Commun. Math. Phys. 79, 529–572 (1981)

Communications in Mathematical Physics

Schrödinger Operators With Magnetic Fields

III. Atoms in Homogeneous Magnetic Field

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Abstract. We prove a large number of results about atoms in constant magnetic field including (i) Asymptotic formula for the ground state energy of Hydrogen in large field, (ii) Proof that the ground state of Hydrogen in an arbitrary constant field has $L_z = 0$ and of the monotonicity of the binding energy as a function of B, (iii) Borel summability of Zeeman series in arbitrary atoms, (iv) Dilation analyticity for arbitrary atoms with infinite nuclear mass, and (v) Proof that every once negatively charged ion has infinitely many bound states in non-zero magnetic field with estimates of the binding energy for small B and large L_z.

1. Introduction

This is the third paper in our series on Schrödinger operators with magnetic field concentrating especially on the case of constant magnetic field where we normally use the gauge

$$\mathbf{a} = \tfrac{1}{2}(\mathbf{B}_0 \times \mathbf{r}) . \tag{1.1}$$

In this paper we consider primarily the physically important case of Coulomb forces and constant B. There turn out to be a number of previously undiscovered phenomena of mathematical and/or physical interest. This is, in part, because of the dearth of previous mathematical literature on the subject and, in part, because the natural units of B are so large (about 10^9 Gauss) that theoretically interesting efforts at large field cannot be seen in the laboratory with present techniques. The natural unit of B is $B^* = \frac{1}{2}mc^2(\alpha^2/\mu_B) = 2.35 \times 10^9$ Gauss; μ_B the Bohr magneton and $\frac{1}{2}mc^2\alpha^2$ the binding energy of Hydrogen. In a field of size B^*, the Landau energy exactly equals the ground state energy.

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* On leave at Department of Mathematics, California Institute of Technology, Pasadena, CA 91125 for 1980/81

** Supported by USNSF Grant MCS-78-00101

*** Supported by USNSF Grant MCS-78-01885; on leave at Department of Mathematics, California Institute of Technology, Pasadena, CA 91125 for 1980/81

0010-3616/81/0079/0529/$08.80

The other papers in our series deal with the following subjects: Paper I [9] discussed features of general interactions: both general B's and constant B with general potential. The paper dealt primarily with the two body case. The techniques and ideas of [9] are especially relevant to the present work. In particular, the stability method of that paper ([9], Sect. 6) will be useful here as it has been useful in the study of constant electric field [22, 23]. Moreover, the general scattering and spectral properties of Hydrogen in a constant field are treated in [9]. If [a given by (1.1)]

$$H=(-i\nabla-a)^2-r^{-1}$$

then H has no singular continuous spectrum (Theorem 4.7 of [9]) and modified Dollard-type scattering operators exist and are complete (Theorem 4.3 of [9]). Paper II [10] deals with certain special features of the reduction of center of mass and Paper IV [11] with numerical calculation of the ground state of Hydrogen in large magnetic fields.

In the present paper, there are points of direct relevance to the other papers in the series. First, there is an error in our discussion of dilation analyticity in [9] which fortunately is not major. The main consequences [(a) and (b)] and proof of Theorem 4.7 in [9] are correct but we do not quite prove precisely what is stated. This is further discussed in Sect. 6 of this paper. With regard to Paper II [10], we have found an interesting formula for the quasimomentum dependence of general N-body systems with total charge $Q=0$ after reduction of the center of mass. While this formula is only marginally relevant to the main thrust of the present paper, we have included it here (Appendix 2) since II has already been published. Finally, Sect. 2 is directly related to Paper IV [11].

The contents of the paper are as follows. We begin with consideration of one electron systems. In Sect. 2, Hydrogen in large B field is studied by reducing it to a one dimensional weakly coupled system. Such systems have been discussed in [43, 14, 27] but only for potentials $V=O(|x|^{-1-\varepsilon})$ at infinity. Since we need $V=O(|x|^{-1})$ at infinity, we begin by studying such one dimensional systems.

In Sects. 3 and 4 the main results are that the ground state in Hydrogen has $L_z=0$ and a binding energy which is monotone increasing in B_0. The main technical tool is the use of correlation inequalities. Such inequalities were originally proven by Griffiths [19] for statistical mechanical models and their applicability for Euclidean quantum field theories was first noted by Guerra et al. [20]. Here we exploit them to study non-relativistic quantum theory with potentials V vanishing at infinity. Motivated by our work, Lieb and Simon [32] have found another application to Born-Oppenheimer curves.

In Sect. 5, we prove Borel summability of the perturbation series for the Zeeman effect in hydrogen in constant field. Our method of estimating the $N!$ growth in the perturbation coefficients has been borrowed in related contexts: for the Stark problem by Herbst and Simon [22, 23] and for the R^{-1} expansion in molecules by Morgan and Simon [34].

In Sect. 6, we begin our treatment of multielectron systems by discussing dilation analyticity, extending our results for the case of Hydrogen in [9]. In Sect. 7, we extend the Borel summability results of Sect. 5 after extending the stability results of [9, Sect. 6]. In Sect. 8, we discuss falloff of bound state wave functions.

In Sect. 9, we discuss in detail a subject we sketched in [8], namely the fact that negative ions always form in magnetic fields; indeed for any atom A, the ion A^- has infinitely many eigenvalues below the continuum in $B_0 \neq 0$ field. Our proof uses the fact that polarization of the atom produces a net attractive force between A and the extra electron, an idea which does not appear in [8]. The importance of polarization has also been emphysized by Larsen [29] who was motivated, in part, by [8]. We also discuss the behavior of the binding energy as $B \downarrow 0$ and as $L_z \uparrow \infty$.

Appendix 1 contains some results on quadrupole moments of atoms in $B_0 \neq 0$ fields and Appendix 2 some new results on reduction of the center of mass.

The reader will note that two one-body topics have not been discussed in N-body contexts: correlation inequalities and strong field. Because of the Pauli principle, correlation inqualities are generally not applicable; indeed L_z may not be zero in the ground state of atoms. It might be possible to treat Helium in large field but this would be premature before the 3-body analog of Simon's result [43] on one dimensional short range potentials is obtained. The latter appears to be non-trivial.

The bulk of the results in this paper were obtained by us in the Spring of 1977 and announced in [7, 8]; the major exceptions are the dilation analyticity material in Sect. 6, the material in Sect. 8, the improved results using polarization in Sect. 9 and the discussion in Appendix 2. Since 1977, some subsets of us have used our methods elsewhere [22, 23, 32, 34]; we emphasize that the work here predates that in the last references. Moreover, Simon [45] has a pedagogical discussion of some of the material in Sects. 3 and 4. We also note that unaware of our work, some of the results in Sect. 3 were found using very different methods by Rosner et al. [39]; see the discussion in Sect. 3.

PART A: Hydrogen

2. Large Field Asymptotics

Let $a(B) = \frac{B}{2}(\hat{z} \times r)$ with $\hat{z} = (0, 0, 1)$ and let

$$H(B) = (-i\nabla - a(B))^2 - \frac{1}{r} \tag{2.1}$$

and define $E_m(B)$ to be the lowest point of the spectrum of $H(B)$ restricted to functions with $L_z = m$. By general principles (Theorem 5.1 of [9]), $E_m(B)$ is an eigenvalue. In this section, we obtain the first few terms in an asymptotic expansion of $E_m(B)$ about $B = \infty$. The expansion is in a parameter like $\ln_2 B/\ln B$ and thus in the region of astro-physical interest, $B \sim 10$–1000, the expansion itself is of limited value. However the implicit equations used to obtain the series are of calculational value, see [11]. The reader may also consult [11] for previous work on large B behavior. Prior to our work [7], Hasegawa and Howard [47] had found the $\ln B$ and $\ln_2 B$ terms in the asymptotic expansion of $\sqrt{-E+B}$. They analyzed the one dimensional problem without showing that the effect of the "latent two dimensiona" is small on this $\ln_2 B$ level. We emphasize that with a finite amount of effort one could carry the series to arbitrarily high order.

Physically, for large B, the electron will move in a tight Landau orbit in the x–y plane and will be bound in the z-direction by the Coulomb potential. The problem is thus essentially one dimensional. Moreover, by scaling, large B can be replaced by B fixed and $\frac{1}{r}$ changed to $\frac{\lambda}{r}$ with λ small. The problem is thus a weak coupling one dimensional one with a long range $|x|^{-1}$ potential. Such one dimensional problems for $O(|x|^{-3-\varepsilon})$ potentials were treated in [43] and extended to $O(|x|^{-1-\varepsilon})$ potentials in [14, 27]. We therefore begin by analyzing one dimensional problems with long range $|x|^{-1}$ potentials. (See Haeringen [21] for other discussion of such long range one dimensional potentials.)

Theorem 2.1. *Let $V(x)$ be a function on $(-\infty, \infty)$ obeying*

$$|V(x)| \leqq D_1(1+|x|)^{-1}\,, \tag{2.2}$$

$$|V(x)+|x|^{-1}| \leqq D_2(1+|x|)^{-1-\varepsilon};\ |x| \geqq 1\,. \tag{2.3}$$

Then for small positive λ, $-d^2/dx^2+\lambda V$ has exactly one eigenvalue, $e(\lambda)$, of energy below $-\lambda^2 D_1^2/4$ and for λ small and positive:

$$\begin{aligned} e(\lambda) = -\lambda^2\{&[\ln(\lambda^{-1})]^2 - 2[\ln(\lambda^{-1})\ln_2(\lambda^{-1})] + 2C[\ln(\lambda^{-1})] \\ &+ [\ln_2(\lambda^{-1})]^2 - 2(C-1)[\ln_2(\lambda^{-1})] + O(1)\}\,, \end{aligned} \tag{2.4}$$

where $\ln_2(x) = \ln[\ln(x)]$ *and*

$$\begin{aligned} C = &\int_1^\infty e^{-y}y^{-1}dy + \int_0^1 y^{-1}(e^{-y}-1)dy - \ln 2 - \tfrac{1}{2}\int_{-1}^{1} V(x)dx \\ &-\tfrac{1}{2}\int_{|x|\geqq 1}(V(x)+|x|^{-1})dx\,. \end{aligned} \tag{2.5}$$

We begin the proof of the theorem by noting that (2.4) is equivalent to $e(\lambda) = -[\alpha(\lambda)]^2$ with

$$\alpha(\lambda) = \lambda\ln(\lambda^{-1}) - \lambda\ln_2(\lambda^{-1}) + \lambda C + \lambda[\ln\lambda^{-1}]^{-1}\ln_2(\lambda^{-1}) + O(\lambda[\ln(\lambda^{-1})]^{-1}) \tag{2.6}$$

and this is what we will prove.

Following the basic scheme of [43], we isolate a rank one divergent piece of the Birman-Schwinger kernel; the particular decomposition is taken from [14] and is better suited to long range interactions than the one in [43]. Define $V(x)^{1/2} \equiv |V(x)^{1/2}|\,\mathrm{sgn}(V(x))$ and let P_α, Q_α be the operators with integral kernels

$$P_\alpha(x,y) = -\tfrac{1}{2}V(x)^{1/2}e^{-\alpha|x|}e^{-\alpha|y|}|V(y)|^{1/2}\,, \tag{2.7}$$

$$Q_\alpha(x,y) = -\tfrac{1}{2}V(x)^{1/2}[e^{-\alpha|x-y|} - e^{-\alpha|x|}e^{-\alpha|y|}]|V(y)|^{1/2}\,. \tag{2.8}$$

Then $\alpha^{-1}[P_\alpha+Q_\alpha]$ is the operator $-V^{1/2}(-d^2/dx^2+\alpha^2)^{-1}|V|^{1/2}$ and so the Birman-Schwinger principle (see [37]) asserts that $-d^2/dx^2+\lambda V(x)$ has eigenvalue $-\alpha^2$ if and only if $P_\alpha+Q_\alpha$ has eigenvalue $\alpha\lambda^{-1}$ or equivalently if and only if $1-\lambda\alpha^{-1}(P_\alpha+Q_\alpha)$ is not invertible.

Lemma 2.2. *Let $\tilde{Q}_\alpha$ have the integral kernel* (2.8) *with $V(x)$ replaced by $-|x|^{-1}$. Then*

$$\|Q_\alpha\| \leqq D_1 \|\tilde{Q}_\alpha\| = \tfrac{1}{2} D_1 \,. \tag{2.9}$$

Remark. The equality $\|\tilde{Q}_\alpha\| = \frac{1}{2}$ improves the estimate $\|\tilde{Q}_\alpha\| \leqq \sqrt{3}$ which we obtained in [11] by more straightforward calculation.

Proof. Since $\|Q_\alpha \phi\| \leqq D_1 \|\hat{Q}_\alpha |\phi|\,\|$, the first half of (2.9) is trivial. Now $\alpha^{-1}\hat{Q}_\alpha = |x|^{-1/2}(h_0+\alpha^2)^{-1}|x|^{-1/2}$ where h_0 is $-d^2/dx^2$ with a Dirichlet boundary condition at $x=0$. Thus by the self-adjointness of $\tilde{Q}_\alpha$ and the Birman-Schwinger principle

$$\|\alpha^{-1}\tilde{Q}_\alpha\| = \sup\{\lambda^{-1} | h_0 - \lambda|x|^{-1} \text{ has eigenvalue } -\alpha^2\} \,.$$

But the eigenvalues of $h_0-\lambda|x|^{-1}$ are $-(4n^2)^{-1}\lambda^2$ by the analysis of Hydrogen. So

$$\|\alpha^{-1}\tilde{Q}_\alpha\| = \sup\{(2n)^{-1}\alpha^{-1} | n=1,2,\dots\} = \tfrac{1}{2}\alpha^{-1} \,. \quad \Box$$

Lemma 2.2 implies that so long as $\lambda D_1/2\alpha < 1$,

$$1-\lambda\alpha^{-1}(P_\alpha+Q_\alpha) = (1-\lambda\alpha^{-1}Q_\alpha)(1-\lambda\alpha^{-1}(1-\lambda\alpha^{-1}Q_\alpha)^{-1}P_\alpha) \tag{2.10}$$

is non-invertible if and only if the last factor in (2.10) is non-invertible. Since P_α is rank 1, the condition for this is

$$\alpha = \lambda \operatorname{Tr}(P_\alpha(1-\lambda\alpha^{-1}Q_\alpha)^{-1} \tag{2.11}$$

or

$$\alpha = \lambda \operatorname{Tr}(P_\alpha) + \lambda^2\alpha^{-1} \operatorname{Tr}(P_\alpha Q_\alpha) + \lambda^3\alpha^{-2} \operatorname{Tr}(P_\alpha Q_\alpha^2(1-\lambda\alpha^{-1}Q_\alpha)^{-1}) \,. \tag{2.12}$$

Lemma 2.3.

