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HEAVY ATOMS IN THE STRONG MAGNETIC FIELD OF A NEUTRON STAR

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Abstract: The ground state energy of an atom of nuclear charge Ze and in a magnetic field B is evaluated exactly in the asymptotic regime $Z \to \infty$. We show rigorously that there are 5 regions as $Z \to \infty$: $B \ll Z^{4/3}$, $B \approx Z^{4/3}$, $Z^{4/3} \ll B \ll Z^3$, $B \approx Z^3$, $B \gg Z^3$. Different regions have different physics and different asymptotic theories. Regions 1,2,3,5 are described exactly by a simple density functional theory, but only in regions 1,2,3 is it of the semiclassical Thomas-Fermi form. Region 4 cannot be described exactly by any simple density functional theory; surprisingly, it can be described by a simple *density matrix* functional theory.

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This letter is concerned with the effect on large atoms of ultra-strong magnetic fields $\mathbf{B}$, which are constant in space and time. The prototypical applications of our results is to atoms on the surface of neutron stars, some of which are believed to have surface fields of $10^{12} - 10^{13}$ Gauss. The atoms on the surface are mostly iron for which $Z = 26$, which is a large number because ordinary Thomas-Fermi (TF) theory is reasonably accurate for this Z when $\mathbf{B} = \mathbf{0}$.

In natural units in which $\hbar = c = m_e = e = 1$, the unit of magnetic field is $m_e^2 e^3 c \hbar^{-3} = 2.4 \times 10^9$ Gauss. For this field the magnetic length, $\sqrt{c\hbar/eB}$, equals the Bohr radius $\hbar^2/m_e e^2$. Thus, 10^{13} Gauss is certainly a large field.

The Hamiltonian for an atom with nuclear charge Ze and N electrons (charge $-e$) will be taken to be

$$H = \sum\nolimits_{i=1}^{N} \tfrac{1}{2}(\mathbf{p}_i + \mathbf{A}(\mathbf{r}_i))^2 + \tfrac{1}{2}\mathbf{B} \cdot \boldsymbol{\sigma}_i - Z{r_i}^{-1} + \sum\nolimits_{i<j} |\mathbf{r}_i - \mathbf{r}_j|^{-1} \tag{1}$$

where $\boldsymbol{\sigma}$ denotes the Pauli matrices and $\mathbf{A}(\mathbf{r}) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$ is the vector potential. The quantum ground state energy of H is denoted by $E^{\mathrm{Q}}(N, Z, B)$. We are also interested in the ground state density $\rho^{\mathrm{Q}}(\mathbf{r}) = \sum_\sigma \int |\psi(\mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N; \sigma_1, \ldots, \sigma_N)|^2 d^3r_2 \ldots d^3r_N$, where ψ is a ground state wave function and where we suppress explicit dependence on N, Z, B.

Given the above facts about Z and B it is sensible to develop an asymptotic theory for $E^{\mathrm{Q}}(N, Z, B)$ as Z and B tend to infinity and with the ratio N/Z held fixed. For the case $B = 0$ this asymptotic theory is known. It is TF theory which was proved [1] to be exact in 1973.

The $B \neq 0$ case has been investigated since the early 70's by several authors [2–9] who studied different parameter regimes and developed various approximation schemes such as TF and Hartree-Fock theories. To the best of our knowledge, however, a precise statement about asymptotics was never actually made, much less proved, except for the case treated in [10]. Additionally, it is difficult to find a precise statement in the literature about the qualitatively different regimes of B versus Z. Our contribution below consists primarily in bringing precision, rigor and definiteness to this question.

It turns out that there are exactly five regimes to be considered, which differ from each other both in mathematical treatment and in physical content.

Before giving our results in detail we begin with an overview and some general remarks. The five regions are described as follows: (1) $B \ll Z^{4/3}$; (2) $B \approx Z^{4/3}$; (3) $Z^{4/3} \ll B \ll Z^3$; (4) $B \approx Z^3$; (5) $B \gg Z^3$. The symbol $\ll$ in region 1 means that $B/Z^{4/3} \to 0$ as $Z \to \infty$, and similarly for regions 3 and 5. The symbol $\approx$ in region (2) means that $B/Z^{4/3}$ is held fixed as $Z \to \infty$. In the following an assertion about the atom is always to be understood as "to leading order as $Z \to \infty$". Details of our work on regions 1,2,3 and on 4,5 will be given in two publications.

