PreXiv:260513.4t95pk [math.MP] 13 May 2026

Finite exterior-power stability and the Dirac exchange constant

Dong Bai*

May 13, 2026

Abstract

A spectral gap above the closed-shell Fermi sea would, if it persisted in the thermodynamic limit, immediately give the Dirac exchange constant. It does not persist: the one-particle gap at the Fermi surface collapses. This paper develops a thin-shell substitute and uses it to bound the indirect Coulomb energy of arbitrary states. In a finite cell, small kinetic excess above the closed-shell determinant forces overlap with the Fermi sea and closeness of any bounded observable to its Fermi-sea expectation. In the thermodynamic limit, the same mechanism with a thin Fermi shell forces all gapless fluctuations into a shell of $O(\eta L^3)$ orbitals; arbitrary correlations inside that shell, including non-quasi-free states, change the Dirac exchange density only by lower-order terms in η. We supplement the analytic estimates with a Lean-verified core that checks the underlying configuration-basis inequalities.

1 Introduction

The Dirac exchange constant $C_D(q)$ is the natural lower-bound benchmark for homogeneous fermion gases. For closed-shell Fermi seas it can be computed directly; for general many-body states with comparable kinetic energy, the question is whether kinetic closeness to a Fermi determinant translates into closeness of all Coulomb expectations. The cleanest version of this is a spectral-gap argument: a positive gap g between occupied and unoccupied one-particle energies makes the closed-shell determinant a stable ground state, in the sense that an ℓ^2-small kinetic excess forces overlap of order $1 - \Delta/g$ with the determinant, and hence closeness of every bounded observable.

The difficulty is that the one-particle gap at the Fermi surface vanishes in the thermodynamic limit. The clean finite-cell stability statement therefore collapses as $L \to \infty$, and a direct application to the Lieb–Oxford problem fails.

This paper supplies a thin-shell replacement and bounds the indirect Coulomb energy of arbitrary correlated states inside that shell. The strategy is:

1. In a finite cell with a spectral gap, prove that small kinetic excess forces overlap with the closed-shell determinant; this gives the bound on any bounded observable, including the projected periodic Coulomb interaction (Section 2).
2. In the gapless thermodynamic regime, split the Fermi configuration into a deep core, a thin Fermi shell, and a high exterior, and prove that kinetic excess forces all weight into configurations that fix the core and the exterior (Section 3).
3. Show that the closed-shell Fermi sea over the core realises the Dirac constant in the Riemann-sum limit (Section 5).

*College of Mechanics and Engineering Science, Hohai University, Nanjing 211100, China. E-mail: bydonfancy@gmail.com.

4. Combine these with a Lieb–Oxford bound inside the shell and a near-diagonal cross-exchange estimate to prove a Dirac lower bound for arbitrary states of the form $\Phi_- \wedge \Xi$, where Ξ lives in the thin shell and may be fully correlated (Section 6).

The thin-shell theorem (Theorem 6.1) is stronger than the finite-gap statement: inside the shell, the state need not be quasi-free or close to any determinant. The Dirac constant survives because the fluctuating shell carries $O(\eta L^3)$ orbitals, so both its Lieb–Oxford cost and its cross-exchange with the core are lower order in η. We do not claim to solve the Lieb local open problem; we identify and prove a nontrivial mechanism beyond the finite-cell gap argument.

A short final section (Section 7) records the configuration-basis inequalities verified in the accompanying Lean file `StabilityCore.lean`.

Plan of the paper. Section 2 states and proves the finite exterior-power stability theorem in a gapped setting. Section 3 replaces the collapsing gap with a thin-shell projector and proves the gapless analog. Section 4 applies the stability theorem to a projected finite-cell periodic Coulomb interaction. Section 5 computes the exchange energy of a closed-shell Fermi sea in the Riemann-sum limit. Section 6 contains the main Dirac bound for correlated thin-shell states. Section 7 records the Lean checks.

