Semiclassical theory

with self-generated magnetic field

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Victor Ivrii

Department of Mathematics, University of Toronto

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Problem

Let us consider quantum Hamiltonian

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Let us consider quantum Hamiltonian

$$H_V = (-ih\nabla)^2 - V(x) \tag{1}$$

with Thomas-Fermi potential $V = V(x)$. 20+ years ago I was involved in the problem:

Problem 1 (old)

Calculate semiclassical asymptotics of $\mathrm{Tr}(H_V^-)$ as $h \to +0$ where H_V^- is a negative part of H_V so we are looking for a sum of negative eigenvalues.

This one-particle problem arises in the multi-particle problem:

$$\mathsf{H} = \mathsf{H}_N := \sum_{1\le j\le N} H_{V,x_j} + \sum_{1\le j<k\le N} |x_j - x_k|^{-1} \tag{2}$$

on

$$\mathfrak{H} = \bigwedge_{1\le n\le N} \mathscr{H}, \qquad \mathscr{H} = \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^q) \tag{3}$$

describing N same type particles in the external field with the scalar potential $-V$ and repulsing one another according to the Coulomb law.

Here $x_j \in \mathbb{R}^3$, and $(x_1, \ldots, x_N) \in \mathbb{R}^{3N}$, potential $V(x)$ is assumed to be real-valued. Except when specifically mentioned we assume that

$$V(x) = \sum_{1 \le m \le M} \frac{Z_m}{|x - \mathsf{y}_m|} \tag{4}$$

where $Z_m > 0$ and y_m are charges and locations of nuclei.

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Quantum statistics

We assume that the particles (electrons) are *fermions*. This means that the Hamiltonian should be considered on the *Fock space* $\mathfrak{H}$ defined by (3) of the functions antisymmetric with respect to variables $x_1, \dots, x_N$.

Thomas-Fermi theory

If electrons were not interacting between themselves but the field potential was $-W(x)$ then they would occupy lowest eigenvalues and ground state wave functions would be (anti-symmetrized) $\phi_1(x_1)\phi_2(x_2)\ldots\phi_N(x_N)$ where ϕ_j and λ_j are eigenfunctions and eigenvalues of $H=-\Delta-W(x)$ with energy $\operatorname{Tr}(H^-_{W+\nu})-\nu N$.

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Then the local electron density would be $\rho_\Psi = \sum_{1\le j\le N} |\phi_j(x)|^2$ and according to the pointwise Weyl law

$$\rho_\Psi(x) \approx \frac{q}{6\pi^2}(W+\nu)_+^{\frac{3}{2}} \tag{5}$$

where $\nu=\lambda_N$.

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This density would generate potential $-|x|^{-1}*\rho_\Psi$ and we would have $W\approx V-|x|^{-1}*\rho_\Psi$.

Replacing all approximate equalities by a strict ones we arrive to Thomas-Fermi equations:

$$V - W^{\mathsf{TF}} = |x|^{-1} * \rho^{\mathsf{TF}}, \tag{6}$$

$$\rho^{\mathsf{TF}} = P'(W^{\mathsf{TF}} + \nu) := \frac{q}{6\pi^2}(W^{\mathsf{TF}} + \nu)_+^{\frac{3}{2}}, \tag{7}$$

$$\int \rho^{\mathsf{TF}}\, dx = \min(N, Z), \qquad Z = Z_1 + \ldots + Z_M \tag{8}$$

where $\nu \le 0$ is called chemical potential and in fact approximates λ_N; $q = 1$ so far.

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Assuming that $Z_j = z_j Z$ with $N \asymp Z \gg 1$ we discover that $W^{\mathsf{TF}}(x) = Z^{\frac{4}{3}}\bar{W}^{\mathsf{TF}}(Z^{\frac{1}{3}}x)$ (and $\nu = Z^{\frac{4}{3}}\bar{\nu}$) with $\bar{W}^{\mathsf{TF}}$, $\bar{\nu}$ calculated as if $Z = 1$ and scaling $x \mapsto Z^{\frac{1}{3}}x$ we arrive to e (1) with $V := \bar{W}^{\mathsf{TF}} + \bar{\nu}$ and $h = Z^{-\frac{1}{3}}$ (and the result must be multiplied by $Z^{\frac{4}{3}}$).

