Estimates on the Two-Dimensional Indirect Coulomb Energy

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based on a joint work with R.D. Benguria†

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Basic notions

- Consider a system of N particles with charges $e_1, \ldots, e_N > 0$.

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of N variables $x_i \in \mathbb{R}^d$, $d \in \{2, 3\}$.
- The (permutation symmetric) **probability density**, P_N, is given by
$$P_N(x_1, \dots, x_N) = |\psi(x_1, \dots, x_N)|^2.$$

Electrostatic energy and charge density

- The expectation value of the **electrostatic energy**, I_P, is given by

$$I_P = \sum_{1 \le i < j \le N} e_i e_j \int_{\mathbb{R}^{dN}} \frac{P_N(x_1, \ldots, x_N)}{|x_i - x_j|} \, \mathrm{d}x_1 \ldots \mathrm{d}x_N.$$

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- We define the **charge density of the *i*th particle**, ρ_i, by

$$\rho_i(x) = e_i \int_{\mathbb{R}^{d(N-1)}} P_N(x_1, \dots, x_{i-1}, x, x_{i+1}, \dots, x_N) \, \mathrm{d}x_1 \dots \hat{\mathrm{d}x_i} \dots \mathrm{d}x_N$$

and the so-called **single particle charge density**, ρ, by

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$$\rho(x) = \sum_{i=1}^{N} \rho_i(x).$$

- Note that due to the normalization condition on P_N, we have

$$\int_{\mathbb{R}^d} \rho_i = e_i, \quad \int_{\mathbb{R}^d} \rho = \sum_{i=1}^{N} e_i = \text{the total charge}.$$

Direct and indirect part of Coulomb energy

- One may approximate the electrostatic energy I_P by the **classical** electrostatic energy, $D(\rho, \rho)$, associated with the charge density ρ,

$$D(\rho, \rho) = \frac{1}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{\rho(x)\rho(y)}{|x - y|} \, \mathrm{d}x \, \mathrm{d}y.$$

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- Remark that in general there is no close form expression for E_P.
- The aim of this talk is to give a lower bound on E_P in terms of the charge density ρ for $d = 2$. (*To what extent can particles avoid each other and yet be constrained to have a given single particle charge density?* E. Lieb)

Structure of the bound

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$$E_P \approx -0.93\; e^{2/3} q^{-1/3} \int_{\mathbb{R}^3} \rho(x)^{4/3}\,\mathrm{d}x$$

(q spin states, $\rho = eN/|\Lambda|$)
$\Rightarrow$ a reasonable lower bound:

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5. Under homogeneous scaling of the coordinates, $x \mapsto \gamma x$:

$$E_P \geq -Ce^{2/3} \int_{\mathbb{R}^d} \rho(x)^{\alpha}\,\mathrm{d}x \quad \mapsto \quad \gamma E_P \geq -Ce^{2/3}\gamma^{d(\alpha-1)} \int_{\mathbb{R}^d} \rho(x)^{\alpha}\,\mathrm{d}x$$

which implies

$$\alpha = \frac{1}{d} + 1 = \begin{cases} 4/3 & \text{for } d = 3 \\ 3/2 & \text{for } d = 2. \end{cases}$$

History of the three-dimensional case ($e = 1$)

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3. Slightly improved by G. Chan and C. Handy (1999) using some numerical optimization:

$$E_P \geq -1.636 \int_{\mathbb{R}^3} \rho(x)^{4/3} \, \mathrm{d}x$$

4. The first bound with a **gradient correction** by R. Benguria, G. Bley, and M. Loss (2011):

$$E_P \geq -1.4508\ (1+\varepsilon) \int_{\mathbb{R}^3} \rho(x)^{4/3}\, \mathrm{d}x - \frac{3}{2\varepsilon} \langle \sqrt{\rho}, |p| \sqrt{\rho} \rangle$$

where $\varepsilon > 0$ and

$$\langle \sqrt{\rho}, |p| \sqrt{\rho} \rangle := \int_{\mathbb{R}^3} |\widehat{\sqrt{\rho}}(k)|^2 |2\pi k|\ \mathrm{d}k = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\sqrt{\rho(x)} - \sqrt{\rho(y)}|^2}{|x-y|^4}\ \mathrm{d}x\, \mathrm{d}y.$$

