

A Nonlinear Model for Relativistic Electrons at Positive Temperature

Christian HAINZL^a, Mathieu LEWIN^b & Robert SEIRINGER^c

^aDepartment of Mathematics, UAB, Birmingham, AL 35294-1170, USA.
hainzl@math.uab.edu

^bCNRS & Department of Mathematics (CNRS UMR8088), University of Cergy-Pontoise, 2 avenue Adolphe Chauvin, 95302 Cergy-Pontoise Cedex, FRANCE.

Mathieu.Lewin@math.cnrs.fr

^cDepartment of Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, New Jersey 08544, USA.

rseiring@math.princeton.edu

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Abstract

We study the relativistic electron-positron field at positive temperature in the Hartree-Fock-approximation. We consider both the case with and without exchange term, and investigate the existence and properties of minimizers. Our approach is non-perturbative in the sense that the relevant electron subspace is determined in a self-consistent way. The present work is an extension of previous work by Hainzl, Lewin, Séré, and Solovej where the case of zero temperature was considered.

Contents

Introduction	2
1 The reduced Bogoliubov-Dirac-Fock free energy	7
1.1 Relative entropy	7
1.2 Existence of a minimizer and Debye screening	11
2 The Bogoliubov-Dirac-Fock free energy	12
2.1 Definition of the free vacuum	12
2.2 The external field case	14

3 Proofs	15
3.1 Proof of Theorem 3	15
3.2 Proof of Proposition 1	17
3.3 Proof of Theorem 4	19
3.4 Proof of Theorem 5	23
A Appendix: Integral Representation of Relative Entropy	24
References	25

Introduction

In Coulomb gauge and when photons are neglected, the Hamiltonian of Quantum Electrodynamics (QED) reads formally [16, 2, 14, 13]

$$\mathbb{H}^\varphi = \int \Psi^*(x) D^0 \Psi(x) dx - \int \varphi(x) \rho(x) dx + \frac{\alpha}{2} \iint \frac{\rho(x) \rho(y)}{|x-y|} dx dy. \quad (1)$$

Here $\Psi(x)$ is the second-quantized field operator satisfying the usual anti-commutation relations, and $\rho(x)$ is the density operator

$$\rho(x) = \frac{\sum_{\sigma=1}^4 [\Psi^*(x)_\sigma, \Psi(x)_\sigma]}{2} = \frac{\sum_{\sigma=1}^4 \{\Psi^*(x)_\sigma \Psi(x)_\sigma - \Psi(x)_\sigma \Psi^*(x)_\sigma\}}{2}, \quad (2)$$

where σ is the spin variable. In (1), $D^0 = -i\boldsymbol{\alpha} \cdot \nabla + \beta$ is the usual free Dirac operator, α is the *bare* Sommerfeld fine structure constant and φ is the external potential. The matrices $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are the usual 4×4 anti-commuting Dirac matrices. We have chosen a system of units such that $\hbar = c = m = 1$. In QED, one main issue is the minimization of the Hamiltonian (1). However, even if we implement an UV-cutoff, the Hamiltonian is unbounded from below, since the particle number can be arbitrary.

In a formal sense this problem was first overcome by Dirac, who suggested that the vacuum is filled with infinitely many particles occupying the negative energy states of the free Dirac operator D^0 . With this axiom Dirac was able to conjecture the existence of holes in the Dirac sea which he interpreted as *anti-electrons* or *positrons*. His prediction was verified by Anderson in 1932. Dirac also predicted [6, 7] the phenomenon of vacuum polarization: in the presence of an electric field, the virtual electrons are displaced and the vacuum acquires a non-uniform charge density.

In Quantum Electrodynamics Dirac's assumption is sometimes implemented via *normal ordering* which essentially consists of subtracting the kinetic energy of the negative free Dirac sea, in such a way that the kinetic energy of electrons as well as positrons (holes) becomes positive. With this procedure the distinction between electrons and positrons is put in by hand.

It was pointed out in [14] (see also the review [13]), however, that normal ordering is probably not well suited to the case $\alpha \neq 0$ of interacting particles (the interaction is the last term of (1)). Instead a procedure was presented where the distinction between electrons and positrons is not an input but rather a consequence of the theory. The approach of [14] is rigorous and fully non-perturbative, but so far it was only applied to the mean-field (Hartree-Fock) approximation, with the photon field neglected. It allowed to justify the use of the Bogoliubov-Dirac-Fock model (BDF) [4], studied previously in [10, 11, 12]. The purpose of the present paper is to extend these results to the nonzero temperature case.

The methodology of [14] is a two steps procedure. First, the free vacuum is constructed by minimizing the Hamiltonian (1) over Hartree-Fock states in a box with an ultraviolet cut-off, and then taking the thermodynamic limit when the size of the box goes to infinity. The limit is a Hartree-Fock state \mathcal{P}_-^0 describing the (Hartree-Fock) free vacuum [14, 13]. It has an infinite energy, since it contains infinitely many virtual particles forming the (self-consistent) Dirac sea. We remark that this state is not the usual sea of negative electrons of the free Dirac operator because all interactions between particles are taken into account, but it corresponds to filling negative energies of an effective mean-field translation invariant operator.

The second step of [14] consists of constructing an energy functional that is bounded from below in the presence of an external field, by subtracting the (infinite) energy of the free self-consistent Dirac sea. The key observation is that the difference of the energy of a general state P minus the (infinite) energy of the free vacuum \mathcal{P}_-^0 can be represented by an effective functional (called Bogoliubov-Dirac-Fock (BDF) [4]) which only depends on $Q = P - \mathcal{P}_-^0$, describing the variations with respect to the free Dirac sea. The BDF energy was studied in [10, 11, 12]. The existence of ground states was shown for the vacuum case in [10, 11] and in charge sectors in [12]. For a detailed review of all these results, we refer to [13]. An associated time-dependent evolution equation, which is in the spirit of Dirac's original paper [6], was studied in [15].

Let us now turn to the case of a non zero temperature $T = 1/\beta > 0$. We consider a Hartree-Fock state with one-particle density matrix $0 \leq P \leq 1$. Because of the definition of the Hamiltonian (1) and the anticommutator in (2), it is more convenient to consider as variable the *renormalized density matrix* $\gamma = P - 1/2$. We remark that the anticommutator in (2) is a kind of renormalization which does not depend on any reference as normal ordering does (it just corresponds to subtracting the identity divided by 2). The anticommutator of (2) is due to Heisenberg [16] (see also [18, Eq. (96)]) and it is necessary for a covariant formulation of QED, see [22, Eq. (1.14)] and [8, Eq. (38)].

Computing the free energy of our Hartree-Fock state using (1) (and

ignoring infinite constant terms) one arrives at the following free energy functional [14, 3]

$$\begin{aligned} \mathcal{F}_T^{\text{QED}}(\gamma) = \text{tr}(D^0\gamma) - \alpha \int \varphi(x)\rho_\gamma(x) + \frac{\alpha}{2} \iint \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|} \\ - \frac{\alpha}{2} \iint \frac{\text{tr}_{\mathbb{C}^4} |\gamma(x,y)|^2}{|x-y|} - TS(\gamma) \end{aligned} \quad (3)$$

where the *entropy* is given by the formula

$$S(\gamma) = -\text{tr}\left(\left(\frac{1}{2} + \gamma\right) \ln\left(\frac{1}{2} + \gamma\right)\right) - \text{tr}\left(\left(\frac{1}{2} - \gamma\right) \ln\left(\frac{1}{2} - \gamma\right)\right). \quad (4)$$

The (matrix-valued) function $\gamma(x, y)$ is the formal integral kernel of the operator γ and $\rho_\gamma(x) := \text{tr}_{\mathbb{C}^4} \gamma(x, x)$ is the associated charge density. The above formulas are purely formal; they only make sense in a finite box with an ultraviolet cut-off, in general.

As in [14] the first step is to define the free vacuum at temperature T , which is the formal minimizer of (3) when $\varphi = 0$. Following [14], one can first confine the system to a box, then study the limit as the size of the box goes to infinity and identify the free vacuum as the limit of the sequence of ground states. Alternatively, it was proved in [14] that the free vacuum can also be obtained as the unique minimizer of the free energy per unit volume. In the nonzero temperature case, this energy reads

$$\begin{aligned} \mathcal{I}_T(\gamma) = \\ \frac{1}{(2\pi)^3} \int_{B(0,\Lambda)} \text{tr}_{\mathbb{C}^4} [D^0(p)\gamma(p)] dp - \frac{\alpha}{(2\pi)^5} \iint_{B(0,\Lambda)^2} \frac{\text{tr}_{\mathbb{C}^4} [\gamma(p)\gamma(q)]}{|p-q|^2} dp dq \\ + \frac{T}{(2\pi)^3} \int_{B(0,\Lambda)} \text{tr}_{\mathbb{C}^4} \left[\left(\frac{1}{2} + \gamma(p)\right) \ln\left(\frac{1}{2} + \gamma(p)\right) + \left(\frac{1}{2} - \gamma(p)\right) \ln\left(\frac{1}{2} - \gamma(p)\right) \right] dp \end{aligned}$$

and it is defined for translation-invariant states $\gamma = \gamma(p)$ only, under the constraint $-1/2 \leq \gamma \leq 1/2$. Here, $B(0, \Lambda)$ denotes the ball of radius Λ centered at the origin. The real number $\Lambda > 0$ is the ultraviolet cut-off. We shall prove in Theorem 4 that the above energy has a unique minimizer $\tilde{\gamma}^0$, and prove several interesting properties of it. In particular, we shall see that it satisfies a nonlinear equation of the form

$$\tilde{\gamma}^0 = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_{\tilde{\gamma}^0}}} - \frac{1}{1 + e^{-\beta D_{\tilde{\gamma}^0}}} \right) \quad (5)$$

i.e. it is the Fermi-Dirac distribution of a (self-consistent) free Dirac operator, defined as

$$D_{\tilde{\gamma}^0} = D^0 - \alpha \frac{\tilde{\gamma}^0(x, y)}{|x - y|}.$$

(The last term stands for the operator having this integral kernel.) This extends results of [14] to the $T > 0$ case.

