A gapless kinetic-to-Dirac theorem for homogeneous occupation states

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Abstract

We prove that the Dirac exchange constant is the correct asymptotic indirect-energy lower bound, in the thermodynamic limit, for a broad class of homogeneous fermionic occupation states with controlled kinetic excess and *without* any spectral gap assumption at the Fermi surface. The states considered are occupation-diagonal density matrices Γ_L in the plane-wave basis of a periodic box, with arbitrarily correlated occupation probabilities. Writing ε_L for the per-volume kinetic excess above the finite-volume Fermi sea, normalized by $k_F^2 \rho L^3$, we show that for every small $\alpha > 0$ the per-volume indirect energy is bounded below by $-C_D(q)\rho^{4/3} - A_{q,\rho}(\alpha + \varepsilon_L/\alpha)\rho^{4/3} - o_\alpha(1)$. Optimizing in α gives the interpolation $\liminf_{L\to\infty} L^{-3} I_L(\Gamma_L) \geq -(C_D(q) + 2A_{q,\rho}\sqrt{\varepsilon})\rho^{4/3}$, where $\varepsilon = \limsup \varepsilon_L$. In particular, sub-extensive kinetic excess forces the sharp Dirac bound. The proof factors into an abstract finite shell-exchange principle and two elementary lattice-Coulomb marginal estimates; the spectral gap is replaced by a shell argument that survives the gapless thermodynamic limit.

1 Setting and main theorem

In the thermodynamic limit of a homogeneous fermion gas, the per-volume indirect Coulomb energy of a filled Fermi sea is asymptotically $-C_D(q)\rho^{4/3}$, with

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

the Dirac exchange constant. A natural and physically important question is how robust this asymptotic is under correlations: how much can one deform a Fermi sea while keeping the indirect energy close to $-C_D(q)\rho^{4/3}$? Finite-gap theorems answer a related question by showing that a fixed spectral gap forces closeness to a single Slater determinant. In the gapless thermodynamic limit, however, the one-particle spectrum has no gap and the spectral approach breaks down.

The result of this paper replaces the spectral-gap mechanism by a shell mechanism. We work with *occupation-diagonal* states—density matrices that are mixtures of plane-wave Slater determinants with arbitrarily correlated occupation numbers—and prove that low kinetic excess alone is enough to force the Dirac lower bound on the indirect energy. The kinetic excess controls a thin Fermi shell where the occupation deviates from the kinetic minimizer; the Coulomb cost of populating that shell is bounded by a marginal estimate.

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

$$\mathcal{K}_L = \frac{2\pi}{L}\mathbb{Z}^3.$$

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The spin degeneracy is q. A spin-momentum orbital is denoted $(k,\sigma) \in \mathcal{K}_L \times \{1,\dots,q\}$. For an N-element set S of spin-momenta let Φ_S be the corresponding plane-wave Slater determinant and put

$$K(S) = \sum_{(k,\sigma)\in S} |k|^2.$$

Let F_L be an N-element minimizer of $K(S)$. Thus F_L is a finite-volume Fermi sea, with an arbitrary choice inside the last degenerate shell.

We consider occupation-diagonal density matrices

$$\Gamma_L = \sum_{|S|=N} p_S |\Phi_S\rangle\langle\Phi_S|, \qquad p_S \geq 0, \qquad \sum_S p_S = 1.$$

The probabilities p_S are arbitrary; in particular this is not a quasi-free assumption, and the occupation variables may carry arbitrary correlations.