2 A finite exterior-power theorem

Let $\mathfrak{h}_M$ be an M-dimensional one-particle Hilbert space with orthonormal basis $u_1, \dots, u_M$. Fix $N < M$. The N-fermion space $\bigwedge^N \mathfrak{h}_M$ has the orthonormal occupation basis

$$e_S = u_{i_1} \wedge \cdots \wedge u_{i_N}, \qquad S = \{i_1 < \cdots < i_N\} \subset \{1, \dots, M\}.$$

Write

$$\mathcal{C}_{M,N} = \{S \subset \{1, \dots, M\} : |S| = N\}.$$

Let

$$F = \{1, \dots, N\}$$

be the closed-shell Fermi configuration. Let the one-particle Hamiltonian be diagonal,

$$hu_i = \varepsilon_i u_i,$$

and assume there are $\lambda_F \in \mathbb{R}$ and $g > 0$ such that

$$\varepsilon_i \le \lambda_F \quad (i \in F), \qquad \varepsilon_i \ge \lambda_F + g \quad (i \notin F).$$

Let

$$H_0 = \sum_{j=1}^{N} h_j$$

on $\bigwedge^N \mathfrak{h}_M$, and set

$$\Phi_F = e_F, \qquad E_F = \sum_{i \in F} \varepsilon_i.$$

Theorem 2.1 (Closed-shell stability in the exterior power)**.** *Let*

$$\Psi = \sum_{S \in \mathcal{C}_{M,N}} c_S e_S, \qquad \sum_S |c_S|^2 = 1,$$

and define

$$\Delta = \langle \Psi, H_0 \Psi \rangle - E_F.$$

Then

$$\sum_{S\in\mathcal{C}_{M,N}} |c_S|^2\,|S\setminus F| \le \frac{\Delta}{g},$$

and

$$\sum_{S\neq F} |c_S|^2 \le \frac{\Delta}{g}.$$

Consequently

$$|\langle \Phi_F, \Psi\rangle|^2 \ge 1 - \frac{\Delta}{g},$$

and

$$\inf_{\theta\in\mathbb{R}} \|\Psi - e^{i\theta}\Phi_F\|^2 \le 2\frac{\Delta}{g}.$$

Moreover, if A is any bounded self-adjoint operator on $\bigwedge^N \mathfrak{h}_M$, then

$$|\langle \Psi, A\Psi\rangle - \langle \Phi_F, A\Phi_F\rangle| \le 2\|A\|\sqrt{2\Delta/g}.$$

Proof. For $S \in \mathcal{C}_{M,N}$, put

$$K(S) = \sum_{i\in S} \varepsilon_i, \qquad r(S) = |S\setminus F|.$$

Since $|S| = |F| = N$, one also has

$$|F\setminus S| = |S\setminus F| = r(S).$$

Therefore

$$\begin{aligned} K(S) - K(F) &= \sum_{i\in S\setminus F} \varepsilon_i - \sum_{j\in F\setminus S} \varepsilon_j \\ &\ge (\lambda_F + g)r(S) - \lambda_F r(S) = g r(S). \end{aligned}$$

Multiplying by $|c_S|^2$ and summing gives

$$\Delta = \sum_S |c_S|^2\big(K(S) - K(F)\big) \ge g\sum_S |c_S|^2 r(S).$$

This proves the first estimate. Since $r(S) \ge 1$ whenever $S \neq F$,

$$\sum_{S\neq F} |c_S|^2 \le \sum_S |c_S|^2 r(S) \le \frac{\Delta}{g}.$$

But

$$|\langle \Phi_F, \Psi\rangle|^2 = |c_F|^2 = 1 - \sum_{S\neq F} |c_S|^2,$$

which proves the overlap bound.

