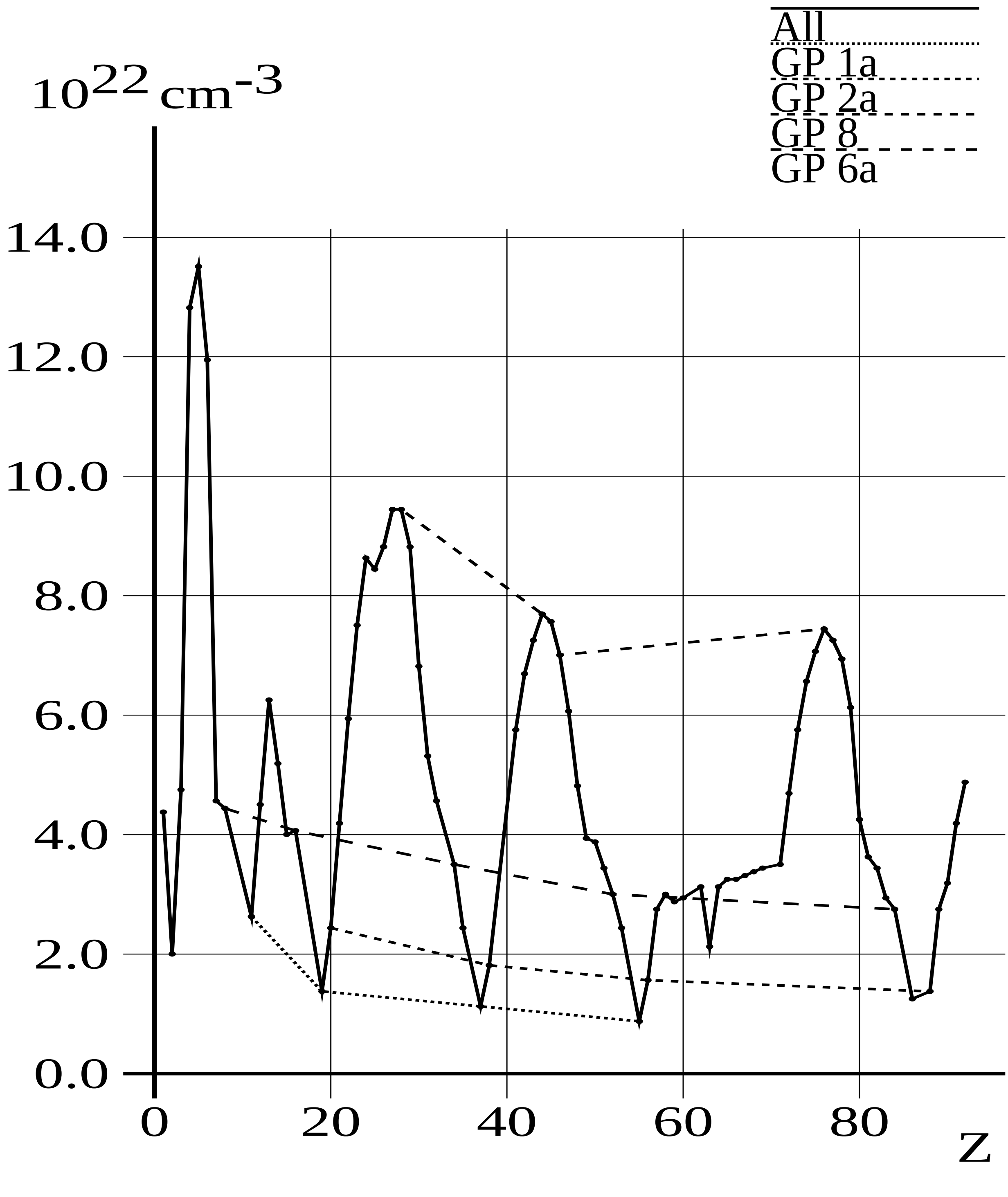
Nuclear Number Densities



I. PROPERTIES OF THE COULOMB POTENTIAL

(A) NEWTON'S THEOREM: If ν 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 ν:

