Multiparticle equations for interacting Dirac fermions in magnetically confined graphene quantum dots

2010 J. Phys. A: Math. Theor. 43 215202

(http://iopscience.iop.org/1751-8121/43/21/215202)

IOP PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND THEORETICAL

J. Phys. A: Math. Theor. **43** (2010) 215202 (18pp) doi:10.1088/1751-8113/43/21/215202

Multiparticle equations for interacting Dirac fermions in magnetically confined graphene quantum dots

Reinhold Egger[1], Alessandro De Martino[2], Heinz Siedentop[3] and Edgardo Stockmeyer[3]

[1] Institut für Theoretische Physik, Heinrich-Heine-Universität, Universitätsstraße 1, D-40225 Düsseldorf, Germany
[2] Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany
[3] Mathematisches Institut, Ludwigs-Maximilians-Universität München, Theresienstraße 39, D-80333 München, Germany

E-mail: egger@thphy.uni-duesseldorf.de, ademarti@thp.uni-koeln.de, h.s@lmu.de and stock@math.lmu.de

Received 20 January 2010, in final form 31 March 2010
Published 4 May 2010
Online at stacks.iop.org/JPhysA/43/215202

Abstract
We study the energy of quasi-particles in graphene within the Hartree–Fock approximation. The quasi-particles are confined via an inhomogeneous magnetic field and interact via the Coulomb potential. We show that the associated functional has a minimizer and determines the stability conditions for the N-particle problem in such a graphene quantum dot.

PACS numbers: 03.65.Pm, 73.22.Pr, 71.15.Rf

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The electronic properties of graphene—a two-dimensional monolayer of graphite made of carbon atoms only—have recently attracted a lot of interest [1–3]. For energies close to the charge neutrality point, noninteracting quasi-particles in graphene (henceforth called 'electrons') are well described by the Dirac–Weyl Hamiltonian of massless relativistic fermions. This suggests an easily accessible condensed-matter realization of relativistic quantum mechanics. Recent interest has turned to Coulomb interaction effects, in particular to the case when N electrons are confined to a finite region (a so-called quantum dot) in the graphene layer. Using electrostatic confinement potentials, such Coulomb-correlated artificial atoms have been studied in detail for the two-dimensional electron gas in semiconductors [4], where the non-relativistic Schrödinger equation describes the single-particle sector. In graphene, however, the Klein tunneling phenomenon [2] of relativistic Dirac fermions renders

the standard electrostatic confinement method experimentally difficult or even impossible to apply, and usually only resonances can be expected [5–9]. As an alternative, confinement by inhomogeneous orbital magnetic fields has been suggested [10], and the electronic structure of two interacting electrons in such a magnetic quantum dot in graphene was recently studied using exact diagonalization [11]. Experimentally, up to now, lithographically fabricated quantum dots were mostly studied [12], where the boundary is rather disordered, the confinement potential cannot be tuned and a detailed comparison of experimental data to theory is difficult. On the other hand, inhomogeneous magnetic fields have been experimentally generated and studied in semiconductor devices by using suitable lithographically deposited ferromagnetic layers [13], and the generalization to graphene should pose no fundamental obstacle. Concrete experimentally relevant profiles for quantum dot confinement by such fields were also theoretically studied in [14]. We note that an artificial vector potential giving rise to the same mathematical model can also be generated by applying mechanical forces, producing appropriate strain in the sample [2, 3].

In this paper, given the widespread interest in understanding and usefully employing the electronic structure of graphene quantum dots, we address the definition and the stability of the relativistic interacting N-particle system in such a magnetic graphene dot, primarily from a mathematically oriented perspective. To that end, we analyze in detail the Hartree–Fock functional and show that under certain conditions, a minimizer exists. The maximum number N_c of particles is computed and shown to depend on the interaction strength. When $N \leqslant N_c$ we solve the Hartree–Fock equations numerically. For $N > N_c$, no minimizer with a particle number N exists. The excess particles are not localized and appear, numerically, occupying bulk Landau states centered far away from the dot region to lower the repulsive interaction energy.

It is well known that for relativistic N-particle problems, the presence of interactions implies that one should use a projection scheme [15–17], whose integrity for graphene dots—despite the fact that bulk graphene corresponds to a gapless model—has been shown in [11]. At first sight, an inclusion of the entire Dirac sea along the more fundamental lines of Hainzl *et al* (see [18] and the references therein) might seem desirable. However, this would complicate matters unduly, since—after all—the description of graphene by a two-dimensional Dirac equation emerges from a non-relativistic band structure calculation. Moreover, in the presence of a finite gap separating occupied and empty states—which is the case below—it is not only reasonable to freeze the Dirac sea as given by the external field (Furry picture), but also to assume that no electron–positron pairs are created. It should be remarked that this strategy is not only supported by [11] but is a standard procedure in quantum chemistry [19]. Because of this we will limit this work to the no-pair model, more precisely to the no-pair model in the Furry picture with the given electron number N.

In this model, the electronic states of graphene in the presence of a magnetic field $\nabla \times \tilde{\mathbf{A}}$ are the unit vectors in $\chi_{(0,\infty)}\big(v\boldsymbol{\sigma}\cdot\big(-\mathrm{i}\hbar\nabla+\frac{e}{c}\tilde{\mathbf{A}}\big)\big)[L^2(\mathbb{R}^2:\mathbb{C}^2)]$, where $\tilde{\mathbf{A}}$ is the magnetic vector potential, v is the Fermi velocity in graphene, $\boldsymbol{\sigma} = (\sigma_1, \sigma_2)$ are the first two Pauli matrices, $-e < 0$ is the charge of the electron and $\hbar$ is the Planck constant. We introduce convenient units by scaling the momentum $\mathbf{p} \mapsto \mathbf{p}/(v\hbar)$ and the coordinates $\mathbf{x} \mapsto v\hbar\mathbf{x}$, which generates a unitary transform. N Coulomb-interacting electrons in graphene are then formally described by the Hamiltonian

$$\sum_{n=1}^{N}[\boldsymbol{\sigma}_n\cdot(\mathbf{p}_n+\mathbf{A}(\mathbf{x}_n))-\varphi(\mathbf{x}_n)]+\sum_{1\leqslant m<n\leqslant N}\frac{\alpha}{|\mathbf{x}_m-\mathbf{x}_n|} \tag{1}$$

projected onto the antisymmetric tensor product of the above space. Here $\mathbf{A}(\mathbf{x}) := (ev/c)\tilde{\mathbf{A}}(v\hbar\mathbf{x})$ and we have added an external electrostatic potential φ. The interaction

strength is encoded in the dimensionless fine structure constant $\alpha = e^2/(v\kappa\hbar)$. Physical values in graphene are $0 < \alpha < 2$, with the precise value depending on the dielectric constant κ of the environment (e.g. the substrate on which graphene is deposited). The upper limit for α is approached only for suspended samples. It is well known that quasi-particles in graphene have additional valley ('K point') and electronic spin degrees of freedom. For field configurations that are smooth on the scale of graphene's lattice constant $a_0 = 0.246$ nm, however, no valley mixing is expected, and our simpler description with just one K point and full spin polarization is sufficient [11]. This is the situation considered in our paper. In any case, the generalizations necessary to go beyond the single-spin and the single-valley model (1) are conceptually unproblematic. A similar approach is also expected to apply for magnetic dots in bilayer graphene, where the linear dispersion relation of monolayer graphene is modified [2].

The outline of the remainder of this paper is as follows. In section 2, we specify and explain the mathematical model. In section 3, the Hartree–Fock functional is considered, and we prove the existence of a minimizer. For the benefit of the mathematically oriented reader, we have included all proofs in detail. To make the abstract discussion in section 3 concrete, we describe a specific magnetic field profile $\mathbf{A}(\mathbf{x})$ in section 4, modeling a circular magnetic dot of radius R around the origin. The confinement here is generated by a constant magnetic field B for $r > R$ but a zero field for $r < R$. The relativistic interacting N-particle problem for a magnetic dot in graphene is then studied for this field profile in section 4 by numerically solving the Hartree–Fock equations discussed in section 3. This calculation also yields quantitative predictions concerning the stability of the N-electron system. We conclude with an outlook in section 5. Some technical details have been relegated to two appendices.

2. Model

To describe the physical situation where electrons are bound to a magnetic quantum dot, the magnetic vector potential $\mathbf{A} = \mathbf{A}_0 + \mathbf{A}_1$ is expressed as the sum of a homogeneous magnetic field of strength $B > 0$ perpendicular to the graphene plane, $\mathbf{A}_0(\mathbf{x}) = (B/2)(-x_2, x_1)$, and a perturbation $\mathbf{A}_1$. For the total external electromagnetic field $A := (\varphi, \mathbf{A})$, using $\not{\mathbf{p}}_0 := \boldsymbol{\sigma} \cdot (\mathbf{p} + \mathbf{A}_0)$, we define

$$D_A := \not{\mathbf{p}} - \varphi := \boldsymbol{\sigma} \cdot (\mathbf{p} + \mathbf{A}) - \varphi = \not{\mathbf{p}}_0 + P, \tag{2}$$

with the 'perturbation' $P := \boldsymbol{\sigma} \cdot \mathbf{A}_1 - \varphi$. We define the one-electron Hilbert space with respect to A as

$$\mathfrak{H}_A := \Lambda_A^+[L^2(\mathbb{R}^2 : \mathbb{C}^2)], \qquad \Lambda_A^+ := \chi_{(0,\infty)}(D_A). \tag{3}$$

Although more general cases can be treated, we assume for simplicity that P is a bounded operator which is sufficient for the application discussed and minimizes the amount of technical arguments needed. In the same spirit, we require relative compactness of the perturbation[4]

$$P \in \mathfrak{B}(\mathfrak{H}_A) \qquad \text{and} \qquad |P|^{\frac{1}{2}} |\not{\mathbf{p}}_0 - \mu|^{-\frac{1}{2}} \in \mathfrak{S}^\infty(\mathfrak{H}_A). \tag{4}$$

Physically, this means that the perturbing electromagnetic potential decays at infinity and has only moderate singularities whose Fourier coefficients can be controlled by the kinetic energy. At the same time, P is responsible for creating bound states that define the quantum dot.