(i) $\operatorname{Tr}(P_\alpha) = \ln\alpha^{-1} + C + O(\alpha^\delta)$, $\quad (\delta>0)$ (2.13)

with C given by (2.5).

(ii) $\operatorname{Tr}(|P_\alpha|) = O(\ln\alpha^{-1})$. (2.14)

Proof. We prove (2.13). (2.14) follows by replacing V by $|V|$.

$$\operatorname{Tr}(P_\alpha) = -\tfrac{1}{2}\int_{-\infty}^{\infty} e^{-2\alpha|x|}V(x)dx = I + II + III \,,$$

where

$$I = -\tfrac{1}{2}\int_{-1}^{1} e^{-2\alpha|x|}V(x)dx = -\tfrac{1}{2}\int_{-1}^{1} V(x)dx + O(\alpha) \,,$$

$$II = -\tfrac{1}{2}\int_{|x|\geqq 1} e^{-2\alpha|x|}\left[V(x)+\frac{1}{|x|}\right]dx = -\tfrac{1}{2}\int_{|x|\geqq 1}\left[V(x)+\frac{1}{|x|}\right]dx + O(\alpha^\delta) \,,$$

using $|e^{-2\alpha|x|}-1| \leqq 2^{(1-\delta)}(2\alpha)^\delta |x|^\delta (0\leqq\delta\leqq 1)$ and (2.3).

$$III = \int_1^\infty e^{-2\alpha|x|}|x|^{-1}dx = \int_{2\alpha}^\infty e^{-y}y^{-1}dy$$
$$= \int_1^\infty e^{-y}y^{-1}dy + \int_0^1 (e^{-y}-1)y^{-1}dy + \ln(2\alpha)^{-1} + O(\alpha)\,.$$

Consulting (2.5), we have proven (2.13). □

Lemma 2.4.

$$\mathrm{Tr}(P_\alpha Q_\alpha) \leqq D_1^2\,. \tag{2.15}$$

Proof. Using (2.2) and then scaling

$$|\mathrm{Tr}(P_\alpha Q_\alpha)| \leqq \frac{D_1^2}{4} 2 \int_0^\infty dx \int_0^\infty dy x^{-1}y^{-1}e^{-\alpha x}e^{-\alpha y}[e^{-\alpha|x-y|} - e^{-\alpha|x|}e^{-\alpha|y|}]$$
$$= D_1^2 \int_0^\infty x^{-1}e^{-2x}dx \int_0^x y^{-1}(1-e^{-2y})dy\,. \tag{2.16}$$

Using

$$(1-e^{-2y}) \leqq 2y \tag{2.17}$$

(2.15) results.

Remark. By using (2.17) we give up a little bit. The right side of (2.16) is exactly $D_1^2(\pi^2/12)$; see [11].

Proof of Theorem 2.1. Clearly, by Lemma 2.4

$$\frac{\lambda^2}{\alpha}\mathrm{Tr}(P_\alpha Q_\alpha) = O\left(\frac{\lambda^2}{\alpha}\right)$$

and by using Lemma 2.2 which implies $\|Q_\alpha(1-\lambda Q_\alpha \alpha^{-1})^{-1}\|$ is bounded in the region λ/α small,

$$\frac{\lambda^3}{\alpha^2}\mathrm{Tr}(P_\alpha Q_\alpha^2(1-\lambda Q_\alpha \alpha^{-1})^{-1}) = O\left(\frac{\lambda^3}{\alpha^2}\mathrm{Tr}(|P_\alpha|)\right) = O\left(\frac{\lambda^3}{\alpha^2}\ln\alpha^{-1}\right)$$

by Lemma 2.3. [Actually, $\mathrm{Tr}(P_\alpha Q_\alpha^2)$ is finite and this term is $O(\lambda^3/\alpha^2)$ in the regions $\lambda/\alpha \sim 1/\ln\alpha^{-1}$.] Thus, by (2.12) and Lemma 2.2:

$$\alpha = \lambda(\ln\alpha^{-1} + C + O(\alpha^\delta)) + O(\lambda^2/\alpha) + O(\lambda^3\ln(\alpha^{-1})/\alpha^2)\,.$$

The simple estimate $-d^2/dx^2 + \lambda V \geqq -c\lambda$ gives $-\alpha^2 \geqq -c\lambda$ or $\alpha \leqq \mathrm{const}\sqrt{\lambda}$ while a crude trial wave function $\psi = \sqrt{\lambda}e^{-\lambda|x|}$ gives $\alpha \geqq \mathrm{const}\,\lambda(\ln\lambda^{-1})^{1/2}$. Using these estimates, the above equation implies

$$c_1\lambda\ln\lambda^{-1} \leqq \alpha \leqq c_2\lambda\ln\lambda^{-1}$$

for small λ and positive constants c_1 and c_2. Thus

$$\alpha = \lambda\ln\alpha^{-1} + \lambda C + O(\lambda[\ln(\lambda^{-1})]^{-1}\,. \tag{2.18}$$

Taking ln's twice

$$\ln \alpha^{-1} = \ln \lambda^{-1} - \ln_2 \alpha^{-1} + O([\ln(\alpha^{-1})]^{-1}), \tag{2.19}$$

$$\begin{aligned}\ln_2 \alpha^{-1} &= \ln_2 \lambda^{-1} + \ln[1 - \ln_2(\alpha^{-1})/\ln(\lambda^{-1})] + O([\ln(\alpha^{-1})\ln(\lambda^{-1})]^{-1}) \\ &= \ln_2 \lambda^{-1} - \ln_2(\alpha^{-1})/\ln(\lambda^{-1}) + O([\ln_2(\alpha^{-1})/\ln(\lambda^{-1})]^2)\end{aligned} \tag{2.20}$$

(2.18)–(2.20) imply (2.6). □

Remark. Klaus [28] has noted that r^{-1} falloff is the slowest where the ground and excited states are distinguished in one dimension: for

$$-\frac{d^2}{dx^2} + \lambda V(x)$$

is unitary equivalent to:

$$\lambda^{2\alpha}(p^2 + \lambda^{1-2\alpha} V(\lambda^{-\alpha} x)) \equiv \tilde{h}(\lambda) .$$

If $V(x) \sim -C|x|^{-\delta}$ at infinity, we pick $\alpha = (2-\delta)^{-1}$ and, using the fact that $x^{-\delta}$ is p^2-bounded if (and only if) $\delta < 1$, we see that $\tilde{h}(\lambda)\lambda^{-2\alpha}$ converges in norm resolvent sense to $p^2 - C|x|^{-\delta}$. Thus, if $0 < \delta < 1$,

$$\varepsilon_m(\lambda) \sim D_m \lambda^{2/(2-\delta)}$$

for *all* eigenvalues.

We are now ready for the main result of this section:

Theorem 2.5. *Let $E_m(B)$ be the ground state energy of* (2.1) *restricted to $L_z = m$. Then for $m \geqq 0$:*

$$\begin{aligned}E_m(B) = B - \tfrac{1}{4}\left[\ln\left(\frac{B}{2}\right)\right]^2 + \left[\ln\left(\frac{B}{2}\right)\ln^2\left(\frac{B}{2}\right)\right] - \left[(C_m + \ln 2)\ln\left(\frac{B}{2}\right)\right] \\ - \left[\ln_2\left(\frac{B}{2}\right)\right]^2 + 2(C_m - 1 + \ln 2)\left[\ln^2\left(\frac{B}{2}\right)\right] + O(1) ,\end{aligned} \tag{2.21}$$

where C_m is the constant C in (2.5) *with the potential*

$$V_m(x) = -(m!)^{-1} \int_0^\infty t^m e^{-t}(t + x^2)^{-1/2} dt . \tag{2.22}$$

Remarks. 1) C_m is evaluated explicitly in [11]; its value is

$$C_m = -\tfrac{1}{2}(\gamma_E + q_m) ,$$

where γ_E is Euler's constant and $q_m = m^{-1} + q_{m-1}$; $q_0 = 0$.

2) Notice that for B large our expansion suggests

$$E_0 < E_1 < E_2 < \dots$$

although since (2.21) is not claimed to be uniform in m this cannot be concluded rigorously from Theorem 2.5. However, we will prove this for all B in Sect. 4.

Proof. Let $H(B, \lambda)$ be the object obtained from (2.1) by replacing $-1/r$ by $-\lambda/r$, and let $\varepsilon_m(B, \lambda)$ be its ground state energy when restricted to $L_z = m$. Then since the scaling $p \to \gamma^{-1} p$, $r \to \gamma r$ is unitarily implementable $H(B,\lambda)$ and $\gamma^{-2} H(\gamma^2 B, \gamma\lambda)$ are unitarily equivalent. Thus

$$\varepsilon_m(B,\lambda) = \gamma^{-2} \varepsilon_m(\gamma^2 B, \gamma^1 \lambda)$$

so taking $\gamma = (2/B)^{1/2}$, $\lambda = 1$

$$E_m(B) = \gamma^{-2} \varepsilon_m(2,\gamma)\,;\, \gamma = (2/B)^{1/2}\,. \tag{2.23}$$

Now

$$H(2,\gamma) = h_0 - 2L_z + \left(-\frac{d^2}{dz^2}\right) - \gamma r^{-1} + 2$$

with

$$h_0 = -\frac{d^2}{dx^2} - \frac{d^2}{dy^2} + x^2 + y^2 - 2.$$

On $L_z = m$, h_0 has simple spectrum at $2|m|, 2|m|+4, \ldots$. Let $\Phi_m(x,y)$ be the ground state of $h_0 \restriction (L_z = m)$, and let

$$(\tilde{P}_m f)(x,y,z) = \Phi_m(x,y) \int \bar{\Phi}_m(x',y') f(x',y',z) dx' dy'\,.$$

Let $H_m(2,0) = H(2,0) \restriction (L_z = m)$, $h_{0,m} = h_0 \restriction (L_z = m)$. Then for $m \geqq 0$

$$(H_m(2,0) - 2 + \alpha^2)^{-1} = A_\alpha + B_\alpha\,,$$

where

$$A_\alpha = \tilde{P}_m \left[-\frac{d^2}{dz^2} + \alpha^2\right]^{-1}$$

$$B_\alpha = (1 - \tilde{P}_m)\left(-\frac{d^2}{dz^2} + h_{0,m} - 2m + \alpha^2\right)^{-1}.$$

The Birman-Schwinger kernels,

$$r^{-1/2}(H_m(2,0) - 2 + \alpha^2)^{-1} r^{-1/2}$$

for $H(2,\gamma)|(L_z = m)$ is a sum of two terms; the $r^{-1/2} B_\alpha r^{-1/2}$ term has a nice limit as $\alpha \downarrow 0$ since

$$(H(2,0) - 2) \restriction (1 - \tilde{P}_m)\mathscr{H} \geqq \tfrac{2}{5}(H(2,0) + 1) \restriction (1 - \tilde{P}_m)\mathscr{H}$$

so that

$$r^{-1/2} B_\alpha r^{-1/2} \leqq \tfrac{5}{2} r^{-1/2}(H_m(2,0) + 1)^{-1} r^{-1/2}$$

and

$$\begin{aligned} \|r^{-1/2}(H_m(2,0)+1)^{-1} r^{-1/2}\| &\leqq \|r^{-1/2}(H(2,0)+1)^{-1} r^{-1/2}\| \\ &\leqq \|r^{-1/2}(-\Delta + 1)^{-1} r^{-1/2}\|\,, \end{aligned}$$

which is finite by standard results [36].

The $r^{-1/2} A_\alpha r^{-1/2}$ term can be analyzed exactly as we analyzed the one dimensional case. In computing $\mathrm{Tr}(P_\alpha)$, the potential that enters will be

$$V_m(z) = \int |\Phi_m(x,y)|^2 (x^2 + y^2 + z^2)^{-1/2} dx dy$$

which, given the explicit formula for Φ_m, is given by (2.21). V_m obeys (2.2), (2.3) with $D_1=1$ and $\varepsilon=2$. $\alpha(\gamma)$, defined by $2-\alpha(\gamma)^2=\varepsilon_m(2,\gamma)$, still obeys an implicit equation

$$\alpha=\gamma\ln\alpha^{-1}+C_m\gamma+O(\gamma[\ln\alpha^{-1}]^{-1}) .$$

The $r^{-1/2}B_m r^{-1/2}$ terms first contribute at order γ^2. Noting that with $\gamma=\left(\frac{2}{B}\right)^{1/2}$,

$$\ln\gamma^{-1}=\tfrac{1}{2}\ln\left(\frac{B}{2}\right)$$

$$\ln_2\gamma^{-1}=\ln_2\left(\frac{B}{2}\right)-\ln 2$$

we obtain (2.21) from (2.4). □

3. GKS Inequalities and Wave Function Collapse

One of our main goals in the next two sections is the proof that $L_z=0$ for the ground state of Hydrogen in a magnetic field. In the absence of a magnetic field, such a result is very general: the ground state for an arbitrary potential is strictly positive [37], hence it must be $L_z=0$ if the potential is azimuthally symmetric. The magnetic field destroys the positivity of the integral kernel of e^{-tH} on which the general result depends and so the result becomes non-trivial. Indeed, Lavine and O'Carroll [30] proved the existence of spherically symmetric potentials, V, so that with a given by (1.1), $(-i\nabla-a)^2+V$ has a ground state with $L_z\neq 0$. In [9], we gave further examples and a picture of why this can happen. Since this picture is also the key to solving the problem for hydrogen, we next describe it in some detail.

