Harmonic moment stability and quantitative Coulomb extension

Research development supplement for Yicheng Pan

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Abstract

The low-particle Lieb–Oxford gap manuscript can be strengthened by separating its finite-configuration mechanism from optimizer localization. We give a self-contained, explicit inverse bound for the first N harmonic moment tensors of N equal-weight points in three dimensions, without a separation assumption. The Hölder exponent $1/N$ is optimal on bounded configurations. A single bounded marginal then forces moment variance. We propagate this to an exact exterior Coulomb covariance estimate after arbitrary small-volume deletion, and to a conditional, all-particle one-particle extension theorem. These results generalize the supplied manuscript's three-point bridge; they do not furnish the missing uniform optimizer localization, improve a sharp Lieb–Oxford constant, or establish a new all-N numerical gap recursion. The underlying projection, polynomial and extension methods are credited to prior work.

Status and scope. This is an AI-assisted candidate mathematical development, not a submission-ready or externally validated paper. The proofs and novelty assessment require human expert review. No priority or acceptance claim is made. The original 49-page manuscript and its bibliography are unchanged. This supplement inspects and extends its harmonic-moment section and three-to-four-particle extension; it does not certify the original foundational or localization arguments.

1 Contribution and primary literature

Rosenzweig [1] states attainment and strict monotonicity of the fixed-particle Riesz constants for every particle number. Sections 6.2–6.3 supply the non-product extension and diffuse completion, while Section 7.2 identifies quantitative control of normalized optimizers as the missing ingredient. Di Marino–Lelotte [2] supply compact support conditional on existence. Thus neither qualitative strict monotonicity nor compact support is a new contribution of the supplied manuscript or this supplement.

Wang–Lü [3, Lemma 0.4.3] construct configuration-dependent complex-isotropic projections and annihilating polynomials. Their source-recovery application assumes within-configuration separation. Here equal known weights permit a degree-N Newton-identity argument and a collision-uniform Hölder estimate. This extends the supplied manuscript's degree-three calculation; it is not a claim to invent harmonic reconstruction or Prony-type methods. Broader antecedents include multivariate Prony recovery [5], so an inverse-problems literature clearance is still needed. Lewin–Lieb–Seiringer [4] give the published universal bound $C_N \leq 1.58$; the new formulas do not improve it.

Proposed revised contribution statement. We quantify the existing finite-particle extension mechanism through a collision-uniform harmonic-moment theorem for equal-weight configurations and a deletion-stable exterior covariance estimate. The inverse exponent is sharp. A modular extension theorem isolates the optimizer information actually needed: a bounded conditional marginal, a positive-probability bounded core, and finite occupied volume. The original low-particle localization estimates provide worked instances, conditional on the stated external attainment input. The general theorem does not itself bound these inputs uniformly in particle number.

2 An all-particle harmonic inverse theorem

For $N \geq 1$, $R > 0$, and $X = (x_1, \dots, x_N) \in (B_R)^N$, let

$$M_k(X) = \sum_{i=1}^{N} \mathrm{STF}(x_i^{\otimes k}), \qquad e_R(X,Y)^2 = \sum_{k=1}^{N} R^{2-2k} \|M_k(X) - M_k(Y)\|_F^2.$$

Here STF is the orthogonal projection onto symmetric trace-free tensors, and $\|\cdot\|_F$ is the full Frobenius norm. Put

$$c_N = \sqrt{1 - (1 - 1/(2N))^2}, \tag{1}$$

$$K_N = c_N^{-N} \left[\sum_{j=1}^{N} \frac{2^{j-1}}{j^2} \binom{2N-j}{N-j}^2 \right]^{1/2}. \tag{2}$$

Theorem 2.1. *For any $X, Y \in (B_R)^N$,*

$$\max_i \operatorname{dist}(x_i, \{y_1, \dots, y_N\})^N \leq K_N R^{N-1} e_R(X,Y).$$

The reverse estimate also holds. If all M_k, $1 \leq k \leq N$, agree, the point multisets agree including multiplicity. No collision separation is assumed.

