A sector-coherent gapless Dirac lower bound

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Abstract

We prove that the Dirac exchange constant is the correct asymptotic lower bound on the indirect Coulomb energy for a broad class of correlated fermionic states in the thermodynamic limit, without invoking a spectral gap at the Fermi surface. The states considered are *sector-coherent*: the macroscopic Fermi core is filled sector by sector, while the active Fermi shell of width αk_F may carry arbitrary many-body correlations and coherent superpositions. We show that every such state Γ_L on a periodic box Λ_L satisfies the per-volume bound $L^{-3}I_L(\Gamma_L) \geq -C_D(q)\rho^{4/3} - A_{\rho,q}(\alpha + \alpha^{4/3}) - o_\alpha(1)$, so that letting $L \to \infty$ and then $\alpha \to 0$ recovers the sharp Dirac constant. The proof combines an elementary Riemann-sum calculation for the filled-core exchange, a Pauli-bound estimate on the active-shell density, and a lattice-Coulomb cross-exchange bound. This is the Coulomb side of the gapless kinetic-to-Dirac programme: once the kinetic data have confined excitations to a thin Fermi shell, residual correlations in the shell are harmless at leading order.

1 Introduction and the main theorem

The Dirac approximation to the indirect Coulomb energy of a homogeneous fermion gas is the workhorse of density functional theory. In rigorous mathematical-physics terms, the question is whether the per-volume indirect energy of an N_L-fermion state on a periodic box $\Lambda_L = [0, L]^3$ is bounded below, in the limit $N_L/L^3 \to \rho$, by $-C_D(q)\rho^{4/3}$, where

$$C_D(q) = \tfrac{3}{4}(6/\pi)^{1/3}q^{-1/3}$$

is the Dirac constant for spin multiplicity q. The Lieb–Oxford inequality [1, 2] gives a universal upper bound on $-I_L/L^3$ that is roughly 80% too large. Bridging that gap calls for some form of *kinetic* input: states with bounded kinetic excess above the Fermi sea should, in some sense, look enough like a filled determinant for the Dirac mechanism to operate.

The natural conjecture is that the gap to Dirac is bridged for states whose kinetic excess is sub-extensive. A direct attack on the full conjecture meets a structural difficulty: in the gapless thermodynamic limit the one-particle spectrum has no spectral gap at the Fermi level, so standard finite-gap stability arguments do not apply. In this paper we prove the Coulomb half of the bridge, in a form which makes no spectral-gap or quasi-free assumption on the shell.

We work in a periodic cube $\Lambda_L = [0, L]^3$ with momentum lattice $\mathcal{K}_L = (2\pi/L)\mathbb{Z}^3$; the spin degeneracy is q. A one-particle orbital is a spin plane wave (k, σ) with $k \in \mathcal{K}_L$ and $\sigma \in \{1, \dots, q\}$; we work with the periodic Coulomb potential with the zero Fourier mode removed. Fix a target density $\rho > 0$ and set

$$k_F = \left(\frac{6\pi^2\rho}{q}\right)^{1/3}, \qquad C_D(q) = \frac{3}{4}\left(\frac{6}{\pi}\right)^{1/3} q^{-1/3}.$$

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Let $N_L/L^3 \to \rho$. For $0 < \alpha < 1/2$ define the deep core and the active Fermi shell by the momentum sets

$$\mathcal{C}_L^\alpha = \{k \in \mathcal{K}_L : |k| \le k_F(1-\alpha)\},$$

and

$$\mathcal{Q}_L^\alpha = \{k \in \mathcal{K}_L : k_F(1-\alpha) < |k| < k_F(1+\alpha)\}.$$

Let P_L^α and Q_L^α be the corresponding spin projections. For a spin-momentum set

$$C \subset \mathcal{C}_L^\alpha \times \{1, \dots, q\},$$

let Φ_C be the filled determinant over C.

We call a mixed N_L-particle state sector-coherent in the shell if it has the form

$$\Gamma_L = \sum_\nu p_\nu |\Phi_{C_\nu} \wedge \Xi_\nu\rangle\langle\Phi_{C_\nu} \wedge \Xi_\nu|, \qquad p_\nu \ge 0, \quad \sum_\nu p_\nu = 1,$$

where

$$C_\nu \subset \mathcal{C}_L^\alpha \times \{1, \dots, q\}, \qquad \Xi_\nu \in \bigwedge^{N_L - |C_\nu|} Q_L^\alpha L^2(\Lambda_L; \mathbb{C}^q).$$

Inside Q_L^α no diagonality or quasi-free assumption is imposed: Ξ_ν is an arbitrary correlated shell wavefunction.