Let

$$T_L(\Gamma_L) = \sum_S p_S K(S), \qquad \Delta_L = T_L(\Gamma_L) - K(F_L).$$

For $N/L^3 \to \rho > 0$, define

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

Theorem 1.1 (Homogeneous kinetic–Dirac interpolation)**.** *Assume $N_L/L^3 \to \rho > 0$ and let Γ_L be any occupation-diagonal N_L-fermion state as above. Set*

$$\varepsilon_L = \frac{\Delta_L}{k_F^2 \rho L^3}.$$

Then there is a constant $A_{q,\rho} < \infty$, independent of L, Γ_L, and the occupation correlations, such that for every fixed $0 < \alpha < 1/2$,

$$\frac{I_L(\Gamma_L)}{L^3} \geq -C_D(q)\rho^{4/3} - A_{q,\rho}\left(\alpha + \frac{\varepsilon_L}{\alpha}\right)\rho^{4/3} - o_\alpha(1).$$

Consequently, if $\limsup_{L\to\infty} \varepsilon_L = \varepsilon$, then

$$\liminf_{L\to\infty} \frac{I_L(\Gamma_L)}{L^3} \geq -\left(C_D(q) + 2A_{q,\rho}\sqrt{\varepsilon}\right)\rho^{4/3}$$

for $0 < \varepsilon < 1/4$, after optimizing $\alpha = \sqrt{\varepsilon}$. Combining this with Lieb–Oxford gives the interpolation

$$\liminf_{L\to\infty} \frac{I_L(\Gamma_L)}{L^3} \geq -\min\left\{C_{\mathrm{LO}}, C_D(q) + 2A_{q,\rho}\sqrt{\varepsilon}\right\}\rho^{4/3}.$$

In particular, kinetic excess $o(L^3)$ forces the sharp Dirac lower bound

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

Remark 1.2. This is gapless: the one-particle spacing at the Fermi surface may collapse to zero. The theorem replaces a spectral-gap argument by a shell argument. The remaining assumption is occupation diagonality in the plane-wave basis; removing that coherence restriction is an independent problem, not a finite-gap artifact.

Plan of the paper. Section 2 formulates the abstract *shell-exchange principle* (Theorem 2.1): for any occupation-diagonal state, kinetic excess upper-bounds the expected core-hole/high-particle count, and a marginal exchange bound converts that into an indirect-energy estimate. Section 3 establishes the two elementary lattice-Coulomb estimates required to apply the shell-exchange principle in the periodic Coulomb setting (Theorems 3.1 and 3.2). Section 4 assembles the proof of Theorem 1.1. Section 5 closes with a short interpretation that highlights how the shell mechanism replaces a finite spectral gap.

2 The finite shell principle

The next theorem is the abstract finite mechanism. It is useful because it separates the kinetic part from the Coulomb estimates.

Let F be a reference N-element set of orbitals with one-particle energies ε_i. Choose a chemical level μ and a shell width satisfying $s > 0$. Define

$$C = \{i \in F : \varepsilon_i \le \mu - s\}, \qquad B = \{i : |\varepsilon_i - \mu| < s\}, \qquad H = \{i \notin F : \varepsilon_i \ge \mu + s\}.$$

For an N-element configuration S, put

$$b(S) = |C \setminus S| + |S \cap H|.$$

Let $X(S) \ge 0$ be an exchange magnitude, so that the indirect energy of Φ_S is $-X(S)$. Assume that X has the following marginal bound: there is $\Lambda < \infty$ such that

$$X(S) \le X(C) + \Lambda |S \setminus C| \qquad \text{for all } |S| = N.$$

Theorem 2.1 (Abstract shell-exchange principle)**.** *Let* $\Gamma = \sum_S p_S |\Phi_S\rangle\langle\Phi_S|$ *be an occupation-diagonal state and*

$$\Delta = \sum_S p_S (K(S) - K(F)).$$

Assume

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

Then

$$I(\Gamma) \ge -X(C) - \Lambda \left(|B| + \frac{\Delta}{s} \right).$$

Proof. For a fixed configuration S, write

$$h_c = |C \setminus S|, \qquad h_b = |(F \cap B) \setminus S|, \qquad p_b = |S \cap (B \setminus F)|, \qquad p_h = |S \cap H|.$$