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

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

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

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

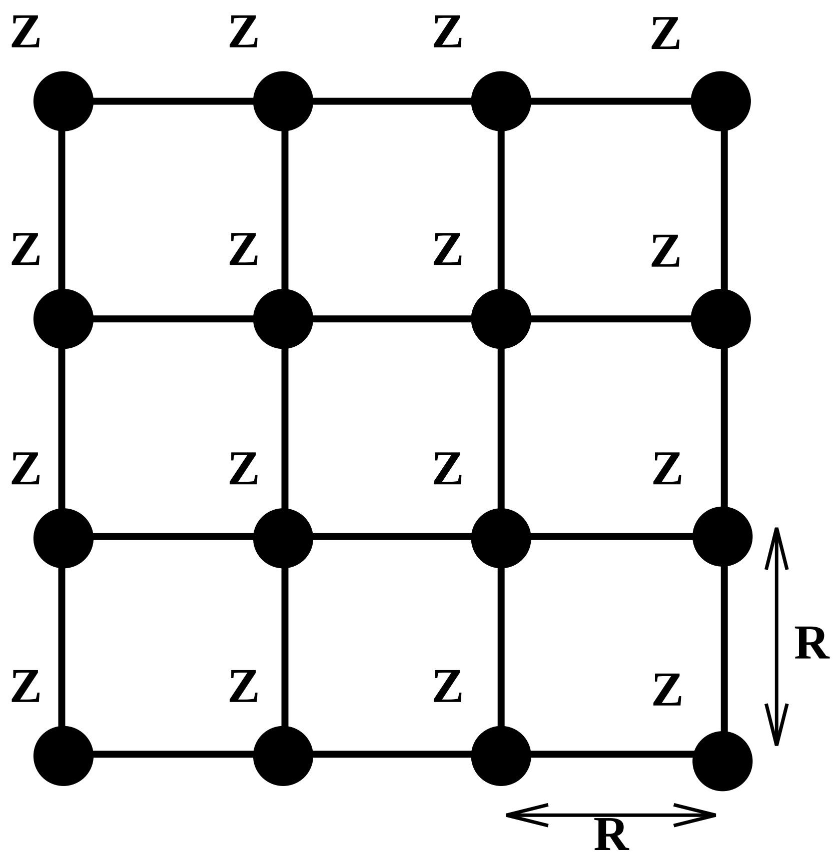
II. THE MEAN FIELD MODEL

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

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

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

$$V^{\rm nuc}(x) = -\sum_{k=1}^{K} \frac{Z}{|x - \mathcal{R}_k|}$$



If the electronic density is $\rho(x)$ we define the *mean field potential*

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

and the N-particle *mean field operator*

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

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

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

DEFINITION: ***We say that ρ 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 ρ.***

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* $N \le N_c(V)$*. 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 $N_c(V^{\mathrm{nuc}}) \ge KZ$.

(ii) POSITIVE TYPE $\Longrightarrow$ **UNIQUENESS**

The ENERGY as a function of R**:**

$$E(R) = \overbrace{\inf\ \mathrm{Spec}\ H_\rho^{(N)}}^{\text{Electronic Energy}} + \overbrace{\sum_{1\le k<\ell\le K} \frac{Z^2}{|\mathcal{R}_k - \mathcal{R}_\ell|}}^{\text{Nuclear Repulsion}}.$$