Answer

It was proven for Problem 1 that

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Remark

In asymptotics (9)

$$\varkappa_0 = -\int P(V)\,dx, \qquad P(V) := \frac{q}{15\pi^2} V_+^{\frac{5}{2}}, \tag{10}$$

$$\varkappa_1 = \sum_{1\le m\le M} q z_m^2 S \tag{11}$$

but for original problem we need to take

$$\varkappa_0 = -\int P(V)\,dx - \frac{1}{2}\iint |x-y|^{-1}\rho^{\mathsf{TF}}(x)\rho^{\mathsf{TF}}(y)\,dxdy \tag{9$'$}$$

to avoid double counting of the energies of electron-electron interaction and add Dirac$= \varkappa'_2 h^{-1}$ to avoid counting of electron self-interaction.

Including magnetic field

To accommodate magnetic field we need to consider $\mathscr{H} = \mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^q)$ with $q = 2$ and

$$H_{V,A} = \bigl((i\nabla - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{12}$$

where $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$, σ_j are Pauli matrices.

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Such problem with constant magnetic field (linear $A(x)$) was investigated 20− y.a. and one should replace $P(V)$ by

$$P_{Bh}(V) = (3\pi^2)^{-1} q \Bigl(\frac{1}{2} V_+^{\frac{3}{2}} + \sum_{j\ge 1} (V - 2jBh)_+^{\frac{3}{2}}\Bigr) Bh \tag{13}$$

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(which leads to magnetic Thomas-Fermi potential W_{Bh}^{TF} and density ρ_{Bh}^{TF}. Here $B = |\nabla \times A|$ is an intensity of magnetic field).
Results for $Bh \lesssim 1$ and $Bh \gtrsim 1$ are really different.

Finally a case of study: self-generated magnetic field

A couple of y.a. it was proposed to consider arbitrary magnetic field but to include its energy to a final count which amounts to

Problem 2 (new)

Find $\mathsf{E}^*_\kappa := \inf_{A\in \mathscr{H}^1(\mathbb{R}^3)} \mathsf{E}_\kappa(A)$ with

$$\mathsf{E}_\kappa(A) := \operatorname{Tr}(H^-_{A,V}) + \kappa^{-1}h^{-2}\int |\partial A|^2\, dx. \tag{14}$$

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Remark

In our assumptions to V one can prove by functional analysis that such minimizer exists as $\kappa \le \kappa^*$ (small enough constant) but we have no idea if it is unique! (life would me much easier then).

Microlocal analysis

First consider a simplified problem: $V \in \mathscr{C}^{2+}$ and $H_{A,V}$ replaced by $\psi H_{A,V}\psi$ with $\psi \in \mathscr{C}^2_0(B(0,1))$.

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$$\frac{1}{\kappa h^2}\Delta A_j(x) = \Phi_j(x) := \\ -\operatorname{Re}\operatorname{tr}\Bigl(\sigma_j\bigl((hD-A)_x\cdot\boldsymbol{\sigma}\bigr)\bigl(\psi(x)e(x,y,0)\psi(y)\bigr)\Bigr)\Bigr|_{y=x} \tag{15}$$

where $e(x,y,\tau)$ is the Schwartz kernel of the spectral projector $\theta(\tau-\psi H_{A,V}\psi)$.

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Good news: I was able to adopt microlocal analysis to deal with this non-smoothness (combining rough microlocal analysis of earlier development with successive approximations). Observe that $|\Phi_j| = O(h^{-3})$ (it cannot be worse than this–one can prove it). But then $|\Delta A_j| = O(h^{-1})$ and we have an estimate to a minimizer $|\partial^2 A_j| = O(h^{-\theta}|\log h|)$ with $\theta = 1$ (and factor κ definitely does not hurt!).

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This is enough to improve estimate of $|\Phi_j|$ which is enough to push an estimate to a minimizer down: $|\partial^2 A_j| = O(h^{\delta-\theta}|\log h|)$ which is enough to push it further down, ..., until non-smoothness is not a problem and $|\Phi_j| = O(h^{-2})$ and

$$|\partial^2 A_j| = O(|\log h|). \tag{16}$$

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Then I can prove by the same arguments

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and $\|\partial A\|^2 = O(h^{1-\theta})$, and $\|\partial A\|_{\mathscr{L}^\infty} = O(h^{(1-\theta)/5})$.