Let $a = |\langle \Phi_F, \Psi\rangle|$. Choosing the phase so that $\langle e^{i\theta}\Phi_F, \Psi\rangle = a \ge 0$, one gets

$$\|\Psi - e^{i\theta}\Phi_F\|^2 = 2(1-a) \le 2(1-a^2) \le 2\Delta/g.$$

Finally,

$$\begin{aligned} &|\langle \Psi, A\Psi\rangle - \langle \Phi_F, A\Phi_F\rangle| \\ &\quad \le |\langle \Psi - \Phi_F^\theta, A\Psi\rangle| + |\langle \Phi_F^\theta, A(\Psi - \Phi_F^\theta)\rangle| \\ &\quad \le 2\|A\|\,\|\Psi - \Phi_F^\theta\| \le 2\|A\|\sqrt{2\Delta/g}, \end{aligned}$$

where $\Phi_F^\theta = e^{i\theta}\Phi_F$. □

Remark 2.2. Theorem 2.1 is the finite-dimensional exterior-power version of the spectral-gap argument. It is not a quasi-free assumption: Ψ is an arbitrary vector in the full N-fermion Hilbert space.

3 Gapless thin-shell stability

Theorem 2.1 cannot survive unchanged in the thermodynamic limit: the one-particle gap at the Fermi surface collapses. The replacement we use is stability not to one determinant, but to the subspace in which only a thin Fermi shell is allowed to fluctuate.

Let $F = \{1, \dots, N\}$ as above. Choose a "chemical level" μ and a width $\eta > 0$. Decompose

$$F = F_{\mathrm{c}} \cup F_{\mathrm{s}}, \qquad F_{\mathrm{c}} = \{i \in F : \varepsilon_i \leq \mu - \eta\},$$

and

$$F^c = U_{\mathrm{s}} \cup U_{\mathrm{h}}, \qquad U_{\mathrm{h}} = \{i \notin F : \varepsilon_i \geq \mu + \eta\}.$$

The active shell is

$$B_\eta = F_{\mathrm{s}} \cup U_{\mathrm{s}}.$$

Let Π_η be the projection onto the span of all configurations S such that

$$S \cap B_\eta^c = F \cap B_\eta^c.$$

Thus Π_η fixes the deep Fermi core as occupied and the high exterior as empty, but allows arbitrary fermionic states in the shell.

Theorem 3.1 (Gapless shell stability)**.** *Assume*

$$\varepsilon_i \leq \mu - \eta \quad (i \in F_{\mathrm{c}}), \qquad \varepsilon_j \geq \mu + \eta \quad (j \in U_{\mathrm{h}}),$$

and also

$$\varepsilon_i \leq \mu \quad (i \in F), \qquad \varepsilon_j \geq \mu \quad (j \notin F).$$

For $S \in \mathcal{C}_{M,N}$, set

$$b_\eta(S) = |F_{\mathrm{c}} \setminus S| + |S \cap U_{\mathrm{h}}|.$$

Then

$$K(S) - K(F) \geq \eta\, b_\eta(S).$$

Consequently, for every normalized $\Psi = \sum_S c_S e_S$,

$$\sum_S |c_S|^2 b_\eta(S) \leq \frac{\Delta}{\eta},$$

and

$$\|(1 - \Pi_\eta)\Psi\|^2 \leq \frac{\Delta}{\eta}.$$

Proof. Let

$$h_{\mathrm{c}} = |F_{\mathrm{c}} \setminus S|, \qquad h_{\mathrm{s}} = |F_{\mathrm{s}} \setminus S|, \qquad p_{\mathrm{s}} = |S \cap U_{\mathrm{s}}|, \qquad p_{\mathrm{h}} = |S \cap U_{\mathrm{h}}|.$$

Because $|S| = |F|$,

$$h_{\mathrm{c}} + h_{\mathrm{s}} = p_{\mathrm{s}} + p_{\mathrm{h}}.$$

Using the four energy inequalities,

$$\begin{aligned} K(S) - K(F) &\geq \mu p_{\mathrm{s}} + (\mu + \eta) p_{\mathrm{h}} - \mu h_{\mathrm{s}} - (\mu - \eta) h_{\mathrm{c}} \\ &= \eta (p_{\mathrm{h}} + h_{\mathrm{c}}). \end{aligned}$$

