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Relativistic Scott correction in self-generated magnetic field

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Based on joint work with L. Erdös and J.P. Solovej

Munich 2012

The model

Kinetic energy of a single electron:

$$\mathcal{T}^{(\alpha)}(A) := \sqrt{\alpha^{-2}\,T(A) + \alpha^{-4}} - \alpha^{-2},$$

where $\alpha > 0$ is a parameter (fine structure constant).

$$T(A) := \begin{cases} [\sigma \cdot (-i\nabla + A)]^2 & \text{(Pauli)} \\ (-i\nabla + A)^2 & \text{(Schrödinger).} \end{cases}$$

Magnetic field $B = \nabla \times A$ and $\sigma =$ Pauli matrices.

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Magnetic field $B = \nabla \times A$ and $\sigma =$ Pauli matrices.

$$H(\mathbf{Z}, \mathbf{R}, \alpha, A) := \sum_{j=1}^{Z} \Big(\mathcal{T}_j^{(\alpha)}(A) - \sum_{k=1}^{M} \frac{Z_k}{|x_j - R_k|} \Big) + \sum_{j<k} \frac{1}{|x_j - x_k|},$$

The Hilbert space

$$\mathcal{H} = \bigwedge_{j=1}^{Z} L^2(\mathbb{R}^3, \mathbb{C}^2).$$

• Stability requires

$$Z_k\alpha \leq 2/\pi, \qquad \text{all } k.$$

We will study $Z \to \infty$, $\alpha \to 0$.

• For a given vector potential A, the ground state energy of the electrons is given by

$$E_0(\mathbf{Z}, \mathbf{R}, \alpha, A) := \inf \operatorname{Spec} H(\mathbf{Z}, \mathbf{R}, \alpha, A).$$

• Minimal total energy

$$E_0(\mathbf{Z}, \mathbf{R}, \alpha) := \inf_A \Big\{ E_0(\mathbf{Z}, \mathbf{R}, \alpha, A) + \frac{1}{8\pi\alpha^2}\int_{\mathbb{R}^3} |\nabla \times A|^2 \Big\}.$$

Energy in large Z limit. Non-relativistic, no A-field

$$H := \sum_{j=1}^{Z} \Big(-\frac{1}{2}\Delta_j - \sum_{k=1}^{M} \frac{Z_k}{|x_j - R_k|} \Big) + \sum_{j<k} \frac{1}{|x_j - x_k|},$$

Leading energy term of order $Z^{7/3}$ given by Thomas-Fermi theory (proved by Lieb-Simon (1977)).
Next term—the Scott correction– predicted by Scott (1952), proved by Siedentop-Weikard (1987) for atoms, Ivrii-Sigal (1993) for molecules,

$$2 \cdot \frac{1}{4} \sum_{k=1}^{M} Z_k^2.$$

In the atomic case also the next (Dirac-Schwinger) term of order $Z^{5/3}$ is known. Proved by Fefferman-Seco (90's).

Relativistic, no A-field

Kinetic energy $\mathcal{T}^{(\alpha)}(0) = \sqrt{\alpha^{-2}(-\Delta) + \alpha^{-4}} - \alpha^{-2}$.
Nuclear charges/positions $Z_k = Zz_k$, $R_k = Z^{-1/3} r_k$.
Scott correction proved by Solovej-Spitzer-Sørensen (alternative proof by Frank-Siedentop-Warzel).

Theorem

There exists a continuous, non-increasing function S on $[0, 2/\pi]$ with $S(0) = 1/4$ such that as $Z \to \infty$ and $\alpha \to 0$ with $\max_k\{Z_k\alpha\} \leq 2/\pi$ we have

$$E_0(\mathbf{Z}, \mathbf{R}; \alpha, A = 0) = Z^{7/3} E^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}) + 2 \sum_{1 \leq k \leq M} Z_k^2 S(Z_k\alpha) + \mathcal{O}(Z^{2-1/30}) .$$

Questions for full operator

Kinetic energy $\mathcal{T}^{(\alpha)}(A) := \sqrt{\alpha^{-2}T(A)+\alpha^{-4}} - \alpha^{-2}$,
self-generated magnetic field.

$$H(\mathbf{Z},\mathbf{R},\alpha,A) := \sum_{j=1}^{Z}\Big(\mathcal{T}_j^{(\alpha)}(A) - \sum_{k=1}^{M}\frac{Z_k}{|x_j - R_k|}\Big) + \sum_{j<k}\frac{1}{|x_j - x_k|},$$

$$E_0(\mathbf{Z},\mathbf{R},\alpha) := \inf_A\Big\{E_0(\mathbf{Z},\mathbf{R},\alpha,A) + \frac{1}{8\pi\alpha^2}\int_{\mathbb{R}^3}|\nabla\times A|^2\Big\}.$$

- Does there exist a Scott correction?
- Is the Scott correction the same as without magnetic field?