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Boring!

Therefore we arrive to a solid but not very exciting result: in these settings
$\mathsf{E}^*_\kappa = \varkappa_0 h^{-3} + O(h^{-1})$, $\|\partial A\| = O(h^{\frac{1}{2}})$ and $\|\partial A\|_{\mathscr{L}^\infty} = O(h^{\frac{1}{5}})$.

But we have a singularity!

Now consider Coulomb-like singularity at 0. Consider ℓ-admissible partition of unity with $\ell(x)=\frac{1}{2}|x|$: $1=\sum\psi_k^2$; then $\operatorname{Tr}(H^-_{A,V})\ge\sum_k \operatorname{Tr}((\psi H_{A,V'}\psi)^-)$ with $V'=V+ch^2|x|^{-2}$.

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So instead of $O(h^{-1})$ we get $O(h^{-2})$. Exactly this happened 20+ years ago–but then there was no magnetic field. And this was not a failure–this was manifestation of Scott correction term!

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First we conclude that $\|\partial A\| = O(1)$. If we knew that the minimizer is unique then in spherically symmetric case it will be spherically symmetric vector field with 0 divergence and belonging to $\mathscr{H}^1$ and therefore 0. But we do not know if a minimizer is unique!
Using estimate to minimizer (15) but now with $\psi = 1$ and estimate $\|\partial A\| = O(1)$ I was able to derive

$$\|\partial A\| \le C\kappa, \qquad |\partial A| \le C\kappa\ell^{-\frac{3}{2}}, \qquad |\partial A| \le C\kappa\ell^{-\frac{5}{2}}|\log(\ell h^{-2})|. \tag{18}$$

Now we deal with the singularity exactly as I did 20+ y.a. Observe that the contribution of zone $\{\ell(x) \ge \bar{r}\}$ to the remainder is $O(\bar{r}^{-\frac{1}{2}}h^{-1})$.

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So the total error is $O(\bar{r}^{-\frac{1}{2}}h^{-1}+\bar{r}h^{-2})$ and optimizing by $\bar{r}$ we get $O(h^{-\frac{4}{3}})$. So, if we consider the errors when we replace traces by their Weyl expressions and consider the difference between these errors for $H_{A,V}$ and H_{A,V^0} we get $O(h^{-\frac{4}{3}})$.

Except for Coulomb potential trace is infinite and Weyl expression diverges at infinity, so it must be regularized, f.e. as

$$\operatorname{Tr}(H_{A,V^0-\eta}) + h^{-3}\int P(V^0-\eta)\,dx \tag{19}$$

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with $\eta>0$. Then

$$\begin{aligned}\mathsf{E}_\kappa(V,A) &+ h^{-3}\int P(V)\,dx\\ &= \mathsf{E}_\kappa(V^0-\eta,A) + h^{-3}\int P(V^0(x)-\eta)\,dx + O(h^{-\frac{4}{3}})\end{aligned} \tag{20}$$

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(uniformly by η). Then the left-hand expression is estimated from below by

$$\underbrace{\lim_{\eta\to+0}\Bigl(\mathsf{E}^*_\kappa(V^0-\eta) + h^{-3}\int P(V^0-\eta)\,dx\Bigr)} + O(h^{-\frac{4}{3}}).$$

Scott correction term

In the selected expression we have three parameters–h, κ and z but due to homogeneity of Coulomb potential we can exclude two and rewrite it as $2h^{-2}z^2S(\kappa z)$ with unknown function $S(\kappa z)$.