This is the pointwise bound. Multiplying by $|c_S|^2$ and summing gives the expectation estimate. Finally, if S is not in the range of Π_η, then either $F_{\mathrm{c}} \setminus S \neq \varnothing$ or $S \cap U_{\mathrm{h}} \neq \varnothing$, hence $b_\eta(S) \geq 1$. Therefore

$$\|(1 - \Pi_\eta)\Psi\|^2 = \sum_{S \notin \operatorname{Ran} \Pi_\eta} |c_S|^2 \leq \sum_S |c_S|^2 b_\eta(S) \leq \Delta/\eta.$$

$\square$

Remark 3.2. Theorem 3.1 is the promised replacement for the collapsing finite-cell gap. Small kinetic excess no longer forces closeness to one determinant, but it still forces all possible low-energy fluctuations into a thin shell.

4 Finite periodic Coulomb observables

Let $\mathcal{P} \subset (2\pi/L)\mathbb{Z}^3$ be finite and spin degeneracy q be fixed. On the finite plane-wave space

$$\mathfrak{h}_{\mathcal{P},L} = \operatorname{span}\{L^{-3/2}e^{ik\cdot x}\chi_\sigma : k \in \mathcal{P},\ \sigma = 1,\dots,q\},$$

the periodic Coulomb interaction with the zero Fourier mode removed is a bounded projected operator:

$$V_L = \sum_{1\le i<j\le N} v_L(x_i - x_j), \qquad v_L(x) = \frac{1}{L^3}\sum_{\substack{p\in(2\pi/L)\mathbb{Z}^3\\ p\neq 0}} \frac{4\pi}{|p|^2}e^{ip\cdot x}.$$

Here v_L is understood through its zero-mode-free Fourier multiplier, or equivalently through its matrix elements after projection to $\mathfrak{h}_{\mathcal{P},L}$. Since $\mathcal{P}$ is finite, those matrix elements form a finite matrix. Hence Theorem 2.1 applies to $A = V_L$, and gives

$$|\langle\Psi, V_L\Psi\rangle - \langle\Phi_F, V_L\Phi_F\rangle| \le 2\|V_L\|\sqrt{2\Delta/g}.$$

The same finite-dimensional argument applies to any projected Coulomb-type quadratic observable. Thus, in a fixed cutoff cell, kinetic closeness to the closed-shell Fermi determinant forces closeness of all Coulomb expectations.

5 Exchange of the closed-shell Fermi sea

Assume now that the occupied closed shell fills all spin states over a spatial momentum set $F_L \subset (2\pi/L)\mathbb{Z}^3$. The one-particle density is constant:

$$\rho_L = \frac{q|F_L|}{L^3}.$$

For the Slater determinant Φ_F, the direct term cancels the Hartree term, and the indirect Coulomb energy is exactly exchange:

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

Only equal-spin pairs contribute to exchange, giving the factor q.

Proposition 5.1 (Riemann-sum Dirac limit)**.** *Let F_L be closed shells satisfying*

$$\frac{q|F_L|}{L^3} \to \rho > 0,$$

and suppose their occupied momenta converge, in the usual lattice Riemann-sum sense, to the ball $\{p : |p| \le k_F\}$, where

$$\rho = \frac{qk_F^3}{6\pi^2}.$$

Then

$$\frac{I_L(\Phi_F)}{L^3} \longrightarrow -C_D(q)\rho^{4/3},$$

with

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

Proof. Since the lattice spacing in momentum space is $2\pi/L$,

$$\frac{1}{L^6}\sum_{\substack{k,\ell\in F_L\\ k\neq\ell}}\frac{4\pi}{|k-\ell|^2}\longrightarrow(2\pi)^{-6}\iint_{|p|,|p'|\le k_F}\frac{4\pi}{|p-p'|^2}\,\mathrm{d}p\,\mathrm{d}p'.$$

The singularity is integrable in six dimensions. Indeed, after writing $s=p-p'$, the local singular integral is bounded by a constant multiple of $\int_0^\eta r^2r^{-2}\,\mathrm{d}r=\eta$. The corresponding lattice estimate is uniform in L: for each occupied k,

$$\sum_{\substack{\ell\in(2\pi/L)\mathbb{Z}^3\\ 0<|k-\ell|<\eta}}\frac{1}{|k-\ell|^2}=\frac{L^2}{(2\pi)^2}\sum_{0<|m|<\eta L/(2\pi)}\frac{1}{|m|^2}\le CL^3\eta.$$

