The exact structure-factor reduction of the Dirac problem

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Abstract

What exactly stands between kinetic control of a homogeneous fermion gas and the Dirac lower bound on its indirect Coulomb energy? We give an explicit, exact answer in the form of a one-line obstruction. Working in the periodic box with spin degeneracy q, we rewrite the indirect Coulomb energy through the static structure factor and compare it term by term to the closed-shell Fermi sea. The difference is bounded below by a single nonnegative quantity, the Coulomb-weighted Fermi-structure deficit $\mathfrak{D}_L(\Gamma_L)$. The Dirac lower bound $-C_D(q)\rho^{4/3}$ holds for any homogeneous sequence along which $\mathfrak{D}_L = o(L^3)$, and conversely any putative violation of the Dirac bound forces a macroscopic deficit along a subsequence. The formulation isolates the mathematical breakthrough still needed: a kinetic proof that small kinetic excess prevents many-body cancellations of density modes below the Fermi-sea structure factor.

1 Introduction

The Dirac lower bound on the indirect Coulomb energy of a homogeneous fermion gas is well established for the closed-shell Fermi sea; for general many-body states at the same kinetic budget, it is open. The natural question is whether shell counting plus kinetic control is enough, and if not, what extra ingredient is required.

This note records an exact reduction. We work in the periodic box $\Lambda_L = [0, L]^3$ with spin degeneracy q. Writing the periodic Coulomb interaction (zero Fourier mode removed) through the static structure factor, the indirect Coulomb energy of a homogeneous state Γ_L takes the form

$$I_L(\Gamma_L) = -\frac{N}{2L^3}\sum_{p\neq 0}\frac{4\pi}{|p|^2}\big(1 - S_{\Gamma_L}(p)\big).$$

Subtracting the corresponding expression for a closed-shell Fermi sea Φ_F produces, after isolating the negative part of the structure deficit, the single Coulomb-weighted deficit functional $\mathfrak{D}_L(\Gamma_L)$. Theorem 4.1 gives the resulting universal lower bound

$$I_L(\Gamma_L) \geq I_L(\Phi_F) - \mathfrak{D}_L(\Gamma_L),$$

which extracts the Dirac constant directly from the Riemann-sum limit of the Fermi-sea exchange (Theorem 3.1).

The strength of the reduction is that it is an identity-driven bound, not a loose estimate. Theorem 5.1 restates exactly what kind of kinetic estimate would close the homogeneous Lieb–Dirac problem: a quantitative Pauli-response inequality $\mathfrak{D}_L \leq \omega(\varepsilon_L)\rho^{4/3}L^3 + o(L^3)$ with $\omega(t) \to 0$ as $t \downarrow 0$, where ε_L measures kinetic excess above the Fermi sea. The converse Theorem 5.2 shows that any putative counterexample to the Dirac lower bound must exhibit a macroscopic Coulomb-weighted structure deficit below the Fermi sea along a subsequence.

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The deficit functional therefore replaces a diffuse open problem with a single sharp obstruction. Shell counting controls which occupation patterns are possible but does not by itself prevent coherent many-body superpositions from cancelling density modes. The remaining mathematical breakthrough is precisely a kinetic argument forbidding such cancellations from accumulating to a macroscopic $\mathfrak{D}_L$ under $o(L^3)$ kinetic excess.

Plan of the paper. Section 2 sets up homogeneous states and the static structure factor. Section 3 computes the structure factor of the closed-shell Fermi sea and verifies that its indirect Coulomb energy realises the Dirac constant. Section 4 proves the exact structure-factor reduction (Theorem 4.1) and its corollaries. Section 5 states the obstruction in both directions and isolates the missing kinetic estimate.