For simplicity, add an εz^2 term to $H_0(B)=(-i\nabla-a)^2$, i.e. consider $\tilde{H}_0(B)\equiv H_0(B))\varepsilon z^2$. Then, for $B\neq 0$, $\tilde{H}_0(B)$ has purely point spectrum and its ground state is infinitely degenerated having states with $L_z=0,1,\dots$ (if $B>0$). If the potential $V\leqq 0$ lives in the region where the state with $L_z=27$ lives, then clearly $\tilde{H}_0(B)+V$ will have a ground state with $L_z=27$. This leads to the natural conjecture (made already by Lavine and O'Carroll [30]) that if V is spherically symmetric and monotone increasing in $|r|$, then $H_0(B)+V$ will have a ground state with $L_z=0$. This is what we will prove in the next section.

Now consider a potential $V(\varrho,z)$ which is azimuthilly symmetric. By making a cylindrical coordinate expansion one sees that:

Proposition 3.1. *The ground state energy, $E_m(B_0,V)$, of $(-i\nabla-\frac{1}{2}B_0(\hat{z}\times r))^2+V$ restricted to $L_z=m$, is identical to the ground state energy of*

$$-\Delta+\tfrac{1}{4}B_0^2\varrho^2+m^2\varrho^{-2}-mB_0+V \tag{3.1}$$

since the ground state of (3.1) *has $L_z=0$.*

One advantage of this reduction is that m can now be varied continuously. Imagine adding an εz^2 term to stabilize the problem by forcing a discrete ground state then

$$\frac{\partial E_m}{\partial m}=2m\langle\varrho^{-2}\rangle-B_0 \tag{3.2}$$

with $\langle\ \rangle$ the expectation value in the ground state. When $V=0$, this derivative is zero for $m>0$. Thus the monotonicity of E_m in m ($m\geqq 0$) will follow from the fact that $\langle\varrho^{-2}\rangle$ increases when V is added, i.e., that the wave function gets "pulled-in" by an attractive potential. In this section, as a warm-up, we prove the following:

Theorem 3.2. *Let V, W be even functions on $(-\infty,\infty)$ so that $\frac{dW}{dx}\geqq 0$ for $x\geqq 0$. Let Ω_V, (respectively Ω_{V+W}) be the normalized ground state eigenfunctions for $-\frac{d^2}{dx^2}+V\left(\text{respectively } -\frac{d^2}{dx^2}+V+W\right)$ (we suppose such exist). Then for any a*

$$\int_{-a}^{a}|\Omega_{V+W}(x)|^2dx\geqq\int_{-a}^{a}|\Omega_V(x)|^2dx\,. \tag{3.3}$$

Remarks. 1) Independently of us and using very different methods, this result was proven by Rosner et al. [39]; we discuss this further at the conclusion of this section.

2) It is natural to use the language of path integrals to describe the proof below but since the correlation inequalities are proven via a lattice approximation which is equivalent to a Trotter product approximation we avoid that language.

We require the following result of Ginibre [18] which generalizes inequalities of Griffiths et al. (GKS inequalities).

Lemma 3.3. *Let A consist of those functions, $\mathscr{G}$, of the form $\mathscr{G}=\mathscr{G}_e+\mathscr{G}_0$ with $\mathscr{G}_e$ even, $\mathscr{G}_0$ odd and both $\mathscr{G}_e$ and $\mathscr{G}_0$ monotone increasing on $(0,\infty)$. Given positive, even functions $f_1,\dots,f_m$ on R and $J_{ij}\geqq 0$ $(i,j=1,\dots,)$, define a probability measure $d\nu$ on R^m by*

$$d\nu=N^{-1}e^{\Sigma J_{ij}x_ix_j}\prod_i f_i(x_i)dx_i \tag{3.4}$$

with N a normalization factor. (Below N denotes a suitable, but changing normalization factor.) Then for any $g,h\in\mathscr{A}$ and i,j

$$\int g(x_i)h(x_j)d\nu\geqq\left[\int g(x_i)d\nu\right]\left[\int h(x_j)d\nu\right]\,.$$

Proof of Theorem 3.2. Let $\Omega_{V+\lambda W}$ be the ground state for $-\frac{d^2}{dx^2}+V+\lambda W$ and let $h=-\chi_{(-a,a)}$, the negative of the characteristic function of $(-a,a)$. Notice that $h\in\mathscr{A}$. Define

$$F(\lambda)=(\Omega_{V+\lambda W},h\Omega_{V+\lambda W})\,.$$

Clearly, we want to show that F is monotone non-increasing in λ. Write $H_\lambda=-\frac{d^2}{dx}+V+\lambda W$ and let

$$F_T(\lambda)=(e^{-TH_\lambda}\psi,he^{-TH_\lambda})/(\psi,e^{-2TH_\lambda}\psi)$$

with $\psi(x)=e^{-x^2}$. Since $\lim_{T\to\infty}F_T(\lambda)=F(\lambda)$, we need only show that $F_T(\lambda)$ is monotone non-increasing. Next let

$$F_{T,n}(\lambda)=((e^{-TH_0/n}e^{-TV(\lambda)/n})^n\psi,h(e^{-TH_0/n}e^{-TV(\lambda)/n})^n\psi)/N\,,$$

where $H_0 = -d^2/dx^2$, $V(\lambda) = V + \lambda W$, and N is the numerator with $h=1$. By the Trotter product formula, $\lim_{n\to\infty} F_{T,n}(\lambda) = F_T(\lambda)$, so we only need to show that

$$\frac{d}{d\lambda} F_{T,n}(\lambda) \leqq 0 \,. \tag{3.5}$$

But $F_{T,n}$ is of the form $\int h dv$ with v obeying (3.4) where $m=2n+1$, and the $f_i(x_i)$ are products of three kinds of factors: (i) ψ's for $i=1, 2n+1$; (ii) $e^{-(V+\lambda W)(x)}$ for $i=1,\dots,m$, $n+2,\dots,2n+1$; (iii) Gaussians from the kernel of $e^{-sH_0} = ce^{-ax^2}e^{-ay^2}e^{+2axy}$. The e^{-ax^2} and e^{-ay^2} are absorbed into f's and the e^{2axy} into the $e^{\Sigma J_{ij}x_ix_j}$. Clearly the f_i's are even. Moreover, $dF_{T,n}/d\lambda$ is a sum of terms of the form

$$-\{[\int W(x_i)h(x_n)dv] - [\int h(x_n)dv]\,[\int W(x_i)dv]\}$$

so by Ginibre's lemma, $dF/d\lambda \leqq 0$. □

Ginibre's result is prowen for more general conditions than f_i even; what he really requires is that $f_i(x) = a_i(x)e^{b_i(x)}$ with a_i even and positive and b_i odd and monotone increasing on $[0,\infty)$ (see [45]). Thus, the above proof shows that:

Theorem 3.4. *Equation* (3.3) *remains true for* $V = V_o + V_e$, $W = W_o + W_e$ *(*V_o, W_o *odd, etc.) so lang as:*

(i) W_o *and* W_e *are monotone increasing on* $[0,\infty)$.

(ii) $-V_o$ *and* $-V_o - W_o$ *are monotone increasing on* $[0,\infty)$.

Remarks. 1) By symmetry, we can replace *all* monotone increasing for odd parts by monotone decreasing.

2) It is clear that an analogous result is also true for the Gibb's state

$$\langle A\rangle = \mathrm{tr}(e^{-\beta H}A)(\mathrm{tr}\, e^{-\beta H})^{-1}$$

using the same technique.

3) One might think intuitively that no restrictions on V are needed for (3.3) to hold if, say $W_o = 0$ and W_e is monotone on $[0,\infty)$. Here is a counterexample to this construction which we owe to Joel Feldman: Let

$$\begin{aligned} V(x) &= A && -1<x<1;\ x<-2,\ x>3 \\ &= 0 && 1<x<3 \\ &= -\pi^2 && -2<x<-1 \\ W(x) &= -A && -1<x<1 \\ &= 0 && |x| \geqq 1\,. \end{aligned}$$

In the limit as $A\to\infty$, the ground state of $-\frac{d^2}{dx^2} + V$ will lie entirely to the left of 0 so, $\int_{-2}^{2} |\psi_V|^2 dx = 1$ while for $-\frac{d^2}{dx^2} + V + W$, the wave function will be non-vanishing in all of $(-2,3)$, so $\int_{-2}^{2} |\psi_{V+W}|^2 dx < 1$. Thus by an approximation argument $\int_{-2}^{2} |\psi_V|^2 dx > \int_{-2}^{2} |\psi_{V+W}|^2 dx$ for all large enough A.

In June of 1977, one of us (B.S.) lectured at CERN on Theorem 3.2 and remarked that he knew of no "elementary" proof of the result. Within several hours, Martin supplied such a proof which we now give with his kind permission. We note that this methods are sufficiently one dimensional that if appears unlikely that one can prove the results of the next section with them. We also note that Martin's proof is a close relative of the proof that Rosner et al. [39] (see also Leung and Rosner [31] and Rosner and Quigg [38]) subsequently found of the result (they were unaware of our or Martin's work); their proof is essentially a "differential" version of Martin's. For yet another proof and a discussion of what happens for excited states, see [48].

Alternate Proof of Theorem 3.2 (Martin [33]). Let $g=\Omega_{V+W}$, $u=\Omega_V$ and add constants to V, W so that both ground state energies are zero. By a limiting argument we can also suppose that $dW/dx>0$ on $(0,\infty)$ so that there is a unique $x_0>0$ with $W(x)<0$ on $(0,x_0)$ and $W(x)>0$ on (x_0,∞). Let $h(x)=u(x)g'(x)-g'(x)u(x)$. By symmetry $u'(0)=g'(0)=0$, so $h(0)=h(\infty)=0$. Since

$$h'(x)=W(x)u(x)g(x)$$

we have that $h'(x)<0$ on $(0,x_0)$ and $h'(x)>0$ on (x_0,∞). Thus $h(x)<0$ on $(0,\infty)$ so that if $u(y_0)=g(y_0)$, then $g'(y_0)<u'(y_0)$. This implies there is a unique such point y_0 and $g(x)>u(x)$ on $(0,y_0)$, $g(x)<u(x)$ on (y_0,∞). Thus $F(y)\equiv\int_0^y[|g(x)|^2-|h(x)|^2]dx$ is increasing on $(0,y_0)$, decreasing on (y_0,∞). Since $F(0)=F(\infty)=0$, $F(a)>0$ for all a. □

4. FKG Inequalities, Wave Function Collaps and $L_z=0$ in Hydrogen

In this section, we will need the following version of the FKG (for Fortuin, Kastely and Ginibre [17]) inequalities. We use the notation

$$\mathbb{R}^m_+=\{x\in\mathbb{R}^m: x_i\geqq 0,\ i=1,\dots,m\}$$

and $(\mathbb{R}^m_+)^\circ$ for the interior of this set and let $\tilde{\mathscr{B}}$ consist of the bounded functions on $(\mathbb{R}^m_+)^\circ$ which are monotone non-decreasing in each x_i for $x_1,\dots,x_{i-1},x_{i+1},\dots,x_m$ fixed

Proposition 4.1. *Let $d\mu_1,\dots,d\mu_m$ be arbitrary (positive) measures on $\mathbb{R}_+$ with $\mu_j(\{0\})=0$, and let F be positive and C^2 in $(\mathbb{R}^m_+)^\circ$ with*

$$\partial^2\ln F/\partial x_i\partial x_j\geqq 0\,,\qquad x\in(\mathbb{R}^m_+)^\circ,\ i\neq j\,. \tag{4.1}$$

Suppose $N=\int F d\mu_1\dots d\mu_m<\infty$ and define

$$d\nu(x)=N^{-1}F(x_1,\dots,x_m)d\mu_1(x_1)\dots d\mu_m(x_m)\,.$$

Then if $f,g\in\tilde{\mathscr{B}}$

$$\int fg d\nu\geqq\int f d\nu\int g d\nu\,. \tag{4.2}$$

Remarks. 1) The condition $\partial^2\ln F/\partial x_i\partial x_j\geqq 0$, $i\neq j$ is equivalent to the FKG condition $F(x\vee y)F(x\wedge y)\geqq F(x)F(y)$. This result appears in the unpublished

Princeton senior thesis of Sax [40] and in a recent review article of Kemperman [26]. A direct proof of the FKG inequalities which does not go through the FKG condition has been found by Battle and Rosen [13]. Our proof of the equivalence to the FKG condition can be found in [45].

2) Proposition 4.1 can be reduced to the FKG inequalities on $\mathbb{R}^m$ by the device of introducing a C^∞ function ϕ_ε on $\mathbb{R}$ with values in $[\varepsilon, \infty)$ and such that $\lim_{\varepsilon\downarrow 0} \phi_\varepsilon(x) = x$ for all $x>0$ and $\phi'_\varepsilon(x) \geqq 0$. Defining

$$F_\varepsilon(x) = F(\phi_\varepsilon(x_1), \dots, \phi_\varepsilon(x_m))$$

produces a positive C^2 function on $\mathbb{R}^m$ satisfying $\partial^2 \ln F/\partial x_i \partial x_j \geqq 0$, $i \neq j$, all $x \in \mathbb{R}^m$. Then by replacing $d\mu_j(x)$ by $\chi_{[n^{-1}, n]}(x) d\mu_j(x)$ and suitably redefining f and g on all of $\mathbb{R}^m$ to be monotone non-decreasing in each variable, we can use the usual FKG inequalities. We then first let $\varepsilon \downarrow 0$ and then $n \to \infty$.

3) The condition that F be positive (and not just non-negative) is essential. We give the following example (shown to us by Brydges) to warn the reader: Let $d\mu_j = e^{-x_j^2} dx_j$, $j=1,2$ and $F(x_1, x_2) = (x_1 - x_2)^2$. Then

$$\partial^2 \ln F/\partial x_1 \partial x_2 = 2(x_1 - x_2)^{-2} > 0$$

but by explicit computation

$$\int x_1 x_2 d\nu - \int x_1 d\nu \int x_2 d\nu = -1/2 \, .$$

(See [26] for further discussion.)