In all five regions the limit $Z \to \infty$ causes correlation effects to vanish rigorously to leading order. Hence, in each region a kind of mean field theory is rigorously exact to leading order, but the nature of this theory depends on the region. Regions 1, 2 and 3 are characterized by a semiclassical theory, i.e., a modified TF theory. The density here is spherical. Regions 3, 4 and 5 are characterized by all the electrons being in the lowest Landau band - a fact that is not true for regions 1 and 2. In particular, this means that all the spins are polarized toward the field $\mathbf{B}$. It is in region 4 that the atom becomes non-spherical and in region 5 it has degenerated to a "needle". The ratio B/Z^3 is like an effective Planck's constant and therefore region 5 corresponds to the opposite of a semiclassical limit (someone called it a "post-modern" limit).

Relativistic effects are neglected here and it is believed [5] that they do not play an important role at least until $B = \alpha^{-2} = (137)^2 \approx (26)^3$, which is the value of B for which $m_e c^2 = \hbar\times$(cyclotron frequency). It can be argued, however, that relativistic effects are not crucial even for very much larger values of B because the interesting electronic motion is in the direction parallel to the field; the energy of this motion depends on B only in the combination $\ln(B/Z^3)$ for large B. The perpendicular motion is frozen into the lowest Landau level (which anyway is largely insensitive to relativistic corrections).

A noteworthy feature of our analysis – from the point of view of density functional theory – is the introduction of a *density matrix functional*. Regions 1,2,3 and 5 can be exactly described in the limit $Z \to \infty$ by a functional of the density $\rho(x)$. (This functional involves $\nabla\rho$ in region 5, but it is nevertheless a density functional theory.) Region 4 is special. Although a $\mathbf{B}$ dependent density functional exists theoretically (by the Hohenberg-Kohn-Sham Theorem) it does not exist in the realm of anything we, at least, can compute. However, we can display a simple functional of a one-body density *matrix*, γ, that is exact as $Z \to \infty$. This matrix γ is *not* the full one-body density matrix $\Gamma^{(1)}$ (which would be unmanageable, since $N \to \infty$). Rather, it equals the diagonal part of $\Gamma^{(1)}$ with respect to the variables perpendicular to $\mathbf{B}$. I.e., if $\mathbf{r} \equiv (x, y, z)$ and $x_\perp \equiv (x, y)$ then

$$\gamma_{x_\perp}(z, z') \equiv \Gamma^{(1)}(x_\perp, z; x_\perp, z') \quad . \tag{2}$$

The reason this γ is manageable is that it has a *finite rank* (independent of N as $N \to \infty$) for each value of the parameter $x_\perp$ (provided B/Z^3 is bounded away from zero as $Z \to \infty$). To our knowledge an exact density *matrix* functional of this kind is novel.

Finally, we should also remark about ionizability and atom-atom binding. In the semiclassical regions 1,2 and 3 atoms neither bind together nor support negative ionization to leading order. This is the same as in ordinary TF theory. In regions 4 and 5 both atom-atom binding and ionization become possible *to leading order*. This means that binding energies of excess electrons to atoms and of atoms to atoms is of the order of the total atomic energy itself. The structure of matter therefore will be vastly different from what we normally see.

We now present a more detailed description of the five regions. We emphasize that all these results are rigorous; the proofs will be presented elsewhere. Our results extend also to the case of molecules.

First let us recall the definition of a Thomas-Fermi (TF) type theory [11]. It begins with a functional $\mathcal{E}(\rho)$ of a one-particle density $\rho(\mathbf{r})$ given by

$$\mathcal{E}(\rho) = \int \tau(\rho(\mathbf{r}))d^3r - Z\int r^{-1}\rho(\mathbf{r})d^3r + \tfrac{1}{2}\int\int \rho(\mathbf{r})\rho(\mathbf{r}')|\mathbf{r}-\mathbf{r}'|^{-1}d^3rd^3r', \qquad (3)$$

in which τ is some positive convex function that satisfies $\tau(0) = \tau'(0) = 0$. It is assumed that for some $\epsilon > 0$, $\tau(\rho)$ is greater than $\rho^{3/2+\epsilon}$ for large ρ (to ensure that $\mathcal{E}(\rho)$ is bounded below) and smaller than $\rho^{4/3+\epsilon}$ for small ρ (to ensure that as many as Z electrons can be bound).

