T^\text{gauge} \chi : (\gamma, \alpha, a) \to (e^{i\chi} e^{-i\gamma} e^{i\alpha} a + \nabla \chi), \quad (6.5)$$

where $\chi \in H^2(\mathbb{R}^d, \mathbb{R})$. (This defines a natural equivalence relation one should keep in mind.) To preserve the Coulomb gauge, we could take $\chi$ linear in $x$.

Thus, we define the gauge (magnetically) translationally (MT) invariant states as states whose translations stay in the same gauge-equivalence class, i.e. which are invariant under the transformations

$$T_s : (\gamma, \alpha, a) \to (T^\text{gauge}_\chi)^{-1} T^\text{transl}_s (\gamma, \alpha, a),$$

for any $s \in \mathbb{R}^d$, with $d = 2, 3$, and for some (linear) functions $\chi_s(x)$. Here $T^\text{transl}_s$, $s \in \mathbb{R}^d$, is the group of translations. We require $T_s$ to be a projective group representation of $\mathbb{R}^d$. Then, the function $\chi_s(x)$ (of $x$ and $s$) satisfies the co-cycle relation

$$\chi_{s+t}(x) - \chi_s(x + t) - \chi_t(x) = \frac{1}{2} b(s, t), \quad (6.6)$$

$\forall s, t \in \mathbb{R}^d$, where $b(s, t)$ is a constant two-form on $\mathbb{R}^d$. Two-forms on $\mathbb{R}^d$, $d = 2, 3$, are gauge equivalent to the 2-form $b \cdot (s \wedge t)$, where $b$ is a constant vector if $d = 3$ and a scalar if $d = 2$. The function $\chi_s(x) := \frac{1}{2} b \cdot (x \wedge s)$ clearly solves the equation (6.6). (This fixes a special - symmetric - gauge.) The two-form $b(s, t)$, or vector/scalar $b$, is identified with a constant external magnetic field.

This extends the translational symmetry to the curl $a \neq 0$ regime. For curl $a \neq 0$, gauge-translationally invariant states yield the simplest solutions and candidates for the ground state for the BdG system.

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13 In this case, $T_s$ is, in general, a non-abelian group with the generators which are the components of the operator-vector $i(-i\nabla - \frac{1}{2} b \wedge x)$.

14 $b \cdot (t \wedge s)$ is the flux of the constant vector field $b$ through the area $t \wedge s$ spanned by the vectors $s$ and $t$. 
Ground state. As was alluded to above, typically, the ground state (GS) has the maximal symmetry. Hence, depending on the magnetic field $b$, one expects that:

GS is translationally invariant for $b = 0$,

GS is magnetically translationally invariant for $b \neq 0$.

Candidates for the ground (or equilibrium Gibbs) state are:

1) Normal states: $(\gamma, \alpha, a)$, with $\alpha = 0$ (⇒ $\gamma$ is ‘Gibbs state’).

2) Superconducting states: $(\gamma, \alpha, a)$, with $\alpha \neq 0$ and $a = 0$ (‘Meissner states’).

Theorem 6.1. For $b = 0$, there is a superconducting, normal, translationally invariant solution.

Theorem 6.2. For $b \neq 0$, the MT-invariance implies the normality ($\alpha = 0$).

Corollary 6.3. For $b \neq 0$, the superconductivity ($\alpha \neq 0$) implies the symmetry breaking.

An addendum to the maximal symmetry paradigm formulated above could be stated as: in the ground state, whenever the maximal symmetry is broken, it is broken in the most minimal way. For the simplest and most important case of the translationally invariant systems, breaking of the translational invariance leads to formation of crystalline structures with lattice symmetries.

We are far from being able to prove that this happens in reasonable models. However, the natural problem at one level below - the existence and stability of such structures - is possibly approachable. Note that the stability would imply that a crystalline solution is a local minimizer (but not necessarily minimizing locally) of a ‘renormalized’ energy. Though it does not give the global minimizing property, one might say that it is the next best thing.

Vortex lattices. Physical experiments show (see below) that most of superconductors in magnetic fields have, in their lowest (locally) energy states, lattice symmetry, yielding minimal symmetry breaking as discussed above. Here we define and discuss such states.