Let $\mathscr{E}(\mathbb{R}^m)$ be the family of all real valued measurable functions $f(x_1, \dots, x_m) = f(|x_1|, \dots, |x_m|)$ defined everywhere in $\mathbb{R}^m$ except perhaps on the hyperplanes $x_j = 0$. Let $\mathscr{E}_+(\mathbb{R}^m)$ be those f in $\mathscr{E}(\mathbb{R}^m)$ such that on $(\mathbb{R}^m_+)^\circ$, f is monotone non-decreasing in each x_i when the others are held fixed.

We prove the following preliminary version of a theorem we will use to show that the ground state of Hydrogen has $L_z = 0$ in a homogeneous magnetic field:

Proposition 4.2. *Suppose $V \in \mathscr{E}(\mathbb{R}_\nu)$, continuous on $\mathbb{R}^\nu$, bounded below, C^2 in $(\mathbb{R}^\nu_+)^\circ$ with*

$$\partial^2 V/\partial x_i \partial x_j \leqq 0 \, , \qquad i \neq j \, , \; x \in (\mathbb{R}^\nu_+)^\circ \, . \tag{4.3}$$

Suppose W and $-G$ are in $\mathscr{E}_+(\mathbb{R}^\nu)$ with G bounded and W continuous and bounded below on $\mathbb{R}^m$. For $\varepsilon > 0$ let

$$\begin{aligned} H(V) &= -\Delta + V + \varepsilon |x|^2 \\ H(V+W) &= -\Delta + V + W + \varepsilon |x|^2 \, . \end{aligned} \tag{4.4}$$

Then for any $\beta > 0$

$$\operatorname{tr}(G e^{-\beta H(V+W)}) (\operatorname{tr} e^{-\beta H(V+W)})^{-1} \geqq \operatorname{tr}(G e^{-\beta H(V)}) (\operatorname{tr} e^{-\beta H(V)})^{-1} \, . \tag{4.5}$$

Proof. Equation (4.5) is equivalent to

$$N(V)^{-1} \operatorname{tr}(G e^{-\beta H(V+W)}) \geqq [N(V)^{-1} \operatorname{tr}(G e^{-\beta H(V)})] [N(V)^{-1} \operatorname{tr}(e^{-\beta H(V+W)})] \, ,$$

where $N(V) = \operatorname{tr} e^{-\beta H(V)}$. As usual we make a discrete approximation in the path integral for the trace. This is justified by a probability argument using the continuity of V and W and their boundedness below. We omit the proof. It is thus sufficient to show that for all n

$$\int \exp\left(-\frac{\beta}{n}\sum_{i=1}^{n} W(\mathbf{x}_i)\right) G(\mathbf{x}_1)dv \geqq \int \exp\left(-\frac{\beta}{n}\sum_{i=1}^{n} W(\mathbf{x}_i)\right) dv \int G(\mathbf{x}_1)dv\,, \tag{4.6}$$

where

$$dv(\mathbf{x}_1,\dots,\mathbf{x}_n)=N^{-1}\exp\left\{-\frac{\beta}{n}\left(\sum_{i=1}^{n} V(\mathbf{x}_i)+\varepsilon|x_i|^2\right)-(4\beta)^{-1}n\sum_{i=1}^{n}|\mathbf{x}_i-\mathbf{x}_{i+1}|^2\right\}\prod_{i=1}^{n} d\mathbf{x}_i$$

and $\mathbf{x}_{n+1}=\mathbf{x}_1$. If we write $(\mathbf{x}_i)_\lambda=x_{i\lambda}$, $i=1,\dots,n$; $\lambda=1,\dots,v$ and $x=(x_{11},x_{12},\dots,x_{n1},\dots,x_{nv})$ then

$$dv(x)=N^{-1}F(x)K(|x_{11}|,\dots,|x_{nv}|)\prod g_{j\lambda}(|x_{j\lambda}|)dx_{j\lambda}\,,$$

where

$$F(x)=\exp\left(\sum J_{ij\lambda}x_{i\lambda}x_{j\lambda}\right); \qquad J_{ij\lambda}\geqq 0$$

$$K(x)=\exp\left\{-\frac{\beta}{n}\sum_{i=1}^{n} V(\mathbf{x}_i)\right\}.$$

We convert the integrals in Eq. (4.6) which are over $\mathbb{R}^{nv}$ to integrals over $\mathbb{R}^{nv}_+$ by replacing dv with the measure

$$d\mu(x)=N^{-1}\tilde F(|x_{11}|,\dots,|x_{nv}|)K(x)\prod g_{j\lambda}(|x_{j\lambda}|)dx_{j\lambda}\,,$$

where

$$\tilde F(x)=\sum_{\sigma_{\alpha\gamma}=\pm 1}\exp\sum J_{ij\lambda}x_{i\lambda}x_{j\lambda}\sigma_{i\lambda}\sigma_{j\lambda}\,.$$

Since Eq. (4.3) implies

$$\frac{\partial^2}{\partial x_{i\lambda}\partial x_{j\lambda}}\ln K(x)\geqq 0\,, \qquad x\in(\mathbb{R}^{nv}_+)^\circ,\ (i,\lambda)\neq(j,\gamma)$$

we must only prove the same inequality for $\tilde F$. Let

$$\langle f(\sigma)\rangle=\tilde F(x)^{-1}\sum_{\sigma_{\alpha\gamma}=\pm 1} f(\sigma)\exp\left(\sum J_{ij\lambda}x_{i\lambda}x_{j\lambda}\sigma_{i\lambda}\sigma_{j\lambda}\right).$$

Then

$$\begin{aligned}\frac{\partial^2}{\partial x_{i\lambda}\partial x_{j\lambda}}\ln\tilde F(x)&=\tilde F(x)^{-1}\frac{\partial^2\tilde F(x)}{\partial x_{i\lambda}\partial x_{j\lambda}}-\left(\tilde F(x)^{-1}\frac{\partial\tilde F(x)}{\partial x_{i\lambda}}\right)\left(\tilde F(x)^{-1}\frac{\partial\tilde F(x)}{\partial x_{j\gamma}}\right)\\&=\langle p_1(\sigma)p_2(\sigma)\rangle-\langle p_1(\sigma)\rangle\langle p_2(\sigma)\rangle+\langle p_3(\sigma)\rangle\,,\end{aligned}$$

where the $p_k(\sigma)$ are polynomials of second degree in the $\sigma_{i\lambda}$'s with non-negative coefficients (if $x\in\mathbb{R}^{nv}_+$). Thus by Griffith's first and second inequalities

$$\frac{\partial^2}{\partial x_{i\lambda}\partial x_{j\lambda}}\ln\tilde F(x)\geqq 0\,, \qquad x\in\mathbb{R}^{nv}_+\,.$$

Since $-\exp\left(-\frac{\beta}{n}\{W(x_{11},\dots,x_{1v})+\dots+W(x_{n1},\dots,x_{nv})\}\right)$ and $-G(x_{11},\dots,x_{1v})$ are in $\mathscr{E}_+(\mathbb{R}^{nv})$, the result follows. □

It is not obvious how to prove Proposition 4.2 for singular V and W because a regularization must be found which preserves the inequalities in Eq. (4.3). Thus we present an approximation argument.

The following result will prove useful. Its proof can be found in [49].

Lemma 4.3. *Suppose $\{H_n\}_{n=1}^{\infty}$ is a sequence of self-adjoint operators converging to H in strong resolvent sense. Suppose K is a self-adjoint operator bounded from below such that for each n, $H_n \geqq K$. Then*

a) *if K has compact resolvent, $H_n \to H$ in norm resolvent sense;*

b) *if $e^{-\beta K/2}$ is trace class, then $e^{-\beta H_n}$ converges to $e^{-\beta H}$ in trace norm.*

In the next theorem, when we say that distributional derivatives $\partial^2 V/\partial x_i \partial x_j \leqq 0$ for $x \in (\mathbb{R}^\nu_+)^\circ$ and $i \neq j$ we mean that given any non-negative $\phi \in C_0^\infty((\mathbb{R}^\nu_+)^\circ)$ we have

$$\int (\partial^2 \phi/\partial x_i \partial x_j) V d^\nu x \leqq 0 \qquad i \neq j.$$

V will be in $L^1_{\text{loc}}(\mathbb{R}^\nu)$ so that the above integral makes sense.

Theorem 4.4. *Suppose $V(x) = V(|x_1|, \ldots, |x_\nu|)$, $W(x) = W(|x_1|, \ldots, |x_\nu|)$ and*

a) *V and W can each be written as a sum of two functions f_1 and f_2 with $f_1 \in L^p(\mathbb{R}^\nu)$ with $p=1$ if $\nu=1$, $\infty > p > 1$ if $\nu=2$, $p=\nu/2$ if $\nu \geqq 3$ and f_2 bounded below and in $L^1_{\text{loc}}(\mathbb{R}^\nu)$.*

b) *The distributional derivatives of V satisfy $\dfrac{\partial^2}{\partial x_i \partial x_j} V(x) \leqq 0$, $x \in (\mathbb{R}^\nu_+)^\circ$, $i \neq j$.*

c) *$W \in \mathscr{E}_+(\mathbb{R}^\nu)$.*

Then for any bounded G with $-G$ in $\mathscr{E}_+(\mathbb{R}^\nu)$, Eq. (4.5) *holds.*

Proof. We approximate V and W by functions satisfying the conditions of Proposition (4.2) and then prove convergence of the traces using Lemma 4.3.

Let j be a non-negative C^∞ function in $\mathscr{E}(\mathbb{R}^\nu)$ with $\int j dx = 1$ and supp j in the unit ball. Let $j_\delta(x) = j(x/\delta)$. With $e = (1, 1, \ldots, 1)$ let $\tilde{V}_\varepsilon(x) = V(x + \varepsilon e)$ and

$$\tilde{V}_{\varepsilon,\delta}(x) = j_\delta * \tilde{V}_\varepsilon(x) = \int j_\delta(x + \varepsilon e - y) V(y) dy.$$

If we take $\delta < \varepsilon$ then for $x \in (\mathbb{R}^\nu_+)^\circ$ the function

$$\phi_x(y) = j_\delta(x + \varepsilon e - y) = j_\delta(y - x - \varepsilon e)$$

is in $C_0^\infty((\mathbb{R}^\nu_+)^\circ)$ and thus

$$V_\delta(x) \equiv \tilde{V}_{2\delta,\delta}(|x_1|, \ldots, |x_\nu|)$$

satisfies the conditions of Proposition (4.2). To approximate W we define

$$\tilde{W}_\delta(x) = 2^\nu \int_{y \in \mathbb{R}^\nu_+} j_\delta(y) W(x+y) dy, \qquad W_\delta(x) = W_\delta(|x_1|, \ldots, |x_\nu|).$$

Then W_δ is in $\mathscr{E}_+(\mathbb{R}^\nu)$ and continuous.

We first show that if χ_N is the indicator function of $\{x : |x_i| \leqq N \text{ all } i\}$ where $N \geqq 1$, then

$$\|\chi_N(V - V_\delta)\|_1 + \|\chi_N(W - W_\delta)\|_1 \to 0. \tag{4.7}$$

For V we have (if $\delta<1$)

$$\begin{aligned}\|(V-V_\delta)\chi_N\|_1 &= 2^\nu\|(V-V_\delta)\chi_N\chi_{\mathbb{R}^\nu_+}\|_1\\ &\leqq 2^\nu\|(V-\tilde{V}_\delta)\chi_N\|_1+2^\nu\|(\tilde{V}_\delta-j_{2\delta}*\tilde{V}_\delta)\chi_N\|_1\\ &\leqq 2^\nu\|(V-\tilde{V}_\delta)\chi_N\|_1+2^\nu\|V\chi_{2N}-j_{2\delta}*(V\chi_{2N})\|_1\end{aligned}$$

$\to 0$ as $\delta\downarrow 0$. For W we have

$$\begin{aligned}\|\chi_N(W-W_\delta)\|_1 &\leqq 2^\nu\|\chi_N(W-\tilde{W}_\delta)\|_1\\ &\leqq 4^\nu\int_{y\in\mathbb{R}^\nu_+} j_\delta(y)\|(W\chi_{2N})(\cdot+y)-W\chi_{2N}\|_1 dy\end{aligned}$$

$\to 0$ as $\delta\downarrow 0$ because of the continuity of translations on L^1.

We will show that $e^{-tH(V_\delta)}\xrightarrow{s} e^{-tH(V)}$ which implies the strong resolvent convergence of $H(V_\delta)$ to $H(V)$. $V_\delta+W_\delta$ is handled similarly. We then apply Lemma 4.3 to get convergence of the relevant traces. We use the Feynman-Kac formula and break up V into V_1 and V_2 and correspondingly write $V_\delta=(V_1)_\delta+(V_2)_\delta$. Thus

$$\begin{aligned}&|(\phi,[e^{-tH(V_\delta)}-e^{-tH(V_1+(V_2)_\delta)}]\psi)|^2\\ &\leqq \Big|\int dx\bar{\phi}(x)\int d\mu_x(\omega)\left[e^{-\int_0^t (V_1)_\delta(\omega(s))ds}-e^{-\int_0^t V_1(\omega(s))ds}\right]\\ &\quad\cdot e^{-\int_0^t[(V_2)_\delta(\omega(s))+\varepsilon|\omega(s)|^2]ds}\psi(\omega(t))\Big|^2 \qquad (4.8)\\ &\leqq (|\phi|,[e^{-t(-\Delta+(2V_1)_\delta)}+e^{-t(-\Delta+2V_1)}-2e^{-t(-\Delta+V_1+(V_1)_\delta)}]|\psi|)\\ &\quad\cdot(|\phi|,|\psi|)e^{\alpha t}. \qquad (4.9)\end{aligned}$$

Here $d\mu_x(\omega)$ is Wiener measure on paths ω with $\omega(0)=x$ and we have used the Schwarz innequality to get from (4.8) to (4.9) coupled with $(V_2)_\delta\geqq-\alpha$. Thus taking the sup over ϕ's with $\|\phi\|=1$ we have

$$\begin{aligned}&\|(e^{-tH(V_\delta)}-e^{-tH(V_1+(V_2)_\delta)})\psi\|^2\\ &\leqq e^{\alpha t}\|\psi\|\,\|(e^{-t(-\Delta+2(V_1)_\delta)}+e^{-t(-\Delta+2V_1)}-2e^{-t(-\Delta+V_1+(V_1)_\delta)})|\psi|\,\|. \qquad (4.10)\end{aligned}$$

By arguments identical to those used to prove (4.7) we have $\|(V_1)_\delta-V_1\|_p\to 0$ and this gives, by standard arguments, the norm resolvent convergence of $-\Delta+2(V_1)_\delta$ and $-\Delta+V_1+(V_1)_\delta$ to $-\Delta+2V_1$. Thus $e^{-tH(V_\delta)}-e^{-tH(V_1+(V_2)_\delta)}\to 0$ in norm.