The function $\tau(\rho)$ is supposed to be the kinetic energy density of an appropriate but ideal Fermi gas. The TF energy E^{TF} for a particle number N is defined to be the infimum of $\mathcal{E}(\rho)$ under the condition that $\int \rho(\mathbf{r})d^3r = N$. It is a basic theorem [11] that there is a ρ that minimizes $\mathcal{E}(\rho)$ under these conditions if and only if $N \leq Z$. When $N > Z$ the TF energy is equal to the energy at $N = Z$. The minimizing ρ is unique and satisfies the TF equation $\tau'(\rho(\mathbf{r})) = Zr^{-1} - \int \rho(\mathbf{r}')|\mathbf{r}-\mathbf{r}'|^{-1}d^3r' - \mu$, whenever the right side is positive and $\rho(\mathbf{r}) = 0$ otherwise. Here, $-\mu \leq 0$ is a chemical potential (that vanishes when $N = Z$). Since $\rho(\mathbf{r})$ is unique it is necessarily spherically symmetric, i.e., ρ depends only on r.

In each of the first three regions there is a TF theory that is asymptotically exact. The differences among the three theories lie in the function τ.

Region 1, $B \ll Z^{4/3}$: The function τ is the same as in standard TF theory, i.e. $\tau_0(\rho) \equiv \frac{3}{10}(3\pi^2)^{2/3}\rho^{5/3}$. Thus, to leading order, the value of B plays no role. More precisely, if $E_0^{\rm TF}(N,Z)$ denotes the usual TF energy, and $B/Z^{4/3}\to 0$ with N/Z fixed as $Z\to\infty$, then $E^{\rm Q}(N,Z,B)/E_0^{\rm TF}(N,Z)\to 1$. There is only one nontrivial parameter, $\lambda\equiv N/Z$, in the theory because of the scaling $E_0^{\rm TF}(N,Z)=Z^{7/3}E_0^{\rm TF}(\lambda,1)$. For fixed value of λ the TF density has the form $Z^2\rho_0^{\rm TF}(Z^{1/3}\mathbf{r})$. The quantum density $\rho^{\rm Q}$ converges (in the sense of weak $L^1_{\rm loc}(\mathbf{R}^3)$) to this TF density after appropriate scaling, i.e., $Z^{-2}\rho^{\rm Q}(Z^{-1/3}\mathbf{r})\to\rho_0^{\rm TF}(\mathbf{r})$. The atomic radius thus behaves as $Z^{-1/3}$.

Region 2, $B/Z^{4/3}$ =constant: This is the case treated in [10] (see also [12] and [13]). The function τ now depends on B in a complicated way; we denote it by τ_B. It is the Legendre transform of the pressure of a free electron gas in the magnetic field $\mathbf{B}$ as a function of its chemical potential v (not to be confused with the chemical potential $-\mu$ of the TF atom), i.e., $\tau_B(\rho)=\sup_v(\rho v-P_B(v))$ with $P_B(v)=2^{1/2}(3\pi^2)^{-1}B[v^{3/2}+2\sum_{\nu\geq 1}(v-B\nu)^{3/2}]$. The terms in the sum correspond to different Landau bands and the sum extends only over bands ν for which $v-B\nu\geq 0$. Note that $\tau_B(\rho)\approx\frac{3}{10}(3\pi^2)^{2/3}\rho^{5/3}$ for large ρ and $\tau_B(\rho)\approx\frac{2}{3}\pi^4\rho^3/B^2$ for small ρ.

In this region there is a second non-trivial parameter $\beta=B/Z^{4/3}$. The scaling of the energy is $E^{\rm TF}(N,Z,B)=Z^{7/3}E^{\rm TF}(\lambda,1,\beta)$. The density is a function $Z^2\rho_\beta^{\rm TF}(Z^{1/3}\mathbf{r})$ depending on the parameter β as well as on λ. When $\beta\to 0$ the energy and density agree with the energy and density in region 1.