[4] For $p \in [1, \infty)$, we set $\mathfrak{S}^p(\mathfrak{H}_A) = \{A \in \mathcal{B}(\mathfrak{H}_A) | \mathrm{tr}|A|^p < \infty\}$, and write $\mathfrak{S}^\infty(\mathfrak{H}_A)$ for the space of compact and $\mathfrak{B}(\mathfrak{H}_A)$ for the bounded operators on $\mathfrak{H}_A$.

The energy of an N-particle state $\psi \in \mathcal{S}(\mathbb{R}^{2N} : \mathbb{C}^{2^N}) \cap \mathfrak{H}_{\mathbf{A}}^{(N)}$ [5] is then given by

$$\mathcal{E}(\psi) := \left(\psi, \left[\sum_{n=1}^{N} (D_{A,n} - \mu) + \sum_{1 \leqslant m < n \leqslant N} \frac{\alpha}{|\mathbf{x}_m - \mathbf{x}_n|} \right] \psi \right). \tag{5}$$

Throughout this paper, μ is a positive constant smaller than the first positive eigenvalue (first bulk Landau level) of $\not{\mathbf{p}}_0$. Of course, since μ is just a constant, the energy is shifted merely by $-\mu \operatorname{tr} \gamma$. However, this shift serves an important technical purpose: it will allow us to replace the minimization under the constraint $\operatorname{tr} \gamma \leqslant N$ instead of $\operatorname{tr} \gamma = N$. If the minimizer γ has a trace N, then the problem with the N electron constraints has been solved. Note that it may happen that the trace of the minimizer, $\operatorname{tr} \gamma$, stays always below some n_c, even if μ is close to the Landau level. Then the smallest such n_c—call it N_c—is the maximal number of electrons which can be captured by the dot, see section 4. For $N > N_c$, there are $N - N_c$ unbound electrons. The case that there is no minimizer with the trace equal to N corresponds exactly to the situation, where those $N - N_c$ electrons float away to infinity and cannot be bounded by the dot.

Form (5) is obviously bounded from below and closable. This allows us to define the Hamiltonian B_A as its Friedrichs extension. The Friedrichs extension is the canonical way to construct a self-adjoint Hamiltonian out of a symmetric operator which is bounded from below, see, e.g. [20, Satz 4.15] or [21, theorem X.23].

3. The Hartree–Fock functional

3.1. The Hartree–Fock functional

We are now interested in the Hartree–Fock approximation for the ground state of the Hamiltonian B_A. The Hartree–Fock method is a standard tool to access interaction effects in atomic, molecular or condensed-matter systems [19, 22]. The Hartree–Fock ground-state energy provides an upper bound for the true ground-state energy corresponding to equation (5), and it can be used to assess the stability of the N-particle problem [23]. We mention that a different variational approach based on the so-called Müller functional can yield lower bounds for the ground-state energy [24, 25], and very useful results can be obtained by combining both methods.

With the above choice for μ, let us denote by d the distance of μ to the nearest spectral point of $\not{\mathbf{p}}_0$. We start our analysis by defining the basic class of operators (γ) that enter the Hartree–Fock functional. In physical terms, γ is the density operator.

Definition 1. *We define the Banach space as*

$$F := \{\gamma \in \mathfrak{B}(\mathfrak{H}_A) | \|\gamma\|_F := \| |\not{\mathbf{p}}_0 - \mu|^{1/2} \gamma |\not{\mathbf{p}}_0 - \mu|^{1/2} \|_1 < \infty, \gamma = \gamma^* \}.$$

Here, as customary, $\|a\|_1 := \operatorname{tr} \sqrt{a^* a}$ denotes the trace norm of the operator a. This definition of F is motivated[6] by the fact that the state represented by γ should have finite kinetic

[5] Here $\mathcal{S}$ denotes the space of Schwartz functions, and $\mathfrak{H}_{\mathbf{A}}^{(N)}$ is the N-fold antisymmetric tensor product of the one-electron Hilbert space $\mathfrak{H}_{\mathbf{A}}$, i.e. the canonical N electron space.

[6] For later use of the Banach–Alaoglu theorem, we also note that

$$F_* := \left\{ \delta \in \mathfrak{B}(\mathfrak{H}_A) \middle| |\not{\mathbf{p}}_0 - \mu|^{-\frac{1}{2}} \delta |\not{\mathbf{p}}_0 - \mu|^{-\frac{1}{2}} \in \mathfrak{S}^{\infty}(\mathfrak{H}_A) \right\}$$

is a Banach space for which F is the dual space. The duality is given naturally as

$$\langle \gamma, \delta \rangle := \operatorname{tr} \left(|\not{\mathbf{p}}_0 - \mu|^{\frac{1}{2}} \gamma |\not{\mathbf{p}}_0 - \mu|^{\frac{1}{2}} |\not{\mathbf{p}}_0 - \mu|^{-\frac{1}{2}} \delta |\not{\mathbf{p}}_0 - \mu|^{-\frac{1}{2}} \right) = \operatorname{tr}(\gamma \delta).$$

energy, finite particle number and real occupation numbers, the latter being the eigenvalues of γ. Note that $\mathfrak{S}^1(\mathfrak{H}_A) \supset F$ since

$$\begin{aligned}\|\gamma\|_F &= \operatorname{tr}\sqrt{|\not{\mathbf{p}}_0 - \mu|^{\frac{1}{2}}\gamma|\not{\mathbf{p}}_0 - \mu|\gamma|\not{\mathbf{p}}_0 - \mu|^{\frac{1}{2}}} \\ &\geqslant d^{\frac{1}{2}}\operatorname{tr}\sqrt{|\not{\mathbf{p}}_0 - \mu|^{\frac{1}{2}}|\gamma||\gamma||\not{\mathbf{p}}_0 - \mu|^{\frac{1}{2}}} \\ &= d^{\frac{1}{2}}\operatorname{tr}\sqrt{|\gamma||\not{\mathbf{p}}_0 - \mu||\gamma|} \geqslant d\operatorname{tr}|\gamma|.\end{aligned}$$

For a given element $\delta \in F$, we denote its eigenvalues by λ_n and its eigenspinors by ξ_n. The associated integral kernel $\delta(x, y)$ is[7]

$$\delta(x, y) := \sum_n \lambda_n \xi_n(x)\overline{\xi_n(y)}. \tag{6}$$

Associated with δ is its one-particle density

$$\rho_\delta(\mathbf{x}) := \sum_{s=1}^{2}\sum_n \lambda_n |\xi_n(x)|^2,$$

its electric potential $\varphi^{(\delta)}(\mathbf{x}) := \int \mathrm{d}\mathbf{y}\, \rho_\delta(\mathbf{y})/|\mathbf{x} - \mathbf{y}|$ and its exchange operator $X^{(\delta)}$ in terms of the integral kernel $X^{(\delta)}(x, y) = \delta(x, y)|\mathbf{x} - \mathbf{y}|^{-1}$. Then $W^{(\delta)} = \varphi^{(\delta)} - X^{(\delta)}$ is the mean field potential, and the Weyl operator associated with δ is

$$h_{\mathrm{HF}}^{(\delta)} := D_A - \mu + \alpha W^{(\delta)}. \tag{7}$$

The Coulomb scalar product is defined as

$$D(\rho, \sigma) := \frac{1}{2}\int_{\mathbb{R}^2} \mathrm{d}\mathbf{x} \int_{\mathbb{R}^2} \mathrm{d}\mathbf{y} \frac{\overline{\rho(\mathbf{x})}\sigma(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|}, \tag{8}$$

and the exchange scalar product for $\gamma, \gamma' \in F$ is

$$X(\gamma, \gamma') := \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}y \frac{\overline{\gamma(x, y)}\gamma'(x, y)}{|\mathbf{x} - \mathbf{y}|}. \tag{9}$$

Indicating the quadratic forms of sesquilinear forms by brackets, e.g. $X(\gamma, \gamma) = X[\gamma]$, we set $Q[\gamma] := D[\rho_\gamma] - X[\gamma]$.

We now discuss inequalities which will allow us to define the Hartree–Fock energy functional.