For $b \neq 0$, we define states, which we call the vortex lattice states (or just vortex lattices), as

- Vortex lattice: $(\gamma, \alpha, a)$ s.t. $T_s^{\text{trans}}(\gamma, \alpha, a) = T_s^{\text{gauge}}(\gamma, \alpha, a)$, $\forall s \in \mathcal{L}$ (some lattice in $\mathbb{R}^2$), with $\chi_s: \mathcal{L} \times \mathbb{R}^2 \to \mathbb{R}$, and $\alpha \neq 0$.

The fact that $T_s^{\text{trans}}$ is a group representation implies that the map $\chi_s$ satisfies the co-cycle relation (see (6.6)):

$$\chi_{s+t}(x) - \chi_s(x + t) - \chi_t(x) \in 2\pi \mathbb{Z}, \forall s, t \in \mathcal{L}. \tag{6.7}$$

Co-cycle relation (6.7) implies that the magnetic flux is quantized:

$$\frac{1}{2\pi} \int_{\Omega^{\mathcal{E}}}\text{curl} \, a \in \mathbb{Z}. $$
Here $\Omega^L$ is a fundamental cell of $\mathcal{L}$ and the left-hand side is the 1st Chern number. The latter can be expressed directly in terms of $\chi$.

The existence result for such solutions is recorded in the following

**Theorem 6.4.** For the BdG system without the self-interaction term:

(i) $\forall n, T > 0$ and $\mathcal{L}$ there is a static solution $u_{TnL} := (\gamma, \alpha, a)$ satisfying

$$u_{TnL} \text{ is } \mathcal{L}\text{-equivariant: } T^\text{trans}_s u_{TnL} = T^\text{gauge}_s u_{TnL}, \forall s \in \mathcal{L},$$

the 1st Chern number is $n$:

$$\int_{\Omega^L} \text{curl} a = 2\pi n,$$

$u_{nTL}$ minimizes the free energy\footnote{For the definition of the free energy see Appendix C.} $F_T = E - TS - \mu N$ on $\Omega^L$ for $c_1 = n$;

(ii) For the pair potential $v \leq 0, v \not\equiv 0$ and $T$ and $b$ sufficiently small, $u_{TnL}$ is a vortex lattice (i.e. $\alpha \neq 0$);

(iii) For $n > 1$, there is a finer lattice, $\mathcal{L}' \supset \mathcal{L}$ for which $u_{TnL} = u_{T1L'}$, i.e. $u_{TnL}$ is $\mathcal{L}'\text{-equivariant with } c_1 = 1$.

*Open problem:* Show that for superconductors of Type II and for $n = 1$, the vortex lattice solution is stable. (For discussion of Type I and II superconductors and the notion of stability in the context of the BdG, see [74]. These notions as well as the notion of self-duality still need to be elucidated in the BdG theory.)

On the first step, one could address stability w.r. to symmetry preserving (periodic) perturbations is usually accessible. Showing that a crystalline solution is stable under general perturbations (deforming the lattice in various ways) is a rather subtle, highly non-trivial matter.

7. **Ginzburg-Landau equations**

In the leading approximation (close to the critical temperature and after ‘integrating out’ $\gamma$ and the relative coordinate $x - y$ of $\alpha(x, y)$), the BdG system leads to the time-dependent Ginzburg-Landau equations

$$\gamma \partial_t \psi = \Delta_a \psi + \kappa^2 (1 - |\psi|^2) \psi,$$

$$\nu \partial_t a = - \text{curl}^2 a + \text{Im}(\bar{\psi} \nabla_a \psi).$$

Here $\text{Re} \gamma, \text{Re} \nu \geq 0$ are constants arising in the approximation. In the application to superconductivity\footnote{Besides describing equilibrium states of superconductors (mesoscopically), the static GLE describe also the (static) $U(1)$ Yang-Mills-Higgs model of particle physics (a part of Weinberg-Salam model of electro-weak interactions/a standard model). In particle physics, $\psi$ and $a$ are the Higgs and $U(1)$ gauge (electro-magnetic) fields, respectively.} $|\psi|^2$ is the density of superconducting electrons;
a : \mathbb{R}^{d+1} \rightarrow \mathbb{R}^d is the magnetic potential;

\text{Im}(\bar{\psi} \nabla_a \psi) is the superconducting current.

The second GLE equation comes from two Maxwell equations (Ampère’s and Faraday’s laws).

**Vortex lattices.** As with the BdG and HFB systems, the major open problem is the symmetry of the ground state. Experiments show that the ground state of a superconductor of Type II in a constant magnetic field is in the form of the hexagonal vortex lattice (see Figure 1).