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Thomas-Fermi density of neutral atom of nuclear charge Z: $\rho(x) = Z^2\tilde{\rho}(Z^{1/3}x)$

$$\int_{\mathbb{R}^3} \rho^{4/3} = Z^{5/3}\int_{\mathbb{R}^3} \tilde{\rho}^{4/3}, \quad \langle\sqrt{\rho}, |\nabla|\sqrt{\rho}\rangle = Z^{4/3}\langle\sqrt{\tilde{\rho}}, |\nabla|\sqrt{\tilde{\rho}}\rangle$$

$$\int_{\mathbb{R}^3} |\nabla\rho| = Z^{4/3}\int_{\mathbb{R}^3} |\nabla\tilde{\rho}|, \quad \int_{\mathbb{R}^3} |\nabla\rho^{1/3}|^2 = Z\int_{\mathbb{R}^3} |\nabla\tilde{\rho}^{1/3}|^2$$

History of the two-dimensional case ($e = 1$)

1. The first lower bound for the indirect part by E. Lieb, J. Solovej, and J. Yngvason as an auxiliary result when investigating large quantum dots in magnetic fields (1995):

$$E_P \geq -192\sqrt{2\pi} \int_{\mathbb{R}^2} \rho(x)^{3/2} \, \mathrm{d}x.$$

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where $\beta = \mathbf{5.9045}$ and $\varepsilon > 0$.

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3. Generalization of the previous result by R. Benguria and M. T. (2012):

$$E_P \geq -(1+\varepsilon)\beta \int_{\mathbb{R}^2} \rho(x)^{3/2} \, \mathrm{d}x - \tilde{C}(\gamma) \int_{\mathbb{R}^2} |\nabla(\rho^{\alpha})|^{\gamma} \, \mathrm{d}x,$$

where $1 < \gamma < 3$, $\alpha = (3-\gamma)/(2\gamma), 1 \leq C(\gamma) \leq 2$, and

$$\tilde{C}(\gamma) = \frac{2^{\gamma} C(\gamma)}{3-\gamma} \left(\frac{1}{\beta \epsilon} \frac{\gamma - 1}{3-\gamma} C\left(\frac{\gamma}{\gamma-1}\right)\right)^{\gamma-1} \quad (\xrightarrow{\gamma \to 1+} \sqrt{2}).$$

Idea of the proof

- In the three-dimensional case, the best estimates on the indirect energy (with or without gradient terms) were obtained with the help of *Onsager's electrostatic inequality* which in turn relies on *Newton's Theorem* that does not hold true in the two-dimensional case (with the *three-dimensional Coulomb potential*).

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- Instead of it, we use a stability of matter result for an auxiliary many particle system introduced through the following *energy functional* of the electronic density $\rho \geq 0$ (cf. R. Benguria, M. Loss, H. Siedentop (2007)–Stability of UTFW model),

$$\xi(\rho) = a^2 \int_{\mathbb{R}^2} |\nabla(\rho^\alpha)|^\gamma \, \mathrm{d}x + b^2 \int_{\mathbb{R}^2} \rho^{3/2} \, \mathrm{d}x - \int_{\mathbb{R}^2} V(x)\rho(x) \, \mathrm{d}x + D(\rho, \rho) + U.$$

Here, with $Z > 0$ and $R_i \in \mathbb{R}^2$,

$$V(x) = \sum_{i=1}^{K} \frac{Z}{|x - R_i|} \ldots \text{potential generated by nuclei}$$

$$U = \sum_{1 \leq i < j \leq K} \frac{Z^2}{|R_i - R_j|} \ldots \text{repulsion of nuclei}$$

$$D(\rho, \rho) = \frac{1}{2} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \frac{\rho(x)\rho(y)}{|x - y|} \, \mathrm{d}x \, \mathrm{d}y \ldots \text{electronic repulsion.}$$

Theorem (The stability result)