In treating the quantity $(\phi,(e^{-tH(V_1+(V_2)_\delta)}-e^{-tH(V)})\psi)$ we again use the Schwartz inequality and find

$$\begin{aligned}&\|(e^{-tH(V_1+(V_2)_\delta)}-e^{-tH(V)})\psi\|^2\\ &\leqq\|e^{-t(-\Delta+2V_1)}|\psi|\,\|\,\|(e^{-tH(2(V_2)_\delta)}+e^{-tH(2V_2)}-2e^{-tH(V_2+(V_2)_\delta)})|\psi|\,\|. \qquad (4.11)\end{aligned}$$

As proved in [50], if $U_n\geqq 0$, $U\geqq 0$ and $U_n\to U$ in L^1_{loc}, then $-\Delta+U_n\to-\Delta+U$ in the strong resolvent sense. Thus $e^{-tH(V_1+(V_2)_\delta)}\xrightarrow{s} e^{-tH(V)}$ and hence $e^{-tH(V_\delta)}\xrightarrow{s} e^{-tH(V)}$. This implies $H(V_\delta)\to H(V)$ in the strong resolvent sense. To apply Lemma 4.3 note that

$$\begin{aligned} H(V_\delta) &\geqq -\Delta + (V_1)_\delta + \varepsilon|x|^2 - \alpha \\ &= -\tfrac{1}{2}\Delta + (V_1)_\delta - \tfrac{1}{2}\Delta + \varepsilon|x|^2 - \alpha \\ &\geqq -\tfrac{1}{2}\Delta + \varepsilon|x|^2 - \text{const} \equiv K . \quad \square \end{aligned}$$

Theorem 4.4 is not quite suitable for our purposes because of the $m^2\varrho^{-2}$ term in Eq. (3.1) which has the property that $\partial^2\varrho^{-2}/\partial x_1\partial x_2 = 8\varrho^{-6}x_1x_2 \geqq 0$ in $\mathbb{R}^3_+$, where $\varrho = \sqrt{x_1^2 + x_2}$. There are two ways out of this difficulty. The first (sketched by one of us at Oberwolfach in 1977) uses the fact that if $V = V(\varrho, |z|)$ we really have a two-variable problem and only the derivatives $\frac{\partial^2}{\partial\varrho\partial z}$ should enter. In fact after a suitable (unitary) coordinate change the operator $(-i\nabla - \frac{1}{2}B_0(\hat{z} \times r))^2 + V(\varrho, |z|)$ restricted to $L_z = m$ can be written (after subtracting a constant)

$$-\frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial \varrho^2} + (m^2 - \tfrac{1}{4})\varrho^{-2} + \tfrac{1}{4}B_0^2\varrho^2 + V(\varrho, |z|),$$

where $-\partial^2/\partial\varrho^2$ has Dirichlet boundary conditions at 0 (for $|m| > 0$) and we work in the half-space $\varrho \geqq 0$, $z \in \mathbb{R}$.

We will instead prove a new result. We restrict ourselves to $\mathbb{R}^3$ and for the purposes of the following theorem use the notations: $\varrho = \varrho(x) = \sqrt{x_1^2 + x_2^2}$, $\boldsymbol{\varrho} = (x_1, x_2, 0)$, $\Omega = \{x \in \mathbb{R}^3 : \varrho > 0, x_3 > 0\}$, $\tilde{\mathscr{E}}$ = set of all almost everywhere defined functions f with f real, measurable and only a function of ϱ and $|x_3|$. We define $\tilde{\mathscr{E}}_+$ = set of all f in $\tilde{\mathscr{E}}$ such that for $x \in \Omega$, $f(x)$ is monotone non-decreasing in each of the variables ϱ and x_3 for the other held fixed.

For a function $f \in L^1_{\text{loc}}(\mathbb{R}^3)$ we say that the distributional derivatives $\frac{\partial^2 f(x)}{\partial\varrho\partial x_3} \leqq 0$ for $x \in \Omega$ if for every non-negative $\phi \in C_0^\infty(\Omega)$ we have

$$\int \left[\frac{\partial}{\partial x_3} \nabla \cdot (\boldsymbol{\varrho}\phi)\right] f d^3x \leqq 0 .$$

Note that a formal integration by parts gives

$$\int \left[\frac{\partial}{\partial x_3} \nabla \cdot (\boldsymbol{\varrho}\phi)\right] f d^3x = \int \phi(\boldsymbol{\varrho} \cdot \nabla) \frac{\partial f}{\partial x_3} d^3x \quad \text{and that} \quad \boldsymbol{\varrho} \cdot \nabla = \varrho \frac{\partial}{\partial \varrho} .$$

Theorem 4.5. *Suppose V and W are in $\tilde{\mathscr{E}}$ and*

a) *V and W can each be written as a sum of functions f_1 and f_2 with $f_1 \in L^{3/2}(\mathbb{R}^3)$ and f_2 bounded below and in $L^1_{\text{loc}}(\mathbb{R}^3)$.*

b) *The distributional derivatives of V satisfy*

$$\frac{\partial^2 V(x)}{\partial\varrho\partial x_3} \leqq 0 \quad \text{for} \quad x \in \Omega .$$

c) *$W \in \tilde{\mathscr{E}}_+$.*

Then for any bounded G with $-G$ in $\tilde{\mathscr{E}}_+$, Eq. (4.5) holds.

We begin the proof of Theoem 4.5 by first proving the analog of Proposition 4.2. We thus assume that V and W are continuous and bounded below and V is C^2 in Ω. We must prove Eq. (4.6). We write $\mathbf{x}_i=(\varrho_i\cos\theta_i, \varrho_i\sin\theta_i, z_i)$ and convert (4.6) from an integral over $\mathbb{R}^{3n}$ to an integral over $(\mathbb{R}^2_+)^n$ by replacing dv with the measure [on $(\mathbb{R}^2_+)^n$]

$$d\mu(\varrho_1, z_1, \ldots, \varrho_n, z_n)=N^{-1}K_1K_2\prod_i (d\varrho_i dz_i f_i(\varrho_i)g_i(z_i)),$$

where

$$K_1=\exp\left(-\frac{\beta}{n}\sum_i V(\mathbf{x}_i)\right)$$

and

$$K_2(\varrho_1, z_1, \ldots, \varrho_n, z_n)=\sum_{\sigma_i=\pm 1}\left[\int_0^{2\pi}\prod_i d\theta_i\right] \cdot\exp\left(\sum_{i<j} J_{ij}(\varrho_i\varrho_j\cos(\theta_i-\theta_j)+z_iz_j\sigma_i\sigma_j)\right).$$

By assumption $\partial^2\ln K_1/\partial\varrho_i\partial z_i \geqq 0$ in $(\mathbb{R}^{2n}_+)^\circ$ with $\partial^2\ln K_1/\partial\varrho_i\partial\varrho_j=\partial^2\ln K_1/\partial z_i\partial z_j =\partial^2\ln K_1/\partial z_i\partial\varrho_j=0$. It suffices to prove that the mixed second partial derivatives of $\ln K_2$ are non-negative. By symmetry, the $\partial^2/\partial\varrho_i\partial z_j$ derivatives are zero while

$$\partial^2\ln K_2/\partial\varrho_i\partial\varrho_j=J_{ij}\langle\cos(\theta_i-\theta_j)\rangle+\sum_{k,\ell} J_{ik}J_{j\ell}\varrho_k\varrho_\ell A(i,k;j,\ell),$$

where

$$A(i,k;j,\ell)=\langle\cos(\theta_i-\theta_k)\cos(\theta_j-\theta_\ell)\rangle-\langle\cos(\theta_i-\theta_k)\rangle\langle\cos(\theta_j-\theta_\ell)\rangle$$

and $\langle\cdot\rangle=N^{-1}\int\cdot\exp\left(\sum_{i<j} J_{ij}\varrho_i\varrho_j\cos(\theta_i-\theta_j)\right)\prod_i d\theta_i$. Since the $J_{ij}=J_{ji}\geqq 0$, by the GKS inequalities for plane rotors (proved by Ginibre [18]), $A(i,k;j,\ell)\geqq 0$ and $\langle\cos(\theta_i-\theta_j)\rangle\geqq 0$. Thus $\partial^2\ln K_2/\partial\varrho_i\partial\varrho_j\geqq 0$. The proof that $\partial^2\ln K_2/\partial z_i\partial z_j\geqq 0$ in $\mathbb{R}^{2n}_+$ is as in the proof of Proposition 4.2.

We now proceed to approximate V and W by smooth functions. Let $V(x)=\tilde{V}(\varrho, x_3)$, $W(x)=\tilde{W}(\varrho, x_3)$. Choose $j\geqq 0$ in $C_0^\infty(\mathbb{R})$ such that $\operatorname{supp} j\subsetneqq(-1,1)$ and $\int j(x)dx=1$. Set $j_\delta(x)=j(x/\delta)$. For $0<\delta<\varepsilon$ let

$$\tilde{V}_{\varepsilon,\delta}(x)=\int j_\delta(\lambda)j_\delta(x_3-y_3)\tilde{V}((\varrho+\varepsilon)e^\lambda, y_3+\varepsilon)d\lambda \tag{4.12}$$

and define $V_{\varepsilon,\delta}(x)=\tilde{V}_{\varepsilon,\delta}(x_1,x_2,|x_3|)$, $V_\delta(x)=V_{2\delta,\delta}(x)$.

We define $\tilde{W}_{\varepsilon,\delta}(x)$ in the same way:

$$\tilde{W}_{\varepsilon,\delta}(x)=\int j_\delta(\lambda)j_\delta(a)\tilde{W}((\varrho+\varepsilon)e^\lambda, x_3-a+\varepsilon)d\lambda da \tag{4.13}$$

and $W_\delta(x)=\tilde{W}_{2\delta,\delta}(x_1,x_2\,|x_3|)$.

If $V=V_1+V_2$ with $V_1\in L^{3/2}(\mathbb{R}^3)$, $V_2\in L^1_{\text{loc}}(\mathbb{R}^3)$ and bounded below, we define $(V_1)_\delta$ and $(V_2)_\delta$ as above. Similarly for W. It is easy to check that

$$\|(V_1)_\delta-V_1\|_{3/2}+\|(W_1)_\delta-W_1\|_{3/2}\to 0$$

and that $(V_2)_\delta\to V_2$, $(W_2)_\delta\to W_2$ in $L^1_{\text{loc}}(\mathbb{R}^3)$ with $(V_2)_\delta\geqq-\text{const}$, $(W_2)_\delta\geqq-\text{const}$. In addition, V_δ and W_δ are continuous with $V_\delta\in C^2(\Omega)$. From (4.13) it is clear that

$W_\delta \in \tilde{\mathscr{E}}_+$. To see more clearly the structure of V_δ we make a change of variable and rewrite (4.12):

$$\tilde{V}_{\varepsilon,\delta}(x) = \int j_\delta(\ln(\xi/\varrho+\varepsilon)) j_\delta(x_3+\varepsilon-y_3)\tilde{V}(\xi, y_3)\frac{d\xi}{\xi}dy_3 \tag{4.14}$$

from which the smoothness of V_δ is clear. Introducing the function

$$\tilde{\phi}_x(\xi, y_3) = \xi^{-2} j_\delta(\ln(\xi/\varrho+\varepsilon)) j_\delta(x_3-y_3+\varepsilon)(2\pi)^{-1}$$

we see that

$$\tilde{V}_{\varepsilon,\delta}(x) = \int \phi_x(y)V(y)d^3y,$$

where $\phi_x(y) = \tilde{\phi}_x(\xi, y_3)$ with the identification $\xi = (y_1^2+y_2^2)^{1/2}$. For each $x \in \Omega$, $\phi_x \in C_0^\infty(\Omega)$ (if $\delta < \varepsilon$) and a bit of algebra shows that

$$\partial^2 \tilde{V}_{\varepsilon,\delta}(x)/\partial\varrho\partial x_3 = (\varrho+\varepsilon)^{-1}\int V(y)\frac{\partial}{\partial y_3}\nabla_y \cdot (\boldsymbol{\varrho}(y)\phi_x(y))d^3y$$

so that for $x \in \Omega$, $\partial^2 V_\delta(x)/\partial\varrho\partial x_3 \leqq 0$.

Thus using the convergence argument given in the proof of Theorem 4.4, Theoem 4.5 follows. □

We now get back to Hydrogen-like atoms in constant field. All potentials V which occur in our discussion will be assumed to obey the regularity property a) of Theorem 4.5. We also write $V(x) = V(\varrho, |z|)$ for a function in $\tilde{\mathscr{E}}$.

Theorem 4.6. *Let $V(\varrho, |z|) \in \tilde{\mathscr{E}}_+$. Let a be given by Eq. (1.1) and let E_m be the ground state energy of $(-i\nabla - a)^2 + V(\varrho, |z|)$ restricted to $L_z = m$. Then*

$$E_0 \leqq E_1 \leqq \ldots \leqq E_m \leqq \ldots, \tag{4.15}$$

If either $V(\varrho, |z|) < 0 = \lim V(\varrho, |z|)$ or $V(\varrho, |z|) \to \infty$ at infinity, then the inequalities in (4.15) are strict. In particular, for hydrogen, $L_z = 0$ in the ground state.

