Nuclear Number Densities

$10^{22} \text{cm}^{-3}$

- **All**
- **GP 1a**
- **GP 2a**
- **GP 8**
- **GP 6a**

$Z$

- 0.0
- 2.0
- 4.0
- 6.0
- 8.0
- 10.0
- 12.0
- 14.0

$Z$

- 0
- 20
- 40
- 60
- 80
I. PROPERTIES OF THE COULOMB POTENTIAL

(A) NEWTON’S THEOREM: If $\nu$ is a spherically symmetric (signed) measure supported in a ball of radius $R$ then for $|x| > R$

$$\int_{|y|<R} \frac{d\nu(y)}{|x-y|} = \frac{\nu(\mathbb{R}^3)}{|x|}$$

(B) POSITIVE TYPE: As a kernel $|x-y|^{-1}$ is positive, i.e., for all (signed) measures $\nu$:

$$\int\int \frac{1}{|x-y|}d\nu(x)d\nu(y) \geq 0$$

equality holds if and only if $\nu \equiv 0$.

(C) REFLECTION POSITIVE: If the signed measure $\nu$ is supported in the half-space $x_1 > 0$ and if $\tilde{\nu}$ denotes the reflection of $\nu$ on the half-space $x_1 < 0$ then

$$\int\int \frac{1}{|x-y|}d\nu(x)d\tilde{\nu}(y) \geq 0$$
II. THE MEAN FIELD MODEL

We consider a NEUTRAL system of $N = ZK$ electrons and $K = L^3$ nuclei of charge $Z$ at positions

$$\mathcal{R}_k \in \mathbb{R}Z^3 \cap (0, RL)^3, \ k = 1, 2, \ldots, K,$$

where $L = 2^p$ for some $p$. The potential from the nuclei is

$$V_{\text{nuc}}(x) = - \sum_{k=1}^{K} \frac{Z}{|x - \mathcal{R}_k|}$$
If the electronic density is $\rho(x)$ we define the mean field potential

$$V_{\rho}(x) = V^{\text{nuc}}(x) + \int \rho(y)|x - y|^{-1}dy$$

and the $N$-particle mean field operator

$$H_{\rho}^{(N)} = \sum_{i=1}^{N} \left(-\Delta_i + V_{\rho}(x_i)\right) = \sum_{i=1}^{N} h_{\rho,i}$$

acting on the fermionic space $\mathcal{H}_N = \bigwedge L^2(\mathbb{R}^3; \mathbb{C}^2)$. Here $h_{\rho}$ is the one-particle mean-field operator

$$h_{\rho} = -\Delta + V^{\text{nuc}}(x) + \int \rho(y)|x - y|^{-1}dy.$$ 

**DEFINITION:** We say that $\rho$ is mean field self-consistent if there is a ground state of $H_{\rho}^{(N)}$ on $\mathcal{H}_N$ with one-particle density equal to $\rho$. 
THEOREM (Existence + uniqueness): If \( V \in L^{5/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3) \) with \( V(x) \to 0 \) as \( |x| \to \infty \) there is a “critical electron number” \( N_c(V) \) such that there exists a mean field self-consistent density if and only if \( N \leq N_c(V) \). Moreover, for fixed \( N \) and \( V \) the mean field self-consistent density is UNIQUE.

REMARKS: (i) In the case of interest here we do have a solution since \( N_c(V^{\text{nuc}}) \geq KZ \).

(ii) POSITIVE TYPE \( \implies \) UNIQUENESS

The ENERGY as a function of \( R \):

\[
E(R) = \inf \text{ Spec } H^{(N)}_\rho + \sum_{1 \leq k < \ell \leq K} \frac{Z^2}{|\mathcal{R}_k - \mathcal{R}_\ell|}.
\]
MAIN THEOREM: There is a constant $D$ independent of $K$ and $Z$ such that

$$R < D \implies E(R) > \inf_{R} E(R),$$

$$\frac{\text{VOLUME}}{K} \geq D^3.$$

More precisely, for $0 < R \leq D$

$$cK \leq \frac{E(R) - KE(\text{atom})}{\min \{R^{-7}, Z^2R^{-1}\}} \leq CK$$

The upper bound is for $R$ not too small $R > Z^{-1/3}$

![Equilibrium Position](image)
“STABILITY OF MATTER” [Dyson & Lenard, Lieb & Thirring, Federbush]

\[ \Rightarrow \frac{\text{VOLUME}}{K} \geq CZ^{-1}, \ Z \text{ dependence!!} \]

(No mean field assumption nor a-priori assumptions on the positions of the nuclei. Only POSITIVE TYPE needed.)

THEOREM: Mean field atomic case $K = 1$. $\rho^{at}$ self-consistent density for $N = Z$ (neutrality). For $r$ small (independently of $Z$)

\[ \int_{|x| \geq r} \rho^{at}(x) \, dx = 324\pi^2 r^{-3} + o(r^{-3}) \]

III. UPPER BOUND ON $E(R)$

The mean field problem has a variational formulation. Using NEWTON’S THEOREM we can construct a trial state of noninteracting neutral atoms:

Each atom is constructed by squeezing $Z$ electrons into a ball of radius $R/2$. Putting the extra electrons between $R/4$ and $R/2$. This costs ENERGY:

\[
\text{Fermi Energy} \quad n(R) \frac{5}{3} R^{-2} = (R^{-3}) \frac{5}{3} R^{-2} = R^{-7},
\]

\[n(R) = \# \text{squeezed electrons} = R^3 \text{ (atomic theorem).}\]
IV. LOWER BOUND ON $E(R)$

LIEB-THIRRING INEQUALITY

$$\left\langle \sum_i -\Delta_i \right\rangle \geq K \int \rho^{5/3}, \quad \rho = \text{Density of } \langle \cdot \rangle$$

Combine this with localization to get

$$\langle H\rho \rangle \geq \langle H\rho \rangle_{\text{res}} + \int \tilde{\rho}^{5/3} + \int V\rho\tilde{\rho} - \int \phi_{\text{loc}}\rho.$$  

Self-consistent $\rho$ is a sum of two parts:

$$\rho = \text{Density of } \langle \cdot \rangle = \text{Density of } \langle \cdot \rangle_{\text{res}} + \tilde{\rho}$$

$\tilde{\rho}$ supported close to the shaded area $\langle \cdot \rangle_{\text{res}}$ supported away from the shaded area. The localization potential $\phi_{\text{loc}}$ is supported close to the boundary of the shaded area.
Using REFLECTION POSITIVITY:
Finally, using the atomic theorem we can estimate that the energy of the squeezed atom is greater than

\[ E(\text{atom}) + R^{-7} - lR^{-8} - l^{-2}R^{-3}, \]

(as for the lower bound squeezing costs an energy \( R^{-7} \)). Here \( l \) is the localization length. The optimal choice is \( l = R^{5/3} \ll R \). We then get

\[ E(\text{atom}) + R^{-7} - R^{-7+2/3}. \]