The next step is to formally subtract the (infinite) energy of $\tilde{\gamma}^0$ from the energy of any state γ . In this way one obtains a Bogoliubov-Dirac-Fock free energy at temperature $T = 1/\beta$ which can be formally written as

$$\begin{aligned}\mathcal{F}_T(\gamma) &= \text{“}\mathcal{F}_T^{\text{QED}}(\gamma) - \mathcal{F}_T^{\text{QED}}(\tilde{\gamma}^0)\text{”} \\ &= TH(\gamma, \tilde{\gamma}^0) - \alpha \int \varphi(x) \rho_{[\gamma - \tilde{\gamma}^0]}(x) + \frac{\alpha}{2} \iint \frac{\rho_{[\gamma - \tilde{\gamma}^0]}(x) \rho_{[\gamma - \tilde{\gamma}^0]}(y)}{|x - y|} \\ &\quad - \frac{\alpha}{2} \iint \frac{\text{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|}\end{aligned}\quad (6)$$

where H is the *relative entropy* formally defined as

$$TH(\gamma, \tilde{\gamma}^0) = \text{“}\text{tr}(D_{\tilde{\gamma}^0}(\gamma - \tilde{\gamma}^0)) - TS(\gamma) + TS(\tilde{\gamma}^0)\text{”}.$$

We shall consider external field of the form $\varphi = \nu * \frac{1}{|x|}$, where ν represents the density distribution of the external particles, like nuclei, or molecules.

In Section 2.2, we show how to give a correct mathematical meaning to the previous formulas and we prove that the BDF free energy is bounded from below. An important tool is the following inequality

$$TH(\gamma, \tilde{\gamma}^0) \geq \text{tr} [|D_{\tilde{\gamma}^0}(\gamma - \tilde{\gamma}^0)|^2] \geq \text{tr} [|D^0(\gamma - \tilde{\gamma}^0)|^2]. \quad (7)$$

This implies that the relative entropy can control the exchange term and enables us to show that \mathcal{F}_T is bounded from below.

Unfortunately, like for the $T = 0$ case, the free BDF energy is not convex, which makes it a difficult task to prove the existence of a minimizer. Although we leave this question open, we derive some properties for a potential minimizer in Section 2.2. In particular we prove that any minimizer γ satisfies the following nonlinear equation

$$\gamma = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_\gamma}} - \frac{1}{1 + e^{-\beta D_\gamma}} \right) \quad (8)$$

where the (self-consistent) Dirac operator reads

$$D_\gamma = D^0 + \alpha \rho_\gamma * |\cdot|^{-1} - \alpha \varphi - \alpha \frac{\gamma^0(x, y)}{|x - y|}.$$

Compared with the zero temperature case, the main difficulty in proving the existence of a minimizer comes from localization issues of the relative entropy which are more involved than in the zero temperature case.

As a slight simplification, we thoroughly study the *reduced* Hartree Fock case for $T > 0$, where the exchange term (the first term of the second line of (3)) is neglected. In the zero-temperature case, this model was already studied in detail in [11] and [9]. The corresponding free vacuum is now

simple: it is the Fermi-Dirac distribution corresponding to the usual free Dirac operator D^0 ,

$$\gamma^0 = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D^0}} - \frac{1}{1 + e^{-\beta D^0}} \right).$$

The *reduced Bogoliubov-Dirac-Fock* free energy is obtained in the same way as before by subtracting the infinite energy of the free Dirac see γ^0 to the (reduced) Hartree-Fock energy. It is given by

$$\mathcal{F}_T^{\text{red}}(\gamma) = TH(\gamma, \gamma^0) - \alpha \int \varphi \rho_{[\gamma - \gamma^0]} + \frac{\alpha}{2} \iint \frac{\rho_{[\gamma - \gamma^0]}(x) \rho_{[\gamma - \gamma^0]}(y)}{|x - y|} dx dy,$$

$H(\gamma, \gamma^0)$ being defined similarly as before. As this functional is now convex, we can prove in Theorem 2 that it has a unique minimizer $\bar{\gamma}$, which satisfies the self-consistent equation

$$\bar{\gamma} = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_{\bar{\gamma}}}} - \frac{1}{1 + e^{-\beta D_{\bar{\gamma}}}} \right)$$

where

$$D_{\bar{\gamma}} := D^0 + \alpha \rho_{\bar{\gamma} - \gamma^0} * |\cdot|^{-1} - \alpha \varphi$$

in this case.

Additionally we show in Theorem 3 that this minimizer has two interesting properties. First, $\bar{\gamma} - \gamma^0$ is a trace-class operator. In the zero temperature case, on the other hand, it was proved in [11] that the minimizer is never trace-class for $\alpha > 0$. This was indeed the source of complications concerning the definition of the trace (and hence of the charge) of Hartree-Fock states [10] when $T = 0$. This is related to the issue of renormalization [11, 14, 9]. Although we do not minimize in the trace-class in the case $T \neq 0$ but rather in the Hilbert-Schmidt class because the free energy is only coercive for the Hilbert-Schmidt norm, it turns out that the minimizer is trace-class nevertheless.

The second (and related) interesting property shown in Theorem 3 below is that the total electrostatic potential created by the density ν and the polarized Dirac sea decays very fast. More precisely we prove that

$$\rho_{\bar{\gamma}} - \nu \in L^1(\mathbb{R}^3) \quad \text{and} \quad (\rho_{\bar{\gamma}} - \nu) * \frac{1}{|x|} \in L^1(\mathbb{R}^3).$$

Necessarily, the charge of $\rho_{\bar{\gamma}}$ and the charge of the external sources have to be equal. More precisely the *effective* potential has a much faster decay at infinity than $1/|x|$, which shows that the *effective* potential is screened. In other words due to the positive temperature, the particles occupying the Dirac-sea have enough freedom to rearrange in such a way that the external sources are totally shielded. Within non-relativistic fermionic plasma

this effect is known as *Debye-screening*. Let us emphasize that in order to recover such a screening, it is essential to calculate the Gibbs-state in a self-consistent way.

These two properties of the minimizer of the reduced theory probably also hold for the full BDF model with exchange term. However, like for the case $T = 0$, the generalization does not seem to be straightforward.

The paper is organized as follows. The first section is devoted to the presentation of our results for the *reduced* model which is simpler and for which we can prove much more than for the general case. In the second section, we consider the original Hartree-Fock model with exchange term. We prove the existence and uniqueness of the free Hartree-Fock vacuum, define the BDF free energy in the presence of an external field and provide some interesting properties of potential minimizers. In the last section we provide some details of proofs which are a too lengthy to be put in the main text.

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1 The reduced Bogoliubov-Dirac-Fock free energy

1.1 Relative entropy

Throughout this paper, we shall denote by $\mathfrak{S}_p(\mathfrak{H})$ the usual Schatten class of operators Q acting on a Hilbert space \mathfrak{H} and such that $\text{tr}(|Q|^p) < \infty$. The UV cut-off is implemented like in [10, 11, 12, 14] in Fourier space by considering the Hilbert space

$$\mathfrak{H}_\Lambda := \left\{ \psi \in L^2(\mathbb{R}^3, \mathbb{C}^4) \mid \text{supp } \hat{\psi} \subset B(0, \Lambda) \right\}, \quad (9)$$

with $B(0, \Lambda)$ denoting the ball of radius Λ centered at the origin. We denote by ‘tr’ the usual trace functional on $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$. Within the reduced theory, the free vacuum at temperature $T = \beta^{-1} > 0$ is the self-adjoint operator acting on \mathfrak{H}_Λ defined by

$$\gamma^0 = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D^0}} - \frac{1}{1 + e^{-\beta D^0}} \right). \quad (10)$$

Notice when $T \rightarrow 0$ ($\beta \rightarrow \infty$), we recover the usual formula [10, 11, 9] $\gamma^0 = -D^0/2|D^0|$.

We assume that $T > 0$ henceforth. Notice that thanks to the cut-off in Fourier space and the gap in the spectrum of D^0 , the spectrum of γ^0 does

not include 0 or $\pm 1/2$. In fact, it is given by

$$\sigma(\gamma^0) = \left[-\frac{1}{2} + \frac{e^{-\beta E(\Lambda)}}{1 + e^{-\beta E(\Lambda)}}, -\frac{1}{2} + \frac{e^{-\beta}}{1 + e^{-\beta}} \right] \cup \left[\frac{1}{2} - \frac{e^{-\beta}}{1 + e^{-\beta}}, \frac{1}{2} - \frac{e^{-\beta E(\Lambda)}}{1 + e^{-\beta E(\Lambda)}} \right] \quad (11)$$

where $E(\Lambda) = \sqrt{1 + \Lambda^2}$. Also the charge density of the free vacuum γ^0 at temperature T vanishes:

$$\rho_{\gamma^0} = \frac{1}{2(2\pi)^3} \int_{B(0, \Lambda)} \text{tr}_{\mathbb{C}^4} \left(\frac{1}{1 + e^{\beta D^0(k)}} - \frac{1}{1 + e^{-\beta D^0(k)}} \right) dk = 0. \quad (12)$$

We shall denote the class of Hilbert-Schmidt perturbations of γ^0 by \mathcal{K} :

$$\mathcal{K} := \left\{ \gamma \in \mathcal{B}(\mathfrak{H}_\Lambda) \mid \gamma^* = \gamma, -\frac{1}{2} \leq \gamma \leq \frac{1}{2}, \gamma - \gamma^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \right\}. \quad (13)$$

The *relative entropy* reads

$$H(\gamma, \gamma^0) = \text{tr} \left[\left(\frac{1}{2} + \gamma \right) \left(\ln \left(\frac{1}{2} + \gamma \right) - \ln \left(\frac{1}{2} + \gamma^0 \right) \right) + \left(\frac{1}{2} - \gamma \right) \left(\ln \left(\frac{1}{2} - \gamma \right) - \ln \left(\frac{1}{2} - \gamma^0 \right) \right) \right]. \quad (14)$$

Note that since $\gamma \in \mathcal{K}$ is a compact perturbation of γ^0 , we always have $\sigma_{\text{ess}}(\gamma) = \sigma_{\text{ess}}(\gamma^0)$. Hence $\sigma(\gamma)$ only contains eigenvalues of finite multiplicity in the neighborhood of $\pm 1/2$. Using the integral formula

$$\ln a - \ln b = - \int_0^\infty \left[\frac{1}{a+t} - \frac{1}{b+t} \right] dt = \int_0^\infty \frac{1}{a+t} (a-b) \frac{1}{b+t} dt, \quad (15)$$

we easily see that Eq. (14) is well defined as soon as $\gamma \in \mathcal{K}$, $\gamma - \gamma^0 \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$, since the spectrum of γ^0 does not contain $\pm 1/2$.