Since $|S| = |F|$,

$$h_c + h_b = p_b + p_h.$$

Using the four energy inequalities,

$$\begin{aligned} K(S) - K(F) &\ge \mu p_b + (\mu + s) p_h - \mu h_b - (\mu - s) h_c \\ &= s(p_h + h_c) = s\, b(S). \end{aligned}$$

Thus

$$\sum_S p_S b(S) \le \Delta / s.$$

Moreover

$$S \setminus C \subset B \cup (S \cap H),$$

and hence

$$|S \setminus C| \le |B| + b(S).$$

By the marginal exchange bound,

$$X(S) \le X(C) + \Lambda(|B| + b(S)).$$

Averaging over p_S gives

$$\sum_S p_S X(S) \le X(C) + \Lambda\left(|B| + \Delta/s\right).$$

For occupation-diagonal plane-wave states all determinants have constant one-particle density N/L^3, so the Hartree term is the same for every component and the indirect energy is the average of the determinant indirect energies:

$$I(\Gamma) = -\sum_S p_S X(S).$$

This proves the theorem. □

3 Coulomb exchange marginal bounds

For a spin-momentum set A, define its exchange magnitude by

$$X_L(A) = \frac{1}{2L^3} \sum_{\sigma=1}^{q} \sum_{\substack{k,\ell \in A_\sigma \\ k \neq \ell}} \frac{4\pi}{|k-\ell|^2},$$

where $A_\sigma = \{k : (k,\sigma) \in A\}$. For a plane-wave determinant Φ_A, the periodic indirect energy with the zero Fourier mode removed is

$$I_L(\Phi_A) = -X_L(A).$$

Lemma 3.1 (Uniform lattice Coulomb bounds). *Fix $R_0 < \infty$. There is $C_{R_0} < \infty$ such that for all sufficiently large L:*

$$\sup_{\ell \in \mathcal{K}_L} \frac{1}{L^3} \sum_{\substack{k \in \mathcal{K}_L \\ |k| \le R_0 \\ k \neq \ell}} \frac{4\pi}{|k-\ell|^2} \le C_{R_0};$$

and, for every finite $A \subset \mathcal{K}_L \times \{1, \ldots, q\}$ with $|A| \le ML^3$,

$$X_L(A) \le C_{M,q}|A|.$$

Proof. The first estimate is a lattice version of the local integrability of $|x|^{-2}$ in three dimensions. Split the sum into cubes of side $2\pi/L$. Away from the cube containing ℓ, the sum is bounded by a constant times

$$\int_{|p| \le R_0+1} \frac{\mathrm{d}p}{|p-\ell|^2},$$

uniformly in ℓ. The cube containing ℓ contributes at most

$$\frac{1}{L^3} \frac{4\pi}{(2\pi/L)^2} = O(L^{-1}),$$

after omitting $k = \ell$. This proves the first bound.

For the second estimate, fix one occupied momentum ℓ. Among all subsets of $\mathcal{K}_L$ with m points, the sum of $|k-\ell|^{-2}$ is bounded by filling the m lattice points closest to ℓ. If

$$r_m = C(m/L^3)^{1/3},$$

then this nearest-neighbour sum is bounded by

$$CL^3 \int_{|p|\le r_m} \frac{\mathrm{d}p}{|p|^2} + O(L^2) \le CL^3 r_m + O(L^2).$$

After multiplying by L^{-3}, the contribution per occupied orbital is

$$O\big((m/L^3)^{1/3}\big) + O(L^{-1}).$$

For $|A| \le ML^3$ this is bounded uniformly. Summing over occupied orbitals and spin components gives $X_L(A) \le C_{M,q}|A|$. □

Lemma 3.2 (Fermi-core marginal bound)**.** *Let C_L be any spin-momentum set contained in $\{|k| \le R_0\}$, and let $|S| \le ML^3$. Then*

$$X_L(S) \le X_L(C_L) + \Lambda_{M,q,R_0}|S \setminus C_L|$$

for all sufficiently large L.