![Figure 1. Experimental picture of the Abrikosov lattice obtained using a tunnelling microscope. Different colours signify different densities of superconducting electrons. Theoretical description of this experiment is given solving the BdG system based on the coarse-scale approximation given by the Ginzburg-Landau system.](image)

For the GLE, the vortex lattice is defined as a *static* solution equivariant under the lattice translations in the sense that

\[ T_s^{\text{transl}}(\psi, a) = T_s^{\text{gauge}}(\psi, a), \]

for every \( s \in \mathcal{L} \) (some lattice in \( \mathbb{R}^2 \)), with \( \chi_s : \mathcal{L} \times \mathbb{R}^2 \rightarrow \mathbb{R} \) (satisfying (6.7)).

A vortex lattice solution is formed by *magnetic vortices* (localized finite energy solutions of a fixed degree, see Fig. 2), arranged in a (mesoscopic) lattice \( \mathcal{L} \).

As for the BdG system, we are far from being able to prove that the ground state of the GLE is given by a vortex lattice. One step below it is the problem of existence and *stability* of vortex lattice solutions.

The *existence* of vortex lattice solutions is well known by now. Thus, we are left with the problem:

- Stability of vortex lattice solutions.

Since the VL *are not localized*, the *stability is a delicate matter.*
Figure 2. The left figure is a 2-dimensional section of a picture of a line vortex center. The figure on the right shows density of the superconducting electrons $|\psi|^2 = n_s$, the magnitude of the magnetic field and the circulation of the superconducting current.

Theorem 7.1. The vortex lattices are stable under lattice-periodic and local perturbations of the same parity as the vortex lattice.

Open problem: Show stability/instability under more general lattice deformations.

8. Summary

- We reviewed some basic properties of the Schrödinger equation which encodes all the information about quantum systems.\textsuperscript{17}

- While we learned much about the general structure\textsuperscript{18} of this equation, our understanding of specific quantum systems with the number of particles $\geq 3$ is spotty and the progress, with some notable exceptions like the stability of matter and the derivation of mean-field type equations, is very slow.

- However, there is one important direction where robust progress is possible – ‘effective’ equations for quantum systems of large number of identical particles (quantum gases), especially, those describing quantum fluids (i.e. quantum gases exhibiting some quantum behaviour at the macroscopic scale) such as superconductors, superfluids and Bose-Einstein condensates – the HFB and BdG equations.

- We (a) formulated some key mathematical problems related to the HFB and BdG equations, (b) described the key stationary solutions of BdG equations, the competitors for the ground/Gibbs state: normal, superconducting and mixed (or intermediate) states, and (c) presented an important class of the mixed states – the vortex lattices – demonstrating the symmetry breaking.

\textsuperscript{17}Extraction of the physical information from the solutions is done according to a fixed quantum mechanical procedure. The theoretical results agree to remarkable precision with experimental ones, while the physical theory connecting the two, initiated by J. von Neumann soon after advent of Quantum Mechanics, remains largely under construction.

\textsuperscript{18}Such as the structure of the spectrum, scattering theory, theory of resonances.
9. Remarks on literature

\textit{n–particle scattering.} Theorem 2.1 is due to A. Soffer and I.M. Sigal ($\mu > 1$), and J. Dereziński ($\sqrt{3} - 1 < \mu < 1$) ([99], see also [265]). The proofs use important earlier results and ideas of P. Deift and B. Simon, V. Enss, C. Gérard, G.M. Graf, E. Mourre, D. Yafaev ([98, 116, 138, 158, 152, 163, 267, 268, 273, 274, 282, 285, 286, 288]), see [100, 157, 201] for books and a review.

For some of the extensions, see [22, 188, 189, 273, 274, 276, 266]. Many ideas and techniques from this field successfully entered Quantum Electrodynamics (QED), see below, nonlinear evolution equations ([56, 57, 84, 85, 105, 106, 231, 232, 232, 256, 259, 277]), wave propagation ([88, 89, 90]) and the energy transfer in the non-autonomous Schrödinger equations ([45, 47, 46, 48, 54, 236, 237, 238, 239]). For an important parallel development see [285, 286].