Remarks. 1) If $(-i\nabla - a)^2 + V(\varrho, |z|)$ has no ground state when restricted to $L_z = m$, E_m is by definition the lowest point in the spectrum.

2) If $V < 0 = \lim_{x \to \infty} V(\varrho, |z|)$ it follows from [9] that E_m is an eigenvalue. If $V \to \infty$ at infinity the spectrum of $((-i\nabla - a)^2 + V(\varrho, |z|)) \upharpoonright (L_z = m)$ is discrete.

Proof. By a monotone convergence argument Eq. (4.5) holds when V in Eq. (4.4) is replaced with $m^2/\varrho^2 + B_0^2\varrho^2/4 - mB_0$ and W is replaced with V. [One needs to cutoff the $1/\varrho^2$ term since it is not in $L^1_{\text{loc}}(\mathbb{R}^3)$.] We then (again by a monotone convergence argument) replace $\varepsilon|x|^2$ with εz^2. We next take the limit $\beta \to \infty$ and find

$$\langle G \rangle_V \geqq \langle G \rangle_{V=0}, \tag{4.16}$$

where $\langle \cdot \rangle_{\lambda V}$ is expectation in the ground state of

$$-\Delta + B_0^2\varrho^2/4 + m^2/\varrho^2 + \lambda V - mB_0 + \varepsilon z^2$$

and G is a bounded function with $-G$ in $\tilde{\mathscr{E}}_+$. By Eq. (3.2). to prove Eq. (4.15) we need only show that

$$\langle \varrho^{-2}\rangle_V \geqq \langle \varrho^{-2}\rangle_{V=0}$$

and this follows from (4.16) by first cutting off ϱ^{-2}.

To get strict inequality, we argue as follows. If $V\to\infty$, E_m is certainly discrete and if $V<0$, then by [9], $E_m < \inf\sigma_{\text{ess}}(H)$ for all m so E_m is discrete. Thus, in either case, E_m is analytic in m for m in $(0,\infty)$. Thus, if $E_m = E_{m-1}$, since $dE_m/dm \geqq 0$, we conclude that E_m is constant. This violates the fact that $\lim_{m\to\infty} E_m = \infty$ if $V\to\infty$ and $\lim_{m\to\infty} E_m = \inf\sigma_{\text{ess}}(H)$ if $V \leqq 0$. □

The above argument compares $V=0$ and V rather than looking at the derivative with respect to λ for $\langle\cdot\rangle_{\lambda V}$. To look at this derivative, we only need that V obey the hypotheses of Theorem 4.5.

Theorem 4.7. *Let $E_m(\lambda)$ denote the ground state energy of* (3.1) *with V replaced by λV. Suppose that*

$$\partial^2 V(\varrho,|z|)/\partial\varrho\partial|z| \leqq 0, \quad \textit{all} \quad \varrho, |z|. \tag{4.17}$$

Then $E_m(\lambda) - E_{m-1}(\lambda)$ increases as λ does.

To apply this, it is useful to note that

Lemma 4.8. *If V is a function, f, of $r=(\varrho^2+z^2)^{1/2}$ and f is monotone in r and concave* ($f'\geqq 0, f''\leqq 0$), *then* (4.17) *holds. In particular,* (4.17) *holds for* $V(\varrho,|z|) = -r^{-1}$.

Proof. A straightforward differentiation. □

Given the scaling relation, (2.22).

Corollary 4.9. *For hydrogen, $B^{-1}[E_m(B)-E_{m-1}(B)]$ decreases as B increases.*

Let $E(B) = \min_m E_m(B)$ be the ground state energy. Let

$$e(B) = |B| - E(B)$$

be the binding energy. In [9], we gave Lieb's proof of his result that

$$e(B) \geqq e(B=0)$$

(to be contrasted with $E(B) \geqq E(B=0)$, [44]) for arbitrary potentials. Here we strengthen this for monotone potentials:

Theorem 4.10. *If $V(\varrho,|z|)$ is monotone increasing, then $e(B)$ is increasing in $|B|$.*

Proof. By Theorem 4.6, $e(B) = B - E_{m=0}(B)$. Thus

$$\frac{de}{dB} = -2B\langle\varrho^2\rangle_V + 1$$

in the region $B \geqq 0$. As, in the proof of Theorem 4.6,

$$\langle\varrho^2\rangle_V \leqq \langle\varrho^2\rangle_{V=0}$$

so

$$\frac{de}{dB}(V) \geqq \frac{de}{dB}(V=0)=0. \quad \square$$

5. Borel Summability

Our goal in this section is to prove:

Theorem 5.1. *Let E be an eigenvalue of $-\Delta - |r|^{-1}$ which is non-degenerate on a subspace of fixed $L_z = m$. Let $E(B)$ be the energy level of $(-i\nabla - \frac{1}{2}B \times r)^2 - |r|^{-1}$ near E for B small and real. Then for each $\delta > 0$, there is an $R_\delta > 0$ so that*

(1) *$E(B)$ has an analytic continuation to $\{B | 0 < |B| < R_\delta ; |\arg B| < \pi - \delta\} \equiv D_\delta$.*

(2) *Let a_{2n} be the Rayleigh-Schrödinger coefficients for $E(B)$. Then for some A and all n:*

$$\left| E(B) + mB - \sum_{k=0}^{n} a_{2k} B^{2k} \right| \leqq (2n+2)! \, |B|^{2n+2} A^{n+1} \tag{5.1}$$

for all $B \in D_\delta$.

Remarks. 1) It is proven in [9, Sect. 6] that there is a unique eigenvalue $E(B)$ of $H(B)$ near E for B small and real.

2) This result is also true so long as any degeneracies are removed to order B^2 (and this is presumably true for *all* levels in hydrogen). Since this proof in quite a bit more complicated and its analog in the Strak problem is described elsewhere [23], we restrict ourselves to the non-degenerate case.

3) If $|r|^{-1}$ is replaced by $V(|r|)$, the result holds true so long as V is dilation analytic in $\mathscr{F}_{\pi/2}$. If $V \in \mathscr{F}_\alpha$, the result is true with $\pi - \delta$ replaced by $\frac{\pi}{2} + \alpha - \delta$.

4) We will see shortly that this result cannot hold [both analyticity and the bound (5.1)] in a (multivalued) sector of opening angle more than π.

The importance of (5.1) comes from Watson's theorem [37, 41] which, given the fact that $E(B) + mB$ has perturbation series in B^2, implies:

Theorem 5.2. *Under the hypotheses of Theorem 5.1, the Borel transform $f(B) = \sum_{n=0}^{\infty} \frac{a_{2n}}{(2n)!} B^{2n}$ is analytic in the whole plane with two cuts (iB_0, ∞) and $(-\infty, -iB_0)$ removed. Moreover, for B small and real*

$$E(B) = -mB + \int_0^\infty f(xB) e^{-x} dx .$$

Remarks. 1) The analytic structure is somewhat reminiscent of that in the Stark problem; see [23].

2) If the sector in Theorem 5.1 were $\pi + \varepsilon$, then $f(B)$ would be entire. In fact, there is considerable evidence, both numerical and (non-rigorous) theoretical that the nearest singularity is on the imaginary axis with $B_0 = \pi/4$; see [5, 6].

Proof of Theorem 5.1. The necessary stability part of the proof is already contained in [9, Sect. 6] which we use freely. $\tilde{E}(B) \equiv E(B) - mB$ is an eigenvalue of the operator

$$\tilde{H}(B) = -\Delta - |r|^{-1} + \tfrac{1}{4}B^2\varrho^2. \tag{5.2}$$

Direct use of Theorem 6.2 on $\tilde{H}(B)$ implies analyticity in opening angle $\frac{\pi}{2} - \delta$. We use the idea [42] of scaling some of the argument of B onto $|r|^{-1}$. We therefore consider the operator

$$\tilde{H}_\omega(B) = -e^{-2i\omega}\Delta - e^{-i\omega}|r|^{-1} + \tfrac{1}{4}e^{2i\omega}B^2\varrho^2.$$

Let $B = |B|e^{i\phi}$ and take $0 < \omega$. We would like to know when $E(B)$ is an eigenvalue of $\tilde{H}_\omega(B)$. We want to be sure that the point $E < 0$ stays out of the sector formed by the lines $\{e^{-2i\omega}p^2 | p^2 \geqq 0\}$ and $\{e^{2i\omega}B^2\varrho^2 | \varrho^2 \geqq 0\}$. To keep the first line away from E, we need

$$0 < \omega < \frac{\pi}{2}.$$

The second line must stay away from the negative axis and in the positive direction cannot swing past the opposite direction to the first line, so:

$$-\pi < 2\omega + 2\phi < \pi - 2\omega.$$

By varying ω, we see that one can have

$$-\pi < \phi < \frac{\pi}{2}.$$

By also taking $\omega < 0$ we can get

$$-\pi < \phi < \pi$$

and thus in the standard way (independence of eigenvalue on ω) [42, 1], $E(B)$ is analytic in D_δ by the stabilty result, Theorem 6.2 of [9].

We describe how to get the bound (5.1) in the region $|\arg B| < \frac{\pi}{2} - \delta$. By using $\tilde{H}_\omega$, we can get (5.1) in any R_δ. There is a standard way of proving bounds of the type (5.1) (see [37], Sect. XI.4): it reduces the bound to proving that

$$\|(H_0 + B^2W - \lambda)^{-1}[W(H_0 - \lambda)^{-1}]^n\Omega\| \leqq C^{2n+1}(2n)! \tag{5.3}$$

for small B and λ with $|\lambda - E| = \varepsilon$. Here $W = \varrho^2/4$, $H_0 = -\Delta - r^{-1}$ and Ω is the vector with $H_0\Omega = E\Omega$. By the stability result, $(H_0 + B^2W - \lambda)^{-1}$ is bounded in the region in question. Now write

$$\|[W(H_0 - \lambda)^{-1}]^n\Omega\| \leqq \prod_{j=1}^{n} [\|We^{-\delta|r|/n}\| \, \|e^{i\delta|r|/n}(H_0 - \lambda)^{-1}e^{-j\delta|r|/n}\| \, \|e^{\delta|r|}\Omega\|$$

and notice that $\|e^{\alpha|r|}(H_0 - \lambda)^{-1}e^{-\alpha|r|}\|$ is uniformly bounded for $|\alpha| \leqq \delta$ by results of Combes and Thomas [15] and that by results of the same authors $\|e^{\delta|r|}\Omega\| < \infty$. Obviously, $\|We^{-\delta|r|/n}\| \leqq C_0 n^2$ so the left side of (5.3) is bounded by $D^{2n+1}n^{2n}$.

We make a remark on the proof of stability needed above when $\tilde{H}(B)$ is replaced by $\tilde{H}_\omega(B)$: Let $\tilde{H}_{\omega,0}(B) = \tilde{H}_\omega(B) + e^{-i\omega}|r|^{-1}$. Then following [9] one only needs to show that as $B \to 0$

$$|r|^{-1}(z-\tilde{H}_{\omega,0}(B))^{-1} \xrightarrow{\|\cdot\|} |r|^{-1}(z-\tilde{H}_{\omega,0}(0))^{-1} \tag{5.4}$$

uniformly in z for z near E. By a quadratic estimate one can show that $(-\Delta+1)(z-\tilde{H}_{\omega,0}(B)^{-1}$ is uniformly bounded for z in this region as $B \to 0$ so we need only prove (5.4) when $|r|^{-1}$ is replaced by $\phi(x)$ with $\phi \in C_0^\infty(\mathbb{R}^3)$. Now

$$\phi[(z-\tilde{H}_{\omega,0}(B))^{-1}-(z-\tilde{H}_{\omega,0}(0))^{-1}] = \tfrac{1}{4}B^2 e^{2i\omega}\phi(z-\tilde{H}_{\omega,0}(0))^{-1}\varrho^2(z-\tilde{H}_{\omega,0}(B))^{-1}.$$

Thus we need only show

$$\phi(x)(z-\tilde{H}_{\omega,0}(0))^{-1}\varrho^2$$

is a bounded operator. But the x-space kernel of this operator is bounded by

$$|\phi(x)|\frac{e^{-\gamma|x-y|}}{|x-y|}|y|^2,$$

where $\gamma > 0$. Using $|y|^2 \leqq 2(|x|^2+|x-y|^2)$ the result follows. □

Part B: Multielectron Atoms

6. Dilation Analyticity

In this section, we discuss dilation analyticity for systems of electrons interacting with an infinitely heavy nucleus. In particular, we will show that the Hamiltonian for such a system has empty singular continuous spectrum. We begin by mentioning what is true in the one electron case, correcting an error in [9].

Let **B** point in the z-direction. Then the scaled Hamiltonian is, for θ real.

$$U(\theta)HU(\theta)^{-1} = -e^{-2\theta}\Delta + e^{2\theta}\frac{B^2}{4}\varrho^2 + V(e^\theta r) - BL_z. \tag{6.1}$$

In [9], we showed that for L_z-*fixed* and V axially symmetric and dilation analytic, this operator could be reasonably defined for $|\mathrm{Im}\,\theta| < \frac{\pi}{4}$ and its essential spectrum is for $L_z = m$:

$$\bigcup_{n=\max(0,-m)}^{\infty} \{(2n+1)B_0 + e^{-2\theta}\lambda \mid \lambda \in [0,\infty)\}. \tag{6.2}$$

In the usual way [1] this implies that $\sigma_{\mathrm{s.c.}}(H)$, the singular continuous spectrum, is empty and on each fixed L_z-subspace, the only accumulation points of the point spectrum of H could be $\{(2n+1)B_0\}$.