Lemma 1. *We have*

$$|\mathbf{p} + \mathbf{A}_0| \leqslant |\not{\mathbf{p}}_0| + B^{1/2} \leqslant |\not{\mathbf{p}}_0 - \mu| + \mu + B^{1/2}.$$

Proof. We have

$$(\psi, (\mathbf{p} + \mathbf{A}_0)^2\psi) \leqslant (\psi, ((\mathbf{p} + \mathbf{A}_0)^2 + \boldsymbol{\sigma}\cdot\mathbf{B} + B)\psi) = (\psi, (\not{\mathbf{p}}_0^2 + B)\psi).$$

Using that the root is operator monotone and $\sqrt{\not{\mathbf{p}}_0^2 + B} \leqslant |\not{\mathbf{p}}_0| + B^{1/2}$, the first inequality follows. The second inequality is then clear. □

Lemma 2. *Assume that $\gamma, |\gamma'| \in F$. Then*

$$|D(\rho_\gamma, \rho_{\gamma'})| \leqslant (2h)^{-1}\|\gamma\|_1\big[\||\gamma'|\|_F + \big(\mu + B^{\frac{1}{2}}\big)\|\gamma'\|_1\big], \tag{10}$$

[7] We use the notation $x = (\mathbf{x}, s)$ for an element of $G := \mathbb{R}^2 \times \{1, 2\}$ and $\mathrm{d}x$ for the product of the Lebesgue measure on $\mathbb{R}^2$ with the counting measure in $\{1, 2\}$.

$$|X(\gamma,\gamma')| \leqslant D(\rho_{|\gamma|},\rho_{|\gamma'|}). \tag{11}$$

Proof. Expanding γ and γ' in eigenfunctions, see equation (6), we get by the Schwarz inequality

$$\begin{aligned}
&\left|\iint \frac{\overline{\gamma(x,y)}\gamma'(x,y)}{|\mathbf{x}-\mathbf{y}|}\,\mathrm{d}x\,\mathrm{d}y\right| \\
&\quad= \left|\iint \sum_\mu \lambda_\mu \sum_\nu \lambda'_\nu \frac{\overline{\xi_\mu(x)}\xi_\mu(y)\xi'_\nu(x)\overline{\xi'_\nu(y)}}{|\mathbf{x}-\mathbf{y}|}\,\mathrm{d}x\,\mathrm{d}y\right| \\
&\quad\leqslant \iint \frac{\sum_\mu |\lambda_\mu||\xi_\mu(x)|^2 \sum_\nu |\lambda'_\nu||\xi'_\nu(y)|^2}{|\mathbf{x}-\mathbf{y}|}\,\mathrm{d}x\,\mathrm{d}y \\
&\quad= \int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \frac{\rho_{|\gamma|}(\mathbf{x})\rho_{|\gamma'|}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{y},
\end{aligned}$$

which shows equation (11). To prove equation (10), we remark that by Hilbert's inequality in two dimensions, i.e. $|\nabla| \geqslant h|x|^{-1}$ with $h := 4\pi^2/(\Gamma(1/4))^4$, and the diamagnetic inequality [26], we have

$$\int \mathrm{d}x|\xi_\mu(x)|^2 \int \mathrm{d}y \frac{|\xi'_\nu(y)|^2}{|\mathbf{x}-\mathbf{y}|} \leqslant h^{-1}(\xi'_\nu, |-\mathrm{i}\nabla + \mathbf{A}_0|\xi'_\nu). \tag{12}$$

The claimed bound follows now by multiplication with $|\lambda_\mu\lambda'_\nu|$ and summation over μ and ν. □

We note that because of equation (10) and lemma 1:

Lemma 3. *For $\gamma \in F$, we have*

$$(2h)^{-1}\|\gamma\|_1[\|\gamma\|_F + (\mu + B^{1/2})\|\gamma\|_1] \geqslant Q[|\gamma|] \geqslant 0.$$

In a mean-field picture, relativistic electrons are described by one-particle density matrices γ with certain additional properties. In particular, since electrons are fermions, they obey the Pauli principle and cannot occupy states in the Dirac sea which is given by the negative spectral subspace of a one-particle Dirac operator $D_{\mathcal{A}}$ with the electromagnetic vector potential $\mathcal{A}$. Mathematically, this is implemented by requiring that $0 \leqslant \gamma \leqslant \Lambda^+_{\mathcal{A}} := \chi_{(0,\infty)}(D_{\mathcal{A}})$. As indicated already above, we will choose $\mathcal{A} := A$, a choice known as the Furry picture. It is then useful to introduce several sets of one-particle density matrices γ for the subsequent discussion.

Definition 2. *We define the following sets of one-particle density matrices for given (maximal) particle number $q \in \mathbb{R}_+$*

$$S^{(A)} := \left\{\gamma \in F \,|\, 0 \leqslant \gamma \leqslant \Lambda^+_A\right\}, \tag{13}$$

$$S^{(A)}_q := \{\gamma \in S^{(A)} \,|\, 0 \leqslant \mathrm{tr}(\gamma) \leqslant q\}, \tag{14}$$

$$S^{(A)}_{\partial q} := \{\gamma \in S^{(A)} \,|\, \mathrm{tr}(\gamma) = q\}. \tag{15}$$

We note that all sets are closed subsets of F. Furthermore, the first two are convex. They are only of technical importance, whereas we are ultimately interested in describing a system with a fixed number of electrons q, i.e. in minimizing the energy over the set $S^{(A)}_{\partial q}$, eventually for

the quantized case $q = N \in \mathbb{N}$. In physical terms, the projection $1 - \Lambda_A^+$ can be interpreted as the one-particle density matrix of the Dirac sea which we consider frozen. The energy of such a system in Hartree–Fock approximation is given by the functional $\mathcal{E} : F \to \mathbb{R}$ as

$$\mathcal{E}(\gamma) = \mathrm{tr}[(D_A - \mu)\gamma] + \alpha Q[\gamma]. \tag{16}$$

The corresponding relativistic model has been successfully used in atomic and molecular physics [15–17, 19]. This projection approach implies that all negative-energy states and the zero modes are occupied, and N additional particles are then added on top of the filled Dirac sea, see also [11].

We now address the mathematical properties of $\mathcal{E}(\gamma)$ in a magnetically confined graphene nanostructure.

Lemma 4. *The energy functional $\mathcal{E}$ is well defined and continuous in the $\|\cdot\|_F$ norm. Furthermore, $\mathcal{E}(\gamma) \geqslant -\mu q$ for $\gamma \in S_q^{(A)}$.*

Proof. The first two claims follow from the definition of the norm, lemma 3. The lower bound is immediate since the only negative term is $-\mu \,\mathrm{tr}\,\gamma$. □

Lemma 5. *The energy functional $\mathcal{E}$ is coercive on $S_q^{(A)}$, i.e. $\mathcal{E}(\gamma_n) \to \infty$ if $\gamma_n \in S_q^{(A)}$ and $\|\gamma_n\|_F \to \infty$.*

Proof. For ψ in the domain of D_A, which equals the one of $\not{p}_0 - \mu$, we have because of the relative compactness of the perturbing term P that

$$\|D_A\psi\| \geqslant \|(\not{p}_0 - \mu)\psi\| - \|P\psi\| \geqslant (1-\epsilon)\|(\not{p}_0 - \mu)\psi\| - M\|\psi\|$$

for an arbitrarily small positive ϵ and some $M \in \mathbb{R}$. Thus, squaring the inequality and taking operator square roots, we get $|D_A| \geqslant c_1|\not{p}_0 - \mu| - c_2$ for some positive constants c_1 and c_2. Thus, for $\gamma \in S^{(A)}$,

$$\mathrm{tr}[(D_A - \mu)\gamma] = \mathrm{tr}((|D_A| - \mu)\gamma) \geqslant c_1\|\gamma\|_F - (c_2 + \mu)q,$$

which implies the coercivity, since Q is non-negative on $S^{(A)}$. □

In order to fulfill the relative compactness requirement (4), it is in fact sufficient to show relative compactness with respect to the free Weyl operator (without the magnetic field). Since the following discussion does not rely on this result, it has been relegated to the appendices.

3.2. Minimization of the energy

We now follow Barbaroux *et al* [27] and wish to show the existence of a minimizer for the Hartree–Fock energy functional (16). Here we will consider only particle numbers q which are so small that always

$$\inf \mathcal{E}\big(S_q^{(A)}\big) = \inf \mathcal{E}\big(S_{\partial q}^{(A)}\big), \tag{17}$$

i.e. the magnetic dot is not yet saturated with electrons. Our proof strategy is standard: first we show that it is enough to minimize over density matrices of finite rank and then we show that there is a projection with the same particle number yielding a lower energy unless it is itself a projection. Moreover, the particle number is automatically quantized so that it is enough to require $q \in \mathbb{N}$. Equation (17) thus corresponds to the case $N \leqslant N_c$ discussed in the introduction. Finally, the existence of a minimizer follows from a compactness argument. Let us now go through the steps of the proof.

3.2.1. Reduction to density matrices with a finite spectrum.

Lemma 6. *Assume $\gamma \in S^{(A)}_{\partial q}$. Then there exists a sequence of finite rank density matrices $\gamma_K \in S^{(A)}_{\partial q}$ such that $\|\gamma_K - \gamma\|_F \to 0$ as $K \to \infty$.*

Proof. Let $\xi_k, k \in \mathbb{N}$ be a complete set of eigenfunctions of γ. If all eigenvalues are 0 or 1, the claim is immediate because then γ is of finite rank itself, and γ is the trace class. Thus, we can assume that there is an eigenvalue $\lambda_n \in (0, 1)$. Now set $\epsilon_K := q - \sum_{k=1}^{K} \lambda_k$. Then ϵ_K is a non-negative monotone decreasing sequence tending to zero. Define $\gamma_K := \sum_{k=1}^{K} \lambda_k |\xi_k\rangle\langle\xi_k| + \epsilon_K |\xi_n\rangle\langle\xi_n|$. We now assume $n \leqslant K$ and K so big that $\lambda_n + \epsilon_K < 1$. Obviously, $0 \leqslant \gamma_K \in S^{(A)}_{\partial q}$ and each γ_K has a finite rank. We now show that $\gamma_K \to \gamma$ in the F-norm as $K \to \infty$. We have

$$\gamma - \gamma_K = \sum_{k=K+1}^{\infty} \lambda_k |\xi_k\rangle\langle\xi_k| - \epsilon_K |\xi_n\rangle\langle\xi_n|.$$

Thus, we obtain

$$\|\gamma - \gamma_K\|_F \leqslant \sum_{k=K+1}^{\infty} \lambda_k \operatorname{tr}(|\not{p} - \mu||\xi_k\rangle\langle\xi_k|) + \epsilon_K (\xi_n, |\not{p} - \mu|\xi_n).$$

The first term tends to zero since $|\not{p} - \mu|^{1/2} \gamma |\not{p} - \mu|^{1/2} \in \mathfrak{S}_1(\mathfrak{H}_A)$, and the second tends to zero since $\epsilon_K \to 0$. □

The following is an immediate consequence of the continuity of $\mathcal{E}$ in the F-norm and the preceding density result.