\textit{NR QED, Radiation.} Theorem 3.1 was proven by V. Bach, J. Fröhlich and I.M. Sigal ([37, 38, 39]). Many important extensions and improvements were obtained in [14, 15, 21, 36, 49, 111, 66, 73, 91, 93, 145, 167, 159, 172, 152, 167, 175, 177, 178, 180, 181, 182, 183, 185, 187, 191, 192, 225, 226, 281], to mention some of more recent results, see e.g [20, 166, 262, 264, 173, 281] for reviews and book presentations.

The main ingredient in the proof of Theorem 3.1 is the spectral renormalization group introduced in [37, 38]. A different approach was developed by V. Bach, M. Balestros, J. Fröhlich, A. Pizzo, which the authors call the multiscale or Pizzo method ([29, 30, 31, 32]).

The infrared (IR) problem was addressed by Th. Chen, J. Fröhlich and A. Pizzo ([69, 70, 71]). For the renormalization of the electron mass see [67, 35].

Ideas and techniques from the NR QED were extended to the Nelson and spin-boson models of the condensed matter physics in [40, 43, 44, 42, 240, 242, 87, 184, 186, 234, 275, 278, 280].

\textit{NR QED, Asymptotic completeness.} Theorem 3.2 is due to J. Faupin and I.M. Sigal and W. De Roeck, M. Griesemer and A. Kupiainen ([117, 94]). These works used ideas and results of M. Hübner-H. Spohn, J. Dereziński-C. Gérard, J. Fröhlich-M. Griesemer-B. Schlein ([101, 141, 142, 143, 144, 200, 279]) as well as those from the \textit{n–particle scattering} theory discussed above. For further developments [108, 109, 111, 110, 36, 169] and review [264].

The finiteness of mean number of photons for the spin-boson model was proven by W. De Roeck and A. Kupiainen ([94]).

\textsuperscript{19}These models have a form similar to the NR QED, with photons replaced by (acoustic) phonons (quantized (longitudinal) oscillations of the underlying medium) and the interaction somewhat modified. The main problems for these models are exactly the same as those formulated in Section 5. The main difference is that these models do not have the gauge invariance which allows to lower the IR singularity in the QED Hamiltonian.
The HFB and BdG systems. Stationary versions of these systems (written in eigenfunction expansion representations) are used extensively in the physics literature. For the HFB system, one inserts the delta-function potentials and in the BdG case one sets \( a = 0 \). The full, time-dependent systems in the general form as they appear in this paper were written out and formally derived in [33] and [74, 52], respectively.

Clearly, the HFB and BdG systems generalize the Hartree and Hartree-Fock equations. For the relation between the Hartree and Hartree-Fock approximations, on one hand, and quasi-free (Wick) states, on the other, see [51] and Appendix E of [74].

For a rigorous derivation of effective equations similar to the HFB and BdG systems, see the books [228, 51], reviews [211, 245, 257] and some recent articles [50, 79, 75, 96, 97, 103, 170, 171, 244]. The rigorous theory started (from very different perspectives) with works of K. Hepp, E. H. Lieb and B. Simon and P.-L. Lions [190, 229, 230, 233] (see also [160, 161] for early follow up work).

For the HFB system, the static, homogeneous case (i.e. \( V = 0 \) and \( \gamma \) and \( \sigma \) are translation-invariant) was treated rigorously by M. Napiórkowski, R. Reuvers and J.P. Solovej, see [246, 247]. In the general case, general properties and the well-posedness were established in [33].

The BdG system without the (dynamic) electromagnetic field, i.e. with \( a = 0 \). See [179] for an excellent review. Theorem 6.1 was proven by Ch. Hainzl, E. Hamza, R. Seiringer and J.P. Solovej ([176]). The Cauchy problem was investigated by N. Benedikter, J. Sok and J.P. Solovej ([52]).

For the full BdG system, general properties of the system and classification and properties of the ground states (and more generally, static solutions) were established by I. Chenn and I.M. Sigal ([74]). In particular, Theorem 6.2 was proven in [74]. An asymptotic behaviour of critical temperature in weak magnetic fields was established in [131, 102].

For \( \alpha = 0 \), the BdG system leads to the Hartree-Fock equation coupled to the Maxwell equations. Closely related to the Hartree-Fock equation is the important and widely used Kohn-Sham equation, the main tool in the density functional theory (DFT), see [16, 62, 65, 73, 112, 113, 114, 115, 254, 255] and references therein for the former and [212, 214, 215] for the latter.