As before, we have that if β and λ are fixed as $Z\to\infty$ the quantum energy is given to leading order by the TF energy (which now is B-dependent). Likewise, for the density we have as before $Z^{-2}\rho^{\rm Q}(Z^{-1/3}\mathbf{r})\to\rho_\beta^{\rm TF}(\mathbf{r})$. Since $\rho_\beta^{\rm TF}(\mathbf{r})$ *is spherical* we reach the remarkable conclusion also applicable to the next region that *although* $\mathbf{B}$ *affects the energy and density it does not spoil the sphericity.*

In this region as well as in the next we find that unlike the ordinary TF theory of region 1 the TF density always has a finite radius. In ordinary TF theory the density will have a finite radius if $N < Z$ but not if $N = Z$. This difference follows from the fact that τ_B behaves as ρ^3 for small ρ rather than as $\rho^{5/3}$.

Region 3, $Z^{4/3} \ll B \ll Z^3$: This region corresponds to the $\beta \to \infty$ limit of region 2. This means that a TF theory with $\tau(\rho)$ taken to be $\tau_\infty(\rho) \equiv \frac{2}{3}\pi^4\rho^3/B^2$ (which is the asymptotic form of τ_B for large B) is exact to leading order. In this region there is only one non-trivial parameter, λ, because the dependence of the energy $E_\infty^{\rm TF}$ and the density $\rho_\infty^{\rm TF}$ on B can be scaled away. In fact, $E_\infty^{\rm TF}(N,Z,B) = Z^{7/3}\beta^{2/5}E_\infty^{\rm TF}(\lambda,1,1)$. The minimizing density can be written, for fixed λ, as $Z^2\beta^{6/5}\rho_\infty^{\rm TF}(\beta^{2/5}Z^{1/3}\mathbf{r})$. In the limit $Z \to \infty$, $\beta \to \infty$, but $BZ^{-3} \to 0$, the quantum energy and density are given to leading order by the energy and density in this TF model. More precisely, in this limit $E^{\rm Q}(N,Z,B)/E_\infty^{\rm TF}(N,B,Z) \to 1$, and $Z^{-2}\beta^{-6/5}\rho^{\rm Q}(\beta^{-2/5}Z^{-1/3}\mathbf{r}) \to \rho_\infty^{\rm TF}(\mathbf{r})$. The effect of the B field is thus to decrease the energy and decrease the radius, which now behaves like $Z^{-1/3}\beta^{-2/5}$. If this radius is written as $(B/Z^3)^{-2/5}Z^{-1}$ and if we recall that the Bohr radius is $Z^{-1}\hbar^2/m_e e^2$, we see that the TF theory can only be appropriate for $\hbar(B/Z^3)^{1/5} \ll 1$. Stated differently, $(B/Z^3)^{1/5}\hbar$ plays the role of an *effective Planck's constant.*

Region 4, B/Z^3 =constant: As stated before, it is a theorem that if $B/Z^{4/3}$ goes to infinity then we can assume that all the electrons are in the lowest Landau band. Assuming that exchange and correlation energies can be neglected as before (which, like all our other assertions can be proved) the energy as a function of the unknown density matrix γ defined in (1) can be written as

$$\mathcal{E}^{\rm DM}(\gamma) = \int \Big[-\frac{\partial^2}{\partial z^2}\gamma_{x_\perp}(z,z')\Big]_{z=z'} d^3r - \int Zr^{-1}\rho(\mathbf{r})d^3r + \tfrac{1}{2}\int\int \rho(\mathbf{r})\rho(\mathbf{r}')|\mathbf{r}-\mathbf{r}'|^{-1}d^3r d^3r', \tag{4}$$

where $\rho(x,y,z) \equiv \gamma_{x_\perp}(z,z)$ is the one-particle density (DM stands for density matrix).

It is not too difficult to prove that the condition that all the electrons are in the lowest Landau band, together with the Pauli principle, has the consequence that the density matrix γ satisfies

$$0 \leq \gamma_{x_\perp}(z, z') \leq \frac{B}{2\pi}\delta(z - z'), \tag{5}$$

as an operator, i.e., $\int \gamma_{x_\perp}(z, z') f(z) f(z')^* dz dz' \leq \frac{B}{2\pi} \int |f(z)|^2 dz$. The new minimization problem that replaces the TF problem is to minimize $\mathcal{E}^{\mathrm{DM}}$ subject to (5) and to the condition $\int \rho(\mathbf{r}) d^3r = N$. Our main theorem is that a unique energy-minimizing γ exists for this problem and that its energy $E^{\mathrm{DM}}(N, Z, B)$ is asymptotically exact in the sense that $E^{\mathrm{Q}}(N, Z, B)/E^{\mathrm{DM}}(N, Z, B) \to 1$ as $Z \to \infty$, provided $B/Z^{4/3} \to \infty$. Note that this statement includes regions 3,4 and 5 under one umbrella, but regions 3 and 5 can be decribed more simply by their own density functional theories.