Proof. Fix x_i. If it equals a point of Y, its distance is zero. Otherwise let $u_j = (x_i - y_j)/|x_i - y_j|$. For a uniform normal $n \in S^2$, each exceptional set $|n \cdot u_j| > 1 - 1/(2N)$ has probability $1/(2N)$. Their union has probability at most $1/2$. Choose a normal outside the union and orthonormal vectors a, b spanning $n^\perp$. With $z = a + ib$,

$$z \cdot z = 0, \quad |z \cdot v| \leq |v| \ (v \in \mathbb{R}^3), \quad |z \cdot (x_i - y_j)| \geq c_N |x_i - y_j|.$$

The power sums of the projected points are $p_j(X) = \sum_i (z \cdot x_i)^j = z^{\otimes j} : M_j(X)$. The real and imaginary parts of $z^{\otimes j}$ are orthogonal real tensors, both of squared norm 2^{j-1}, because $(z \cdot z)^j = 0$ and $|z|^{2j} = 2^j$. Bessel's inequality gives

$$|p_j(X) - p_j(Y)| \leq 2^{(j-1)/2} \|M_j(X) - M_j(Y)\|_F. \tag{3}$$

Write $\Delta p_j = p_j(Y) - p_j(X)$ and $p_j(t) = (1-t)p_j(X) + t p_j(Y)$ for $0 \leq t \leq 1$ and all $j \geq 1$. As a formal power series set

$$E_t(u) = \exp\left(\sum_{j \geq 1} (-1)^{j-1} p_j(t) u^j / j \right) = \sum_{k \geq 0} e_k(t) u^k.$$

At the endpoints e_k are elementary symmetric functions of the projected roots. Intermediate coefficients need not describe roots inside the disk, and no such assertion is used. Since $|p_j(t)| \le NR^j$, coefficientwise majorization by $\exp(\sum_{j\ge1} NR^j u^j/j) = (1-Ru)^{-N}$ gives

$$|e_l(t)| \le \binom{N+l-1}{l} R^l.$$

Differentiating the formal series and integrating t yields

$$|e_k(1) - e_k(0)| \le \sum_{j=1}^{k} \frac{|\Delta p_j|}{j} \binom{N+k-j-1}{k-j} R^{k-j}.$$

For $F_X(w) = \prod_i (w - z\cdot x_i)$, and $|w| \le R$, summing coefficients and using the hockey-stick identity gives

$$\begin{aligned} |F_X(w) - F_Y(w)| &\le \sum_{j=1}^{N} \frac{|\Delta p_j|}{j} R^{N-j} \sum_{l=0}^{N-j} \binom{N+l-1}{l} \\ &= \sum_{j=1}^{N} \frac{|\Delta p_j|}{j} R^{N-j} \binom{2N-j}{N-j} \\ &\le c_N^N K_N R^{N-1} e_R(X,Y). \end{aligned}$$

The final step is (3) and Cauchy–Schwarz. At $w = z\cdot x_i$, $F_X(w) = 0$, whereas $|F_Y(w)| \ge c_N^N \operatorname{dist}(x_i, \{y_j\})^N$. This proves the estimate. Interchanging X, Y proves its reverse.

If the moments agree, choose a projection whose normal is not parallel to any nonzero difference of distinct points in the combined finite support. The projection is then injective on that support. Its first N power sums agree, so Newton's identities identify its degree-N root multisets. Injectivity gives the original multiplicities as well. □

Proposition 2.2 (Sharpness of the exponent)**.** *On the fixed domain $(B_1)^N$, no bound $d_H(X,Y) \le Ce_1(X,Y)^\alpha$ can hold uniformly with $\alpha > 1/N$.*

Proof. Take N equally spaced points on the circle of radius ε in the xy plane, and rotate the polygon by π/N to obtain Y. Their Hausdorff distance is $2\varepsilon\sin(\pi/(2N))$. For $k < N$, every coordinate polynomial of degree k restricted to the circle is a trigonometric polynomial with frequencies of absolute value at most k. Its sum over the polygon retains only frequency zero and is unchanged by rotation. Thus the full degree-k tensors, hence their STF parts, agree. At degree N the harmonic polynomial $(x+iy)^N$ has sums $N\varepsilon^N$ and $-N\varepsilon^N$, so the degree-N difference is nonzero and scales exactly as ε^N. Consequently $e_1(X,Y) = b_N\varepsilon^N$ for a constant $b_N > 0$. Sending $\varepsilon \downarrow 0$ excludes $N\alpha > 1$. This includes $N = 1$. □

3 Variance and deletion stable exterior covariance

Corollary 3.1. *Let Q be a probability law on $(B_R)^N$ whose first labeled marginal has density at most L. If $r > 0$ and $(4\pi/3)NLr^3 \le 1/2$, then*

$$\sum_{k=1}^{N} R^{2-2k} \operatorname{Var}_Q(M_k) \ge \frac{r^{2N}}{4K_N^2 R^{2N-2}}.$$

Here tensor variance means $\mathbb{E}\|M_k - \mathbb{E}M_k\|_F^2$. Symmetry and independence of coordinates are unnecessary.