When $\gamma - \gamma^0 \in \mathcal{K}$ is merely Hilbert-Schmidt, we may define the relative entropy by the integral formula

$$\boxed{H(\gamma, \gamma^0) = \text{tr} \left(\int_{-1}^1 \frac{2}{1 + 2u\gamma^0} (\gamma - \gamma^0) \frac{1 - |u|}{1 + 2u\gamma} (\gamma - \gamma^0) \frac{1}{1 + 2u\gamma^0} du \right)} \quad (16)$$

It is clear that this provides a well defined object in \mathcal{K} as one has

$$\forall \gamma \in \mathcal{K}, \forall u \in [-1, 1], \quad 0 \leq \frac{1 - |u|}{1 + 2u\gamma} \leq 1 \quad \text{and} \quad 0 \leq \frac{1}{1 + 2u\gamma^0} \leq \frac{1}{\epsilon}$$

for some $\epsilon > 0$, by (11). It is not difficult to see that (16) and (14) coincide when $\gamma - \gamma^0 \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$. We shall discuss this in the appendix. But (16) has the advantage of being well-defined for all $\gamma \in \mathcal{K}$, and hence we use (16) for a *definition* of H henceforth.

Our first result is the

Theorem 1 (Properties of Relative Entropy). *The functional $\gamma \mapsto H(\gamma, \gamma^0)$ defined in (16) is strongly continuous on \mathcal{K} for the topology of $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$. It is convex, hence weakly lower semi-continuous (wlsc). Moreover, it is coercive on \mathcal{K} for the Hilbert-Schmidt norm:*

$$\forall \gamma \in \mathcal{K}, \quad TH(\gamma, \gamma^0) \geq \text{tr}(|D^0|(\gamma - \gamma^0)^2) \quad (17)$$

where we recall that $T = \beta^{-1}$ is the temperature.

Coercive in this context means that $H(\gamma, \gamma^0) \rightarrow \infty$ if $\|\gamma - \gamma^0\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)} \rightarrow \infty$. This follows from (17) since $|D^0| \geq 1$.

Proof of Theorem 1. First we prove that $H(\cdot, \gamma^0)$ is strongly continuous for the $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ topology. This is indeed a consequence of the following

Lemma 1. *Let $\gamma, \gamma' \in \mathcal{K}$. Then we have for some constant C (depending on Λ) and all $0 \leq \eta \leq 1$,*

$$\begin{aligned} |H(\gamma, \gamma^0) - H(\gamma', \gamma^0)| &\leq \frac{C}{\eta} \|\gamma - \gamma'\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)} \\ &\quad + C\eta \left(\|\gamma - \gamma^0\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)}^2 + \|\gamma' - \gamma^0\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)}^2 \right). \end{aligned} \quad (18)$$

Proof. We use Formula (16) and split the integrals as follows:

$$\int_{-1}^1 = \int_{-1}^{-1+\eta} + \int_{-1+\eta}^{1-\eta} + \int_{1-\eta}^1.$$

We estimate

$$\begin{aligned} &\left| \text{tr} \left(\int_{-1+\eta}^{1-\eta} du \left(\frac{1}{1+2u\gamma^0}(\gamma - \gamma^0) \frac{1-|u|}{1+2u\gamma}(\gamma - \gamma^0) \frac{1}{1+2u\gamma^0} \right. \right. \right. \\ &\quad \left. \left. \left. - \frac{1}{1+2u\gamma^0}(\gamma' - \gamma^0) \frac{1-|u|}{1+2u\gamma'}(\gamma' - \gamma^0) \frac{1}{1+2u\gamma^0} \right) \right| \leq \frac{C}{\eta} \|\gamma - \gamma'\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)} \end{aligned}$$

using in particular

$$\frac{1-|u|}{1+2u\gamma} - \frac{1-|u|}{1+2u\gamma'} = 2u \frac{1-|u|}{1+2u\gamma} (\gamma' - \gamma) \frac{1}{1+2u\gamma'}$$

and $0 \leq (1 + 2u\gamma')^{-1} \leq \eta^{-1}$ as $\gamma' \in \mathcal{K}$ and $-1 + \eta \leq u \leq 1 - \eta$. Similarly

$$\left| \operatorname{tr} \int_{1-\eta}^1 du \frac{1}{1+2u\gamma^0} (\gamma - \gamma^0) \frac{1-|u|}{1+2u\gamma} (\gamma - \gamma^0) \frac{1}{1+2u\gamma^0} \right| \leq C\eta \|\gamma - \gamma^0\|_{\mathfrak{S}_2(\mathfrak{H}_\Lambda)}^2.$$

The other terms are treated in the same way. \square

Convexity of $\gamma \mapsto H(\gamma, \gamma_0)$ is a simple consequence of the integral representation (16). In fact, the integrand is convex for any fixed $u \in [-1, 1]$, since

$$\begin{aligned} \gamma \mapsto (\gamma - \gamma^0) \frac{1}{1+2u\gamma} (\gamma - \gamma^0) \\ = \frac{1}{(2u)^2} \left(2u\gamma - 1 - 4u\gamma_0 + (1+2u\gamma_0) \frac{1}{1+2u\gamma} (1+2u\gamma_0) \right) \end{aligned}$$

is clearly convex.

Finally, we prove Formula (17). Consider the following function

$$f(x, y) = \left(\frac{1}{2} + x\right) \left(\ln\left(\frac{1}{2} + x\right) - \ln\left(\frac{1}{2} + y\right)\right) + \left(\frac{1}{2} - x\right) \left(\ln\left(\frac{1}{2} - x\right) - \ln\left(\frac{1}{2} - y\right)\right)$$

defined on $(-1/2, 1/2)^2$. Minimizing over x for fixed y , one finds that $f(x, y) \geq (x - y)^2 C(y)$ where $C(y) = \ln\left(\frac{1/2+y}{1/2-y}\right) / (2y)$. If we write y as

$$y = \frac{1}{2} \left(\frac{1}{1+e^h} - \frac{1}{1+e^{-h}} \right), \quad (19)$$

we obtain $C(y) = h \tanh(h/2)^{-1} \geq \max(|h|, 2)$. Hence if y takes the form (19), we deduce

$$f(x, y) \geq \max\{(x - y)^2 |h|, 2(x - y)^2\}.$$

Assume now that X and Y are self-adjoint operators acting on a Hilbert space \mathfrak{H} , with $-1/2 \leq X, Y \leq 1/2$ and

$$Y = \frac{1}{2} \left(\frac{1}{1+e^H} - \frac{1}{1+e^{-H}} \right)$$

for some H . By Klein's inequality [23, p. 330], one also has

$$H(X, Y) = \operatorname{tr} f(X, Y) \geq \max\{\operatorname{tr}(X - Y)^2 |H|, 2 \operatorname{tr}(X - Y)^2\}. \quad (20)$$

This gives (17), taking $X = \gamma$ and $Y = \gamma^0$. \square

1.2 Existence of a minimizer and Debye screening

Now we are able to define the *reduced Bogoliubov-Dirac-Fock* energy at temperature $T = \beta^{-1}$. For this purpose, we introduce the Coulomb space

$$\mathcal{C} := \{\rho \in \mathcal{S}'(\mathbb{R}^3) \mid D(\rho, \rho) < \infty\} \quad (21)$$

where

$$D(f, g) = 4\pi \int_{\mathbb{R}^3} |k|^{-2} \widehat{f}(k) \overline{\widehat{g}(k)} dk. \quad (22)$$

We remark that the Fourier transform of $Q = \gamma - \gamma^0$ is an L^2 -function with support in $B(0, \Lambda) \times B(0, \Lambda)$. Hence $Q(x, y)$ is a smooth kernel and $\rho_Q(x) = \text{tr}_{\mathbb{C}^4}(Q(x, x))$ is a well defined function. Indeed, the map $\gamma \in \mathcal{K} \mapsto \rho_{\gamma - \gamma^0} \in L^2(\mathbb{R}^3)$ is continuous for the topology of $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$. It is easy to see that the Fourier transform of $\rho_{\gamma - \gamma^0}$ is given by the formula

$$\widehat{\rho_{\gamma - \gamma^0}}(k) = \frac{1}{(2\pi)^{3/2}} \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} \text{tr}_{\mathbb{C}^4} \left[(\widehat{\gamma - \gamma^0})(p + k/2, p - k/2) \right] dp. \quad (23)$$

We also define our variational set by

$$\mathcal{K}_C := \{\gamma \in \mathcal{K} \mid \rho_{\gamma - \gamma^0} \in \mathcal{C}\}. \quad (24)$$