The error in Theorem 4.7 of [9] involved two connected mistatements. First, we stated something about the spectrum of $U(\theta)HU(\theta)^{-1}$ without the restriction $L_z = m$. Of course, $(H(\theta)-z)^{-1} = \bigoplus_{m=-\infty}^{\infty}([H(\theta)\restriction(L_z=m)]-z)^{-1}$ formally but unless one has a bound on $\|([H(\theta)\restriction(L_z=m)]-z)^{-1}\|$ uniform in m, one does not know that $z \notin \sigma(H(\theta))$ just because, $z \notin \sigma(H(\theta)\restriction(L_z=m))$ for all m. Indeed, it might be false that the spectrum of $H(\theta)$ is just $\bigcup_m \sigma(H(\theta)\restriction(L_z=m))$; for example, it is not hard to see that the numerical range of $H(\theta)$ is all of $\mathbb{C}$ if $\mathrm{Im}\,\theta \neq 0$. Secondly, we stated something about accumulation points of the point spectrum of $H(\theta)$ when all we can safely discuss is accumulation points of the point spectrum of $H(\theta)\upharpoonright(L_z=m)$. We can talk about $\sigma_{\text{s.c.}}(H)$, since for self-adjoint $H, \sigma_{\text{s.c.}}(H)=\bigcup_m \sigma_{\text{s.c.}}(H\upharpoonright(L_z=m))$.

With the above in mind, we will discuss dilation analyticity for atoms in magnetic fields by restricting to $L_z=m$ subspaces. For this to work, it will be important that the linear term in B multiply the *total* L_z and thus that the charge/mass ratio of all the finite mass particles be identical. For neutral systems with all masses finite and center of mass motion removed it might well be possible to discuss dilation analyticity on the whole space without restricting to $(L_z=m)$ and thus without any restrictions on charge/mass ratios.

Theorem 6.1. *Let $V_{ij}(r)$ $(0\leqq i<j\leqq n)$ be potentials on $\mathbb{R}^3$ which are azimuthally symmetric and dilation analytic in the usual operator theory sense* [1, 37], *say $V_{ij}(\theta)(-\Delta+1)^{-1}$ compact for all $|\operatorname{Im}\theta|<\theta_0$. Let*

$$H(\theta)=\sum_{j=1}^{n}(-ie^{-\theta}V_j-\tfrac{1}{2}B(\hat{z}\times e^{\theta}r_j))^2+\sum_{1\leqq i\leqq j\leqq n}V_{ij}(e^{\theta}(r_i-r_j))+\sum_{r\leqq i\leqq n}V_{0i}(e^{\theta}r_1). \quad (6.3)$$

Fix $L_z=m$. Then, there is a countable closed set, Σ_m, so that for $|\operatorname{Im}\theta|<\operatorname{Min}\{\pi/4,\theta_0\}$

$$\sigma_{\text{ess}}(H(\theta)\upharpoonright(L_z=m))\subsetneqq\{x+e^{-2\theta}\lambda|x\in\Sigma_m,\lambda\in[0,\infty)\}.$$

In particular,

(a) *The closure of the point spectrum of $H(\theta=0)\upharpoonright(L_z=m)$ is countable.*

(b) *$H(\theta=0)$ has empty singular continuous spectrum.*

Proof. Clearly, on the subspace with $L_z=m$:

$$H(\theta)=\tilde{H}(\theta)-mB$$

with

$$\tilde{H}(\theta)=\sum_{j=1}^{n}[(-e^{-2\theta}\Delta_i)+\tfrac{1}{4}e^{2\theta}B^2\varrho_i^2]+\sum_{i<j}V_{ij}(\theta).$$

We will find a countably closed set Σ so that

$$\sigma_{\text{ess}}(\tilde{H}(\theta))=\{x+e^{-2\theta}\lambda|x\in\Sigma,\lambda\in[0,\infty)\} \quad (6.4)$$

(no restriction to $L_z=m$) from which the results follow.

Let $D=\{C_1,\dots,C_k\}$ be a cluster decomposition and let $\tilde{H}_D(\theta)$ be $\tilde{H}(\theta)$ with intercluster potentials dropped. If $\tilde{H}_{C_i}(\theta)$ is the internal Hamiltonian of cluster C_i and $\zeta_1,\dots,\zeta_{k-1}$ are intercluster coordinates, one see that

$$\tilde{H}_D(\theta)=\sum_k \tilde{H}_{C_i}(\theta)+R_D(\theta)$$

$$R_D(\theta)=\sum_{j=1}^{k-1}(-e^{-2\theta}a_j\Delta_{\zeta_j}+e^{2\theta}B^2b_j\varrho_{\zeta_j}^2)$$

with $a_j, b_j>0$. In the usual way [37], using either a Weinberg-van Winter analysis or the Zhislin-Enss method, one sees that

$$\sigma_{\text{ess}}(\tilde{H}(\theta))=\bigcup_D\{x_1+\dots+x_k+\mu|x_i\in\sigma_{\text{disc}}(\tilde{h}_{C_i}(\theta));\mu\in\sigma(R_D(\theta))\},$$

where $\tilde{H}_{C_i}(\theta)=\tilde{h}_{C_i}(\theta)\otimes I$ and $\tilde{h}_{C_i}(\theta)$ acts on the Hilbert space of internal coordinates for cluster C_i. But for suitable positive numbers $\omega_1, \ldots, \omega_{k-1}$

$$\sigma(R_D(\theta))=\left\{\sum_{i=1}^{k-1} (n_i+\tfrac{1}{2})\omega_i+e^{-2\sigma}\lambda \middle| n_i\in\{0,1,\ldots\}, \lambda\in[0,\infty)\right\}$$

so (6.4) holds with

$$\Sigma=\left\{x_1+\ldots+x_k+\sum_{i=1}^{k-1}(n_i+\tfrac{1}{2})\omega_i\right\}.$$

By a standard inductive argument [12], Σ is closed and countable. □

7. Stability and Borel Summability

We begin by extending the stability criterion of [9, Sect. 6] to multiparticle systems.

Theorem 7.1. *Let $\{V_{ij}\}_{0\leqq i\leqq j\leqq n}$ be real valued functions in $L^2+L^\infty_\varepsilon$. Let*

$$H(B)=\sum_{j=1}^{n}(-i\nabla_j-\mathbf{A}_j)^2+\sum_{1\leqq i\leqq j\leqq n}V_{ij}(r_i-r_j)+\sum_{i=1}^{n}V_{0i}(r_i),\tag{7.1}$$

where $\mathbf{A}_j=\frac{1}{2}B\hat{\mathbf{z}}\times\mathbf{r}_j$. Let $E<\Sigma\equiv\inf\sigma_{\mathrm{ess}}(H(0))$ be a discrete eigenvalue of $H(0)$ of multiplicity m. Then for any B sufficiently small, there are precisely m eigenvalues (counting multiplicity) of $H(B)$ near E and they converge to E. More precisely, there is an $\varepsilon_0>0$ and a $B_0>0$ so that for $|B|<B_0$ the spectrum of $H(B)$ inside $|z-E|<\varepsilon_0$ consists of eigenvalues of combined multiplicity m, and these eigenvalues converge to E as $B\to 0$.

Proof. We freely use the machinery of Weinberg-van Winter equations [37]. We claim that

$$\operatorname*{s-lim}_{B\to 0}D(B,z)=D(z),\tag{7.2}$$

$$\lim_{B\to 0}\|I(B,z)-I(z)\|=0\tag{7.3}$$

uniformly for z in compacts of $\mathbb{C}\backslash[\Sigma,\infty)$ with D and I respectively the disconnected and connected operators occurring in the Weinberg equations for $H(B)$ and $H(0)$.

We claim that (7.2) and (7.3) for an n-particle system imply $(z-H(B))^{-1}\xrightarrow{s}(z-H(0))^{-1}$ uniformly on compacts of $\mathbb{C}\backslash[\inf\sigma(H(0)),\infty)$. To see this write

$$(z-H(B))^{-1}=(1-I(B,z))^{-1}D(B,z).\tag{7.4}$$

Choosing a contour Γ in the region $\mathbb{C}\backslash[\inf\sigma(H(0)),\infty)$ such that $1-I(z)$ is invertible on Γ, we know by 7.2 that for sufficiently small B, $D(B,z)$ is analytic inside Γ so

$$\begin{aligned}\int_\Gamma(z-H(B))^{-1}dz&=\int_\Gamma[(z-H(B))^{-1}-D(B,z)]\,dz\\&=\int_\Gamma I(B,z)(1-I(B,z))^{-1}D(B,z)dz\,.\end{aligned}\tag{7.5}$$

Since $I(B,z)\xrightarrow{\|\cdot\|} I(z)$ uniformly for $z\in\Gamma$ we see that

$$\int_\Gamma (z-H(B))^{-1}dz-\int_\Gamma I(z)(1-I(z))^{-1}D(B,z)dz\xrightarrow{\|\cdot\|}0. \tag{7.6}$$

If $K=(\phi,\cdot)\psi$ then integrating over a subset $\tilde\Gamma\subseteqq\Gamma$

$$\int_{\tilde\Gamma} KD(B,z)dz=\int_{\tilde\Gamma}(D^*(B,z)\psi,\cdot)dz\,\psi.$$

But $D(B,z)$ is a sum of resolvents [35] and thus $D(B,z)^*=D(B,\bar z)$ converges strongly to $D(\bar z)$. Hence

$$\int_{\tilde\Gamma} KD(B,z)dz\xrightarrow{\|\cdot\|}\int_{\tilde\Gamma} KD(z)dz.$$

Approximating $I(z)(1-I(z))^{-1}$ by constant finite rank operators locally on Γ we see from (7.6) that

$$\begin{aligned}\int_\Gamma (z-H(B))^{-1}dz&\xrightarrow{\|\cdot\|}\int_\Gamma I(z)(1-I(z))^{-1}D(z)dz\\&=\int_\Gamma(z-H(0))^{-1}dz=0.\end{aligned}\tag{7.7}$$

The projection $(2\pi i)^{-1}\int_\Gamma(z-H(B))^{-1}dz$ has norm 1 or norm 0; thus for sufficiently small B, $H(B)$ has no spectrum inside Γ. Since (7.3) and (7.4) imply strong convergence of $(z-H(B))^{-1}$ to $(z-H(0))^{-1}$ for all but a discrete set inside Γ [the points where $1-I(z)$ is not invertible], our claim follows.

Since we know (7.2) for one-particle systems (Lemma 6.4 of [9]) we can inductively suppose strong convergence of the resolvents of subsystems on $\mathbb{C}\backslash[\Sigma,\infty)$. Because of the tensor product structure of the H_D's, we get strong convergence of their resolvents and so since $D(B,z)$ is a sum of such resolvents [35], (7.2) follows inductively. This also implies a uniform bound on $\|I(B,z)\|$ on compact subsets of $\mathbb{C}\backslash[\Sigma,\infty)$ (for sufficiently small B) and thus by Vitali's theorem it suffices to prove (7.3) in an open subset of this region. Taking $\operatorname{Re}z$ very negative, we can consider (7.3) in the region where the perturbation series converges. It thus suffices to consider individual diagrams and by a limiting argument we may assume $V_{ij}\in C_0^\infty$. We must thus show that for a connected diagram

$$V_{\alpha_1}(z-H_0(B))^{-1}V_{\alpha_2}\dots V_{\alpha_l}(z-H_0(B))^{-1}\xrightarrow{\|\cdot\|}V_{\alpha_1}(z+\Delta)^{-1}\dots(z+\Delta)^{-1}\tag{7.8}$$

with $H_0(B)=\sum_j(\mathbf{p}_j-\mathbf{A}_j)^2$, $\mathbf{p}_j=-i\nabla_j$, and where $\alpha_k=(i_k,j_k)$. By writing the difference of the two sides of (7.8) as a telescoping sum it suffices to show that

$$\|V_{\alpha_1}(z-H_0(B))^{-1}\dots V_{\alpha_j}[(z-H_0(B))^{-1}-(z+\Delta)^{-1}]V_{\alpha_{j+1}}(z+\Delta)^{-1}\dots\|\tag{7.9}$$

converges to zero. But the factor in brackets is

$$-(z-H_0(B))^{-1}\Big(2\sum_j(\mathbf{p}_j-\mathbf{A}_j)\cdot\mathbf{A}_j+\sum_j|\mathbf{A}_j|^2\Big)(z+\Delta)^{-1}.$$

Let $\varrho_{(k)}$ denote the ϱ for $\mathbf{r}_{i_k}-\mathbf{r}_{j_k}$ where $\mathbf{r}_0=\mathbf{0}$. By the connectedness hypothesis

$$\varrho_i=\sum_k a_{ik}\varrho_{(k)}\,.$$

Thus the components of $\mathbf{A}_j$ can be written as linear combinations of the components of the $\varrho_{(k)}$'s with an explicit factor of B out in front. We use the fact that $(z-H_0(B))^{-1}(\mathbf{p}_j-\mathbf{A}_j)$ is bounded and commute the $\varrho_{(k)}$'s past resolvents $(z-H_0(B))^{-1}$ and $(z+\Delta)^{-1}$ until they reach their corresponding V_{α_k}'s. In this way we see that (7.9) is bounded by (const)$|B|$. This proves (7.3). □

Given (7.2) and (7.3) the theorem follows as in [9] by an argument similar to that directly below (7.4): Choosing small contours Γ to the right and left of E, we see that there is an $\varepsilon>0$ so that given any $\delta>0$

$$\{z:\delta\leqq|z-E|\leqq\varepsilon\}\cap\sigma(H(B))=\emptyset$$

if B is sufficiently small. We can and do choose ε so that $1-I(z)$ is invertible on $|z-E|=\varepsilon$. Then as in (7.7)

$$(2\pi i)^{-1}\int_{|z-E|=\varepsilon}(z-H(B))^{-1}dz\xrightarrow{\|\cdot\|}(2\pi i)^{-1}\int_{|z-E|=\varepsilon}(z-H(0))^{-1}dz$$

and this proves stability (and hence our theorem).