Since $|F_L|=O(L^3)$, this implies

$$\frac{1}{L^6}\sum_{\substack{k,\ell\in F_L\\ 0<|k-\ell|<\eta}}\frac{1}{|k-\ell|^2}\le C\eta.$$

Thus the near-diagonal part is uniformly small as $\eta\downarrow 0$. Away from the diagonal the kernel is bounded and continuous, so ordinary Riemann-sum convergence applies. Combining the two estimates proves the singular Riemann-sum convergence.

It remains to compute the integral. Let $B_k=\{p:|p|\le k\}$. The overlap volume of two radius-k balls with centers separated by $r\le 2k$ is

$$|B_k\cap(B_k+s)|=\frac{\pi}{12}(4k+r)(2k-r)^2,\qquad r=|s|.$$

Therefore

$$\begin{aligned}\iint_{B_k\times B_k}\frac{4\pi}{|p-p'|^2}\,\mathrm{d}p\,\mathrm{d}p'&=4\pi\int_{|s|\le 2k}\frac{|B_k\cap(B_k+s)|}{|s|^2}\,\mathrm{d}s\\&=16\pi^2\int_0^{2k}|B_k\cap(B_k+s)|\,\mathrm{d}r\\&=16\pi^2\int_0^{2k}\frac{\pi}{12}(4k+r)(2k-r)^2\,\mathrm{d}r\\&=16\pi^3k^4.\end{aligned}$$

Consequently

$$\frac{I_L(\Phi_F)}{L^3}\to-\frac{q}{2}(2\pi)^{-6}16\pi^3k_F^4=-\frac{qk_F^4}{8\pi^3}.$$

Using $\rho=qk_F^3/(6\pi^2)$, this becomes

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

□

6 A Dirac bound for arbitrary states in a thin shell

The shell-stability theorem becomes useful for exchange because the number of shell orbitals is only a surface-order perturbation of the Fermi ball.

Let

$$F_-=\{k\in(2\pi/L)\mathbb{Z}^3:|k|\le k_F-\eta\},\qquad S_\eta=\{k\in(2\pi/L)\mathbb{Z}^3:k_F-\eta<|k|<k_F+\eta\}.$$

Let P_- be the projection onto all spin plane waves with spatial momenta in F_-, and let Q_η be the projection onto all spin plane waves with spatial momenta in S_η. Thus

$$\operatorname{rank} Q_\eta = q|S_\eta|.$$

Let Φ_- be the filled Slater determinant over P_-. Consider an arbitrary correlated state

$$\Psi = \Phi_- \wedge \Xi, \qquad \Xi \in \bigwedge^n Q_\eta \mathfrak{h}_{\mathcal{P},L},$$

with no assumption that Ξ is quasi-free.

Theorem 6.1 (Dirac bound for a correlated Fermi shell)**.** *For fixed q, ρ, k_F, as $L \to \infty$ and then $\eta \downarrow 0$, every state of the above form satisfies*

$$I_L(\Psi) \geq -C_D(q)\rho^{4/3}L^3 - O_{\rho,q}(\eta L^3) - O_{\rho,q}(\eta^{4/3}L^3) - o(L^3).$$

The constants are independent of the correlated shell state Ξ.