In a remarkable work, R. Frank, Ch. Hainzl, R. Seiringer, J.P. Solovej ([132]) have shown that, for non-dynamical magnetic fields, the nanoscopic approximation of the BdG system is given by the Ginzburg-Landau one (see also [133, 134, 72]).

Vortex lattices. Existence of vortex lattices for the BdG equations was proven by I. Chenn and I.M. Sigal ([74]).

For the existence results for the Ginzburg-Landau system, see review [261]. Stability of vortex lattices for the Ginzburg-Landau system under lattice-periodic and local perturbations was proven by I. M. Sigal and T. Tzanealas ([269, 270]).
Important results on asymptotic behaviour of solutions, for $\kappa \to \infty$ and applied magnetic fields, $h$, satisfying $h \leq \frac{1}{2} \ln \kappa + \text{const}$ (the London limit), were obtained in \cite{26}. Further extensions to the Ginzburg-Landau equations for anisotropic and high temperature superconductors in the $\kappa \to \infty$ regime can be found in \cite{10, 11}.

For the $\kappa \to \infty$ (the semi-classical) regime in the Ginzburg-Landau equations and the linear eigenvalue problem related to the second critical magnetic field, see the books \cite{258, 20} and \cite{126}, respectively, and see \cite{8, 12, 13, 80, 81, 82, 125, 127, 128, 129, 130}, for some additional and more recent results.

There are many similarities between the Ginzburg-Landau and Gross-Pitaevskii equations and more specifically between the phenomena of superconductivity and the Bose-Einstein condensations (BEC) described by these equations, respectively. The key results for the BEC vortices in the Gross-Pitaevski equation are due to A. Aftalion, R. Jerrard, M. Correggi, N. Rougerie, J. Yngvasson et al, see the book \cite{3} and the more recent papers \cite{4, 5, 6, 7, 9, 83, 77}.

For recent work on vortices in the somewhat similar Landau-Lifshitz-type equations and the Weinberg-Salam model of electro-weak interactions (the $U(2)$ Yang-Mills-Higgs system), see \cite{174, 219, 151}.

The HFB, BdG, GL and GP equations are obtained from the original many-body Schrödinger equation by ‘integrating out’ some degrees of freedom corresponding to finer length scales (the GL and GP equations) or faster dynamics (the HFB and BdG equations). Such equations are called the effective equations and the dynamics described by them, the effective dynamics. One can continue further integrating out degrees of freedom to obtain even coarser (say, nanoscopic) effective equations, see e.g. \cite{60, 76, 61, 64, 63, 83, 77, 92, 112, 113, 114, 115, 123, 121, 122, 146, 149, 150, 204, 205, 207, 195, 196, 197, 198, 199, 287}.

For effective equations approach to other quantum-mechanical problems, see \cite{210, 213, 221, 224, 271, 283} for reviews and books and \cite{17, 18, 59, 147, 135, 136, 137, 227, 235, 243, 249, 250, 251}, for some recent work. Of important aspects of the quantum many-body problem lying further a field and not discussed above, we mention the Coulomb systems, positive temperatures, topological techniques, random Schrödinger operators and perturbation theory. For some general reviews and books in these areas, see \cite{23, 24, 25, 86, 104, 107, 119, 120, 139, 140, 162, 194, 203, 206, 208, 220, 223, 227, 272, 271}.

**Appendix A. The NR QED Hamiltonian**

In this appendix, we define the quantized vector potential and the Hamiltonian of the quantized electromagnetic field entering the Hamiltonian \eqref{3.2}.

First, we mention that the state space $\mathcal{H}_f$ of photons is the bosonic Fock space, $\mathcal{F} := \bigoplus_{n=0}^{\infty} \otimes_n^s \mathfrak{h}$, where $\otimes_n^s \mathfrak{h} := \mathbb{C}$, based on the one-photon space $\mathfrak{h} := L^2(\mathbb{R}^3, \mathbb{C}^2)$ ($\otimes_n^s$ stands for the symmetrized tensor product of $n$ factors, $\mathbb{C}^2$ accounts for the photon polarization).