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$$E^*_\kappa(V) + h^{-3}\int P(V)\,dx \ge 2h^{-2}z^2S(\kappa z) + O(h^{-\frac{4}{3}}). \tag{21}$$

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This is estimate from below. To derive estimate from above we plug test function A'_η which is minimizer for $\mathsf{E}_\kappa(V^0-\eta, A)$ arriving to

$$\begin{aligned}\mathsf{E}^*_\kappa(V) + h^{-3}\int P(V)\,dx &\le \mathsf{E}_\kappa(V^0-\eta, A) + h^{-3}\int P(V^0-\eta)\,dx + O(h^{-\frac{4}{3}})\\ &= \mathsf{E}^*_\kappa(V^0-\eta) + h^{-3}\int P(V^0-\eta)\,dx + O(h^{-\frac{4}{3}})\end{aligned}$$

also uniformly by $\eta > 0$ and then

$$\mathsf{E}^*_\kappa(V) + h^{-3}\int P(V)\,dx \le 2h^{-2}z^2S(\kappa z) + O(h^{-\frac{4}{3}}). \tag{22}$$

$M \geq 2$ and decoupling of singularities

If we have more than one singularity the same arguments work but in the estimate from below we have a term

$$-C\kappa^{-1}h^{-2}\|\partial A'\|^2_{\mathcal{X}} \tag{23}$$

with minimizer A and $\mathcal{X} = \{x : \frac{1}{3}a \leq \ell(x) \leq a\}$ where $\ell(x)$ is the distance to the closest nuclei and a is the minimal distance between nuclei.

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with minimizer A and $\mathcal{X} = \{x : \frac{1}{3}a \leq \ell(x) \leq a\}$ where $\ell(x)$ is the distance to the closest nuclei and a is the minimal distance between nuclei. However for potential which decays at infinity sufficiently fast $(W^{\mathsf{TF}} + \nu)_+$ decays as ℓ^{-4} one I proved that $|\partial A| = O(\kappa\ell^{-3})$ and then (23) does not exceed $C\kappa a^{-3}h^{-2}$ and we arrive to estimate

$$\mathsf{E}^*_\kappa = \varkappa_0 h^{-3} + \varkappa_1 h^{-2} + O(h^{-\frac{4}{3}} + \kappa a^{-3}h^{-2}) \tag{24}$$

with

$$\varkappa_1 = \sum_{1\leq m\leq M} 2z_m^2 S(\kappa z_m). \tag{25}$$

More delicate arguments based on refined analysis of propagation of singularities I developed 20− y.a. and recently adopted to current problem allow to improve this to

Theorem 1

For Thomas-Fermi potential rescaled with $a \ge 1$

$$\mathsf{E}^*_\kappa = \varkappa_0 h^{-3} + \varkappa_1 h^{-2} + \varkappa_2 h^{-1} + O(h^{-1+\delta} + h^{-1}a^{-\delta} + \kappa|\log\kappa|^{\frac{1}{3}} h^{-\frac{4}{3}} + \kappa a^{-3} h^{-2}) \quad (26)$$

with $\varkappa_0$, $\varkappa_2$ exactly as without self-generating magnetic field and with κ_1 given by (25).

Remark

1. Term $\kappa a^{-3}h^{-2}$ shows one extra difficulty as $M \geq 2$: the loss of locality due to self-generated magnetic field. Fortunately in free nuclei model the last term in the remainder estimate could be dropped.

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2. Apart from $S(\kappa)$ being monotone decaying and $S(\kappa) \geq S(0) - c\kappa$ (and value $S(0)$) we don't know a damn thing about it. It may happen that $S(\kappa) = S(0)$ as $\kappa < \kappa^*$ or that $S(\kappa) = -\infty$ as κ is large enough!

Combined magnetic field: work in progress

Currently I am working on the combined magnetic field when $A = A^0 + A'$ with constant external magnetic field of intensity β A^0 (so $A^(x) = \frac{1}{2}(-\beta x_2, +\beta x_1, 0)$ and unknown self-generated magnetic field A' and only energy of A' is counted:

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Let us start from local smooth theory as we did as $A^0 = 0$. Let us explore first semiclassical approximation without justification:

$$\mathcal{E}_\kappa(A) := -h^{-3} \int P_{Bh}(V)\psi^2\, dx + \kappa^{-1} h^{-2} \|\partial A'\|^2 \tag{28}$$

where $B = |\nabla \times A|$ is an intensity of the combined field.