Corollary 1. *Assume that $q > 0$. Then*

$$\inf \mathcal{E}_\mu\big(S^{(A)}_{\partial q}\big) = \inf \big\{\mathcal{E}_\mu(\gamma) | \gamma \in S^{(A)}_{\partial q}, \operatorname{rank}(\gamma) < \infty\big\}.$$

3.2.2. Reduction to projection. In the following we assume $q \geqslant 0$. As customary, $[q] := \max\{k \in \mathbb{Z} | k \leqslant q\}$ denotes the integer part of q, and we set $\epsilon_q := q - [q]$. Following the lines of Bach [28], we get the following.

Lemma 7. *Assume $0 \leqslant \gamma \in S^{(A)}_{\partial q}$ with a finite rank. Then there exists a projection $\Lambda \in S^{(A)}_{\partial [q]}$ and a self-adjoint rank 1 operator R with $\Lambda R = 0$ and $\operatorname{tr} R = \epsilon_q$ such that*

$$\mathcal{E}(\Lambda + R) \leqslant \mathcal{E}(\gamma).$$

Equality holds only if γ is already of that form.

Proof. Suppose that γ is not of that form. Then there exist at least two eigenvalues λ, $\lambda' \in (0, 1)$ of γ; we denote the corresponding normalized eigenvectors by u and v. We set $\tilde{\gamma} := \gamma + \epsilon S$, where $S := |u\rangle\langle u| - |v\rangle\langle v|$. Note that $\tilde{\gamma} \in S^{A}_{\partial q}$ as long as $0 \leqslant \lambda + \epsilon \leqslant 1$ and $0 \leqslant \lambda' - \epsilon \leqslant 1$, which is the case for ϵ in the neighborhood of zero. We get

$$\mathcal{E}(\tilde{\gamma}) - \mathcal{E}(\gamma) = \epsilon[\operatorname{tr}(D_A S) + 2\Re Q(\gamma, S)] + \epsilon^2 Q(S, S).$$

By explicit computation and use of the Schwarz inequality, we find $Q(S, S) < 0$, since S is the difference of two orthogonal rank 1 projections. Now—depending on the sign of the coefficient linear in ϵ—we lower the energy by increasing or decreasing ϵ from zero, until one of the constraints $0 \leqslant \lambda + \epsilon, \lambda' - \epsilon \leqslant 1$ forbids any further increase or decrease of ϵ. This process leaves all the eigenvalues of γ unchanged except for λ and λ', one of which becomes either 0 or 1. Since there are only finitely many eigenvalues of γ strictly between 0 and 1, even if they are counted according to their multiplicity, iterating this process eliminates all eigenvalues that are strictly between 0 and 1, i.e. we have found a density matrix Λ such that $\Lambda^2 = \Lambda$. □

3.2.3. Criterion for maximal charge.

Lemma 8. *Assume that for* $\gamma \in S_q^{(A)}$ *with* $\operatorname{tr}\gamma < q$, *the operator* $\Lambda_A^+ h_{\mathrm{HF}}^{(\gamma)} \Lambda_A^+$ *has at least* q *negative eigenvalues. Then*

$$\inf \mathcal{E}\big(S_{\partial q}^{(A)}\big) = \inf \mathcal{E}\big(S_q^{(A)}\big).$$

If in addition $0 \leqslant \tilde{\gamma}$ *is a minimizer of* $\mathcal{E}$ *in* $S_q^{(A)}$, *it follows that* $\operatorname{tr}\tilde{\gamma} = q$.

Proof. That the left-hand side bounds the right-hand side from above is obvious. To prove the converse inequality, we assume that $0 \leqslant \gamma \in S_q^{(A)}$ with $\operatorname{tr}\gamma < q$. By lemma 7, we can assume that γ is a projection Λ plus a rank 1 operator. In particular, the dimension of the range of Λ is at most $[\operatorname{tr}\gamma]$. Since the dimension of the discrete spectral subspace $\mathfrak{X}$ of $\Lambda_A^+ h_{\mathrm{HF}}^{(\gamma)} \Lambda_A^+$ is larger than q, we can find $u \in \mathfrak{X} \cap \Lambda(\mathfrak{H}_A)^\perp$ with $\|u\| \leqslant 1$ and define $\tilde{\gamma} := \gamma + \omega$ with $\omega := |u\rangle\langle u|$. We then get

$$\mathcal{E}(\gamma + \omega) - \mathcal{E}(\gamma) = \operatorname{tr}[(D_A - \mu)\omega] + 2\Re Q(\gamma, \omega) = \big\langle u, h_{\mathrm{HF}}^{(\gamma)} u\big\rangle < 0.$$

Therefore, this construction yields a density matrix $\tilde{\gamma}$ with strictly smaller energy and a trace that can be made larger by $\min\{1, q - \operatorname{tr}\gamma\}$. Iteration of the construction yields the desired result. This proves both claims. □

3.2.4. Existence of a minimizer. We now show the existence of a minimizer by weak lower semi-continuity of the functional on a minimizing sequence and weak compactness. This has been addressed by Lieb and Simon [29] in the context of orbitals in the non-relativistic setting. For density matrices, it was addressed by Solovej [30] in the non-relativistic context, and by Barbaroux *et al* [27] for relativistic systems.

Theorem 1. *Assume* $0 \leqslant q$ *and let* μ *be in the intersection of the resolvent set of* D_A *and the interval* $(0, l_1)$, *where* l_1 *is the first positive eigenvalue of* $\not{p}_0$. *Then there exists* $\gamma \in S_q^{(A)}$ *such that*

$$\mathcal{E}(\gamma) = \inf \mathcal{E}\left(S_q^{(A)}\right).$$

Moreover, $\gamma = \Lambda + |\xi\rangle\langle\xi|$ *with* Λ *a projection,* $\Lambda\xi = 0$, *and* $\|\xi\| < 1$.

Proof. Let γ_n be a minimizing sequence in $S_q^{(A)}$, i.e. $\mathcal{E}(\gamma_n)$ converges to $\inf \mathcal{E}\left(S_q^{(A)}\right)$. Because of the coercivity of $\mathcal{E}$ on $S_q^{(A)}$ (lemma 5), the sequence γ_n is bounded in F. Thus, according to Banach and Alaoglu, γ_n—if necessary by extracting a subsequence—converges in the weak-$*$ topology, i.e. there exist $\gamma_\infty \in F$ such that for all compact K, we have

$$\operatorname{tr}(K|\not{p}_0 - \mu|^{1/2}\gamma_n|\not{p}_0 - \mu|^{1/2}) \to \operatorname{tr}(K|\not{p}_0 - \mu|^{1/2}\gamma_\infty|\not{p}_0 - \mu|^{1/2}).$$

Since

$$\begin{aligned}\langle\psi, \gamma_\infty\psi\rangle &= \operatorname{tr}(|\not{p}_0 - \mu|^{-1/2}|\psi\rangle\langle\psi||\not{p}_0 - \mu|^{-1/2}|\not{p}_0 - \mu|^{1/2}\gamma_\infty|\not{p}_0 - \mu|^{1/2}) \\ &= \lim_{n\to\infty} \operatorname{tr}(|\not{p}_0 - \mu|^{-1/2}|\psi\rangle\langle\psi||\not{p}_0 - \mu|^{-1/2}|\not{p}_0 - \mu|^{1/2}\gamma_n|\not{p}_0 - \mu|^{1/2}) \\ &= \lim_{n\to\infty} \langle\psi, \gamma_n\psi\rangle \geqslant 0,\end{aligned}$$

we have $\gamma_\infty \geqslant 0$. Similarly, $\gamma_\infty \leqslant \Lambda_A^+$. Picking an orthonormal basis $e_1, e_2, \ldots$, Fatou's lemma gives, possibly under extraction of yet another subsequence,

$$q \geqslant \lim_{n\to\infty} \operatorname{tr}\gamma_n \geqslant \sum_\nu \liminf_{n\to\infty} \operatorname{tr}(|e_\nu\rangle\langle e_\nu|\gamma_n) = \operatorname{tr}\gamma_\infty.$$