\footnote{For the precursor of the development described in this book, see \cite{55}.}
There is a distinguished pair of unbounded, operator-valued distributions, $a_\lambda(k)$ and $a^*_\lambda(k)$, acting on $\mathcal{F}$, called the annihilation and creation operators, which generate the operator algebra on $\mathcal{F}$. They are defined as follows. With each function $f \in \mathfrak{F}$, one associates the operators $a(f)$ and $a^*(f)$ defined, for $u \in \otimes^\infty \mathfrak{h}$, as

$$ a^*(f) : u \to \sqrt{n+1} f \otimes a u \quad \text{and} \quad a(f) : u \to \sqrt{n}\langle f, u \rangle_\mathfrak{h}, $$

with $\langle f, u \rangle_\mathfrak{h} := \sum_{\lambda=1,2} \int dk f(k, \lambda) u(k, \lambda, \lambda_1, \ldots, k_{n-1}, \lambda_{n-1})$. $(a^*(f) = (a(f))^*)$ Since $a(f)$ is anti-linear and $a^*(f)$ is linear in $f$, we can write formally

$$ a(f) = \sum_{\lambda=1,2} \int f(k, \lambda) a_\lambda(k) dk, \quad a^*(f) = \sum_{\lambda=1,2} \int f(k, \lambda) a^*_\lambda(k) dk \quad \text{(A.1)} $$

and consider $a_\lambda(k)$ and $a^*_\lambda(k)$ as formal objects with certain commutation properties.

The operators $A_\xi$ and $H_f$, describing the quantized electromagnetic field and its dynamics, respectively, are given by

$$ A_\xi(y) = \sum_{\lambda=1,2} \int \frac{\xi(k) dk}{\sqrt{2\omega(k)}} \varepsilon_\lambda(k) (e^{ik\gamma}a_\lambda(k) + e^{-ik\gamma}a^*_\lambda(k)), \quad \text{(A.2)} $$

$$ H_f = \sum_{\lambda=1,2} \int \omega(k) a^*_\lambda(k) a_\lambda(k). \quad \text{(A.3)} $$

Here, $\omega(k) = |k|$ denotes the (Einstein) photon dispersion relation (the energy as a function of the wave vector).

To give rigorous meaning to expressions like (A.2) and (A.3), we can express them in terms of $a(f_j)$ and $a^*(f_j)$ for some orthonormal basis $\{f_j\}$ in $\mathfrak{h}$.

**APPENDIX B. HARTREE-FOCK-BOGOLUBOV EQUATIONS**

For the pair interaction potential $v$, the HFB equations are

$$ i\partial_t \phi = h\phi + \lambda|\phi|^2 \phi + 2\lambda\rho_\gamma \phi + \lambda\phi \rho_\alpha, \quad \text{(GP)} $$

$$ i\partial_t \gamma = [h_{\gamma,\phi}, \gamma]_+ + \lambda[w_{\alpha,\phi}, \alpha]_-, \quad \text{(HF)} $$

$$ i\partial_t \alpha = [h_{\gamma,\phi}, \alpha]_+ + \lambda[w_{\alpha,\phi}, \gamma]_+ + \lambda w_{\alpha,\phi}, \quad \text{(Coh)} $$

where $h$ is a one-particle Schrödinger operator, $[A, B]_\pm$ are defined after (6.3) and

$$ \rho_\sigma(x, t) := \sigma(x; x, t), \quad w_{\alpha,\phi} := \rho_\alpha + \phi^2, $$

$$ h_{\gamma,\phi} := h + 2\lambda(\rho_\gamma + |\phi|^2) + ex(\gamma). \quad \text{(B.1)} $$

The last term on the r.h.s. of Eq. (Coh), $\lambda w_{\alpha,\phi} := \lambda(\rho_\alpha + \phi^2)$, is the quantum depletion term. Because of it the system has no solutions of the form $(\phi, 0, 0)$ (100% condensation).

If this term is omitted then the system becomes Hamiltonian and has solutions of the form $(\phi, 0, 0)$, where $\phi$ satisfies the *Gross-Pitaevskii equation*.  

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21\textit{k} is the photon wave vector and $\lambda$ is the photon polarization.
APPENDIX C. BOGOLUBOV-DE GENNES EQUATIONS: DISCUSSION

The BdG equations (6.1)-(6.3) are derived from the von Neumann-Landau equation (4.2) with Hamiltonian (3.2) with \( m_j = m \) and

\[
U(x) = \sum_{i=1}^{n} V(x_i) + \sum_{i<j} v(x_i - x_j).
\]

This Hamiltonian is written in the Coulomb gauge with \( A \) being the quantized transverse vector potential and with the electrostatic potential incorporated into \( \sum_{i<j} v(x_i - x_j) \). To obtain the BdG equations (6.1)-(6.3), we pass to the Wick (or quasifree) approximation as in Section 4, but, in addition, use the coherent states in the vector potential. The effective magnetic potential \( a \) arises from \( A \).