For *non-relativistic operators* with self-generated field, we proved recently that there *is* a Scott correction which depends on $Z\alpha^2$. This motivates the second question.

Affirmative result

Theorem (Relativistic Scott correction with self-generated field)

Assume that there exists $\kappa_0 < 2/\pi$ *such that* $\max_k\{Z_k\alpha\} \leq \kappa_0$. *Then the ground state energy with self-generated magnetic field is given by*

$$E_0(\mathbf{Z}, \mathbf{R}; \alpha) = Z^{7/3} E^{\mathrm{TF}}(\mathbf{z}, \mathbf{r}) + 2\sum_{k=1}^{M} Z_k^2 S(Z_k\alpha) + o(Z^2)$$

in the limit as $Z \to \infty$ *and* $\alpha \to 0$.

Techniques for the proof

Upper bounds as in [SSS] by taking $A = 0$.

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Lower bounds: Local semiclassical analysis combined with multiscaling. In order to localize one needs a new localization inequality

Lemma (Pull-out estimate)

Assume that $g_i \geq 0$ are smooth, $\sum_{i\in I} g_i^2(x) = 1$. Let H_i, $i \in I$, be a family of positive self-adjoint operators on $L^2(\mathbb{R}^3, \mathbb{C}^2)$. Then

$$\sqrt{\sum_{i\in I} g_i H_i g_i} \geq \sum_{i\in I} g_i \sqrt{H_i} g_i.$$

Theorem (Lieb-Thirring inequality for $\mathcal{T}^{(\beta)}(A)$)

There exists a universal constant $C > 0$ such that for any positive number $\beta > 0$, for any potential V with $[V]_+ \in L^{5/2} \cap L^4(\mathbb{R}^3)$, and magnetic field $B = \nabla \times A \in L^2(\mathbb{R}^3)$, we have

$$Tr\Big[\sqrt{\beta^{-2}T(A) + \beta^{-4}} - \beta^{-2} - V(x)\Big]_- \geq -C\Big\{ \int [V]_+^{5/2} + \beta^3 \int [V]_+^4 + \Big(\int B^2 \Big)^{3/4} \Big(\int [V]_+^4 \Big)^{1/4} \Big\}.$$

- If $A = 0$ this is the well-known Daubechies inequality.
- For the Schrödinger case, the Daubechies inequality was generalized (and improved to incorporate a critical Coulomb singularity) to non-zero A by Frank-Lieb-Seiringer using diamagnetic techniques. For the Pauli operator there is no diamagnetic inequality.

Theorem (Local Lieb-Thirring inequality with a Coulomb potential)

Let ϕ_r be a real function satisfying $\operatorname{supp}\phi_r \subset \{|x| \leq r\}$, $\|\phi_r\|_\infty \leq 1$. *There exists a constant $C > 0$ such that if $\beta \in (0, 2/\pi)$, then*

$$Tr\Big[\phi_r\big(\sqrt{\beta^{-2}T(A)+\beta^{-4}}-\beta^{-2}-\frac{1}{|x|}-V\big)\phi_r\Big]_-$$
$$\geq -C\Big\{\eta^{-3/2}\int|\nabla\times A|^2+\eta^{-3}r^3+\eta^{-3/2}\int[V]_+^{5/2}+\eta^{-3}\beta^3\int[V]_+^4$$
$$+\Big(\int|\nabla\times A|^2\Big)^{3/4}\Big(\int[V]_+^4\Big)^{1/4}\Big\},$$

where $\eta := \frac{1}{10}(1-(\pi\beta/2)^2)$.

Reduction to semiclassics

After scaling by $Z^{-1/3}$ and passing to the Thomas-Fermi potential, we find a semiclassical problem

$$\mathrm{Tr}\Big[\sqrt{\beta^{-2}T_h(\widetilde{A})+\beta^{-4}}-\beta^{-2}-\kappa V^{TF}_{\mathbf{z},\mathbf{r}}\Big]_- + \frac{\lambda}{\beta^2 h^3}\int |\nabla\otimes\widetilde{A}|^2$$

with parameters

$$\kappa = \min_k \frac{2}{\pi z_k}, \quad h=\kappa^{1/2}Z^{-1/3}, \quad \beta = Z^{2/3}\alpha\kappa^{-1/2} = \frac{Z\alpha}{\kappa}h.$$

Theorem (Scott corrected semiclassics with self-generated field)