Thus, the trace may only decrease. Joining these results shows that $S_q^{(A)}$ is weakly-$*$ closed, i.e. $\gamma_\infty \in S_q^{(A)}$. We now show lower semi-continuity in the weak-$*$ topology. Concerning the one-particle part, we set $\Lambda_0^- := \chi_{(-\infty,0]}(\not{p}_0)$ and compute, for some $\vartheta > 0$ and smaller than the first positive eigenvalue of D_A,

$$\Lambda_0^- \Lambda_A^+ = \int_{\mathbb{R}} \frac{\mathrm{d}\eta}{2\pi} \Lambda_0^- (\not{p}_0 - \vartheta + P + \mathrm{i}\eta)^{-1} P (\not{p}_0 - \vartheta + \mathrm{i}\eta)^{-1}, \tag{18}$$

where we used [31, lemma 5.6] $\operatorname{sgn} H = \pi^{-1} \int_{-\infty}^{\infty} (\mathrm{i}\eta + H)^{-1}\, \mathrm{d}\eta$, meant as the Cauchy principal value

$$\operatorname{sgn}(H) = \frac{1}{\pi} \lim_{r\to\infty} \int_{-r}^{+r} (\mathrm{i}\eta + H)^{-1}\, \mathrm{d}\eta$$

in the strong topology. Equation (18) shows that the product of these two projections is compact, expressing that the orthogonality of the positive and negative spectral subspaces is not perturbed too much by P, see equation (4). Moreover, it is easy to see that $K_A := |\not{p}_0 - \mu|^{1/2} \Lambda_0^- \Lambda_A^+ |\not{p}_0 - \mu|^{-1/2}$ is also compact. We are now in a position to show the lower semi-continuity of the one-particle part:

$$\begin{aligned}
&\liminf_{n\to\infty} \operatorname{tr}[(D_A - \mu)\gamma_n] \\
&\quad = \liminf_{n\to\infty} \operatorname{tr}\big[(\not{p}_0 - \mu)\gamma_n + |\not{p}_0 - \mu|^{-\frac{1}{2}} P |\not{p}_0 - \mu|^{-\frac{1}{2}} |\not{p}_0 - \mu|^{\frac{1}{2}} \gamma_n |\not{p}_0 - \mu|^{\frac{1}{2}}\big] \\
&\quad = \liminf_{n\to\infty} \operatorname{tr}(|\not{p}_0 - \mu|^{1/2} \gamma_n |\not{p}_0 - \mu|^{1/2}) \\
&\qquad - 2\operatorname{tr}(K_A^* K_A |\not{p}_0 - \mu|^{1/2} \gamma_\infty |\not{p}_0 - \mu|^{1/2}) + \operatorname{tr}(P\gamma_\infty).
\end{aligned} \tag{19}$$

Now, using Fatou's lemma and picking an orthonormal basis $e_1, e_2, \ldots$, we have for the first summand

$$\begin{aligned}
&\liminf_{n\to\infty} \operatorname{tr}(|\not{p}_0 - \mu|^{1/2} \gamma_n |\not{p}_0 - \mu|^{1/2}) \\
&\quad = \liminf_{n\to\infty} \sum_\nu \operatorname{tr}[|e_\nu\rangle\langle e_\nu| |\not{p}_0 - \mu|^{1/2} \gamma_n |\not{p}_0 - \mu|^{1/2}] \\
&\quad \geqslant \sum_\nu \liminf_{n\to\infty} \operatorname{tr}[|e_\nu\rangle\langle e_\nu| |\not{p}_0 - \mu|^{1/2} \gamma_n |\not{p}_0 - \mu|^{1/2}] = \|\gamma_\infty\|_F.
\end{aligned}$$

Inserting this into the last line of equation (19) and undoing the first steps again gives the desired bound $\liminf_{n\to\infty} \operatorname{tr}[(D_A - \mu)\gamma_n] \geqslant \operatorname{tr}[(D_A - \mu)\gamma_\infty]$. It remains to show the lower semi-continuity of the interaction part which is quadratic in the density matrix. Although it is quadratic and positive on $S_q^{(A)}$, it is not a positive quadratic form on a vector space, i.e. its lower semi-continuity does not follow immediately from the Schwarz inequality. However, we can proceed as follows. First, we note that there is some constant C such that $C \geqslant \|\gamma_n\|_F = \sum_\nu \big(\xi_\nu^{(n)}, |\not{p}_0 - \mu| \xi_\nu^{(n)}\big)$, where the $\xi_\nu^{(n)}$ are the eigenfunctions of γ_n with $\|\xi_\nu^{(n)}\| \leqslant 1$. Because of corollary 1 and lemma 7, we can assume that the sum contains at most $[q] + 1$ summands. Thus, by lemma 10, also the standard Sobolev norm of $\chi \xi_\nu^{(n)}$ is bounded uniformly in n (and ν) for any C_0^∞ function χ. Thus, possibly by extracting another subsequence, we can assume that the $\xi_\nu^{(n)} \chi$ converge weakly in the $H^{1/2}$ norm to $\xi_1, \ldots, \xi_{[q]+1}$. Thus, $\xi_\nu^{(n)}(x) \to \xi_n(x)$ almost everywhere pointwise, see, e.g. [32, theorem 16.1]. The pointwise convergence allows us to use Fatou's lemma to show that

$$\liminf_{n\to\infty} Q[\gamma_n] \geqslant Q[|\xi_1\rangle\langle\xi_1| + \cdots + |\xi_{[q]+1}\rangle\langle\xi_{[q]+1}|].$$

We note that the ways of taking the limits—pointwise and in the weak-$*$ sense—agree, i.e. the pointwise limit of $\sum_\nu \xi_\nu^{(n)}(x) \overline{\xi_\nu^{(n)}(y)}$ is an integral kernel of γ_∞ [27]. □

The critical particle number N_c for which the minimizer γ on $S_N^{(A)}$ has a trace N is certainly positive. Unfortunately, for an arbitrary perturbation P, we have not been able to obtain effective bounds neither from below nor from above for N_c. In the next section, we therefore consider a specific choice for the perturbation P, first proposed in [10], and discuss our results for the numerical solution of the self-consistent Hartree–Fock equations.

4. Numerical results

In this section, we consider a circularly symmetric magnetic dot in graphene, defined by a homogeneous background field B with vector potential $\mathbf{A}_0(\mathbf{x}) = (B/2)(-x_2, x_1)$ and a purely magnetic perturbation $P = \boldsymbol{\sigma} \cdot \mathbf{A}_1$ with

$$\mathbf{A}_1(\mathbf{x}) = -(Br/2)[\Theta(R-r) + (R/r)^2\Theta(r-R)] \begin{pmatrix} -\sin\phi \\ \cos\phi \end{pmatrix}, \tag{20}$$

where $x_1 = r\cos\phi$, $x_2 = r\sin\phi$ and Θ is the Heaviside function. This choice implies that the magnetic field vanishes inside a disk of radius R around the origin, while outside this disk the field is constant and given by B. On a semiclassical level, one can expect bound states inside the disk, built by combining the plane-wave solutions inside the disk with the cyclotron orbit solutions outside the disk. The existence of bound states is shown below, under a fully quantum mechanical approach. Note that single-particle states centered far away from this disk ('magnetic dot') represent spatially localized Landau cyclotron orbits. The dimensionless 'missing flux' $\delta := R^2/2l_B^2$, where $l_B := (c/|eB|)^{1/2}$ is the magnetic length, then controls the number of bound positive-energy single-particle states energetically below the first bulk Landau level. In what follows, all energies are given in units of the first Landau level energy, $\sqrt{2}\hbar v/l_B$.

We solve the interacting problem ($\alpha > 0$) numerically within the self-consistent Hartree–Fock approximation discussed in section 3, with density matrices γ with $\mathrm{tr}(\gamma) = N$ constrained to the Hilbert space spanned by positive single-particle energies. The familiar $\delta = 0$ Landau level energies [2], $\varepsilon_s := \sigma\sqrt{n + (j+1/2)\Theta(j)}$, are expressed in terms of the set $s := (j, n, \sigma)$ of quantum numbers $j \in \mathbb{Z} + 1/2$ (angular momentum), $n \in \mathbb{N}_0$ (radial index), and the conduction/valence band index $\sigma = \pm$. (For $n = 0$ and $j < 0$, only $\sigma = -$ is allowed and spans the zero-energy level $\varepsilon = 0$.) The corresponding single-particle eigenspinor $|s\rangle$ has the spatial representation [10]

$$\Psi_{s=(jn\sigma)}(\xi, \phi) := \langle \mathbf{x}|s\rangle = \frac{\mathrm{e}^{\mathrm{i}j\phi}}{\sqrt{2\pi}} \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\phi/2}\psi_{jn}^{+}(\xi) \\ \mathrm{i}\sigma\, \mathrm{e}^{\mathrm{i}\phi/2}\psi_{jn}^{-}(\xi) \end{pmatrix}, \tag{21}$$

where $\xi := r^2/2l_B^2$ is a dimensionless radial coordinate, and we have $\langle s|s'\rangle = \delta_{ss'}$ with $\int_0^\infty \mathrm{d}\xi\big[\big(\psi_{nj}^{+}\big)^2 + \big(\psi_{nj}^{-}\big)^2\big] = 1$. Using the generalized Laguerre polynomials L_n^k, the Landau states (21) contain the real-valued functions

$$\begin{aligned} \psi_{nj}^{+}(\xi) &= A_{jn}^{+}\xi^{\frac{1}{2}|j-\frac{1}{2}|}\,\mathrm{e}^{-\xi/2}L_{n-\Theta(-j)}^{|j-\frac{1}{2}|}(\xi), \\ \psi_{nj}^{-}(\xi) &= A_{jn}^{-}\xi^{\frac{1}{2}|j+\frac{1}{2}|}\,\mathrm{e}^{-\xi/2}L_{n}^{|j+\frac{1}{2}|}(\xi), \end{aligned} \tag{22}$$

with normalization factors

$$A_{jn}^{+} = \sqrt{\frac{(n-\Theta(-j))!}{2\big(n-\Theta(-j)+\big|j-\frac{1}{2}\big|\big)!}}, \qquad A_{jn}^{-} = \mathrm{sgn}(j)\sqrt{\frac{n!}{2\big(n+\big|j+\frac{1}{2}\big|\big)!}}.$$

For $n = 0$ and $j < 0$, we have $A_{jn}^{+} = 0$ and A_{jn}^{-} has to be multiplied by $\sqrt{2}$.