It turns out that it is natural to organize the operators \( \gamma \) and \( \sigma \) into the self-adjoint operator-matrix (called the generalized one-particle reduced density matrix)

\[
\eta := \begin{pmatrix} \gamma & \alpha \\ \alpha^* & 1 - \bar{\gamma} \end{pmatrix}.
\] (C.1)

Similarly to \( \gamma \), one can then show that this the operator-matrix \( \eta \) obeys the inequalities:

\[ 0 \leq \eta = \eta^* \leq 1. \]

These inequalities imply that the bounded operators \( \gamma \) and \( \alpha \) satisfy the relations

\[ 0 \leq \gamma = \gamma^* \leq 1, \quad \alpha^* = \bar{\alpha} \quad \text{and} \quad \alpha \alpha^* \leq \gamma(1 - \gamma), \] (C.2)

where \( \bar{\gamma} := C\gamma C \), with \( C \), the operation of complex conjugation (see [74], Appendix E, and [52]).

Furthermore, the first two equations, (6.1)-(6.2), of the BdG system can be written in the form similar to the HF equation (4.4):

\[
i \partial_t \eta = [H_{a,\eta}, \eta], \quad \text{where} \quad H_{a,\eta} = \begin{pmatrix} h_{a,\gamma} & v^\alpha \\ v^\gamma & -h_{a,\gamma} \end{pmatrix},
\] (C.3)

with \( h_{a,\gamma} \) and \( v^\alpha \) defined in Section 6.

The stationary BdG equations arise as the Euler-Lagrange equations for the (BCS) free energy functional

\[
F_T(\gamma, \alpha, a) := E(\gamma, \alpha, a) - TS(\gamma, \alpha) - \mu N(\gamma),
\] (C.4)

\[ ^{22} \text{The quantum fields (the annihilation and creation operators) } \psi(x) \text{ and } \psi^*(x), \text{ used in Section 4, are operator-valued distributions (cf. Appendix A). If we write them as functionals } \psi(u) = \int \psi(x) u(x) dx \text{ and } \psi^*(u) = \int \psi^*(x) \bar{u}(x) dx \text{ (cf. (A.1))}, \text{ then (4.8)-(4.9)} \text{ can be rewritten as } \chi(\psi^*(v)\psi(u)) = \langle u, \gamma v \rangle \text{ and } \chi(\psi(v)\psi(u)) = \langle \bar{v}, \alpha u \rangle. \text{ Letting } f = (f_1, f_2) \in L^2(\mathbb{R}^d) \oplus L^2(\mathbb{R}^d), \text{ and } A(f) := \psi(f_1) + \psi^*(f_2) \text{ and using the previous equations, one can easily compute that } \chi(A^*(g)A(f)) = \langle f, \eta g \rangle, \text{ which, together with the anti-commutation relation } \{A^*(g), A(f)\} = \langle f, g \rangle, \text{ yields } 0 \leq \eta = \eta^* \leq 1. \]
where $S(\gamma, \alpha) = \text{Tr} g(\Gamma)$, with $g(\lambda) := -\lambda \ln \lambda - (1 - \lambda) \ln(1 - \lambda)$, is the entropy, $N(\gamma) := \text{Tr} \gamma$ is the number of particles, and $E(\gamma, \alpha, a)$ is the conserved energy functional for $\gamma, \alpha$ and $a$ time-independent given by

$$E(\gamma, \alpha, a) = \text{Tr}((-\Delta_a)\gamma) + \frac{1}{2} \text{Tr}((v * \rho_\gamma)\gamma) - \frac{1}{2} \text{Tr}((v^\sharp \gamma)\gamma)$$

$$+ \frac{1}{2} \text{Tr}(\alpha^\sharp(v^\sharp a)) + \int |\text{curl} a|^2. \quad (C.5)$$

Not surprisingly, it turns out that $E(\gamma, \alpha, a) := \chi(H_a)$, where $\chi$ is a Wick (quasi-free) state in question and $H_a$ is the standard many-body Hamiltonian, coupled to the vector potential $a$.

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Israel Michael Sigal, Department of Mathematics, University of Toronto, Toronto, M5S 2E4, Canada
Email address: im.sigal@utoronto.ca