Maximum ionization in Thomas-Fermi-Dirac-Weizsäcker theory

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(joint work with Rupert L. Frank and Hanne Van Den Bosch)

While experiments tell us that a neutral atom can bind at most one or two extra electrons, justifying this fact from the first principles of quantum mechanics is a long standing open problem, often referred to as the *ionization conjecture* (see [10, Chapter 12]). In the full many-body Schrödinger theory, it is known that a nucleus of charge Z can bind at most $\min\{2Z+1, 1.22\,Z+3Z^{1/3}, Z+CZ^{5/7}+C\}$ where C is a universal constant (see [9], [14] and [3, 16] respectively). The uniform bound $Z+C$ is established only in some much simpler theories, such as Thomas-Fermi [11], Thomas-Fermi-von Weizsäcker [2] and Hartree-Fock [17].

In my talk, I have proved the uniform bound $Z+C$ in the Thomas-Fermi-Dirac-von Weizsäcker theory. More precisely, we minimize the TFDW energy functional

$$\int_{\mathbb{R}^3}\Big(c^{\mathrm{TF}}\rho(x)^{5/3}-c^{\mathrm{D}}\rho(x)^{4/3}+c^{\mathrm{W}}|\nabla\sqrt{\rho(x)}|^2-\frac{Z\rho(x)}{|x|}\Big)\mathrm{d}x+\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\rho(x)\rho(y)}{|x-y|}\mathrm{d}x\mathrm{d}y$$

under the constraint

$$0\le\rho\in L^1(\mathbb{R}^3)\cap L^{5/3}(\mathbb{R}^3),\quad \int\rho=N.$$

Our main result in [5] is that for all given positive constants c^{TF}, c^{W} and c^{D}, if the TFDW functional has a minimizer, then

$$N\le Z+C$$

for a constant C independent of Z.

One of the key feature of the Thomas-Fermi-Dirac-von Weizsäcker theory is that some electrons at infinity may form a nontrivial bound state (see [12, 15]). This makes the ionization problem difficult because we cannot apply the standard strategy of 'multiplying the Euler-Lagrange equation by $|x|$' by Benguria and Lieb (see [1, 8, 9]). The ionization problem for 'the infinity model' (the case $Z=0$) has been solved recently by Lu and Otto [13] by a completely different strategy. Unfortunately, the method in [13] relies on the translation-invariance of the model and fails to apply when $Z>0$.

In our work [5], we introduce a novel method to replace the 'multiplying by $|x|$' strategy. This method is inspired by ideas in a recent proof of the nonexistence in the liquid drop model by R. Killip and two of us [4]. Roughly speaking, the argument is to exploit the binding inequality by localizing the minimizer by half-planes and taking the average. This allows us to prove $N\le(2+o(1))Z$ easily.

To achieve the much improved bound $N\le Z+C$, we apply our new technique to control only the particles far from the nucleus. We may still lose a factor 2 but this is not a serious problem because the number of the exterior particles is much smaller than Z. The interior particles are controlled by comparing with the Thomas-Fermi theory, following Solovej's proof of the ionization conjecture in the Hartree-Fock theory [17].

The main technical tool in the whole approach is to show that the screened nuclear potential (i.e. the attraction of the nucleus screened by the electrons in the interior region) is approximated well by the Thomas-Fermi screened potential up to the distance o(1) from the nucleus. In the semi-classical distance $O(Z^{-1/3})$, it is well-known that the Thomas-Fermi theory is valid and the approximation of the screened potentials follows easily. However, to extend this approximation to the much larger distance o(1), we need to combine the new bound on exterior particles with Solovej's delicate bootstrap argument [17].

As a by-product of our approach, we can deduce that the atomic radius in TFDW theory is close to that in Thomas-Fermi theory.

Our approach has been adapted to solve the ionization problem in Müller density-matrix-functional theory [6] and a related theory [7].

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