Proof. For every fixed Y, the first coordinate lies outside the union of the N radius-r balls with probability at least $1/2$. The inverse theorem therefore bounds $e_R(X,Y)$ below by $r^N/(K_N R^{N-1})$ on an event of that probability. Average over an independent copy Y of X and use $\mathbb{E}\|M(X) - M(Y)\|^2 = 2\operatorname{Var}(M)$. □

Let $S = \{T < |y| < 2T\}$, $T \geq R$, with uniform probability ν_0, and put

$$a_k = (2k-1)!!/k!,$$
$$w_k = a_k^2 \frac{k!}{(2k+1)!!} \frac{3(1-2^{1-2k})}{7(2k-1)},$$
$$\beta_N = \min_{1\leq k\leq N} w_k, \qquad H_N = N \max_{1\leq k\leq N} (a_k^2/w_k).$$

For $y = sn$, define the centered degree-N truncation $f(X,y) = \sum_{k=1}^N a_k s^{-k-1} n^{\otimes k} : (M_k(X) - \mathbb{E}_Q M_k)$. Spherical orthogonality and radial integration give exactly

$$\|f\|^2_{L^2(Q\otimes\nu_0)} = \sum_{k=1}^N w_k T^{-2k-2} \operatorname{Var}_Q(M_k) \geq \frac{\beta_N r^{2N}}{4K_N^2 T^{2N+2}}. \tag{4}$$

Indeed, the angular STF factor is $k!/(2k+1)!!$, and $\mathbb{E}_{\nu_0} s^{-2k-2} = 3(1-2^{1-2k})/[7(2k-1)T^{2k+2}]$. For each X, the sum-of-N-squares bound gives $\sup_S |f(X,\cdot)|^2 \leq H_N \|f(X,\cdot)\|^2_{L^2(\nu_0)}$.

Theorem 3.2. *Under Corollary 3.1, let $E \subset S$ be measurable, ν uniform on E, and $\theta = |S \setminus E|/|S| \leq [2(H_N+1)]^{-1}$. If*

$$T \geq \max\left\{2R, \frac{4\sqrt{8}\, N K_N}{\sqrt{\beta_N}} \frac{R^{N+1}}{r^N}\right\},$$

then for $V(X,y) = \sum_i |y - x_i|^{-1}$ and $h = (\mathrm{Id} - \mathbb{E}_Q)(\mathrm{Id} - \mathbb{E}_\nu)V$,

$$\|h\|^2_{L^2(Q\otimes\nu)} \geq \frac{\beta_N r^{2N}}{32 K_N^2 T^{2N+2}}. \tag{5}$$

Proof. For fixed X, write $B_X = \mathbb{E}_{\nu_0} f^2$. Its unmasked mean is zero. Deletion loses at most $H_N \theta B_X$ from the second moment, and its new mean has square at most $H_N \theta^2 B_X/(1-\theta)^2$. Thus

$$\operatorname{Var}_\nu f \geq \frac{1 - (H_N+1)\theta}{(1-\theta)^2} B_X \geq \tfrac{1}{2} B_X.$$

Average and use (4). The Coulomb multipole expansion has coefficients $a_k n^{\otimes k} : \mathrm{STF}(x^{\otimes k})$; equivalently these are $|x|^k P_k(n\cdot x/|x|)$. Since $|P_k| \leq 1$, the remainder beyond degree N, before centering, is at most $2NR^{N+1}/T^{N+2}$ when $T \geq 2R$. Both centering operators are commuting L^2 contractions. The retained norm is at least $\sqrt{\beta_N} r^N/(\sqrt{8} K_N T^{N+1})$; the stated scale makes the remainder at most half this lower bound. Squaring proves (5). □

A useful distinction. With no deletion, all higher harmonic degrees are orthogonal to the first N, and the monopole disappears after Q-centering. Consequently, for $h_0 = (\mathrm{Id} - \mathbb{E}_Q)(\mathrm{Id} - \mathbb{E}_{\nu_0})V$ and every $T > R$,

$$\|h_0\|^2 \geq \sum_{k=1}^N w_k T^{-2k-2} \operatorname{Var}_Q(M_k) \geq \frac{\beta_N r^{2N}}{4K_N^2 T^{2N+2}}.$$

Thus the lower bound in (4) applies to exact unmasked covariance without a remainder-dominance condition. The larger scale in Theorem 3.2 is needed by this proof to survive an arbitrary mask. It is not an intrinsic requirement for observing full-shell Coulomb fluctuations.

4 A modular all-particle extension theorem

Use the original conventions $H(\rho) = \frac{1}{2}\iint \rho(x)\rho(y)|x-y|^{-1}dxdy$, $I(\rho) = \int \rho^{4/3}$, and $C_N = \sup(H - W_N)/I$ at mass N.