The *reduced Bogoliubov-Dirac-Fock energy* reads

$$\boxed{\mathcal{F}_T^{\text{red}}(\gamma) = TH(\gamma, \gamma^0) - \alpha D(\nu, \rho_{\gamma - \gamma^0}) + \frac{\alpha}{2} D(\rho_{\gamma - \gamma^0}, \rho_{\gamma - \gamma^0})} \quad (25)$$

and it is well-defined on \mathcal{K}_C by Theorem 1. In (25), $\nu \in \mathcal{C}$ is an external density creating an electrostatic potential $-\nu * 1/|x|$. The number $\alpha > 0$ is the *fine structure constant*. The following is an easy consequence on Theorem 1:

Theorem 2 (Existence of a minimizer). *Assume $T > 0$, $\alpha \geq 0$ and $\nu \in \mathcal{C}$. Then $\mathcal{F}_T^{\text{red}}$ satisfies*

$$\forall \gamma \in \mathcal{K}_C, \quad \mathcal{F}_T^{\text{red}}(\gamma) \geq -\frac{\alpha}{2} D(\nu, \nu) \quad (26)$$

hence it is bounded below on \mathcal{K}_C . It has a unique minimizer $\bar{\gamma}$ on \mathcal{K}_C . The operator $\bar{\gamma}$ satisfies the self-consistent equation

$$\begin{cases} \bar{\gamma} = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D \bar{\gamma}}} - \frac{1}{1 + e^{-\beta D \bar{\gamma}}} \right), \\ D_{\bar{\gamma}} := D^0 + \alpha(\rho_{\bar{\gamma} - \gamma^0} - \nu) * |\cdot|^{-1}. \end{cases} \quad (27)$$

Remark 1. When $T = 0$, a similar result was proved in [11, Thm 3], but there might be no uniqueness in this case.

Remark 2. If there is no external field, $\nu = 0$, we recover that the optimal state is $\gamma - \gamma^0 = 0$, and its energy is zero, by (26).

Proof of Theorem 2. Eq. (26) is an obvious consequence of positivity of the relative entropy H and positive definiteness of $D(\cdot, \cdot)$. The existence of a minimizer is obtained by noticing that $\mathcal{F}_T^{\text{red}}$ is weakly lower semi-continuous for the topology of $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and \mathcal{C} , by Theorem 1. As $\mathcal{F}_T^{\text{red}}$ is convex¹ and strictly convex with respect to $\rho_{\gamma-\gamma^0}$, we deduce that all the minimizers share the same density. Next we notice that $\pm 1/2 \notin \sigma(\bar{\gamma})$ since the derivative of the relative entropy with respect to variations of an eigenvalue is infinite at these two points. Hence $\bar{\gamma}$ does not saturate the constraint and it is a solution of Eq. (27). This *a fortiori* proves that $\bar{\gamma}$ is unique, since $D_{\bar{\gamma}}$ depends only on the density $\rho_{\bar{\gamma}-\gamma^0}$. \square

Now we provide some interesting properties of any solution of Eq. (27), thus in particular of our minimizer $\bar{\gamma}$.

Theorem 3 (Debye Screening). *Assume $T > 0$, $\alpha > 0$ and $\nu \in \mathcal{C} \cap L^1(\mathbb{R}^3)$. Any $\gamma \in \mathcal{K}$ that solves Eq. (27) is a trace-class perturbation of γ^0 , i.e., $\gamma - \gamma^0 \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$. Its charge density $\rho_{\gamma-\gamma^0}$ is an $L^1(\mathbb{R}^3)$ function which satisfies*

$$\int_{\mathbb{R}^3} \rho_{\gamma-\gamma^0} = \int_{\mathbb{R}^3} \nu \quad \text{and} \quad (\rho_{\gamma-\gamma^0} - \nu) * \frac{1}{|x|} \in L^1(\mathbb{R}^3). \quad (28)$$

This result implies that the particles arrange themselves such that the total effective potential $(\rho_{\gamma-\gamma^0} - \nu) * 1/|x|$ has a decay much faster than $1/|x|$. This implies that the nuclear charge of the external sources is completely screened.

The proof of Theorem 3 is lengthy and is given later in Section 3.1.

2 The Bogoliubov-Dirac-Fock free energy

2.1 Definition of the free vacuum

When the exchange term is not neglected, the free vacuum is no longer described by the operator γ^0 introduced in the previous section. Instead it is another translation-invariant operator $\tilde{\gamma}^0$ that solves a self-consistent equation. Following ideas from [14], we define in this section $\tilde{\gamma}^0$ as the (unique) minimizer of the free energy per unit volume. We consider translation-invariant operators $\gamma = \gamma(p)$ acting on \mathfrak{H}_Λ and such that $-1/2 \leq \gamma \leq 1/2$ which is obviously equivalent to $-1/2 \leq \gamma(p) \leq 1/2$, for a.e. $p \in B(0, \Lambda)$, in

¹It can indeed be proved that $H(\cdot, \gamma^0)$ is strictly convex but we do not need that here.

the sense of $\mathbb{C}^4 \times \mathbb{C}^4$ hermitian matrices. The free energy per unit volume of such a translation-invariant operator γ at temperature T is given by [14]

$$\mathcal{T}_T(\gamma) = \frac{1}{(2\pi)^3} \left(\int_{B(0,\Lambda)} \text{tr}_{\mathbb{C}^4} [D^0(p)\gamma(p)] dp - \frac{\alpha}{(2\pi)^2} \iint_{B(0,\Lambda)^2} \frac{\text{tr}_{\mathbb{C}^4} [\gamma(p)\gamma(q)]}{|p-q|^2} dp dq - TS(\gamma) \right) \quad (29)$$

where the entropy is defined as

$$S(\gamma) = - \int_{B(0,\Lambda)} \text{tr}_{\mathbb{C}^4} \left[\left(\frac{1}{2} + \gamma(p) \right) \ln \left(\frac{1}{2} + \gamma(p) \right) + \left(\frac{1}{2} - \gamma(p) \right) \ln \left(\frac{1}{2} - \gamma(p) \right) \right] dp.$$

The free energy is defined on the convex set of matrix-valued functions, such that, for all $p \in B(0, \Lambda)$, $\gamma(p)$ is a hermitian 4×4 matrix, i.e.

$$\mathcal{A} := \left\{ \gamma : B(0, \Lambda) \rightarrow M^4 \mid \gamma(p)^* = \gamma(p), \right. \\ \left. -1/2 \leq \gamma(p) \leq 1/2 \text{ for all } p \in B(0, \Lambda) \right\}. \quad (30)$$

Theorem 4 (The free vacuum at temperature T). *For all $T > 0$ and all $0 \leq \alpha < 4/\pi$, the free energy per unit volume \mathcal{T}_T in (29) has a unique minimizer $\tilde{\gamma}^0$ on \mathcal{A} . It is a solution of the self-consistent equation*

$$\begin{cases} \tilde{\gamma}^0 = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_{\tilde{\gamma}^0}}} - \frac{1}{1 + e^{-\beta D_{\tilde{\gamma}^0}}} \right) \\ D_{\tilde{\gamma}^0} = D^0 - \alpha \frac{\tilde{\gamma}^0(x,y)}{|x-y|}. \end{cases} \quad (31)$$

Furthermore, $\tilde{\gamma}^0$ has the form

$$\tilde{\gamma}^0(p) = f_1(|p|)\boldsymbol{\alpha} \cdot p + f_0(|p|)\beta \quad (32)$$

with $f_0, f_1 \leq 0$ a.e. on $B(0, \Lambda)$ and $D_{\tilde{\gamma}^0}$ satisfies

$$|D_{\tilde{\gamma}^0}| \geq |D^0|. \quad (33)$$

Here and in the following, we shall identify operators with their integral kernels for simplicity of the notation. That is, the last term in the second line of (31) denotes the operator with integral kernel given by $\frac{(\gamma - \tilde{\gamma}^0)(x,y)}{|x-y|}$, where $(\gamma - \tilde{\gamma}^0)(x, y)$ is the integral kernel of the translation-invariant operator $\gamma - \tilde{\gamma}^0$ (it is a function of $x - y$).

Remark 3. The assumption $\alpha < 4/\pi$ guarantees that the functional (29) is bounded from below, independently of the UV cutoff Λ , which is arbitrary in this paper. This is a consequence of Kato's inequality. For $\alpha > 4/\pi$ this is not the case [5, 17].

For comparison, we note that in the *non-interacting* case $\alpha = 0$, the functions $f_1(|p|)$ and $f_0(|p|)$ appearing in Theorem 4 are given by

$$f_1(|p|) = f_0(|p|) = \frac{1}{2E(p)} \left(\frac{1}{1 + e^{\beta E(p)}} - \frac{1}{1 + e^{-\beta E(p)}} \right).$$

A similar result was proved in the zero temperature case in [14]. As in [14], it is possible to justify the introduction of \mathcal{T}_T by a thermodynamic limit procedure. The proof of Theorem 4 is given in Section 3.3.

Like for the reduced case, we have that

$$\sigma(\tilde{\gamma}^0) \subset \left[-\frac{1}{2} + \epsilon, -\epsilon \right] \cup \left[\epsilon, \frac{1}{2} - \epsilon \right]$$

for some $\epsilon > 0$. This can be seen from (33) and the fact that $D_{\tilde{\gamma}^0}$ is a bounded operator on \mathfrak{H}_Λ due to the presence of the ultraviolet cut-off. Notice also that we have formally $\rho_{\tilde{\gamma}^0} \equiv 0$ by (32), as in (12).