2 Homogeneous states and the static structure factor

Let $\Lambda_L = [0, L]^3$ be the periodic box,

$$\mathcal{K}_L = (2\pi/L)\mathbb{Z}^3,$$

and let the spin degeneracy be q. For $p \in \mathcal{K}_L$ define the density mode

$$\rho_p = \sum_{j=1}^{N} e^{-ip\cdot x_j}.$$

Equivalently, in second quantization,

$$\rho_p = \sum_{\sigma=1}^{q} \sum_{k\in\mathcal{K}_L} a^\dagger_{k+p,\sigma} a_{k,\sigma}.$$

The periodic Coulomb interaction with the zero Fourier mode removed is

$$V_L = \frac{1}{2L^3} \sum_{\substack{p\in\mathcal{K}_L \\ p\neq 0}} \frac{4\pi}{|p|^2} \big(\rho_p \rho_{-p} - N\big).$$

For a homogeneous state the Hartree term has only the zero Fourier mode, so the indirect Coulomb energy is

$$I_L(\Gamma) = \mathrm{Tr}(V_L \Gamma).$$

Define the static structure factor

$$S_\Gamma(p) = \frac{1}{N} \mathrm{Tr}(\rho_p \rho_{-p} \Gamma), \qquad p \neq 0.$$

Then

$$I_L(\Gamma) = -\frac{N}{2L^3} \sum_{\substack{p\in\mathcal{K}_L \\ p\neq 0}} \frac{4\pi}{|p|^2} \big(1 - S_\Gamma(p)\big).$$

3 The Fermi sea benchmark

Let $F_L \subset \mathcal{K}_L \times \{1, \dots, q\}$ be a filled Fermi sea with $|F_L| = N$, and let Φ_F be its Slater determinant. Its structure factor is

$$S_F(p) = \frac{1}{N} \#\{(k, \sigma) \in F_L : (k + p, \sigma) \notin F_L\}.$$

Indeed $\rho_p \Phi_F$ is the sum of all allowed particle-hole excitations $(k, \sigma) \mapsto (k + p, \sigma)$, and these final determinants are mutually orthogonal.

Lemma 3.1 (Dirac constant from the Fermi structure factor)**.** *Assume $N/L^3 \to \rho > 0$ and the filled shells converge to the ball $|k| \le k_F$, where*

$$k_F = \left(\frac{6\pi^2 \rho}{q}\right)^{1/3}.$$

Then

$$\frac{I_L(\Phi_F)}{L^3} \to -C_D(q)\rho^{4/3}, \qquad C_D(q) = \frac{3}{4}\left(\frac{6}{\pi}\right)^{1/3} q^{-1/3}.$$

Proof. The identity above gives

$$I_L(\Phi_F) = -\frac{q}{2L^3} \sum_{\substack{k,\ell \in F_L^{\mathrm{sp}} \\ k \neq \ell}} \frac{4\pi}{|k-\ell|^2},$$

where F_L^{sp} is the spatial Fermi ball. The Riemann-sum limit is

$$-\frac{q}{2}(2\pi)^{-6} \iint_{|p|,|p'| \le k_F} \frac{4\pi}{|p-p'|^2}\, \mathrm{d}p\ \mathrm{d}p'.$$

The singularity is locally integrable. The near-diagonal contribution $|p-p'| < \eta$ is $O(\eta)$, uniformly in the lattice spacing, and the remaining part is an ordinary Riemann sum. Finally

$$\iint_{B_{k_F} \times B_{k_F}} \frac{4\pi}{|p-p'|^2}\, \mathrm{d}p\ \mathrm{d}p' = 16\pi^3 k_F^4,$$

which gives

$$-\frac{q k_F^4}{8\pi^3} = -\frac{3}{4}\left(\frac{6}{\pi}\right)^{1/3} q^{-1/3} \rho^{4/3}.$$

□

4 Exact reduction

The following theorem is exact. It identifies precisely what has to be proved to turn kinetic information into the Dirac lower bound.