MAIN THEOREM: *There is a constant D independent of K and Z such that*

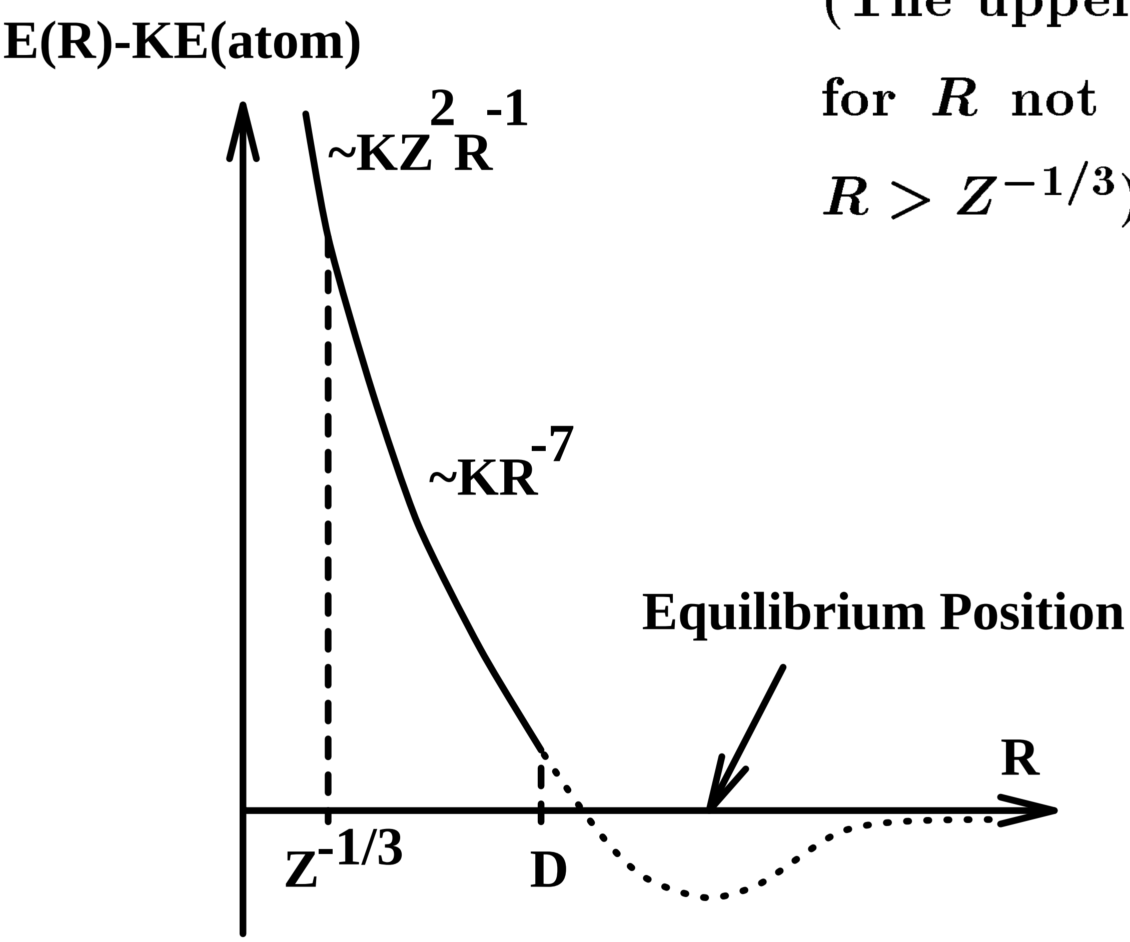
$$R < D \Longrightarrow E(R) > \inf_R E(R),$$

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

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 $R > Z^{-1/3}$)



"STABILITY OF MATTER" [Dyson & Lenard, Lieb & Thirring, Federbush]

$$\Longrightarrow \frac{\text{VOLUME}}{K} \geq CZ^{-1}, \;\; Z \text{ dependence!!}$$

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

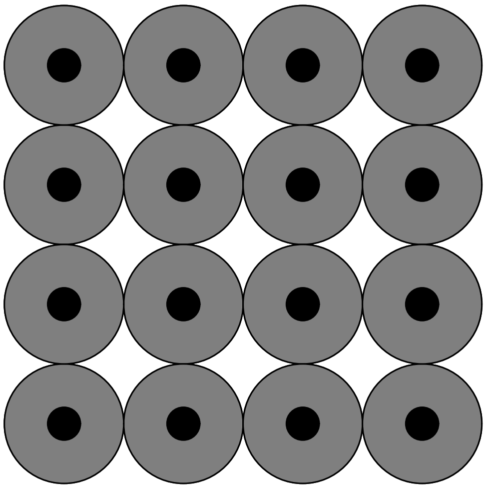
THEOREM: ***Mean field atomic case $K = 1$. ρ^{at} self-consistent density for $N = Z$ (neutrality). For r small (independently of Z)***

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

J.P.S, *Inventiones Math.* 104, 291–311 (1991).