Theorem 1.1 (Sector-coherent Dirac bound)**.** *There is a constant $A_{\rho,q} < \infty$, independent of L, α, and the shell states Ξ_ν, such that every sector-coherent shell state satisfies*

$$I_L(\Gamma_L) \ge -C_D(q)\rho^{4/3}L^3 - A_{\rho,q}(\alpha + \alpha^{4/3})L^3 - o_\alpha(L^3).$$

Consequently,

$$\lim_{\alpha \downarrow 0} \liminf_{L \to \infty} \frac{I_L(\Gamma_L)}{L^3} \ge -C_D(q)\rho^{4/3}.$$

Remark 1.2. This is not a finite-gap theorem and it is not an occupation-diagonal statement. The gap at the Fermi surface is allowed to collapse, and the shell wavefunction may be an arbitrary vector in a many-dimensional exterior power, so the theorem covers coherent superpositions and genuine many-body correlations in the active shell. The only structural restriction is that the macroscopic Fermi core is filled sector by sector, with holes compensated by particles confined to the thin shell.

Plan of the paper. Section 2 collects the two elementary ingredients of the proof: the Riemann-sum evaluation of the filled-core exchange (Theorem 2.1), and the Pauli-bound estimate that controls both the shell density and the core–shell exchange (Theorem 2.2). Section 3 assembles these into the proof of Theorem 1.1. Section 4 closes the discussion by recording the elementary kinetic-confinement lemma that motivates the sector-coherent class and delineating the still-open kinetic side of the programme.

2 Two elementary estimates

Lemma 2.1 (Exchange of a filled core)**.** *Let C_L^α be the completely filled spin core with $|k| \le k_F(1-\alpha)$. Then*

$$\frac{I_L(\Phi_{C_L^\alpha})}{L^3} = -C_D(q)\rho_\alpha^{4/3} + o_\alpha(1), \qquad \rho_\alpha = \frac{qk_F^3(1-\alpha)^3}{6\pi^2}.$$

In particular,

$$I_L(\Phi_{C_L^\alpha}) \ge -C_D(q)\rho^{4/3}L^3 - C_{\rho,q}\alpha L^3 - o_\alpha(L^3).$$

Proof. For a filled plane-wave determinant the indirect energy is exactly exchange:

$$I_L(\Phi_{C_L^\alpha}) = -\frac{q}{2L^3} \sum_{\substack{k,\ell \in \mathcal{C}_L^\alpha \\ k \neq \ell}} \frac{4\pi}{|k-\ell|^2}.$$

The Riemann-sum limit is

$$-\frac{q}{2}(2\pi)^{-6} \iint_{|p|,|p'| \le k_F(1-\alpha)} \frac{4\pi}{|p-p'|^2}\,\mathrm{d}p\,\mathrm{d}p'.$$

The singularity is integrable in three dimensions. More explicitly, the near-diagonal contribution with $|p-p'|<\eta$ is bounded uniformly by $C\eta$, because

$$\int_{|s|<\eta} |s|^{-2}\,\mathrm{d}s = 4\pi\eta,$$

and the remaining part is an ordinary Riemann sum. The ball-overlap calculation gives

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

Substituting $R = k_F(1-\alpha)$ gives the first formula. The second follows from $\rho_\alpha = \rho(1-\alpha)^3$. □

Lemma 2.2 (Shell density and cross-exchange bounds)**.** *Let Q_L^α be the spin projection onto the shell $\mathcal{Q}_L^\alpha$. If $\Xi \in \bigwedge^n Q_L^\alpha L^2(\Lambda_L;\mathbb{C}^q)$ is arbitrary and γ_Ξ is its one-particle density matrix, then*

$$0 \le \gamma_\Xi \le Q_L^\alpha, \qquad \rho_\Xi(x) \le \frac{\operatorname{rank} Q_L^\alpha}{L^3} = O_{\rho,q}(\alpha) + o_\alpha(1).$$

Hence

$$\int_{\Lambda_L} \rho_\Xi(x)^{4/3}\,\mathrm{d}x \le C_{\rho,q}\alpha^{4/3}L^3 + o_\alpha(L^3).$$

Moreover, for every filled subcore

$$C \subset \mathcal{C}_L^\alpha \times \{1,\dots,q\},$$

the core-shell exchange term obeys

$$0 \le X_L(C,\gamma_\Xi) \le C_{\rho,q}\alpha L^3 + o_\alpha(L^3),$$

uniformly in C and Ξ.

Proof. The operator inequality $0 \le \gamma_\Xi \le Q_L^\alpha$ is the Pauli bound for the one-particle density matrix. Since $Q_L^\alpha(x,x)$ is constant,

$$Q_L^\alpha(x,x) = \frac{\operatorname{rank} Q_L^\alpha}{L^3}.$$

The lattice Weyl estimate gives

$$\operatorname{rank} Q_L^\alpha = q|\mathcal{Q}_L^\alpha| = O_{\rho,q}(\alpha L^3) + o_\alpha(L^3),$$

and the density bound follows. Therefore

$$\int \rho_\Xi^{4/3} \le L^3 \|\rho_\Xi\|_\infty^{4/3} \le C_{\rho,q}\alpha^{4/3}L^3 + o_\alpha(L^3).$$

For the exchange term, write it in the plane-wave basis:

$$X_L(C,\gamma_\Xi) = \frac{1}{L^3}\sum_{\sigma=1}^{q}\sum_{\substack{k:(k,\sigma)\in C\\ \ell\in\mathcal{Q}_L^\alpha}}\frac{4\pi}{|k-\ell|^2}\langle \ell,\sigma|\gamma_\Xi|\ell,\sigma\rangle.$$