2.2 The external field case

As in Section 1.2, one can consider the Bogoliubov-Dirac-Fock energy with an external field. It is formally obtained by subtracting the infinite free energy of the free vacuum at temperature $T > 0$ from the free energy of our state γ . This procedure can be justified like in [14] by a thermodynamic limit procedure. Using the same notation as in Section 1.2, the *Bogoliubov-Dirac-Fock free energy* reads

$$\begin{aligned} \mathcal{F}_T(\gamma) = TH(\gamma, \tilde{\gamma}^0) - \alpha D(\nu, \rho_{\gamma - \tilde{\gamma}^0}) + \frac{\alpha}{2} D(\rho_{\gamma - \tilde{\gamma}^0}, \rho_{\gamma - \tilde{\gamma}^0}) \\ - \frac{\alpha}{2} \iint \frac{\text{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|} dx dy, \end{aligned} \quad (34)$$

where H is the relative entropy defined like in Section 1.1. Like for the reduced case, we see that the functional \mathcal{F}_T is well-defined on the following convex set

$$\tilde{\mathcal{K}}_C := \left\{ \gamma \in \mathcal{B}(\mathfrak{H}_\Lambda) \mid \gamma^* = \gamma, -\frac{1}{2} \leq \gamma \leq \frac{1}{2}, \gamma - \tilde{\gamma}^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), \rho_{\gamma - \tilde{\gamma}^0} \in \mathcal{C} \right\}. \quad (35)$$

Note that although the function $\gamma \mapsto H(\gamma, \tilde{\gamma}^0)$ is convex, \mathcal{F}_T is not a convex functional because of the presence of the exchange term. This is of course a great obstacle in proving the existence of a minimizer, and we have to leave this as an open problem. Following the method of Theorem 1, we shall show that

$$\forall \gamma \in \tilde{\mathcal{K}}_C, \quad TH(\gamma, \tilde{\gamma}^0) \geq \text{tr}(|D_{\tilde{\gamma}^0}|(\gamma - \tilde{\gamma}^0)^2). \quad (36)$$

With the aid of this inequality we can prove the

Theorem 5 (Minimizer in External Field). *Assume that $0 \leq \alpha < 4/\pi$ and that $T > 0$. We have*

$$\forall \gamma \in \tilde{\mathcal{K}}_C, \quad \mathcal{F}_T(\gamma) \geq -\frac{\alpha}{2} D(\nu, \nu) \quad (37)$$

and hence \mathcal{F}_T is bounded below on $\tilde{\mathcal{K}}_C$.

Assume that $\gamma \in \tilde{\mathcal{K}}_C$ is a minimizer of \mathcal{F}_T . Then it satisfies the self-consistent equation

$$\begin{cases} \gamma = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_\gamma}} - \frac{1}{1 + e^{-\beta D_\gamma}} \right), \\ D_\gamma := D_{\tilde{\gamma}^0} + \alpha(\rho_{\gamma-\gamma^0} - \nu) * |\cdot|^{-1} - \alpha \frac{(\gamma-\tilde{\gamma}^0)(x,y)}{|x-y|} \end{cases} \quad (38)$$

with $D_{\tilde{\gamma}^0}$ defined in (31). It is unique when

$$0 \leq \alpha \frac{\pi}{4} \left\{ 1 - \alpha \left(\frac{\pi}{2} \sqrt{\frac{\alpha/2}{1 - \alpha\pi/4}} + \pi^{1/6} 2^{11/6} \right) D(\nu, \nu)^{1/2} \right\}^{-1} \leq 1. \quad (39)$$

The proof of Theorem 5 is provided in Section 3.4.

3 Proofs

3.1 Proof of Theorem 3

Let γ be a solution of

$$\begin{cases} \gamma = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_\gamma}} - \frac{1}{1 + e^{-\beta D_\gamma}} \right), \\ D_\gamma := D^0 + \alpha(\rho_{\gamma-\gamma^0} - \nu) * |\cdot|^{-1}. \end{cases} \quad (40)$$

For the sake of simplicity, we define $\rho := \rho_{\gamma-\gamma^0} - \nu$ and $V = \alpha(\rho_{\gamma-\gamma^0} - \nu) * |\cdot|^{-1}$. Note that $\nabla V \in L^2(\mathbb{R}^3)$ as $\rho \in \mathcal{C}$, hence $V \in L^6(\mathbb{R}^3)$. Following [11, p. 4495], we may use the Kato-Seiler-Simon inequality (see [20] and [21, Thm. 4.1])

$$\forall p \geq 2, \quad \|f(-i\nabla)g(x)\|_{\mathfrak{S}_p(L^2(\mathbb{R}^3))} \leq (2\pi)^{-3/p} \|g\|_{L^p(\mathbb{R}^3)} \|f\|_{L^p(\mathbb{R}^3)} \quad (41)$$

to obtain

$$\left\| V \frac{1}{|D^0|} \right\|_{\mathfrak{S}_\infty(\mathfrak{H}_\Lambda)} \leq \left\| V \frac{1}{|D^0|} \right\|_{\mathfrak{S}_6(\mathfrak{H}_\Lambda)} \leq C' \|V\|_{L^6(\mathbb{R}^3)} \leq C \|\rho\|_{\mathcal{C}}.$$

This shows that $|D_\gamma| \leq (1 + \alpha C \|\rho\|_{\mathcal{C}}) |D^0|$. Thanks to the cut-off in Fourier space, we deduce that D_γ is a bounded operator on \mathfrak{H}_Λ . Recall Duhamel's formula

$$e^{\beta D_\gamma} = e^{\beta D^0} + \beta \int_0^1 e^{t\beta D_\gamma} V e^{(1-t)\beta D^0} dt. \quad (42)$$

Denoting $K := \beta \int_0^1 e^{t\beta D_\gamma} V e^{(1-t)\beta D^0} dt$ and using (42), we have

$$\begin{aligned} K &= K_0 + K' \\ &:= \beta \int_0^1 dt e^{t\beta D^0} V e^{(1-t)\beta D^0} + \beta^2 \int_0^1 dt \int_0^t ds e^{s\beta D_\gamma} V e^{(t-s)\beta D^0} V e^{(1-t)\beta D^0}. \end{aligned}$$

We obtain for the self-consistent solution

$$\begin{aligned}
\gamma - \gamma^0 &= \frac{1}{1 + e^{\beta D_\gamma}} - \frac{1}{1 + e^{\beta D^0}} \\
&= -\frac{1}{1 + e^{\beta D^0}} K_0 \frac{1}{1 + e^{\beta D^0}} - \frac{1}{1 + e^{\beta D^0}} K' \frac{1}{1 + e^{\beta D^0}} \\
&\quad + \frac{1}{1 + e^{\beta D^0}} K \frac{1}{1 + e^{\beta D_\gamma}} K \frac{1}{1 + e^{\beta D^0}} \quad (43)
\end{aligned}$$

which we write as $\gamma - \gamma^0 = A + B$ where

$$A = -\frac{1}{1 + e^{\beta D^0}} K_0 \frac{1}{1 + e^{\beta D^0}} = -\beta \int_0^1 \frac{e^{t\beta D^0}}{1 + e^{\beta D^0}} V \frac{e^{(1-t)\beta D^0}}{1 + e^{\beta D^0}} dt.$$

As $V \in L^6(\mathbb{R}^3)$ and D_γ is bounded, using the cut-off in Fourier space and the Kato-Seiler-Simon inequality (41), we have $K \in \mathfrak{S}_6(\mathfrak{H}_\Lambda)$. Hence we obtain that $K' \in \mathfrak{S}_3(\mathfrak{H}_\Lambda)$ and $B \in \mathfrak{S}_3(\mathfrak{H}_\Lambda)$.

The next step is to compute the density of A . The kernel of A is given by

$$\widehat{A}(p, q) = -\beta(2\pi)^{-3/2} \int_0^1 \frac{e^{t\beta D^0(p)}}{1 + e^{\beta D^0(p)}} \widehat{V}(p - q) \frac{e^{(1-t)\beta D^0(q)}}{1 + e^{\beta D^0(q)}} dt.$$

Using (23), we obtain

$$\widehat{\rho}_A(k) = -\frac{\alpha C(|k|)}{|k|^2} \widehat{\rho}(k)$$

where

$$C(|k|) := \frac{\beta}{2\pi^2} \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} dp \int_0^1 dt \operatorname{tr}_{\mathbb{C}^4} \left[\frac{e^{t\beta D^0(p+k/2)}}{1 + e^{\beta D^0(p+k/2)}} \frac{e^{(1-t)\beta D^0(p-k/2)}}{1 + e^{\beta D^0(p-k/2)}} \right]. \quad (44)$$

Inserting this into the self-consistent equation (43) gives

$$\widehat{\rho}(k) = -\widehat{\nu}(k) - \frac{\alpha C(|k|)}{|k|^2} \widehat{\rho}(k) + \widehat{\rho}_B(k) \quad (45)$$

or, equivalently,

$$\widehat{\rho}(k) = \widehat{b}_1(k)(-\widehat{\nu}(k) + \widehat{\rho}_B(k)), \quad (46)$$

and

$$\widehat{V}(k) = 4\pi \widehat{b}_2(k)(-\widehat{\nu}(k) + \widehat{\rho}_B(k)), \quad (47)$$

where

$$b_1 := \mathcal{F}^{-1} \left(\frac{|k|^2}{|k|^2 + \alpha C(|k|)} \right) \quad \text{and} \quad b_2 := \mathcal{F}^{-1} \left(\frac{1}{|k|^2 + \alpha C(|k|)} \right), \quad (48)$$

with \mathcal{F}^{-1} denoting the inverse Fourier transform. Our main tool will be the following

Proposition 1 (Properties of b_1, b_2). *The two functions $b_1(x)$ and $b_2(x)$, defined in (48) and (44), belong to $L^1(\mathbb{R}^3)$.*

We postpone the proof of Proposition 1 to Section 3.2 and first complete the proof of Theorem 3. First we claim that $\rho_B \in L^3(\mathbb{R}^3)$. To see this, we take a function $\xi \in L^{3/2}(\mathbb{R}^3) \cap C_0^\infty(\mathbb{R}^3)$ and compute

$$\begin{aligned} |\operatorname{tr}(B\xi)| &= |\operatorname{tr}(B\mathbb{1}_{B(0,\Lambda)}(p)\xi\mathbb{1}_{B(0,\Lambda)}(p))| \\ &\leq \|B\|_{\mathfrak{S}_3(\mathfrak{H}_\Lambda)} \|\mathbb{1}_{B(0,\Lambda)}(p)\xi\mathbb{1}_{B(0,\Lambda)}(p)\|_{\mathfrak{S}_{3/2}(\mathfrak{H}_\Lambda)}. \end{aligned}$$

Writing $\xi = |\xi|^{1/2} \operatorname{sgn}(\xi) |\xi|^{1/2}$ and using the Kato-Seiler-Simon inequality (41) twice in $\mathfrak{S}_3(\mathfrak{H}_\Lambda)$, we obtain $|\operatorname{tr}(B\xi)| \leq C \|B\|_{\mathfrak{S}_3(\mathfrak{H}_\Lambda)} \|\xi\|_{L^{3/2}(\mathbb{R}^3)}$ where C depends on the cut-off Λ . This proves by duality that $\rho_B \in L^3(\mathbb{R}^3)$.