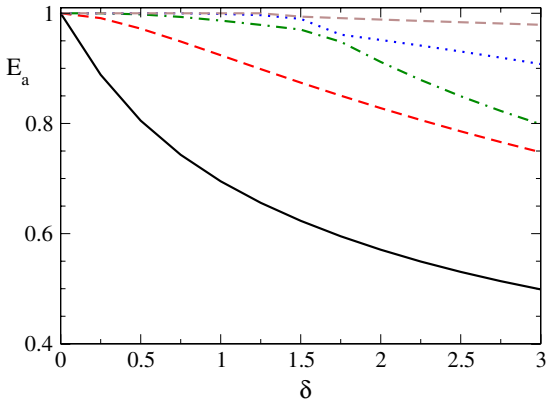

Figure 1. Single-particle spectrum of the circular magnetic dot (20) versus dimensionless missing flux δ. The lowest five positive-energy solutions E_a are shown; E_a is given in units of the first Landau level energy.

It is then straightforward to express the perturbation P in this basis, and to diagonalize the full single-particle problem numerically. Note that j is still a good quantum number, and we label the positive energy solutions $|a\rangle$ with energy E_a by $a = (j, k)$ with $k \in \mathbb{N}$. Numerical diagonalization of the single-particle Hamiltonian yields the orthogonal matrix A in the expansion $|a\rangle = \sum_s A_{s,a}|s\rangle$. Assuming an inert filled Dirac sea, in what follows we only keep states with $E_a > 0$. The zero-energy states are thus included in the filled Dirac sea, i.e. the chemical potential is assumed to be just above zero. The energies E_a are shown as a function of the missing flux δ in figure 1. Bound states correspond to states with energy $0 < E_a < 1$ that are localized near the origin. As shown in [33], there are only finitely many states below μ—note that μ as defined after equation (5) is a constant in $(0, 1)$ which we have not yet specified—whereas there are infinitely many states with energy between μ and 1. These states with energy close to 1 are not localized near the dot and correspond to weakly perturbed Landau states far away from the dot. We will now pick μ such that it implements this intuition. We have checked that under the choice $\mu = 0.99$, all states with $0 < E_a < \mu$ correspond to bound states localized near the dot while those with $\mu < E_a < 1$ correspond to states far away from the dot. From figure 1, we can then read off the number of bound states within the magnetic dot.

Next we address the interacting multiparticle problem, where N electrons are added on top of the filled Dirac sea. With the numerically obtained matrix A, the two-particle interaction matrix elements

$$V_{a_1a_2a_3a_4} := \sum_{s_1,s_2,s_3,s_4} A_{s_1,a_1} A_{s_2,a_2} \tilde{V}_{s_1s_2s_3s_4} A_{s_3,a_3} A_{s_4,a_4}$$

follow from the Landau-state matrix elements

$$\tilde{V}_{s_1s_2s_3s_4} = \frac{\alpha}{\sqrt{2}} \int \frac{\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{x}'}{|\mathbf{x}-\mathbf{x}'|} \left(\Psi^\dagger_{s_4} \cdot \Psi_{s_1}\right)(\mathbf{x}) \left(\Psi^\dagger_{s_3} \cdot \Psi_{s_2}\right)(\mathbf{x}'), \tag{23}$$

where $s_i = (j_i, n_i, \sigma_i)$ and lengths (energies) are expressed in units of l_B (the first Landau level energy). Angular momentum conservation dictates $j_1 + j_2 = j_3 + j_4$, and numerically we find that only momentum exchange processes with $k := |j_4 - j_1| \leqslant 4$ need to be kept,

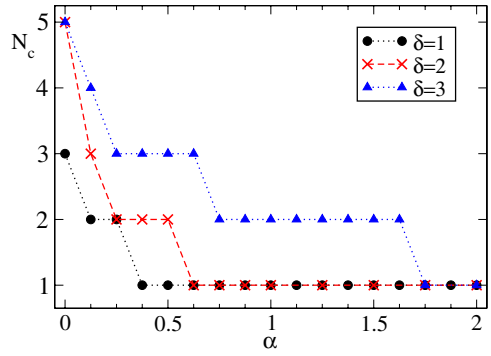

Figure 2. Critical particle number N_c versus interaction strength α for three different values of the missing flux δ. The symbols represent the computed values, and lines connecting them are guides to the eye only.

cf also [11]. A useful but lengthy explicit expression for the matrix elements (23) is given in appendix B.

The Hartree–Fock scheme to determine the ground-state energy E_N for N particles with the given interaction strength α and missing flux δ is then standard [19, 22]. Numerical calculations were carried out by restricting the Hilbert space to $-18 < j < 2$ and $n = 0, 1, 2$, which spans the relevant low-energy sector and very accurately describes all stable (i.e. $N \leqslant N_c$) multiparticle ground-state energies reported below.

The self-consistent numerical solution for the density matrix γ also allows us to read off the number of bound electrons in the interacting dot. In particular, only a maximum number $N_c = N_c(\alpha, \delta)$ of electrons can be bound by the magnetic dot, and for $N > N_c$, we find that $N - N_c$ electrons enter bulk Landau states centered far away from the dot (and from each other) in order to minimize the Coulomb interaction energy. The diagonal elements γ_{aa} yield the occupation probability of state $|a\rangle$, and we can thereby directly infer $N_c(\alpha, \delta)$ from the converged density matrix. The result is shown in figure 2 for several values of δ. Note that $N_c(\delta)$ for $\alpha = 0$ follows directly from figure 1. When increasing the repulsive interaction strength α, electrons tend to be pushed out of the dot, and N_c monotonically decreases with α. For sufficiently strong interactions, $\alpha \geqslant 1.75$, and moderate values of the missing flux, $\delta \leqslant 3$, we find that only a single electron can be bound by such a dot ($N_c = 1$). Coulomb interactions in graphene nanostructures are thus very significant for the physically relevant regime $\alpha < 2$.

Hartree–Fock results for the ground-state energy E_N are shown for several δ and α in figure 3. For $N > N_c$, the shown energies still depend on the chosen Hilbert space dimension, and for a bigger basis size, they move to smaller values. This is clear on physical grounds, since $N - N_c$ electrons will stay as far away as possible from the dot region and from each other in order to minimize the Coulomb energy. In the limit of infinite basis size, the Coulomb interaction energy can be minimized by moving $N - N_c$ electrons to infinity, such that $E_{N+1} - E_N = 1$ for $N \geqslant N_c$. Obviously, for the chosen basis size, the results in figure 3 do not yet match onto this asymptotic form. However, the shown results for E_N with $N \leqslant N_c$ in figure 3, describing the stable multiparticle case, are accurate and do not change when increasing the basis size. This behavior gives an additional criterion to find the number N_c and thereby the sought stability condition.

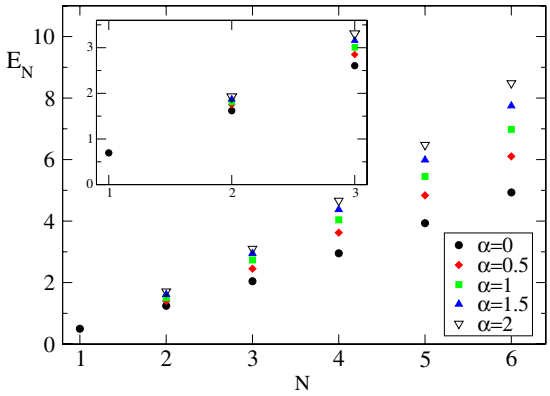

Figure 3. Hartree–Fock ground-state energy E_N versus N for several α with $\delta = 3$. Inset: same for $\delta = 1$.

5. Discussion

In this paper, we have studied the interacting multiparticle problem in graphene quantum dots. Such quantum dots can be created in a tunable way by imposing suitable inhomogeneous magnetic field profiles. After providing the mathematical foundations of Hartree–Fock theory and discussing the conditions for the existence of a minimizer, we have given predictions for the maximum number of bound electrons in a specific example. The Hartree–Fock ground-state energies shown here represent upper bounds for the true ground-state energy. An alternative to Hartree–Fock calculations is to employ the Müller functional [24, 25]. As opposed to the Hartree–Fock functional, the exchange energy is no longer dominated by $D[\rho_\gamma]$ but instead by the kinetic energy. In fact, the Müller correlation energy shares the feature of the Dirac exchange energy $\rho_\gamma^{4/3}$ that it underestimates the correlation energy, resulting in too low energies. We expect that the Müller functional then implies lower bounds for the ground-state energy, and we can thereby get both upper and lower bounds for the exact result. This work is currently in progress.

Acknowledgments

We acknowledge support by the SFB Transregio 12 of the DFG.

Appendix A. Some useful lemmata

The relevance of the following result is that it suffices to show relative (form) compactness with respect to the free Weyl operator to fulfill the compactness requirements (4).

For some $R > 1$ (not to be confused with the radius R used in section 4), we define a smooth cutoff function $\chi_R \in C_0^\infty(\mathbb{R}^2; [0, 1])$ with the property that $\chi_R = 1$ for $|\mathbf{x}| \leqslant R/2$ and $\chi_R = 0$ for $|\mathbf{x}| \geqslant R$; it follows that $\|\nabla\chi_R\|_\infty = \mathcal{O}(1/R)$. We will often use that for $\varphi \in C_0^\infty(\mathbb{R}^2 : \mathbb{C}^2)$,

$$[D_A, \chi_R]\varphi = -\mathrm{i}\boldsymbol{\sigma} \cdot \nabla\chi_R\varphi. \tag{A.1}$$

Lemma 9. *Let $A = (A_1, A_2)$ be a magnetic vector potential with $A_j \in L^\infty_{\rm loc}(\mathbb{R}^2)$ for $j = 1, 2$. Let T be a bounded symmetric (matrix-valued) multiplication operator such that*

- $\|T(\mathbf{x})\| \to 0$ *as* $\|\mathbf{x}\| \to \infty$,
- $T|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2}$ *is a compact operator.*

Then, for any λ in the resolvent set of D_A, the operator $T|D_A + \lambda|^{-1/2}$ is compact.