Theorem 4.1. *Suppose a compactly supported optimizer ρ for C_N has $I(\rho) = 1$, $\rho \le B < \infty$, and occupied volume $|\{\rho > 0\}| \le V_0 < \infty$. Let its symmetric optimal law P satisfy $q = P((B_R)^N) > 0$ after translation. Choose $r > 0$ with $r^3 \le 3q/(8\pi B)$ and*

$$T \ge \max\left\{2R, \frac{4\sqrt{8}\,NK_N}{\sqrt{\beta_N}}\frac{R^{N+1}}{r^N}, \left[\frac{3(H_N+1)V_0}{14\pi}\right]^{1/3}\right\}.$$

Set

$$\delta = \frac{q\beta_N r^{2N}}{512NK_N^2T^{2N+1}}, \qquad \varepsilon = \min\{1, (\delta T/(2\overline{C}))^3\},$$

where $\overline{C} \ge C_{N+1} > 0$ (for example the published 1.58 bound). Then

$$C_{N+1} - C_N \ge \tfrac{1}{2}\varepsilon\delta > 0.$$

No optimizer at $N+1$ is needed.

Proof. Condition P on $C = (B_R)^N$ to obtain Q. Its first marginal is bounded by $L = B/(Nq)$, so the chosen r satisfies Corollary 3.1. Delete the occupied set from S to obtain E. Since $|S| = (28\pi/3)T^3$, the last condition on T gives the required deletion fraction. The resulting $\nu = \mathbf{1}_E/|E|$ has $\rho\nu = 0$ almost everywhere and $A = I(\nu) = |E|^{-1/3} \le T^{-1}$; indeed $H_N \ge 1$ implies $\theta \le 1/4$.

On $C \times E$, $0 \le V \le 2N/T$ and $|h| \le 8N/T$. For $t = T/(16N)$, define

$$d\Gamma(X,y) = [1 - t\mathbf{1}_C(X)h(X,y)]dP(X)d\nu(y).$$

The bracket is between $1/2$ and $3/2$. The two zero-mean conditions on h preserve the whole old law P and the new marginal ν. Its reduction in cross cost is

$$\Delta = tq\mathbb{E}_{Q\otimes\nu}Vh = tq\|h\|^2 \ge \delta.$$

All integrals are finite: bounded compactly supported ρ has bounded Coulomb potential, and the perturbation lies in the bounded region where $V \le 2N/T$.

Mix Γ with $P \otimes \zeta_\ell$ using probabilities ε and $1-\varepsilon$, where ζ_ℓ is a diffuse probability density, disjoint from ρ and E, with $I(\zeta_\ell) \to 0$. Symmetrize all $N+1$ labels. The old–new Hartree cross terms cancel the corresponding pair costs exactly. Positivity of the added density's Hartree energy and the disjoint supports give, on taking $\ell \to \infty$,

$$C_N + \varepsilon\delta \le C_{N+1}(1 + A\varepsilon^{4/3}).$$

Consequently the gap is at least $\varepsilon\delta - \overline{C}T^{-1}\varepsilon^{4/3} \ge \varepsilon\delta/2$. This is the quantitative version of the credited non-product extension and diffuse-completion method [1]. □

5 What this changes and what remains open

Theorem 2.1 and Proposition 2.2 replace a three-point technical statement by an all-particle result with an optimal collision-uniform exponent. Theorem 4.1 packages the harmonic, masking and energy steps into a reusable implication, rather than another isolated enormous numerical constant. Its constants are deliberately explicit, not optimized; at $N = 3$ the original more favorable transverse projection gives a smaller inverse constant. The new contribution is scope and the sharp exponent, not numerical improvement of the original bounds.

This is still insufficient to characterize the project as ready for a leading journal. First, the equal-weight harmonic theorem must be compared in depth with classical point-source and polynomial-root stability results; its explicit formulation may be a useful lemma rather than a standalone novelty. Second, obtaining useful all-N bounds for q, R, B, V_0 is unresolved here. Compact support for an individual optimizer does not give a uniform radius or volume for a normalized family. Third, the original saturated-triple localization, chemical-gap argument and foundational reconstruction still need independent specialist scrutiny. The arithmetic checks here and any AI review cannot certify them.

The most consequential next target is a general optimizer localization theorem that bounds these inputs in terms of N and a preceding binding gap, or a substantially stronger sharp-constant/optimizer-structure result. Until one of these is established and its novelty is verified, the accurate status is a strengthened candidate contribution, not a promised top-journal paper.

References

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