Suppose that $\lambda > 0$*. If* $0 \leq \beta \leq h$*, and* $\widetilde{\kappa} z_k < 2/\pi$*, then*

$$\Big| \inf_{\widetilde{A}} \Big\{ Tr\Big[\sqrt{\beta^{-2} T_h(\widetilde{A}) + \beta^{-4}} - \beta^{-2} - \widetilde{\kappa} V^{TF}_{\mathbf{z},\mathbf{r}}\Big]_- + \frac{\lambda}{\beta^2 h^3} \int |\nabla \otimes \widetilde{A}|^2 \Big\}$$

$$- \frac{2}{(2\pi h)^3} \iint \Big[\frac{1}{2} p^2 - \widetilde{\kappa} V^{TF}_{\mathbf{z},\mathbf{r}}(x)\Big]_- - 2h^{-2} \sum_{k=1}^{M} (z_k \widetilde{\kappa})^2 S(\beta h^{-1} \widetilde{\kappa} z_k)\Big|$$

$$\leq o(h^{-2}).$$

Local semiclassics - no singularity

Theorem

Let $\theta, V \in C_0^\infty(B(1))$, $\lambda > 0$ *be fixed.*

$$\beta \leq Ch.$$

Then

$$\Big| \inf_A \Big\{ Tr[\theta\{\sqrt{\beta^{-2} T_h(A) + \beta^{-4}} - \beta^{-2} - V\}\theta]_- + \frac{\lambda}{\beta^2 h^3} \int_{B(2)} |\nabla \otimes A|^2 \Big\} - \frac{2}{(2\pi h)^3} \iint \theta(x)^2 \Big[\frac{1}{2}p^2 - V(x)\Big]_- dxdp \Big| \leq Ch^{-2+1/11}.$$

Upper bound: $A = 0$ (Solovej-Spitzer-Sørensen).

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Lower bound: By Lieb-Thirring (for suitable vector fields A)

$$\mathcal{B}^2 = \int |\nabla \otimes A|^2 \leq C\beta^2.$$

Also, (using Lieb-Thirring, Hölder and Sobolev)

$$\begin{aligned} T_h(A) &\geq (1-2\epsilon)(-h^2\Delta) + \epsilon(-h^2\Delta - \epsilon^{-2}A^2) \\ &\geq (1-2\epsilon)(-h^2\Delta) - Ch^{-3}\epsilon^{-4}\mathcal{B}^5 \end{aligned}$$

So (with $\gamma^{-4} = \beta^{-4} - Ch^{-3}\epsilon^{-4}\mathcal{B}^5$ and $\tilde{h} = \sqrt{1-2\epsilon}\, h$)

$$\begin{aligned} &\sqrt{\beta^{-2}T_h(A) + \beta^{-4}} - \beta^{-2} - V(x) \\ &\quad \geq \sqrt{\gamma^{-2}(-\tilde{h}^2\Delta) + \gamma^{-4}} - \beta^{-2} - V(x) \\ &\quad \geq \sqrt{\gamma^{-2}(-\tilde{h}^2\Delta) + \gamma^{-4}} - \gamma^{-2} - (V(x) + Ch^{-3}\epsilon^{-4}\mathcal{B}^5). \end{aligned}$$

But with $\epsilon = h$, $\beta \leq h$, we get

$$h^{-3}\epsilon^{-4}\mathcal{B}^5 \leq h^{-2} \qquad \text{TOO LARGE!}$$

Solution: Localize to balls of size $\ell \ll 1$.

Lieb-Thirring

$$\mathcal{B}^2 = \int_{B(2\ell)} |\nabla \otimes A|^2 \leq C\beta^2 \ell^3.$$

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So

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But with $\epsilon = h$, $\beta \leq h$, we get

$$h^{-3}\epsilon^{-4}\mathcal{B}^5\ell^{1/2} \leq h^{-2}\ell^8$$

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$$\geq (1-2\epsilon)(-h^2\Delta) - Ch^{-3}\epsilon^{-4}\mathcal{B}^5\ell^{1/2}$$

So

$$\sqrt{\beta^{-2}T_h(A) + \beta^{-4}} - \beta^{-2} - V(x)$$
$$\geq \sqrt{\gamma^{-2}(-\tilde{h}^2\Delta) + \gamma^{-4}} - \beta^{-2} - V(x)$$
$$\geq \sqrt{\gamma^{-2}(-\tilde{h}^2\Delta) + \gamma^{-4}} - \gamma^{-2} - (V(x) + Ch^{-3}\epsilon^{-4}\mathcal{B}^5\ell^{1/2}).$$

But with $\epsilon = h$, $\beta \leq h$, we get

$$h^{-3}\epsilon^{-4}\mathcal{B}^5\ell^{1/2} \leq h^{-2}\ell^8 = h \text{ for } \ell = h^{3/8}.$$

Units

Length: $h^2/(me^2)$.
Energy: me^4/h^2.
Vector potential: mec/h.