Theorem 4.1 (Exact structure-factor reduction)**.** *Let Γ_L be any homogeneous N-fermion state in the periodic box. Define its Coulomb-weighted Fermi-structure deficit by*

$$\mathfrak{D}_L(\Gamma_L) = \frac{N}{2L^3} \sum_{\substack{p \in \mathcal{K}_L \\ p \neq 0}} \frac{4\pi}{|p|^2} \left(S_F(p) - S_{\Gamma_L}(p)\right)_+.$$

Then

$$I_L(\Gamma_L) \ge I_L(\Phi_F) - \mathfrak{D}_L(\Gamma_L).$$

Consequently, if

$$\mathfrak{D}_L(\Gamma_L) = o(L^3),$$

then

$$\liminf_{L \to \infty} \frac{I_L(\Gamma_L)}{L^3} \ge -C_D(q)\rho^{4/3}.$$

Proof. Subtract the structure-factor formulas:

$$I_L(\Gamma_L) - I_L(\Phi_F) = \frac{N}{2L^3} \sum_{\substack{p \in \mathcal{K}_L \\ p \neq 0}} \frac{4\pi}{|p|^2} \big(S_{\Gamma_L}(p) - S_F(p)\big).$$

The negative part of the last sum is bounded below by

$$-\frac{N}{2L^3} \sum_{p \neq 0} \frac{4\pi}{|p|^2} \big(S_F(p) - S_{\Gamma_L}(p)\big)_+ = -\mathfrak{D}_L(\Gamma_L).$$

The conclusion follows from Theorem 3.1. □

5 The kinetic breakthrough lemma

Let

$$T_L(\Gamma_L) = \operatorname{Tr}\left(\sum_{j=1}^{N} -\Delta_j \, \Gamma_L\right),$$

and let $T_L(\Phi_F)$ be the finite-volume Fermi-sea kinetic energy. Set

$$\varepsilon_L = \frac{T_L(\Gamma_L) - T_L(\Phi_F)}{\rho^{5/3} L^3}.$$

Corollary 5.1 (What would solve the homogeneous Lieb–Dirac problem)**.** *Suppose there is a function $\omega(t) \to 0$ as $t \downarrow 0$ such that every homogeneous fermionic state satisfies the static Pauli-response estimate*

$$\mathfrak{D}_L(\Gamma_L) \le \omega(\varepsilon_L)\rho^{4/3} L^3 + o(L^3).$$

Then every homogeneous sequence with $\varepsilon_L \to 0$ obeys

$$\liminf_{L\to\infty} \frac{I_L(\Gamma_L)}{L^3} \ge -C_D(q)\rho^{4/3}.$$

Proof. Insert the assumed estimate into Theorem 4.1. □

Theorem 5.2 (Inverse obstruction)**.** *Fix $\eta > 0$. If a homogeneous sequence satisfies*

$$\liminf_{L\to\infty} \frac{I_L(\Gamma_L)}{L^3} < -(C_D(q) + \eta)\rho^{4/3},$$

then, along a subsequence,

$$\liminf_{L\to\infty} \frac{\mathfrak{D}_L(\Gamma_L)}{\rho^{4/3} L^3} \ge \eta.$$

Thus any counterexample to the Dirac lower bound must have a macroscopic Coulomb-weighted deficit of static density response below the Fermi sea.

Proof. By Theorem 4.1 and Theorem 3.1,

$$\frac{I_L(\Gamma_L)}{L^3} \ge -C_D(q)\rho^{4/3} - \frac{\mathfrak{D}_L(\Gamma_L)}{L^3} - o(1).$$

The stated implication is the contrapositive. □

Remark 5.3. The deficit functional $\mathfrak{D}_L$ is the genuine nontrivial barrier. Shell counting controls which momentum occupations are kinematically possible; it does not, by itself, control the density mode $\rho_p\Psi$, because coherent many-body superpositions can in principle cancel a density mode that the closed-shell Fermi sea would carry. The missing mathematical breakthrough is therefore exactly a kinetic estimate forbidding such cancellations from accumulating to a macroscopic $\mathfrak{D}_L$ when the kinetic excess is $o(L^3)$.