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:

$$\overbrace{n(R)^{5/3}R^{-2}}^{\text{Fermi Energy}} = (R^{-3})^{5/3}R^{-2} = R^{-7},$$

$n(R) = \#$ squeezed electrons $= R^3$ (atomic theorem).

IV. LOWER BOUND ON $E(R)$

LIEB-THIRRING INEQUALITY

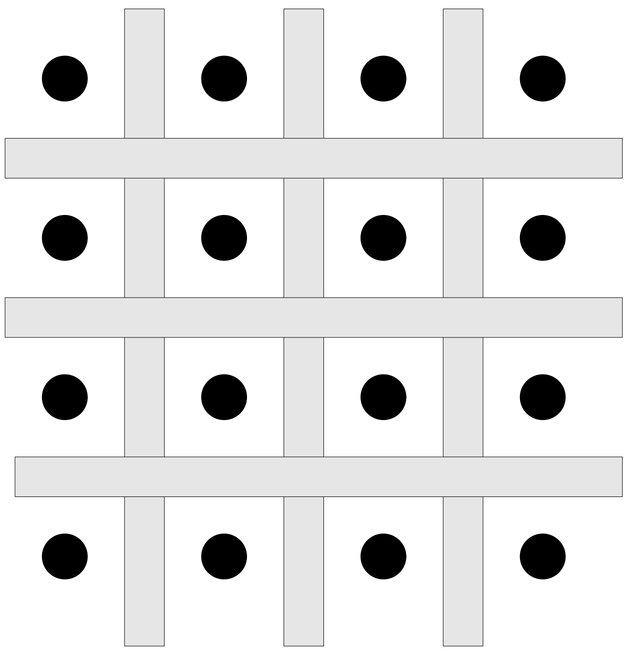
$$\left\langle \sum_i -\Delta_i \right\rangle \geq K \int \rho^{5/3}, \ \rho = \text{ Density of } \langle\ \rangle$$