Next we use a boot-strap argument. As $\nu \in L^1(\mathbb{R}^3)$ and $\rho_B \in L^3(\mathbb{R}^3)$, we get from (47) and Proposition 1 that $V \in L^3(\mathbb{R}^3)$. Inserting in the definition of K' and using (41) once more, we obtain that $K' \in \mathfrak{S}_{3/2}(\mathfrak{H}_\Lambda)$, hence $B \in \mathfrak{S}_2(\mathbb{R}^3)$ and $\rho_B \in L^2(\mathbb{R}^3)$. Using again (47) and Proposition 1, we get that $V \in L^2(\mathbb{R}^3)$, hence $B \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and $\rho_B \in L^1(\mathbb{R}^3)$. This finishes the proof of Theorem 3, by (46), (47) and Proposition 1. \square

3.2 Proof of Proposition 1

The proof proceeds along the same lines as in the Appendix of [9]. In the following we shall denote by P_0^+ and P_0^- the projection onto the positive and negative spectral subspace of D^0 , respectively. As multiplication operators in momentum space,

$$P_0^+(p) = \frac{1}{2} \left(1 + \frac{\alpha \cdot p + \beta}{E(p)} \right), \quad P_0^-(p) = \frac{1}{2} \left(1 - \frac{\alpha \cdot p + \beta}{E(p)} \right).$$

The function C in (44) can be written as

$$\begin{aligned} C(|k|) &= \frac{\beta}{\pi^2} \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} dp \times \\ &\times \int_0^1 dt \left(\operatorname{tr}_{\mathbb{C}^4} \left[\frac{e^{t\beta E(p+k/2)}}{1 + e^{\beta E(p+k/2)}} \frac{e^{(1-t)\beta E(p-k/2)}}{1 + e^{\beta E(p-k/2)}} P_0^+(p+k/2) P_0^+(p-k/2) \right] \right. \\ &\left. + \operatorname{tr}_{\mathbb{C}^4} \left[\frac{e^{t\beta E(p+k/2)}}{1 + e^{\beta E(p+k/2)}} \frac{e^{-(1-t)\beta E(p-k/2)}}{1 + e^{-\beta E(p-k/2)}} P_0^+(p+k/2) P_0^-(p-k/2) \right] \right). \quad (49) \end{aligned}$$

Hence

$$\begin{aligned}
C(|k|) = & \frac{1}{\pi^2} \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} \frac{1}{1 + e^{\beta E(p+k/2)}} \frac{e^{\beta E(p+k/2)} - e^{\beta E(p-k/2)}}{E(p+k/2) - E(p-k/2)} \frac{1}{1 + e^{\beta E(p-k/2)}} \times \\
& \times \left[1 + \frac{(p+k/2) \cdot (p-k/2) + 1}{E(p+k/2)E(p-k/2)} \right] dp \\
+ & \frac{1}{\pi^2} \int_{\substack{|p+k/2| \leq \Lambda \\ |p-k/2| \leq \Lambda}} \frac{1}{1 + e^{\beta E(p+k/2)}} \frac{e^{\beta E(p+k/2)} - e^{-\beta E(p-k/2)}}{E(p+k/2) + E(p-k/2)} \frac{1}{1 + e^{-\beta E(p-k/2)}} \times \\
& \times \left[1 - \frac{(p+k/2) \cdot (p-k/2) + 1}{E(p+k/2)E(p-k/2)} \right] dp.
\end{aligned}$$

For the sake of clarity, we denote by $C_1(|k|)$ (resp. $C_2(|k|)$) the first (resp. second) integral of the previous formula. By the monotonicity of the exponential function, it is easily seen that $C_1(|k|) \geq 0$ and $C_2(|k|) \geq 0$.

The next step is to simplify the above integral formula. We follow a method of Pauli and Rose [19] which was recently used in the appendix of [9]. After two changes of variables, we end up with

$$\begin{aligned}
C_1(|k|) = & \frac{8}{\pi|k|} \int_0^{Z_\Lambda(|k|)} dz \int_0^{\frac{|k|}{2}z} dv \frac{e^{\beta w(k,z)}}{1 + e^{\beta(w(k,z)+v)}} \frac{\sinh(\beta v)}{v} \times \\
& \times \frac{1}{1 + e^{\beta(w(k,z)-v)}} \frac{z w(k,z)^{-1}}{(1 - z^2)^3} \\
+ & \frac{8}{\pi|k|} \int_0^{\frac{|k|}{2}Z_\Lambda(|k|)} dz \int_0^z dv \frac{e^{\beta(E(\Lambda)-z)}}{1 + e^{\beta(E(\Lambda)-z+v)}} \frac{\sinh(\beta v)}{v} \frac{1}{1 + e^{\beta(E(\Lambda)-z-v)}} \times \\
& \times \left((E(\Lambda) - z)^2 - \frac{|k|^2}{4} \right), \quad (50)
\end{aligned}$$

$$\begin{aligned}
C_2(|k|) = & \frac{8}{\pi|k|} \int_0^{Z_\Lambda(|k|)} dz \int_0^{\frac{|k|}{2}z} dv \frac{e^{\beta v}}{1 + e^{\beta(w(k,z)+v)}} \frac{\sinh(\beta w)}{1 + \frac{|k|^2}{4}(1 - z^2)} \times \\
& \times \frac{1}{1 + e^{\beta(v-w(k,z))}} \left(\frac{|k|^2}{4} - v^2 \right) \frac{z}{1 - z^2} \\
+ & \frac{8}{\pi|k|} \int_0^{\frac{|k|}{2}Z_\Lambda(|k|)} dz \int_0^z dv \frac{e^{\beta v}}{1 + e^{\beta(E(\Lambda)-z+v)}} \frac{\sinh(\beta(E(\Lambda) - z))}{E(\Lambda) - z} \times \\
& \times \frac{1}{1 + e^{\beta(v+z-E(\Lambda))}} \left(\frac{|k|^2}{4} - v^2 \right). \quad (51)
\end{aligned}$$

In the above formulas we have used the notation (as in [9])

$$Z_\Lambda(r) = \frac{\sqrt{1 + \Lambda^2} - \sqrt{1 + (\Lambda - r)^2}}{r}.$$

Note that Z_Λ is a decreasing C^∞ function on $[0, 2\Lambda]$ satisfying $Z_\Lambda(0) = \Lambda/E(\Lambda)$, $Z_\Lambda(2\Lambda) = 0$. We have also used the shorthand notation

$$w(k, z) = \sqrt{\frac{1 + |k|^2(1 - z^2)/4}{1 - z^2}}.$$

All integrands of the above formulas are real analytic functions of $r = |k|$ on a neighborhood of $[0, 2\Lambda]$. Also all the integrals vanish at $k = 0$. We deduce that C_1 and C_2 are smooth functions on $[0, 2\Lambda]$. Using $Z_\Lambda(2\Lambda) = 0$, one also sees that $C_1(2\Lambda) = C_1'(2\Lambda) = C_2(2\Lambda) = C_2'(2\Lambda) = 0$. A Taylor expansion of the first integral of C_1 yields

$$C_1(0) = \frac{4}{\pi}\beta \int_1^{E(\Lambda)} \frac{t^2 dt}{(1 + e^{-\beta t})(1 + e^{\beta t})} > 0.$$

The end of the proof of Proposition 1 is then the same as in [9, Prop. 17]. First we notice that as $C(r)$ is bounded and has a compact support, b_1 and b_2 are in $L^\infty(\mathbb{R}^3)$. We now prove that they decay at least like $|x|^{-4}$ at infinity meaning that they also belong to $L^1(\mathbb{R}^3)$. To this end we write for $b = b_1$ or $b = b_2$ the inverse Fourier transform in radial coordinates:

$$\forall x \in \mathbb{R}^3 \setminus \{0\}, \quad b(x) = \frac{1}{\sqrt{2\pi}|x|} \int_0^{2\Lambda} (r\widehat{b}(r)) \sin(r|x|) dr. \quad (52)$$

Integrating by parts and using $\widehat{b}(2\Lambda) = \widehat{b}'(2\Lambda) = 0$ yields

$$\forall x \in \mathbb{R}^3 \setminus \{0\}, \quad b(x) = \frac{1}{\sqrt{2\pi}|x|^4} \left(2\Lambda\widehat{b}''(2\Lambda) \cos(2\Lambda|x|) - 2\widehat{b}'(0) - \int_0^{2\Lambda} (r\widehat{b})^{(3)}(r) \cos(r|x|) dr \right). \quad (53)$$