In this region there are again two non-trivial parameters namely $\lambda = N/Z$ and $\eta \equiv B/Z^3$. The energy scales like $E^{\mathrm{DM}}(N, Z, B) = Z^3 E^{\mathrm{DM}}(\lambda, 1, \eta)$ and the energy-minimizing γ is of the form $Z^4 \gamma^{\mathrm{DM}}_{Zx_\perp}(Zz, Zz')$, where γ^{DM} depends on the parameters λ and η. Thus the density scales like $Z^4 \rho^{\mathrm{DM}}(Z\mathbf{r})$. Our theorem includes the assertion that the true quantum density converges to this density, i.e., $Z^{-4}\rho^{\mathrm{Q}}(Z^{-1}\mathbf{r}) \to \rho^{\mathrm{DM}}(\mathbf{r})$ in the same sense as before.

The density matrix $\gamma_{x_\perp}$ can of course be written in the form $\sum \lambda_j \phi_j(z) \phi_j(z')^*$. The non-negative numbers λ_j and the orthonormal functions ϕ_j depend on $x_\perp$, and $\lambda_j \leq B/2\pi$. In fact, one of our theorems is that for each $x_\perp$ only finitely many λ's are non-zero and these have the value $B/2\pi$. The corresponding $\phi_j(z)$'s satisfy the *one-dimensional* Schrödinger equation, parametrized by $x_\perp$

$$-\frac{\partial^2}{\partial z^2}\phi_j - W_{x_\perp}(z)\phi_j = \mu_j(x_\perp)\phi_j \quad , \tag{6}$$

where $W_{x_\perp}(z) = Zr^{-1} - \int \rho(\mathbf{r}')|\mathbf{r} - \mathbf{r}'|^{-1} d^3r'$ is the Coulomb potential along the fiber $x_\perp$ =constant. Although the directions parallel and perpendicular to the field $\mathbf{B}$ both scale as Z^{-1}, the atom is definitely no longer spherical. It has the shape of a cylinder with a finite radius smaller than $(2N/B)^{1/2}$. This last conclusion follows from a theorem which states that the lowest eigenvalue $\mu_1(x_\perp)$ is a monotone increasing function of $|x_\perp|$.

The one-dimensional problem specified by (6) is amenable to computer calculations and the only difficulty concerns the fact that the one-dimensional potential on each fiber is determined by the global density ρ. We emphasize once again that this is quite different from Hartree-Fock theory because the number of eigenvalues and eigenfunctions needed on each fiber is independent of N and depends only on the parameter B/Z^3. As B/Z^3 tends to zero this number tends to infinity and eventually we obtain the semiclassical limiting theory of region 3.

On the other hand, if B/Z^3 is sufficiently large but finite, only one eigenvalue has to be considered along each fiber. In this case the density matrix and the density contain the same information since $\gamma_{x_\perp}(z,z') = \sqrt{\rho(x_\perp,z)}\sqrt{\rho(x_\perp,z')}$. Then the energy functional depends only on the density and we are led to the analysis of the last region.

Region 5, $B \gg Z^3$: If we substitute the above expression for γ into the energy functional (4) we obtain another functional of the density ρ. Note that it resembles TF theory except that the kinetic energy term $\int \tau(\rho)$ is replaced by a Hartree-like term $\int (\partial\sqrt{\rho}/\partial z)^2 d^3r$ involving the density gradient along the field. This term is not, by itself strong enough to guarantee a bounded energy, but when it is supplemented by the subsidiary condition (5), which now reads $\int \rho dz \leq B/2\pi$ for all $x_\perp$, it does prevent collapse.