Proof. Clearly the claim follows if we prove that $\chi_R T|D_A + \mathrm{i}|^{-1/2}$ is compact for all $R > 1$, since $\chi_R T|D_A + \mathrm{i}|^{-1/2} \to T|D_A + \mathrm{i}|^{-1/2}$ in the operator norm as $R \to \infty$ and the operator $|D_A + \mathrm{i}|^{1/2}|D_A + \lambda|^{-1/2}$ is bounded. We observe that

$$\begin{aligned}\chi_R T|D_A + \mathrm{i}|^{-1/2} &= \chi_R T|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2} \\ &\quad + T|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2}|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{1/2}\chi_R(|D_A + \mathrm{i}|^{-1/2} - |\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2}).\end{aligned}$$

Therefore, it suffices to show that $|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{1/2}\chi_R(|D_A + \mathrm{i}|^{-1/2} - |\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2})$ is a bounded operator. In order to do so, we first note that the following resolvent identity holds in $L^2(\mathbb{R}^2 : \mathbb{C}^2)$. For $z \in \mathrm{i}\mathbb{R}\backslash\{0\}$,

$$R_A(z) = (D_A + z)^{-1}, \qquad R_0(z) = (\boldsymbol{\sigma}\cdot\mathbf{p} + z)^{-1}.$$

Then

$$\begin{aligned}&\chi_R(R_A(z) - R_0(z)) \\ &\quad = R_0(z)(\mathrm{i}\boldsymbol{\sigma}\cdot\nabla\chi_R)(R_A(z) - R_0(z)) - R_0(z)\boldsymbol{\sigma}\cdot A\chi_R R_A(z) \\ &\quad =: R_0(z)\Gamma(z). \qquad (A.2)\end{aligned}$$

Before proving the above equation, using the spectral theorem, we compute

$$\begin{aligned}|D_A + \mathrm{i}|^{-1/2} = \left(D_A^2 + 1\right)^{-1/4} &= \frac{1}{\sqrt{2}\pi}\int_0^\infty \frac{\mathrm{d}t}{t^{1/4}}\frac{1}{D_A^2 + 1 + t} \\ &= \frac{1}{\sqrt{2}\pi}\int_0^\infty \frac{\mathrm{d}t}{2\mathrm{i}t^{1/4}\sqrt{1+t}}[R_A(-\mathrm{i}\sqrt{1+t}) - R_A(\mathrm{i}\sqrt{1+t})].\end{aligned}$$

An analogous formula holds for $|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2}$ with R_A replaced by R_0. Therefore, also using equation (A.2) we get

$$\begin{aligned}&|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{1/2}\chi_R(|D_A + \mathrm{i}|^{-1/2} - |\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{-1/2}) \\ &\quad = \frac{-1}{\sqrt{2}\pi}\sum_{\kappa=-1,1}\kappa\int_0^\infty \frac{\mathrm{d}t}{2\mathrm{i}t^{1/4}\sqrt{1+t}}|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{1/2}R_0(\kappa\mathrm{i}\sqrt{1+t})\Gamma(\kappa\mathrm{i}\sqrt{1+t}).\end{aligned}$$

Noting that $|\boldsymbol{\sigma}\cdot\mathbf{p} + \mathrm{i}|^{1/2}R_0(\kappa\mathrm{i}\sqrt{1+t})$ is bounded and that $\|\Gamma(\kappa\mathrm{i}\sqrt{1+t})\| \leqslant c/\sqrt{1+t}$ for some constant c, we conclude that the operator above is bounded.

It remains to show equation (A.2). For $\phi \in C_0^\infty(\mathbb{R}^2 : \mathbb{C}^2)$, using equation (A.1) we find

$$\begin{aligned}&(R_A(z) - R_0(z))\chi_R(\boldsymbol{\sigma}\cdot\mathbf{p} + z)\phi \\ &\quad = (R_A(z) - R_0(z))[\mathrm{i}\boldsymbol{\sigma}\cdot\nabla\chi_R + (\boldsymbol{\sigma}\cdot\mathbf{p} + z)\chi_R]\phi \\ &\quad = (R_A(z) - R_0(z))\mathrm{i}\boldsymbol{\sigma}\cdot\nabla\chi_R\phi - R_A(z)\boldsymbol{\sigma}\cdot A\chi_R\phi \\ &\quad = [(R_A(z) - R_0(z))\mathrm{i}\boldsymbol{\sigma}\cdot\nabla\chi_R R_0(z) \\ &\qquad - R_A(z)\boldsymbol{\sigma}\cdot A\chi_R R_0(z)](\boldsymbol{\sigma}\cdot\mathbf{p} + z)\phi.\end{aligned}$$

Since the range of $(\boldsymbol{\sigma}\cdot\mathbf{p} + z)|C_0^\infty(\mathbb{R}^2 : \mathbb{C}^2)$ is dense in $L^2(\mathbb{R}^2 : \mathbb{C}^2)$, we obtain the adjoint of equation (A.2) by a limiting argument. □

The next result allows us to use weak $H^{1/2}$ convergence in the proof of the main theorem.

Lemma 10. *Assume for the magnetic field and the magnetic vector potential that their components are locally bounded, i.e.* $A_j, B_j \in L^\infty_{\rm loc}(\mathbb{R}^2)$ *for* $j = 1, 2$. *Then, for any* $\chi \in C^\infty_0(\mathbb{R}^2; [0,1])$, *there exists a constant* $c_\chi > 0$ *such that for all* $\phi \in C^\infty_0(\mathbb{R}^2 : \mathbb{C}^2)$, *we have*

$$(\phi, \chi|\mathbf{p}|\chi\phi) \leqslant 2^{3/2}(\phi, |\not{\mathbf{p}} - \mu|\phi) + c_\chi \|\phi\|^2. \tag{A.3}$$

Proof. A simple application of the inequality $(a+b)^2 \geqslant (1-\delta)a^2 + (1-1/\delta)b^2$ yields, as quadratic forms on $C^\infty_0(\mathbb{R}^2 : \mathbb{C}^2)$,

$$\begin{aligned}\chi(\not{\mathbf{p}} - \mu)^2\chi &\geqslant (1-\delta)\chi[(\mathbf{p}+\mathbf{A})^2 + \boldsymbol{\sigma}\cdot\mathbf{B}]\chi + (1-\delta^{-1})\mu^2\chi^2 \\ &\geqslant (1-\delta)^2\chi\mathbf{p}^2\chi + (1-\delta)(1-\delta^{-1})\chi\mathbf{A}^2\chi \\ &\quad + (1-\delta)\chi\boldsymbol{\sigma}\cdot\mathbf{B}\chi + (1-\delta^{-1})\mu^2\chi^2 \\ &\geqslant \tfrac{1}{4}\chi\mathbf{p}^2\chi - c^2,\end{aligned}$$

where in the last inequality we set $\delta = 1/2$ and $c^2 = \|\chi\mathbf{A}^2\chi\|_\infty + \|\chi|\mathbf{B}|\chi\|_\infty/2 + \mu^2$. With the help of the above inequality and equation (A.1), we obtain, for any $\phi \in C^\infty_0(\mathbb{R}^2 : \mathbb{C}^2)$,

$$\begin{aligned}\tfrac{1}{4}(\phi, [\chi|\mathbf{p}|\chi]^2\phi) &\leqslant \tfrac{1}{4}\||\mathbf{p}|\chi\phi\|^2 \leqslant \|(\not{\mathbf{p}} - \mu)\chi\phi\|^2 + c^2\|\phi\|^2 \\ &\leqslant 2\|(\not{\mathbf{p}} - \mu)\phi\|^2 + 2\|\boldsymbol{\sigma}\cdot\nabla\chi\phi\|^2 + c^2\|\phi\|^2 \\ &\leqslant 2(\phi, (\not{\mathbf{p}} - \mu)^2\phi) + (\phi, [2\|\nabla\chi\|_\infty + c^2]\phi).\end{aligned}$$

Using this last estimate and the fact that the square root is operator monotone, we get equation (A.3) with $c_\chi = 2[2\|\nabla\chi\|_\infty + c^2]^{1/2}$. □

Appendix B. Two-particle matrix elements

In this appendix, we provide the explicit form of the two-particle Coulomb matrix elements (23) in terms of the Landau level spinors (21). With the radial functions (22) and momentum exchange $k = |j_4 - j_1|$, we have

$$\begin{aligned}\tilde{V}_{s_1s_2s_3s_4} = \frac{\alpha}{2\pi}\int_0^\pi \mathrm{d}\phi \int_0^\infty \mathrm{d}\xi \int_0^\infty \mathrm{d}\xi' \frac{\cos(k\phi)}{\sqrt{\xi+\xi'-2\sqrt{\xi\xi'}\cos\phi}} \\ \times \big[\psi_{s_4}\cdot\psi_{s_1}\big](\xi)\big[\psi_{s_3}\cdot\psi_{s_2}\big](\xi'),\end{aligned} \tag{B.1}$$

where $\psi_1\cdot\psi_2 := \psi_1^+\psi_2^+ + \sigma_1\sigma_2\psi_1^-\psi_2^-$. We now employ the expansion formula

$$\frac{1}{\sqrt{\xi+\xi'-2\sqrt{\xi\xi'}\cos\phi}} = \frac{1}{\sqrt{\xi_>}}\sum_{\ell=0}^\infty (\xi_</\xi_>)^{\ell/2}P_\ell(\cos\phi)$$

with Legendre functions $P_\ell(\cos\phi)$, where $\xi_> = \max(\xi,\xi')$ and $\xi_< = \min(\xi,\xi')$. The angular integration can then be performed by using the relation

$$\int_0^\pi \frac{\mathrm{d}\phi}{\pi}\cos(k\phi)P_\ell(\cos\phi) = \frac{(2\ell-1)!!}{2^\ell\ell!}C_{(\ell+k)/2;\ell}. \tag{B.2}$$