This completes the proof of Proposition 1. \square

3.3 Proof of Theorem 4

The proof is inspired by ideas from [14]. We denote $I := \inf_{\gamma \in \mathcal{A}} \mathcal{T}_T(\gamma)$. We start by introducing the following auxiliary minimization problem

$$J = \inf_{\gamma \in \mathcal{B}} \mathcal{T}_T(\gamma) \quad (54)$$

where $\mathcal{B} \subset \mathcal{A}$ is given by

$$\mathcal{B} := \{\gamma \in \mathcal{A}, \gamma(p) = f_1(|p|)\alpha \cdot p + f_0(|p|)\beta, f_0, f_1 \leq 0\}. \quad (55)$$

Lemma 2. *There exists a minimizer $\tilde{\gamma}^0 \in \mathcal{B}$ for (54).*

Proof of Lemma 2. The functional \mathcal{T}_T is weakly lower semi-continuous for the weak-* topology of $L^\infty(B(0, \Lambda))$. This is because $-S$ is convex and the exchange term is continuous for the weak topology of $L^2(B(0, \Lambda))$ as shown in [14]. Also \mathcal{B} is a bounded closed convex subset of $L^\infty(B(0, \Lambda))$. Hence there exists a minimum. \square

Lemma 3. *Let $\tilde{\gamma}^0 \in \mathcal{B}$ be a minimizer of (54). Then there exists an $\epsilon > 0$ such that $|\tilde{\gamma}^0| \leq 1/2 - \epsilon$.*

Proof. For $x \in [1/2, 1/2]$,

$$s(x) := \left(\frac{1}{2} + x\right) \ln \left(\frac{1}{2} + x\right) + \left(\frac{1}{2} - x\right) \ln \left(\frac{1}{2} - x\right)$$

is an even function of x . Because of the special form of $\tilde{\gamma}^0$, we have $\tilde{\gamma}^0(p)^2 = \|\tilde{\gamma}^0(p)\|^2 I_{\mathbb{C}^4}$ for all $p \in B(0, \Lambda)$, where $\|\cdot\|$ denotes the matrix norm. Hence

$$\forall \gamma \in \mathcal{B}, \quad S(\gamma) = -4 \int_{B(0, \Lambda)} s(\|\gamma(p)\|) dp.$$

The derivative of s is infinite at $x = 1/2$ and the derivative of the terms of the first line of (29) stays bounded. It is therefore clear that $\{p \in B(0, \Lambda) \mid 1/2 - \epsilon \leq \|\tilde{\gamma}^0(p)\| \leq 1/2\}$ has zero measure for ϵ small enough. \square

Let us now write the first order condition satisfied by $\tilde{\gamma}^0$. Since $\|\tilde{\gamma}^0(p)\| \leq 1/2 - \epsilon$ for some ϵ small enough, we can consider a perturbation of the form

$$\gamma(p) = \tilde{\gamma}^0(p) + t(g_1(|p|)\alpha \cdot p + g_0(|p|)\beta)$$

with $g_0, g_1 \leq 0$ and $t > 0$ small enough. We obtain

$$\int_{B(0, \Lambda)} \text{tr}_{\mathbb{C}^4} \left[\left(D_{\tilde{\gamma}^0}(p) + T \ln \frac{1/2 + \tilde{\gamma}^0(p)}{1/2 - \tilde{\gamma}^0(p)} \right) (g_1(|p|)\alpha \cdot p + g_0(|p|)\beta) \right] dp \geq 0 \quad (56)$$

for all $g_1, g_0 \leq 0$.

We notice that the function $x \mapsto \ln \left(\frac{1/2+x}{1/2-x} \right)$ is odd, hence

$$\forall \gamma \in \mathcal{B}, \quad \ln \left(\frac{1/2 + \gamma(p)}{1/2 - \gamma(p)} \right) = \text{sgn}(\gamma) \ln \left(\frac{1/2 + \|\gamma(p)\|}{1/2 - \|\gamma(p)\|} \right), \quad (57)$$

with $\text{sgn}(\gamma) = \gamma/|\gamma|$. We obtain that

$$\ln \left(\frac{1/2 + \tilde{\gamma}^0(p)}{1/2 - \tilde{\gamma}^0(p)} \right) = \tilde{\gamma}^0(p) F(\|\tilde{\gamma}^0(p)\|)$$

where $F(x) = \ln \left(\frac{1/2+x}{1/2-x} \right) / x$. On the other hand, we can write

$$D_{\tilde{\gamma}^0} = d_1(|p|)\alpha \cdot p + d_0(|p|)\beta$$

where d_1 and d_0 are given by [14, Eq. (72)-(73)]. Using $f_1, f_0 \leq 0$, we immediately see that

$$d_1(|p|) \geq 1 \quad \text{and} \quad d_0(|p|) \geq 1, \quad (58)$$

which in particular proves that

$$\|D_{\tilde{\gamma}^0}(p)\| \geq \|D^0(p)\| \geq |p|. \quad (59)$$

All this gives

$$D_{\tilde{\gamma}^0} + T \ln \frac{1/2 + \tilde{\gamma}^0}{1/2 - \tilde{\gamma}^0} = (d_1(|p|) + T f_1(|p|) F(\|\tilde{\gamma}^0(p)\|)) \boldsymbol{\alpha} \cdot p \\ + (d_0(|p|) + T f_0(|p|) F(\|\tilde{\gamma}^0(p)\|)) \beta. \quad (60)$$

Inserting this in (56), we obtain the first order conditions

$$\begin{cases} d_1(|p|) + T f_1(|p|) F(\|\tilde{\gamma}^0(p)\|) \leq 0 \\ d_0(|p|) + T f_0(|p|) F(\|\tilde{\gamma}^0(p)\|) \leq 0. \end{cases} \quad (61)$$

In particular, because of (58) we infer that

$$\begin{cases} f_1(|p|) F(\|\tilde{\gamma}^0(p)\|) \leq -1/T \\ f_0(|p|) F(\|\tilde{\gamma}^0(p)\|) \leq -1/T. \end{cases} \quad (62)$$

As $F(\|\tilde{\gamma}^0(p)\|) \geq 0$ and $f_0 \geq -\|\tilde{\gamma}^0(p)\|$, we obtain from (62) the inequality $|\gamma(p)| F(\|\gamma(p)\|) \geq 1/T$. Hence

$$\|\gamma(p)\| \geq \frac{e^{1/T} - 1}{2(1 + e^{1/T})}. \quad (63)$$

This inequality means that f_0 and f_1 cannot vanish simultaneously. But we can indeed prove that each of them cannot vanish, as expressed in the

Lemma 4. *Let $\tilde{\gamma}^0(p) = f_1(|p|)\boldsymbol{\alpha} \cdot p + f_0(|p|)\beta$ be a minimizer of (54). Then there exists an $\epsilon > 0$ such that*

$$f_0 \leq -\epsilon \quad \text{and} \quad f_1 \leq -\epsilon.$$

Proof. By Lemma 3 we know that $\|\tilde{\gamma}^0(p)\| \leq 1/2 - \epsilon$ for some $\epsilon > 0$. By (62) and the monotonicity of F we obtain $f_k \leq -\frac{1}{T F(1/2 - \epsilon)}$ for $k = 0, 1$. \square

Lemma 5. *Let $\tilde{\gamma}^0 \in \mathcal{B}$ be a minimizer of (54). Then it solves the self-consistent equation*

$$\tilde{\gamma}^0 = \frac{1}{2} \left(\frac{1}{1 + e^{\beta D_{\tilde{\gamma}^0}}} - \frac{1}{1 + e^{-\beta D_{\tilde{\gamma}^0}}} \right). \quad (64)$$

Proof. As the constraints are not saturated by Lemmas 3 and 4, we obtain that the derivative vanishes, i.e.

$$\begin{cases} d_1(|p|) + T f_1(|p|) F(\|\tilde{\gamma}^0(p)\|) = 0 \\ d_0(|p|) + T f_0(|p|) F(\|\tilde{\gamma}^0(p)\|) = 0. \end{cases} \quad (65)$$

which means that

$$D_{\tilde{\gamma}^0} + T \ln \frac{1/2 + \tilde{\gamma}^0}{1/2 - \tilde{\gamma}^0} = 0.$$

Hence $\tilde{\gamma}^0$ solves (64). \square

Now we prove that the operator $\tilde{\gamma}^0$ defined in the previous step is the unique minimizer of \mathcal{T}_T on the full space \mathcal{A} defined in (30), not merely on the subset \mathcal{B} in (55). We have

$$\mathcal{T}_T(\gamma) - \mathcal{T}_T(\tilde{\gamma}^0) = TH(\gamma, \tilde{\gamma}^0) - \frac{\alpha}{(2\pi)^5} \iint_{B(0, \Lambda)^2} \frac{\text{tr}_{\mathbb{C}^4}[(\gamma - \tilde{\gamma}^0)(p)(\gamma - \tilde{\gamma}^0)(q)]}{|p - q|^2} dp dq$$

where H is the relative entropy per unit volume

$$\begin{aligned} H(\gamma, \tilde{\gamma}^0) = (2\pi)^{-3} \int_{B(0, \Lambda)} \text{tr}_{\mathbb{C}^4} \left[\left(\frac{1}{2} + \gamma \right) \left(\ln \left(\frac{1}{2} + \gamma \right) - \ln \left(\frac{1}{2} + \tilde{\gamma}^0 \right) \right) \right. \\ \left. + \left(\frac{1}{2} - \gamma \right) \left(\ln \left(\frac{1}{2} - \gamma \right) - \ln \left(\frac{1}{2} - \tilde{\gamma}^0 \right) \right) \right] dp. \end{aligned} \quad (66)$$

We shall use the important

Lemma 6. *For H in (66) the inequality*

$$TH(\gamma, \tilde{\gamma}^0) \geq (2\pi)^{-3} \int_{B(0, \Lambda)} \text{tr}_{\mathbb{C}^4} |D_{\tilde{\gamma}^0}(p)| (\gamma(p) - \tilde{\gamma}^0(p))^2 dp \quad (67)$$

holds for all $\gamma \in \mathcal{A}$.