The lowest eigenvalue of the one-dimensional Schrödinger operator (6) will behave like $\mu_1(x_\perp) \sim -Z^2[\ln(Z|x_\perp|)]^2$ for the small values of $|x_\perp|$ relevant when $B \gg Z^3$ (while the second eigenvalue is larger than $-\frac{1}{4}Z^2$). Since the perpendicular radius of the atom is of order $(2Z/B)^{1/2}$ we see that the asymptotic form of the energy is $Z^3[\ln(\eta)]^2 E^{\mathrm{HS}}(N/Z)$ for large values of the parameter $\eta = B/Z^3$. Our aim is to find the function E^{HS} of the only non-trivial parameter $\lambda = N/Z$ (HS here stands for hyper-strong). The length of the atom determined by the one-dimensional uncertainty principle is of the order of $Z^{-1}[\ln(\eta)]^{-1}$. Thus the length is longer by a factor $(\eta)^{1/2}[\ln(\eta)]^{-1}$ than the width of the atom. For $B \gg Z^3$ the atom has degenerated into a "needle".

¿From the scaling of the energy it is clear that only electrons at a distance $D \equiv Z^{-1}[\ln(\eta)]^{-2}$ or less from the nucleus contribute to the attractive potential energy to leading order. It also means that the Coulomb repulsion contributes to leading order only when electrons are closer than D from each other. Note that this effective range D of the Coulomb potential is shorter by a factor $[\ln(\eta)]^{-1}$ than the length of the atom. Thus, we are led to the conclusion that in Region 5, where $\eta \to \infty$ the atom not only degenerates into an "infinitely thin needle" but *the Coulomb potential can be replaced by a delta function*. Consequently, the function E^{HS} appearing in the asymptotics of the energy can be computed from the following functional of a one-dimensional density $\overline{\rho}(z)$.

$$\mathcal{E}^{\mathrm{HS}}(\overline{\rho}) = \int (\partial\sqrt{\overline{\rho}}/\partial z)^2 dz - \overline{\rho}(0) + \tfrac{1}{2}\int \overline{\rho}(z)^2 dz \quad . \tag{7}$$

The energy $E^{\mathrm{HS}}(\lambda)$ is the minimum of $\mathcal{E}^{\mathrm{HS}}$ over all densities $\overline{\rho}$ with $\int \overline{\rho}(z)dz = \lambda$. Apart from some scaling $\overline{\rho}$ is the cross-sectional integral of $\rho(\mathbf{r})$.

It is remarkable that the functional (7) can be minimized in closed form. The Euler-Lagrange equation is, with $\psi = \sqrt{\overline{\rho}}$

$$-\psi''(z) - \delta(z)\psi(0) + \psi^3(z) = \mu\psi(z) \quad .$$

A minimizer exists if and only if $\lambda \leq 2$. The explicit solution is

$$\begin{aligned} \psi(z) &= \frac{\sqrt{2}(2-\lambda)}{4\sinh[\frac{1}{4}(2-\lambda)|z| + c]} && \text{for } \lambda < 2 \\ \psi(z) &= \sqrt{2}(2+|z|)^{-1} && \text{for } \lambda = 2, \end{aligned}$$

with $\tanh c = (2-\lambda)/2$. For $\lambda \leq 2$ the energy is

$$E^{\rm HS}(\lambda) = \mathcal{E}^{\rm HS}(\psi^2) = -\tfrac{1}{4}\lambda + \tfrac{1}{8}\lambda^2 - \tfrac{1}{48}\lambda^3. \tag{8}$$

Finally, we note the strange fact about ionizability that we alluded to at the beginning. The maximum number of electrons is $N = 2Z$ not Z as we are used to. Not only can we bind that many electrons but the binding energy of the last Z electrons is of the same order of magnitude as the first Z electrons. This is consistent with the fact, which we can also prove, that atom-atom binding energies in this region are of the same order as the internal energy. In fact, we can compute the exact asymptotics of the binding energy of a K atomic molecule since to leading order in the energy we can neglect the nuclear repulsion as long as the nuclear distance is bigger than D. Thus to leading order the energy of a K atomic molecule is the same as the energy of an atom where all K nuclei are on top of each other. Thus the asymptotics (as $Z \to \infty$ and $\eta \to \infty$) of the binding energy of, say, a neutral diatomic molecule with two identical nuclei of charge Z is (using the explicit form (8) of $E^{\rm HS}$) given by

$$((2Z)^3 - 2Z^3)[\ln(\eta)]^2 |E^{\rm HS}(1)| = \tfrac{7}{8} Z^3 [\ln(\eta)]^2 \quad .$$

The effect is dramatic. The binding energy is greater than the energy of the two individual atoms!

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