Proof. Put $E = S \setminus C_L$. Since removing occupied momenta cannot increase exchange,

$$X_L(S) \le X_L(C_L \cup E).$$

Expanding the exchange of $C_L \cup E$,

$$X_L(C_L \cup E) \le X_L(C_L) + X_L(E) + \frac{1}{L^3} \sum_{\sigma=1}^{q} \sum_{\substack{k\in(C_L)_\sigma \\ \ell\in E_\sigma}} \frac{4\pi}{|k-\ell|^2}.$$

The cross term is at most $C_{R_0}|E|$ by the first estimate of Theorem 3.1. The term $X_L(E)$ is at most $C_{M,q}|E|$ by the second estimate. This proves the claim. □

4 Proof of the main theorem

Proof of Theorem 1.1. Let F_L be the kinetic minimizer. There is a chemical level μ_L such that

$$|k|^2 \le \mu_L \quad \text{on } F_L, \qquad |k|^2 \ge \mu_L \quad \text{outside } F_L,$$

where degeneracies at μ_L are assigned arbitrarily to make $|F_L| = N_L$. By the elementary lattice Weyl law,

$$\mu_L \to k_F^2.$$

Fix $0 < \alpha < 1/2$ and set

$$s = \alpha k_F^2.$$

Let C_L, B_L, and H_L be the core, active shell, and high region defined from F_L, μ_L, s as in Theorem 2.1. The shell has surface-order volume:

$$|B_L| \le C_{q,\rho}\alpha L^3 + o_\alpha(L^3).$$

This is again the lattice Weyl law, applied to $\big||k|^2 - \mu_L\big| < s$.

The core C_L is contained in a fixed ball $\{|k| \le R_0\}$, and $|S| = N_L \le M_\rho L^3$. Hence Theorem 3.2 supplies a constant $\Lambda_{q,\rho}$ such that

$$X_L(S) \le X_L(C_L) + \Lambda_{q,\rho}|S \setminus C_L|.$$

The abstract shell-exchange principle gives

$$I_L(\Gamma_L) \ge -X_L(C_L) - \Lambda_{q,\rho}\left(|B_L| + \frac{\Delta_L}{\alpha k_F^2}\right).$$

Dividing by L^3, using the definition of ε_L, and observing that $k_F\rho$ is a constant multiple of $\rho^{4/3}$, the error term is bounded by

$$A_{q,\rho}\rho^{4/3}\left(\alpha + \frac{\varepsilon_L}{\alpha}\right) + o_\alpha(1).$$

It remains only to evaluate the core exchange. The sets C_L converge, in Riemann-sum sense, to the ball $|k|^2 \le k_F^2 - \alpha k_F^2$. Therefore

$$\frac{X_L(C_L)}{L^3} \le C_D(q)\rho^{4/3} + C_{q,\rho}\alpha\rho^{4/3} + o_\alpha(1).$$

This is the usual Dirac Riemann-sum computation; the singularity is harmless because $|p - p'|^{-2}$ is locally integrable in three dimensions, and the near-diagonal lattice contribution is $O(\eta)$ after excluding $|p - p'| < \eta$.

Combining the preceding two estimates proves the first bound. The optimized bound follows by choosing $\alpha = \sqrt{\varepsilon}$. The Lieb–Oxford interpolation follows by taking the better of this estimate and the Lieb–Oxford lower bound. □

5 Interpretation

The finite-gap theorem says that a fixed gap forces closeness to one Slater determinant. Theorem 1.1 is different. The spectral gap is allowed to collapse. Low kinetic excess only forces the state into a thin Fermi shell, and the proof shows that this is enough: the shell has only $O(\alpha L^3)$ orbitals, while the expected number of particles outside the shell is at most $O(\Delta_L/(\alpha k_F^2))$. Coulomb exchange has bounded marginal cost per such orbital, so the total error is

$$O(\alpha L^3) + O(\Delta_L/\alpha).$$

This is the mechanism producing the Dirac constant from kinetic information in the gapless thermodynamic limit.

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