Proof. This is a simple application of (20), taking $X = \gamma(p)$, $Y = \tilde{\gamma}^0(p)$ and integrating over the ball $B(0, \Lambda)$. \square

Using Lemma 6 and the formula

$$\frac{\alpha}{(2\pi)^2} \iint_{B(0, \Lambda)^2} \frac{\text{tr}_{\mathbb{C}^4}[\gamma(p)\gamma(q)]}{|p - q|^2} dp dq = \frac{\alpha}{2} \int_{\mathbb{R}^3} \frac{\text{tr}_{\mathbb{C}^4} |\check{\gamma}(x)|^2}{|x|} dx$$

where $\check{\gamma}(x)$ is the Fourier inverse of the function $\gamma(p)$, we find

$$\begin{aligned} \mathcal{T}_T(\gamma) - \mathcal{T}_T(\tilde{\gamma}^0) \geq (2\pi)^{-3} \left(\int_{B(0, \Lambda)} \text{tr}_{\mathbb{C}^4} |D_{\tilde{\gamma}^0}(p)| (\gamma(p) - \tilde{\gamma}^0(p))^2 dp \right. \\ \left. - \frac{\alpha}{2} \int_{\mathbb{R}^3} \frac{\text{tr}_{\mathbb{C}^4} |(\check{\gamma} - \check{\gamma}^0)(x)|^2}{|x|} dx \right) \end{aligned} \quad (68)$$

for all $\gamma \in \mathcal{A}$. We now use ideas of [1, 10, 14]. Kato's inequality $|x|^{-1} \leq \pi/2|\nabla|$ gives

$$\frac{\alpha}{2} \int_{\mathbb{R}^3} \frac{\operatorname{tr}_{\mathbb{C}^4} |(\tilde{\gamma} - \tilde{\gamma}^0)(x)|^2}{|x|} dx \leq \frac{\alpha\pi}{4} \int_{B(0,\Lambda)} \operatorname{tr}_{\mathbb{C}^4} |p|(\gamma(p) - \tilde{\gamma}^0(p))^2 dp.$$

By (59) we deduce

$$\mathcal{T}_T(\gamma) - \mathcal{T}_T(\tilde{\gamma}^0) \geq (1 - \pi\alpha/4)(2\pi)^{-3} \int_{B(0,\Lambda)} \operatorname{tr}_{\mathbb{C}^4} |D_{\tilde{\gamma}^0}(p)|(\gamma(p) - \tilde{\gamma}^0(p))^2 dp.$$

Hence $\tilde{\gamma}^0$ is the unique minimizer of \mathcal{T}_T on \mathcal{A} when $0 \leq \alpha < 4/\pi$. This completes the proof of Theorem 4. \square

3.4 Proof of Theorem 5

The lower bound (37) is obtained by following an argument of [1, 10]. By (36) we have for all $\gamma \in \tilde{\mathcal{K}}_C$

$$\begin{aligned} \mathcal{F}_T(\gamma) &\geq \operatorname{tr} (|D_{\tilde{\gamma}^0}|(\gamma - \tilde{\gamma}^0)^2) - \frac{\alpha}{2} \iint \frac{\operatorname{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|} dx dy \\ &\quad + \frac{\alpha}{2} D(\rho_{\gamma - \tilde{\gamma}^0} - \nu, \rho_{\gamma - \tilde{\gamma}^0} - \nu) - \frac{\alpha}{2} D(\nu, \nu). \end{aligned} \quad (69)$$

By (33) together with Kato's inequality $|x|^{-1} \leq (\pi/2)|\nabla| \leq (\pi/2)|D^0|$,

$$\iint \frac{\operatorname{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|} dx dy \leq \frac{\pi}{2} \operatorname{tr} (|D_{\tilde{\gamma}^0}|(\gamma - \tilde{\gamma}^0)^2)$$

which yields (37) when $0 \leq \alpha < 4/\pi$.

Assume now that γ is a minimizer of \mathcal{F}_T on $\tilde{\mathcal{K}}_C$. The proof that it satisfies the self-consistent equation (38) is the same as in the case of the reduced BDF functional in Section 1.2. Note that because of (69) and $\inf_{\tilde{\mathcal{K}}_C} \mathcal{F}_T \leq 0$, we obtain

$$\left(\frac{2}{\pi} - \frac{\alpha}{2}\right) \iint \frac{\operatorname{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|} dx dy + \frac{\alpha}{2} D(\rho_{\gamma - \tilde{\gamma}^0}, \rho_{\gamma - \tilde{\gamma}^0}) \leq \frac{\alpha}{2} D(\nu, \nu).$$

It was proved in [11, p. 4495] that this implies (under the condition (39)) that

$$|D_\gamma| \geq d^{-1}|D^0| \quad (70)$$

with

$$d = \left\{ 1 - \alpha \left(\frac{\pi}{2} \sqrt{\frac{\alpha/2}{1 - \alpha\pi/4}} + \pi^{1/6} 2^{11/6} \right) D(\nu, \nu)^{1/2} \right\}^{-1}.$$

Next we fix some $\gamma' \in \tilde{\mathcal{K}}_C$ and use that

$$H(\gamma', \tilde{\gamma}^0) = H(\gamma, \tilde{\gamma}^0) + H(\gamma', \gamma) + \text{tr} \left[(\gamma' - \gamma) \left(\ln \left(\frac{\frac{1}{2} + \gamma}{\frac{1}{2} - \gamma} \right) - \ln \left(\frac{\frac{1}{2} + \tilde{\gamma}^0}{\frac{1}{2} - \tilde{\gamma}^0} \right) \right) \right]. \quad (71)$$

Inserting Eq. (38) for our minimizer γ and Eq. (31) for $\tilde{\gamma}^0$, we obtain for any $\gamma' \in \tilde{\mathcal{K}}_C$ the formula

$$\mathcal{F}_T(\gamma') = \mathcal{F}_T(\gamma) + TH(\gamma', \gamma) + \frac{\alpha}{2} D(\rho_{\gamma' - \gamma}, \rho_{\gamma' - \gamma}) - \frac{\alpha}{2} \iint \frac{\text{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|} dx dy. \quad (72)$$

We may use one more time (15) and the self-consistent equation (38) to obtain

$$TH(\gamma', \gamma) \geq \text{tr} (|D_\gamma|(\gamma' - \gamma)^2).$$

By (70) and Kato's inequality as before, we eventually get

$$\mathcal{F}_T(\gamma') \geq \mathcal{F}_T(\gamma) + \frac{\alpha}{2} D(\rho_{\gamma' - \gamma}, \rho_{\gamma' - \gamma}) + \left(\frac{2}{\pi d} - \frac{\alpha}{2} \right) \iint \frac{\text{tr}_{\mathbb{C}^4} |(\gamma - \tilde{\gamma}^0)(x, y)|^2}{|x - y|} dx dy.$$

Hence we obtain that any minimizer is unique when $\alpha\pi d/4 \leq 1$, as stated. Let us remark that the expression in last term of (71) is indeed a trace-class operator. It would, however, have been sufficient to choose γ' as trace class perturbation of γ^0 and conclude the rest by a density argument. \square

A Appendix: Integral Representation of Relative Entropy

Here we shall prove the claim made in Section 1.1 that (14) and (16) coincide as long as $\gamma - \gamma^0 \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and the spectrum of γ^0 does not contain $\pm 1/2$.

From the integral representation (15), we have

$$a(\ln a - \ln b) = \int_0^\infty \frac{a}{a+t} (a-b) \frac{1}{b+t} dt.$$

We split the first factor as

$$\frac{a}{a+t} = \frac{b}{b+t} + \frac{t}{b+t} (a-b) \frac{1}{a+t}$$

and obtain

$$a(\ln a - \ln b) = \int_0^\infty \frac{t}{b+t} (a-b) \frac{1}{a+t} (a-b) \frac{1}{b+t} dt + \int_0^\infty \frac{b}{b+t} (a-b) \frac{1}{b+t} dt.$$

Now if $a - b$ is trace class and the spectrum of b is contained in $(0, \infty)$, then

$$\operatorname{tr} \int_0^\infty \frac{b}{b+t} (a-b) \frac{1}{b+t} dt = \operatorname{tr} \int_0^\infty (a-b) \frac{b}{(b+t)^2} dt = \operatorname{tr}(a-b).$$

If we apply this reasoning to $a = 1/2 + \gamma$, $b = 1/2 + \gamma^0$ and to $a = 1/2 - \gamma$ and $b = 1/2 - \gamma^0$, respectively, we thus obtain

$$\begin{aligned} H(\gamma, \gamma^0) = \operatorname{tr} & \left(\int_0^\infty \frac{t}{\frac{1}{2} + \gamma + t} (\gamma - \gamma^0) \frac{1}{\frac{1}{2} + \gamma^0 + t} (\gamma - \gamma^0) \frac{1}{\frac{1}{2} + \gamma^0 + t} dt \right. \\ & \left. + \int_0^\infty \frac{t}{\frac{1}{2} - \gamma + t} (\gamma - \gamma^0) \frac{1}{\frac{1}{2} - \gamma^0 + t} (\gamma - \gamma^0) \frac{1}{\frac{1}{2} - \gamma^0 + t} dt \right) \end{aligned}$$

Changing variables from t to $u = 1/(1 + 2t)$ in the first integral and $u = -1/(1 + 2t)$ in the second integral, respectively, we arrive at the integral representation (16).

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