The coefficients $C_{m;\ell}$ with $m \in \mathbb{N}_0$ are the expansion coefficients of a hypergeometric function, and $C_{(\ell+k)/2;\ell} \neq 0$ only for even $k+\ell$ and $\ell \geqslant k$. In particular, $C_{0;\ell} = 1$, while for $0 < m \leqslant \ell$, we have the product representation

$$C_{m;\ell} = \prod_{i=1}^m \frac{(i-1/2)(\ell+1-i)}{i(\ell+1/2-i)}.$$

To perform the ξ, ξ' integrations in equation (B.1), we insert the explicit form of $\psi^{\pm}_{nj}(\xi)$ in equation (22), with the generalized Laguerre polynomials ($n, m \in \mathbb{N}_0$)

$$L_n^m(\xi) = \sum_{i=0}^{n} \frac{1}{i!} \binom{n+m}{n-i} (-\xi)^i .$$

After some algebra, with the ℓ summation only extending over $\ell + k \in 2\mathbb{Z}$, we find the lengthy result

$$\begin{aligned}
\tilde{V}_{s_1 s_2 s_3 s_4} = \alpha \sum_{\eta,\eta'=\pm} \sum_{\ell \geqslant k} & \frac{(2\ell-1)!!}{2^{\ell+1}\ell!} C_{(\ell+k)/2;\ell} \\
& \times (\delta_{\eta,+} + \delta_{\eta,-}\sigma_1\sigma_4)(\delta_{\eta',+} + \delta_{\eta',-}\sigma_2\sigma_3) A^{\eta}_{s_1} A^{\eta'}_{s_2} A^{\eta'}_{s_3} A^{\eta}_{s_4} \\
& \times \sum_{m_1=0}^{\tilde{n}_1} \sum_{m_2=0}^{\tilde{n}_2} \sum_{m_3=0}^{\tilde{n}_3} \sum_{m_4=0}^{\tilde{n}_4} \frac{(-)^{m_1+m_2+m_3+m_4}}{m_1! m_2! m_3! m_4!} \\
& \times \binom{\tilde{n}_1 + |j_1 - \eta/2|}{\tilde{n}_1 - m_1} \binom{\tilde{n}_2 + |j_2 - \eta'/2|}{\tilde{n}_2 - m_2} \\
& \times \binom{\tilde{n}_3 + |j_3 - \eta'/2|}{\tilde{n}_3 - m_3} \binom{\tilde{n}_4 + |j_4 - \eta/2|}{\tilde{n}_4 - m_4} \\
& \times I(M + M', M') + (s_1, s_4) \leftrightarrow (s_2, s_3),
\end{aligned} \tag{B.3}$$

where $\tilde{n}_{1,4} := n_{1,4} - \delta_{\eta,+}\Theta(-j_{1,4})$, $\tilde{n}_{2,3} := n_{2,3} - \delta_{\eta',+}\Theta(-j_{2,3})$, and

$$\begin{aligned}
M &:= m_1 + m_4 + \tfrac{1}{2}\left(|j_1 - \eta/2| + |j_4 - \eta/2| - \ell\right), \\
M' &:= m_2 + m_3 + \tfrac{1}{2}(|j_2 - \eta'/2| + |j_3 - \eta'/2| + \ell).
\end{aligned}$$

Finally, for $n, n' \in \mathbb{N}_0$, we have

$$I(n, n') := \frac{\sqrt{\pi}}{2} \frac{(2n+1)!!}{2^n} \int_0^1 \mathrm{d}y \, \frac{y^{n'}}{(1+y)^{n+3/2}}.$$

This allows for the numerical evaluation of the Coulomb interaction matrix elements, since all summations in equation (B.3) converge rapidly. Finally, note that the matrix elements obey the symmetry relations

$$\tilde{V}_{s_1 s_2 s_3 s_4} = \tilde{V}_{s_2 s_1 s_4 s_3} = \tilde{V}_{s_4 s_3 s_2 s_1}. \tag{B.4}$$

References

[1] Geim A K and Novoselov K S 2007 The rise of graphene *Nature Mater.* **6** 183–91

[2] Castro Neto A H, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 The electronic properties of graphene *Rev. Mod. Phys.* **81** 109–62

[3] Geim A K 2009 Graphene: status and prospects *Science* **324** 1530–4

[4] Reimann S M and Manninen M 2002 Electronic structure of quantum dots *Rev. Mod. Phys.* **74** 1283–342

[5] Pereira J M, Mlinar V, Peeters F M and Vasilopoulos P 2006 Confined states and direction-dependent transmission in graphene quantum wells *Phys. Rev.* B **74** 045424

[6] Silvestrov P G and Efetov K B 2007 Quantum dots in graphene *Phys. Rev. Lett.* **98** 016802

[7] Chen H-Y, Apalkov V and Chakraborty T 2007 Fock–Darwin states of Dirac electrons in graphene-based artificial atoms *Phys. Rev. Lett.* **98** 186803

[8] Matulis A and Peeters F M 2008 Quasibound states of quantum dots in single and bilayer graphene *Phys. Rev.* B **77** 115423

[9] Recher P, Nilsson J, Burkard G and Trauzettel B 2009 Bound states and magnetic field induced valley splitting in gate-tunable graphene quantum dots *Phys. Rev.* B **79** 085407

[10] De Martino A, Dell'Anna L and Egger R 2007 Magnetic confinement of massless Dirac fermions in graphene *Phys. Rev. Lett.* **98** 066802
[11] Häusler W and Egger R 2009 Artificial atoms in interacting graphene quantum dots *Phys. Rev.* B **80** 161402(R)
[12] Stampfer C, Güttinger J, Molitor F, Graf D, Ihn T and Ensslin K 2008 Tunable Coulomb blockade in nanostructured graphene *Appl. Phys. Lett.* **92** 012102
[13] Cerchez M, Hugger S, Heinzel T and Schulz N 2007 Effect of edge transmission and elastic scattering on the resistance of magnetic barriers: experiment and theory *Phys. Rev.* B **75** 035341
[14] Reijniers J, Peeters F M and Matulis A 1999 Quantum states in a magnetic antidot *Phys. Rev.* B **59** 2817–23
[15] Sucher J 1980 Foundations of the relativistic theory of many-electron atoms *Phys. Rev.* A **22** 348–62
[16] Sucher J 1984 Foundations of the relativistic theory of many-electron bound states *Int. J. Quantum Chem.* **25** 3–21
[17] Sucher J 1987 Relativistic many-electron Hamiltonians *Phys. Scr.* **36** 271–81
[18] Hainzl C, Lewin M and Seiringer R 2008 A nonlinear model for relativistic electrons at nonzero temperature *Rev. Math. Phys.* **20** 1283–307
[19] Reiher M and Wolf A 2009 *Relativistic Quantum Chemistry: The Fundamental Theory of Molecular Science* (Weinheim: Wiley-VCH)
[20] Weidmann J 2000 *Linear Operatoren in Hilberträumen, vol I: Grundlagen* (Stuttgart: Teubner Verlag)
[21] Reed M and Simon B 1975 *Methods of Modern Mathematical Physics, vol II: Fourier Analysis and Self-Adjointness* (New York: Academic)
[22] Giuliani G F and Vignale G 2005 *Quantum Theory of the Electron Liquid* (Cambridge: Cambridge University Press)
[23] Lieb E H, Siedentop H and Solovej J P 1997 Stability of relativistic matter with magnetic fields *Phys. Rev. Lett.* **79** 1785–8
[24] Müller A M K 1984 Explicit approximate relation between reduced two- and one-particle density matrices *Phys. Lett.* A **105** 446–52
[25] Frank R L, Lieb E H, Seiringer R and Siedentop H 2007 Müller's exchange-correlation energy in density-matrix-functional theory *Phys. Rev.* A **76** 052517
[26] Frank R L, Lieb E H and Seiringer R 2007 Stability of relativistic matter with magnetic fields for nuclear charges up to the critical value *Commun. Math. Phys.* **275** 479–89
[27] Barbaroux J-M, Farkas W, Helffer B and Siedentop H 2005 On the Hartree–Fock equations of the electron-positron field *Commun. Math. Phys.* **255** 131–59
[28] Bach V 1992 Error bound for the Hartree–Fock energy of atoms and molecules *Commun. Math. Phys.* **147** 527–48
[29] Lieb E H and Simon B 1977 The Hartree–Fock theory for Coulomb systems *Commun. Math. Phys.* **53** 185–94
[30] Solovej J P 1991 Proof of the ionization conjecture in a reduced Hartree–Fock model *Inventions Math.* **104** 291–311
[31] Kato T 1966 *Perturbation Theory for Linear Operators (Grundlehren der mathematischen Wissenschaften* vol 132*)* (Berlin: Springer)
[32] Lions J-L and Magenes E 1972 *Non-Homogeneous Boundary Value Problems and Applications* vol I (New York: Springer)
[33] De Martino A and Egger R 2010 On the spectrum of a magnetic quantum dot in graphene *Semicond. Sci. Technol.* **25** 034006