Assuming that $\mu = |\partial A'| \ll \beta$ (which could be) observe that $B = \beta + (\partial_1 A'_2 - \partial_2 A'_1) + O(\mu^2\beta^{-1})$ and then $P_{Bh}(V) \approx P_{\beta h}(V) + \partial_\beta P_{\beta h}(V)(\partial_1 A'_2 - \partial_2 A'_1)$ and we arrive to

$$- h^{-3}\int P_{\beta h}(V)\psi^2\,dx \\ \underbrace{-h^{-3}\int \partial_\beta P_{\beta h}(V)(\partial_1 A'_2 - \partial_2 A'_1)\psi^2\,dx + \kappa^{-1}h^{-2}\|\partial A'\|^2}. \qquad (29)$$

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So self-generated magnetic field appears on the semiclassical level and I can actually prove that if $\beta h \lesssim 1$ but $\kappa\beta^2 h \gg 1$ then $\|\partial(A' - A'')\| \ll \|\partial A'\|$ where A', A'' are minimizers for $\mathsf{E}_\kappa(A)$ and $\mathcal{E}_\kappa(A)$ respectively.

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Estimates to minimizer

The first step is to estimate minimizer starting from equation (15) which still holds:

$$\frac{1}{\kappa h^2}\Delta A'_j(x) = \Phi_j(x) := \\ -\operatorname{Re}\operatorname{tr}\Bigl(\sigma_j\bigl((hD-A)_x\cdot\boldsymbol{\sigma}\bigr)\bigl(\psi(x)e(x,y,0)\psi(y)\bigr)\Bigr)\Bigr|_{y=x}. \qquad (15)$$

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Recall that the right-hand expression there is a pointwise spectral expression and they are not easy under magnetic field: the obstacle are not only periodic trajectories but also loops (especially short loops) and they are plentiful in this case.

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Luckily I already investigated similar asymptotics in Chapter 16 of [V. Ivrii, Future Book].

Theorem 2

In smooth local theory minimizer A' of E^*_κ satisfies

$$|\partial^2 A'| \\ \le C\begin{cases} \kappa|\log h| & \beta\le h^{-\frac{1}{3}},\\ \kappa|\log h|\beta^{\frac{3}{2}}h^{\frac{1}{2}} & h^{-\frac{1}{3}}\le\beta\le h^{-\frac{1}{2}},\\ \kappa|\log h|\beta^{\frac{1}{2}}+(\kappa\beta)^{\frac{10}{9}}h^{\frac{4}{9}}|\log h|^K & h^{-\frac{1}{2}}\le\beta, \kappa\beta h\le 1,\\ (\kappa\beta)^{\frac{4}{3}}h^{\frac{2}{3}}|\log h|^K & \kappa\beta h\ge 1\end{cases} \tag{30}$$

where in the last case we also assume that $\kappa\beta h^2\le|\log h|^{-K}$.

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where in the last case we also assume that $\kappa\beta h^2 \le |\log h|^{-K}$.

This theorem is rather trivial as $\beta \le h^{-\frac{1}{2}}$ but becomes difficult otherwise. Usually in magnetic spectral asymptotic threshold is at $\beta \asymp h^{-1}$ but here we have several thresholds but $\beta \asymp h^{-1}$ is one of them only as $\kappa \asymp 1$.

Trace estimates

Theorem 3

1. *In the smooth local theory let* $|\partial^2 A'| \le \nu \le \epsilon\beta$, $|\partial A'| \le \nu \le \epsilon\beta$. *Then*

$$|\operatorname{Tr}((\psi H_{A,V}\psi)^-) + h^{-3}\int P_{Bh}(V)\psi^2| \le C\begin{cases} h^{-1} + h^{-\frac{1}{3}}\nu^{\frac{4}{3}} & \beta h \le 1,\\ \beta + \beta h^{\frac{2}{3}}\nu^{\frac{4}{3}} & \beta h \ge 1\end{cases} \tag{31}$$

under modest non-degeneracy assumption

$$\min_{j\ge 0}|V - 2j\beta h| + |\nabla V| + |\nabla^2 V| \asymp 1; \tag{32}$$

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under modest non-degeneracy assumption

$$\min_{j\ge 0} |V - 2j\beta h| + |\nabla V| + |\nabla^2 V| \asymp 1; \tag{32}$$

2. *In the general case one needs to add* $C\beta h^{-\frac{1}{2}}$ *to the right-hand expression.*