For all $\rho \geq 0$,

$$\xi(\rho) \geq 0,$$

provided that

$$Z \leq \max_{\sigma \in (0,1)} h(\sigma)$$

with

$$h(\sigma) := \min \left\{ \frac{1}{2} \left(\frac{2a^2 \alpha \gamma}{C(\gamma)} \right)^{1/\gamma} \left(b^2 \frac{3-\gamma}{\gamma - 1} C \left(\frac{\gamma}{\gamma - 1} \right)^{-1} (1 - \sigma) \right)^{(\gamma-1)/\gamma}, \frac{27}{64} \frac{b^4}{5\pi - 1} \sigma^2 \right\}.$$

Key ingredients of the proof

The Lieb-Yau electrostatic inequality plus

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Lemma

Let D_R stands for the disk of radius R and origin $(0,0)$. Moreover let $u = u(|x|)$ be such that $u(R) = 0$, and $1 < \gamma < 3$. Then the following ***uncertainty principle*** *holds*

$$\left| \int_{D_R} \left[2u(|x|) + |x| u'(|x|)\right] f(x)^{1/\alpha} \right| \leq$$

$$\leq \frac{1}{\alpha} \left(C(\gamma) \int_{D_R} |\nabla f(x)|^\gamma \, \mathrm{d}x \right)^{1/\gamma} \left(C(\delta) \int_{D_R} |x|^\delta |u(|x|)|^\delta |f(x)|^{3/(2\alpha)} \, \mathrm{d}x \right)^{1/\delta},$$

where

$$\frac{1}{\alpha} = \frac{2\gamma}{3-\gamma}, \qquad \frac{1}{\gamma} + \frac{1}{\delta} = 1.$$

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Corollary

Put $u(r) = |x|^{-1} - R^{-1}$ and $f = \rho^\alpha$. Then for any $c, d \in \mathbb{R}$, we have

$$cd\,\alpha \left| \int_{D_R} \left(\frac{1}{|x|} - \frac{2}{R} \right) \rho(x) \, \mathrm{d}x \right| \leq \frac{c^\gamma C(\gamma)}{\gamma} \int_{D_R} |\nabla \rho(x)^\alpha|^\gamma \, \mathrm{d}x + \frac{d^\delta C(\delta)}{\delta} \int_{D_R} \rho^{3/2} \, \mathrm{d}x.$$

Proof of the lower bound-a trick by Lieb and Thirring

- In the functional ξ set
  1. $K = N$ =the number of particles (namely electrons) in the original system
  2. $Z = 1$ =the charge of the electron
  3. $R_i = x_i$
  4. $\rho(x) = N \int_{\mathbb{R}^{2(N-1)}} P_N(x, x_2, \dots, x_N)\, \mathrm{d}x_2 \dots \mathrm{d}x_N$

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  4. $\rho(x) = N \int_{\mathbb{R}^{2(N-1)}} P_N(x, x_2, \dots, x_N)\, \mathrm{d}x_2 \dots \mathrm{d}x_N$
- Multiply $\xi \geq 0$ (the stability result) by $P_N(x_1, \dots, x_N)$ and integrate over all electronic configurations, i.e., over $\mathbb{R}^{2N}$:

$$
\begin{aligned}
& a^2 \int_{\mathbb{R}^2} |\nabla(\rho^\alpha)|^\gamma \, \mathrm{d}x + b^2 \int_{\mathbb{R}^2} \rho^{3/2} \, \mathrm{d}x + D(\rho, \rho) \\
& - \underbrace{\int_{\mathbb{R}^{2(N+1)}} \sum_{i=1}^{N} \frac{P_N(x_1, \dots, x_N)}{|x - x_i|} \rho(x) \, \mathrm{d}x \, \mathrm{d}x_1 \dots \mathrm{d}x_N}_{2D(\rho,\rho)} \\
& + \underbrace{\sum_{1 \leq i < j \leq N} \int_{\mathbb{R}^{2N}} \frac{P_N(x_1, \dots, x_N)}{|x_i - x_j|} \, \mathrm{d}x_1 \dots \mathrm{d}x_N}_{I_P} \geq 0
\end{aligned}
$$

- Thus we have

$$I_P - D(\rho,\rho) = E_P \geq -b^2 \int_{\mathbb{R}^2} \rho^{3/2}\,\mathrm{d}x - a^2 \int_{\mathbb{R}^2} |\nabla(\rho^\alpha)|^\gamma\,\mathrm{d}x$$

provided that the assumption of the stability result, $1 \leq \max_{\sigma\in(0,1)} h(\sigma)$, is fulfilled.