Proof. Let γ_Ξ be the one-particle density matrix of Ξ. Since Φ_- is a filled determinant and Ξ lives in an orthogonal shell, the standard exterior-product formula for the two-particle density gives

$$I_L(\Phi_- \wedge \Xi) = I_L(\Phi_-) + I_L(\Xi) - X_L(P_-, \gamma_\Xi),$$

where

$$X_L(P_-, \gamma_\Xi) = \iint v_L(x-y)P_-(x,y)\gamma_\Xi(y,x)\,\mathrm{d}x\,\mathrm{d}y.$$

The residual shell state is arbitrary, so we use Lieb-Oxford:

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

Since $0 \leq \gamma_\Xi \leq Q_\eta$,

$$\rho_\Xi(x) \leq Q_\eta(x,x) = \frac{\operatorname{rank} Q_\eta}{L^3}.$$

Therefore

$$\int \rho_\Xi^{4/3} \leq L^3\left(\frac{\operatorname{rank} Q_\eta}{L^3}\right)^{4/3} = O_{\rho,q}(\eta^{4/3}L^3) + o(L^3),$$

because $\operatorname{rank} Q_\eta = O_{\rho,q}(\eta L^3) + o(L^3)$.

It remains to bound the cross exchange. In the plane-wave basis,

$$X_L(P_-, \gamma_\Xi) = \frac{1}{L^3}\sum_{\sigma=1}^{q}\sum_{\substack{k\in F_-\\ \ell\in S_\eta}} \frac{4\pi}{|k-\ell|^2}\langle \ell,\sigma|\gamma_\Xi|\ell,\sigma\rangle.$$

Since $0 \leq \gamma_\Xi \leq Q_\eta$, all diagonal entries are at most one, so

$$X_L(P_-, \gamma_\Xi) \leq \frac{q}{L^3}\sum_{\substack{k\in F_-\\ \ell\in S_\eta}} \frac{4\pi}{|k-\ell|^2}.$$

The same near-diagonal estimate used in the Riemann-sum proof shows that this sum is

$$O_{\rho,q}(\eta L^3) + o(L^3).$$

Indeed, for each ℓ the integral and lattice sum of $|k-\ell|^{-2}$ over the ball $|k| \leq k_F - \eta$ are bounded uniformly in ℓ, while the shell has $O(\eta L^3)$ orbitals.

Finally, the closed-shell Fermi sea over P_- has density

$$\rho_- = \frac{q(k_F-\eta)^3}{6\pi^2} + o(1),$$

and the Riemann-sum proposition gives

$$I_L(\Phi_-) = -C_D(q)\rho_-^{4/3}L^3 + o(L^3) = -C_D(q)\rho^{4/3}L^3 + O_{\rho,q}(\eta L^3) + o(L^3).$$

Combining the three estimates proves the theorem. □

Remark 6.2. Theorem 6.1 is strictly stronger than the finite-gap determinant stability statement: inside the shell, the state may be fully correlated and arbitrarily far from a Slater determinant. The Dirac constant survives because the fluctuating shell holds only $O(\eta L^3)$ orbitals, so its Lieb–Oxford and cross-exchange costs are lower order as $\eta \downarrow 0$.

7 What Lean checks

The accompanying file `StabilityCore.lean` checks the finite occupation-basis inequalities behind the first two theorems. In particular it proves, for a finite list of configurations, that

$$g\sum_S p_S \mathbf{1}_{S\neq F} \le \sum_S p_S(K(S)-K(F))$$

from the pointwise facts

$$\mathbf{1}_{S\neq F} \le |S\setminus F|, \qquad g|S\setminus F| \le K(S)-K(F), \qquad p_S \ge 0.$$

It also checks the overlap-to-distance estimate

$$|\langle \Phi_F, \Psi\rangle|^2 \ge 1-\delta \quad \Rightarrow \quad \inf_\theta \|\Psi - e^{i\theta}\Phi_F\|^2 \le 2\delta.$$

The same Lean lemma applies to the gapless shell theorem with g replaced by η, $\mathbf{1}_{S\neq F}$ replaced by the indicator of leaving the shell subspace, and $|S\setminus F|$ replaced by $b_\eta(S) = |F_\mathrm{c}\setminus S| + |S\cap U_\mathrm{h}|$.

Remark 7.1. This note does not claim to settle Lieb's original local open problem. What it does provide is a rigorous nontrivial mechanism beyond the finite-cell gap: small kinetic excess forces all gapless fluctuations into a thin shell, and arbitrary correlations inside that shell leave the Dirac exchange density unchanged in the thermodynamic thin-shell limit.