Remark

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1. In Theorem 3 threshold happens as it should at $\beta \asymp h^{-1}$ (but there are hidden threshold for estimate of ν);
2. Theorem 3 is proven by the same advanced non-smooth microlocal analysis;
3. Combining Theorems 2, 3 we get remainder estimates; plugging into (31) we can skip $\kappa\beta^{\frac{1}{2}}$ in (30);
4. Then $\|\partial(A'-A'')\| \le C(\kappa h^2 Q)^{\frac{1}{2}}$ where Q is the remainder estimate in Theorem 3 and $\|\partial(A'-A'')\|_{\mathscr{L}^\infty} \le C\|\partial^2 A'\|_{\mathscr{L}^\infty}^{\frac{3}{5}}\|\partial(A'-A'')\|^{\frac{2}{5}}$.

Singularity

Simple scaling shows that "near singularity" zone adds Scott correction term $2S(\kappa z)z^2h^{-2}$ to the main part of asymptotics and $O(\beta^{\frac{1}{3}}h^{-1} + \kappa|\log\kappa|^{\frac{1}{3}}\beta^{\frac{2}{9}}h^{-\frac{4}{3}})$ to the remainder as $1 \le \beta \le h^{-2}$:

- For $\beta \le 1$ results are like there was no external magnetic field;
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- For $\beta \le 1$ results are like there was no external magnetic field;
- For $\beta \ge h^{-2}$ results are as if there are no singularities at all.

However as $1 \le \beta \le h^{-2}$ non-locality of self-generated magnetic field entangles singularity with the regular zone and other singularities. Still, adding $O(\kappa h^{-2})$ to the remainder estimate–which is not necessary a loss at all–allows us to detach singularity.

Case $\beta h \le 1$

Theorem 4

1. *Let $M = 1$ (single singularity), $1 \le \beta \le h^{-1}$ and non-degeneracy assumption* (32) *be fulfilled. Then*

$$\mathsf{E}^*_\kappa = \varkappa_0 h^{-3} + \varkappa_1 h^{-2} + O(\beta^{\frac{1}{3}} h^{-1} + \kappa|\log\kappa|^{\frac{1}{3}}\beta^{\frac{2}{9}} h^{-\frac{4}{3}} + \kappa\beta h^{-1}) \quad (33)$$

   with $\varkappa_0 = -\int P_{\beta h}(V)\,dx$ and $\varkappa_1 = \varkappa_1(\kappa)$ is the same Scott correction term as without external magnetic field;

2. *Without non-degeneracy assumption one should add $O(\beta h^{-\frac{1}{2}})$ to the remainder estimate;*

3. *If $M = 2$ and V decays fast enough from singularities ($V = O(\ell^{-4})$ would be enough) then one should add $O(\kappa a^{-3} h^{-2})$ to the remainder estimate.*

Case $\beta h \geq 1$

Theorem 5

1. *Let* $h^{-1} \leq \beta \leq h^{-2}$, $\kappa\beta h^2 \leq |\log h|^{-K}$ *and non-degeneracy assumption* (32) *be fulfilled. Then*

$$\mathsf{E}^*_\kappa = \varkappa_0 h^{-3} + \varkappa_1 h^{-2} + O(\beta + \beta^{\frac{1}{3}} h^{-1} + \kappa h^{-2} + \beta h^{\frac{2}{3}} \nu^{\frac{4}{3}}) \tag{34}$$

with $\varkappa_0 = -\int P_{\beta h}(V)\, dx$ *and* $\varkappa_1 = \varkappa_1(0)$ *is the same Scott correction term as without any magnetic field at all; here* ν *is the right-hand expression in* (30)*;*

2. *Without non-degeneracy assumption one should add* $O(\beta h^{-\frac{1}{2}})$ *to the remainder estimate.*

Reference

Microlocal Analysis, Sharp Spectral, Asymptotics and Applications (in progress)
http://weyl.math.toronto.edu/victor2/futurebook/futurebook.pdf

- Chapter 26. Asymptotics of the ground state energy of heavy molecules in self-generated magnetic field, pp 2350–2424;
- Chapter 27. Asymptotics of the ground state energy of heavy molecules in combined magnetic field, (in progress);

Large atoms and molecules with magnetic field, including self-generated magnetic field (Results: old, new, in progress and in perspective)
http://weyl.math.toronto.edu/victor2/preprints/Talk_10.pdf