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- h depends on a and b. Our lower bound follows if we think of b as a free parameter.

Comparison with numerical results

By non-rigorous but still reasonable arguments by E. Räsänen, S. Pittalis, K. Capelle, C. Proetto (2009):

3D Astonishing correspondence with **analytical** result of E. Lieb, S. Oxford / R. Benguria, G. Bley, and M. Loss:

$$E_P \geq -1.45 \int_{\mathbb{R}^3} \rho(x)^{4/3} \, \mathrm{d}x$$

2D Comparable with our constant (5.90):

$$E_P \geq -1.95 \int_{\mathbb{R}^2} \rho(x)^{3/2} \, \mathrm{d}x$$

Thanks for listening!

1. R.D. Benguria, P. Gallegos, and M. Tušek. New Estimate on the Two-Dimensional Indirect Coulomb Energy. Ann. H. Poincaré, Vol. 13, 2012. arXiv:1106.5772
2. R.D. Benguria and M. Tušek. Indirect Coulomb Energy for Two-Dimensional Atoms. J. Math. Phys., Vol. 53, 2012. arXiv:1205.6926

Newton's Theorem

Let μ be a charge distribution that is **rotationally symmetric** w.r.t. the origin. Then

$$\phi(x) = \int_{\mathbb{R}^3} \frac{1}{|x-y|}\mu(\mathrm{d}y) = \frac{1}{|x|}\int_{|y|\leq|x|}\mu(\mathrm{d}y) + \int_{|y|>|x|}\frac{1}{|y|}\mu(\mathrm{d}y).$$

Onsager's electrostatic inequality

Let $e_i > 0$, $x_i \in \mathbb{R}^3 (x_i \neq x_j$ for $i \neq j)$, and μ_{x_i} be a non-negative bounded function that is spherically symmetric about x_i with $\int \mu_{x_i}\,\mathrm{d}x = 1$. Then for any non-negative integrable function ρ,

$$\sum_{i<j}\frac{e_i e_j}{|x_i - x_j|} \geq -D(\rho,\rho) + 2\sum_i e_i D(\rho,\mu_{x_i}) - \sum_i e_i^2 D(\mu_{x_i},\mu_{x_i})$$

The Lieb-Yau electrostatic inequality

Let $R_i \in \mathbb{R}^3$ ($R_i \neq R_j$ for $i \neq j$), $D_j := \frac{1}{2} \min_{i \neq j} |R_i - R_j|$, and

$$\Phi(x) := \sum_k \frac{Z}{|x - R_k|} - \frac{Z}{\min_i |x - R_i|}.$$

Then for any distribution $\mu = \mu_+ - \mu_-$ with $D(\mu_+, \mu_+), D(\mu_-, \mu_-) < \infty$,

$$D(\mu, \mu) - \int \Phi(x)\mu(\mathrm{d}x) + \sum_{k<l} \frac{Z^2}{|R_k - R_l|} \geq \frac{1}{8} \sum_j \frac{Z^2}{D_j}.$$

Note on the two-dimensional Coulomb potential

- From the first Maxwell equation, $\mathrm{div} E = \sigma$, where σ stands for the planar charge density, is easy to deduce that the two-dimensional Coulomb potential is proportional to $\ln |x|$.
- Nevertheless, P. Duclos, P. Šťovíček, and M.T. (2010) proved that

$$\lim_{a \to 0+} \|(H_a - \xi)^{-1} - (h + (\pi/a)^2 - \xi)^{-1} \oplus 0\| = 0$$

where

$$H_a = -\Delta_{3D} - \frac{1}{|x|} \text{ in } L^2(\mathbb{R}^2 \times (-a/2, a/2))$$
$$h = -\Delta_{2D} - \frac{1}{|x|} \text{ in } L^2(\mathbb{R}^2).$$

- M.T. (2014) generalized the above result to atomic Hamiltonians.