Combine this with localization to get

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

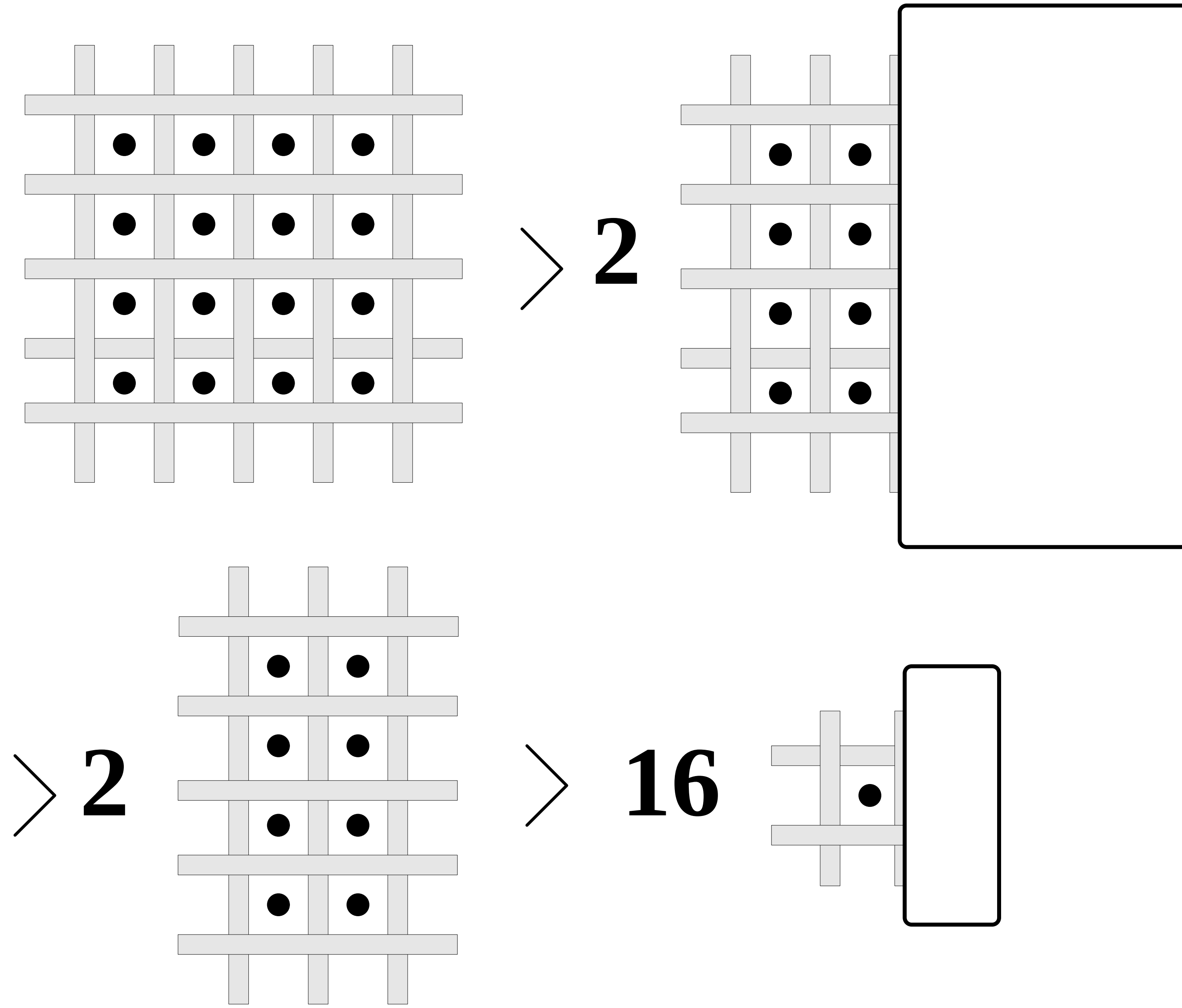
Self-consistent ρ is a sum of two parts:

$$\rho = \text{ Density of } \langle\ \rangle = \text{ Density of } \langle\ \rangle_{\mathrm{res}} + \widetilde{\rho}$$

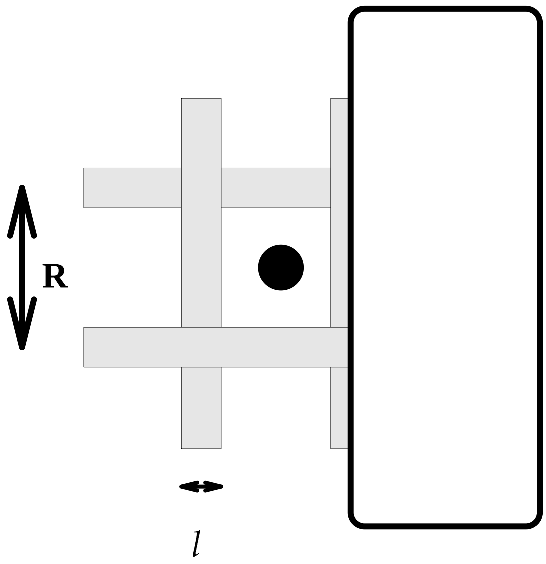


$\widetilde{\rho}$ supported close to the shaded area $\langle\ \rangle_{\mathrm{res}}$ supported away from the shaded area. The localization potential ϕ_{loc} is supported close to the boundary of the shaded area.

Using REFLECTION POSITIVITY:



Finally, using the atomic theorem we can estimate that the energy of the squeezed atom



is greater than

$$E(\text{atom}) + \overbrace{R^{-7}}^{\text{Squeezing}} - \overbrace{lR^{-8}}^{\tilde{\rho}\text{ energy}} - \overbrace{l^{-2}R^{-3}}^{\text{Localization}} ,$$

(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

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