The diagonal entries of γ_Ξ are at most one. For each shell momentum ℓ,

$$\frac{1}{L^3}\sum_{\substack{k\in\mathcal{K}_L\\ |k|\le k_F}}\frac{4\pi}{|k-\ell|^2}\le C_{\rho,q},$$

uniformly in L and ℓ. This is again the lattice version of local integrability of $|p-\ell|^{-2}$. Since the shell has $O_{\rho,q}(\alpha L^3)+o_\alpha(L^3)$ spin orbitals, the claimed bound follows. □

3 Proof of the theorem

Proof of Theorem 1.1. It is enough to prove the bound for one pure sector

$$\Psi = \Phi_C\wedge\Xi,\qquad C\subset\mathcal{C}_L^\alpha\times\{1,\dots,q\},\qquad \Xi\in\bigwedge^{N_L-|C|} Q_L^\alpha L^2(\Lambda_L;\mathbb{C}^q),$$

because the mixed-state indirect energy is bounded below by the average of the pure-sector indirect energies. Indeed, if $\Gamma=\sum_\nu p_\nu|\Psi_\nu\rangle\langle\Psi_\nu|$, then the pair energy is affine in Γ, while the Hartree term is the positive quadratic form $D_L(\rho,\rho)$ with the zero Fourier mode removed. Hence

$$D_L\left(\sum_\nu p_\nu\rho_\nu,\sum_\nu p_\nu\rho_\nu\right)\le\sum_\nu p_\nu D_L(\rho_\nu,\rho_\nu),$$

and therefore

$$I_L(\Gamma)\ge\sum_\nu p_\nu I_L(\Psi_\nu).$$

For $\Psi=\Phi_C\wedge\Xi$, the exterior-product formula for the two-particle density gives

$$I_L(\Psi)=I_L(\Phi_C)+I_L(\Xi)-X_L(C,\gamma_\Xi).$$

Since deleting occupied core orbitals can only make exchange less negative,

$$I_L(\Phi_C)\ge I_L(\Phi_{C_L^\alpha}).$$

The residual shell state is arbitrary, so Lieb–Oxford gives

$$I_L(\Xi)\ge -C_{\mathrm{LO}}\int_{\Lambda_L}\rho_\Xi(x)^{4/3}\,\mathrm{d}x.$$

Applying Theorem 2.2 to this term and to the cross-exchange term gives

$$I_L(\Psi)\ge I_L(\Phi_{C_L^\alpha})-C_{\rho,q}\alpha^{4/3}L^3-C_{\rho,q}\alpha L^3-o_\alpha(L^3).$$

Finally Theorem 2.1 evaluates the filled-core exchange:

$$I_L(\Phi_{C_L^\alpha})\ge -C_D(q)\rho^{4/3}L^3-C_{\rho,q}\alpha L^3-o_\alpha(L^3).$$

Combining the estimates proves the theorem. □

4 Relation to kinetic excess

The theorem is a Coulomb statement: once kinetic information has confined all non-core degrees of freedom to a thin Fermi shell, arbitrary coherent correlations in that shell are harmless at leading order. The elementary gapless kinetic shell estimate is the following.

Lemma 4.1 (Kinetic confinement to the shell)**.** *Let F_L be a finite-volume kinetic minimizer and let the core, shell, and high region be defined by one-particle energies*

$$|k|^2 \le \mu_L - s, \qquad ||k|^2 - \mu_L| < s, \qquad |k|^2 \ge \mu_L + s.$$

For every occupation configuration S,

$$K(S) - K(F_L) \ge s\Big(|\textit{core holes in } S| + |\textit{high particles in } S|\Big).$$

Proof. Let h_c be the number of holes in the deep core, h_s the number of holes in the occupied part of the shell, p_s the number of particles in the unoccupied part of the shell, and p_h the number of high particles. Since $|S| = |F_L|$,

$$h_c + h_s = p_s + p_h.$$

Using the four inequalities

$$\varepsilon_{\text{core}} \le \mu_L - s, \quad \varepsilon_{\text{occupied shell}} \le \mu_L, \quad \varepsilon_{\text{unoccupied shell}} \ge \mu_L, \quad \varepsilon_{\text{high}} \ge \mu_L + s,$$

one obtains

$$\begin{aligned} K(S) - K(F_L) &\ge \mu_L p_s + (\mu_L + s)p_h - \mu_L h_s - (\mu_L - s)h_c \\ &= s(p_h + h_c). \end{aligned}$$

□

Remark 4.2. The missing step for the full Lieb programme can thus be stated sharply: prove that a general low-kinetic-excess state can be pinched to sector-coherent shell form without lowering the indirect Coulomb energy by an order-L^3 amount. Theorem 1.1 delivers the entire Dirac mechanism once that pinching step is in hand, and it does so for genuinely correlated shell wavefunctions, with no spectral-gap assumption.

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