We want to make two comments on an extension of Theorem 7.1 which we will make use of in Sect. 9: If instead of considering the operator of Eq. (7.1) as an operator on $L^2(\mathbb{R}^{3n})$ we instead use the Hilbert space $\mathscr{H}$ appropriate to n spin $\frac{1}{2}$ electrons

$$\mathscr{H}=\wedge^n(L^2(\mathbb{R}^3)\otimes\mathbb{C}^2)$$

the theorem still holds. Here $\wedge^n(K)$ is the antisymmetric subspace of the n-fold tensor product of the Hilbert space K. Here we assume $V_{ij}(r)=|r|^{-1}$ and $V_{0i}(r)=-n|r|^{-1}$. The spectrum of $H(B)$ on $\mathscr{H}$ is of course in general different from its spectrum on $L^2(\mathbb{R}^{3n})$ but because $D(B,z)$ and $I(B,z)$ commute with permutations the proof is essentially the same. One can still consider individual diagrams for $\mathrm{Re}\,z$ very negative, because the norm of an operator on $\mathscr{H}$ is no greater than the norm of the same operator restricted to an invariant subspace.

The second extension is the following: On $L^2(\mathbb{R}^{3n})$ we have [44] $\inf\sigma(H(B))\geqq\inf\sigma(H(0))$, however this is in general false on $\mathscr{H}$. If we replace $L^2(\mathbb{R}^{3n})$ in Theorem 7.1 by $\mathscr{H}$ and E of the theorem is $\inf\sigma(H(0))$ then we claim that $\inf\sigma(H(B))$ is among the m eigenvalues of $H(B)$ which are close to E. This follows as in the argument below Eq. (7.4). We know that $H(B)$ is bounded below uniformly in B thus we need only choose Γ to be a large circle in the region $\mathbb{C}\backslash[\inf\sigma(H(0)),\infty)$; for small enough B, $H(B)$ has no spectrum inside Γ.

Given the stability result, the proof of Borel summability is now easy: using the dilation analyticity ideas of the last section and a mild extension of the above argument, we get analyticity in a region identical to that in Sect. 5. The proof of the $n!$ bound uses ideas in the Combes-Thomas method that easily extend to n-body. While the results extend to arbitrary dilation analytic potentials, for simplicity we state it for atoms:

Theorem 7.2. *Let E be a discrete eigenvalue of* (7.1) *for $B=0$ and $V_{ij}(r)=|r|^{-1}$ $(1\leqq i<j\leqq n)$, $V_{0i}(r)=-Z|r|^{-1}$. Suppose that on $L_z=m$, E is simple. Then for B, small*

and positive, the eigenvalue $E(B)$ *of* $H_m(B) \equiv H(B) \upharpoonright L_z = m$ *is analytic in*

$$\bigcup_{\delta>0} \{B \mid |\arg B| < \pi - \delta; 0 < |B| < R_\delta\}.$$

Moreover, the Borel transform of the Rayleigh-Schrödinger series is analytic in $\{z \mid z \notin [iB_0, i\infty)$ *or* $(-i\infty, -iB_0]\}$, *and for* B *small and positive, the Borel sum is precisely* $E(B)$.

8. The Falloff of Eigenfunctions

In this section we want to prove:

Theorem 8.1. *Let* $H_m(B)$ *be the Hamiltonian of* (7.1) *with* $V_{ij} \in L^2 + L_\varepsilon^\infty$. *Let* $\Sigma = \inf \sigma_{\mathrm{ess}}(H_m(B))$ *and let* ψ *with* $L_z\psi = m\psi$ *obey* $H_m(B)\psi = E\psi$ *with* $E < \Sigma$. *Then for any* ε, *there is a* C_ε *with*

$$|\psi(r_1, \ldots, r_n)| \leqq C_\varepsilon \exp\left\{-(1-\varepsilon)\left[\sum_{i=1}^{n} \frac{B_0}{4}\varrho_i^2 + \sqrt{\Sigma - E}\left[\sum_{i=1}^{n} z_i^2\right]^{1/2}\right]\right\}, \tag{8.1}$$

where $r_i = (\varrho_i \cos\theta_i, \varrho_i \sin\theta, z_i)$.

Remarks. 1) See [37] for references on this general subject of falloff; recent papers include [3, 16, 2].

2) The ϱ-dependence in (8.1) is presumably optimal (modulo ε) but the z_i dependence can probably be improved [16, 2].

Lemma 8.2. $\exp((1-\varepsilon)\sqrt{\Sigma - E}\,[\sum z_i^2]^{1/2})\psi \in L^2$.

Proof. A standard application of the Combes-Thomas method [15]. □

Lemma 8.3. *Let* $\tilde{H}(B)$ *be* $H(B)$ *with the* BL_z *term dropped and let* $\tilde{H}_0(B) = \tilde{H}(B) - \sum V_{ij}$. *Then for any* f, $p > 1$ *and* $q = p/p - 1$:

$$|e^{-t\tilde{H}(B)}f| \leqq [e^{-t\tilde{H}_0(B)}|f|]^{1/q}[e^{-t\ \tilde{H}_0(B) + p\Sigma V_{ij}}\ |f|]^{1/p}. \tag{8.2}$$

Proof. $e^{-tH_0(B)}$ generates a path integral which is Brownian in the z-variables and the oscillator process in the ϱ-variables. (8.2) is just Hölder's inequality for the Feynman-Kac formula (see [24, 45, 16]). □

Lemma 8.4. $e^{-t[\tilde{H}_0(B) + p\Sigma V_{ij}]}$ *maps* L^2 *to* L^∞.

Proof. From the Feynman-Kac formula we see that

$$|e^{-t(\tilde{H}_0(B) + \Sigma V_{ij})}\phi| \leqq e^{-t(-\Delta + \Sigma V_{ij})}|\phi|$$
$$\leqq \prod_{i<j} (e^{-t(-\Delta + \ell V_{ij})}|\phi|)^{1/\ell},$$

where the last inequality is Hölder's inequality on path space and ℓ is the number of potentials V_{ij}. Now use

$$e^{-t(-\Delta + \ell V_{ij})} = e^{t\Delta_\perp} \otimes e^{-t(-\Delta_3 + \ell V_{ij})},$$

where $\Delta = \Delta_\perp + \Delta_3$ and Δ_3 is the 3-dimensional Laplacian. Thus the result follows from $e^{-t(-\Delta + V)} : L^2(\mathbb{R}^3) \to L^\infty(\mathbb{R}^3)$ when $V \in L^2 + L_\varepsilon^\infty$. This is a result of Herbst and Sloan [24]. See also [45]. □

Lemma 8.5. *Let f be a function of r_i obeying*

$\exp((1-\varepsilon)\sqrt{\Sigma-E}[\sum z_i^2]^{1/2})f\in L^2$.

Let $\psi_t=e^{-t\tilde{H}_0(B)}f$. Then for large enough t, ψ_t obeys (8.1).

Proof. Let $K(\varrho_i,\varrho_i';\, z_i,\, z_i')$ be the integral kernel of $e^{-t\tilde{H}_0(B)}$. By Mehler's formula ((3.6) of [9]) and the fact that $\lim_{t\to\infty}[\cosh(\omega t)-1]/\sinh(\omega t)=1$ we can choose t so that

$$K(\varrho_i,\varrho_i';z_i,z_i')\leqq C\exp(-(1-\varepsilon)\sum_{i=1}^{n}\frac{B_0^2}{4}(\varrho_i^2+\varrho_i'^2))\exp\left(-a\sum_i(z_i-z_i')^2\right) \quad (8.3)$$

for some $a>0$. Next notice that

$$\exp\left(-a\sum_i(z_i-z_i')^2+(1-\varepsilon)\sqrt{\Sigma-E}\left\{\left[\sum_i z_i^2\right]^{1/2}-\left[\sum_i z_i'^2\right]^{1/2}\right\}\right)$$

is dominated by

$$\text{const}\exp\left(-\frac{a}{2}\sum_i(z_i-z_i')^2\right)$$

so that

$$\begin{aligned}|\psi_t|&\leqq\int d\varrho'dz'K(\varrho,\varrho';z,z')|f|\\ &\leqq C\exp\left\{-(1-\varepsilon)B_0^2\varrho^2/4-(1-\varepsilon)\sqrt{\Sigma-E}\left(\sum_i z_i^2\right)^{1/2}\right\}\\ &\quad\cdot\int d\varrho'dz'\exp\left(-\frac{a}{2}\sum_i(z_i-z_i')^2-(1-\varepsilon)\frac{B_0^2}{4}\varrho'^2\right)\\ &\quad\cdot[\exp(1-\varepsilon)\sqrt{\Sigma-E}(\textstyle\sum z_i'^2)^{1/2}]|f|\end{aligned}$$

and thus by the Schwarz inequality we immediately conclude (8.1). □

Proof of Theorem 8.1. We have $e^{-t\tilde{H}(B)}\psi=e^{-t\alpha}\psi$ so that by Lemma 8.3

$$|\psi|\leqq e^{t\alpha}[e^{-t\tilde{H}_0(B)}|\psi|]^{1/q}[e^{-t[H_0(B)+p\Sigma V_{ij}]}|\phi|]^{1/p}.$$

By Lemma 8.4

$$|\psi|\leqq c(t,q)[e^{-t\tilde{H}_0(B)}|\psi|]^{1/q}$$

which by Lemmas 8.2 and 8.5 gives Eq. (8.1) for large enough t, since q can be taken arbitrarily close to 1. □

9. Negative Ions

Many atoms do not have stable negative ions. For example, of the 72 elements listed in [25], 18, including all the noble gases are in this class [and it is claimed that most of those not listed (rare earths) probably have no stable negative ions]. Moreover, it is a rigorous theorem [46,4] that the purely Coulombic Hamiltonian for negative ions has at most a finite number of bound states. It is thus somewhat surprising that negative ions in a non-zero constant magnetic field always have an infinity of bound states. As we will explain the binding energy for small fields goes as B^3 and so it is unlikely that these states can be seen with currently available laboratory fields. However they may have astrophysical significance.

The physics behind this phenomenon was discussed by us in [8]: The extra electron moves in a Landau orbit and thus is pinned down in two dimensions. Binding is thus a one-dimensional phenomenon. The net attraction of the neutral atom on the extra electron is greater than that of imperfect shielding because there is an induced polarization of the atom by this extra electron. The importance of polarization has also been recently noted by Larsen [29]. With induced polarization in mind we gave a heuristic argument why the binding should be $O(B^3)$ for B small. We imagine the extra electron feeling a polarization potential $V_{\mathrm{pol}}(r) \sim -r^{-4}$ near infinity. (One can calculate an induced dipole moment $\mathbf{D} \sim \mathbf{r}/r^3$ using perturbation theory.) Thus when it is in a Landau orbit in the directions orthogonal to the field, the effective one dimensional potential is

$$W(z) = \int V_{\mathrm{pol}}(r) |\phi(\boldsymbol{\varrho})|^2 d^2\varrho$$

with ϕ the Landau orbital. Weak coupling one dimensional theory [43] says that the binding energy for small W is $O((\int W dz)^2)$. But $\int V_{\mathrm{pol}}(r) dz \sim -\varrho^{-3}$ at infinity and by scaling $\int_{|\varrho| \geqq 1} \varrho^{-3} |\phi|^2 d^2\varrho$ is $O(B^{3/2})$ for B small. Thus we obtain the $O(B^3)$ estimate on binding.

In our next theorem we will be dealing with the two operators

$$H(B) = \sum_{j=1}^{n} (-i\nabla_j - 1/2 B\mathbf{z} \times \mathbf{r}_j)^2 + \sum_{1 \leqq i < j \leqq n} |\mathbf{r}_i - \mathbf{r}_j|^{-1} - (n-1) \sum_{j=1}^{n} |\mathbf{r}_j|^{-1} \quad (9.1)$$

which is the Hamiltonian of an ion with nuclear charge $n-1$ and n electrons and

$$H^{n-1}(B) = \sum_{j=1}^{n-1} (-i\nabla_j - 1/2 B\hat{\mathbf{z}} \times \mathbf{r}_j)^2 + \sum_{1 \leqq i < j \leqq n-1} |\mathbf{r}_i - \mathbf{r}_j|^{-1} - (n-1) \sum_{j=1}^{n-1} |\mathbf{r}_j|^{-1} \quad (9.2)$$

which is the Hamiltonian of a neutral atom with $n-1$ electrons. Unless otherwise stated $H(B)$ will be considered as an operator in

$$\mathscr{H}_a^n = \wedge^n (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2),$$

the physical subspace of wave functions which are antisymmetric under simultaneous interchange of space and spin variables. Similarly $H^{n-1}(B)$ will be considered as an operator in $\mathscr{H}_a^{n-1} = \wedge^{n-1}(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)$.

Let $E(0)$ be the ground state energy of $H^{n-1}(0)$,

$$E(0) = \inf \sigma(H^{n-1}(0) \restriction \mathscr{H}_a^{n-1})$$

and $\mathscr{K}$ the space of ground states:

$$\mathscr{K} = \{\psi \in \mathscr{H}_a^{n-1} : H^{n-1}(0)\psi = E(0)\psi\}.$$

Before the Pauli principle is accomodated, i.e., on $\bigotimes_{j=1}^{n-1} (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)$, $H^{n-1}(B)$ commutes with a "physical" symmetry group $\mathrm{SO}(3) \times S_{n-1} \times \mathrm{SU}(2) \times S_{n-1}$ corresponding to space rotations, permutations of spatial coordinates, electron spin rotations, and permutations of electron spin coordinates. Because there is no spin dependence, this is a subgroup of an even larger group commuting with $H^{n-1}(B)$, $SO(3)\times S_{n-1}\times SU(2n-2)\equiv\mathscr{G}$ incorporating arbitrary unitary maps in spin space. A group theoretic analysis [52] shows that if $\mathscr{G}$ acts irreducibly on an eigenspace, then $SO(3)\times SU(2)$ (space plus spin rotations) acts irreducibly on the corresponding subspace of $\mathscr{H}_a^{n-1}$. (Moreover, the representation of S_{n-1} = coordinate permutations, determines the total electron spin, S.)

Thus if all degeneracies are due to $\mathscr{G}$-symmetries a single L and single S will enter (and each only once) in the natural decomposition of $\mathscr{K}$ induced by the action of the symmetry group $SO(3)\times SU(2)$:

$$\mathscr{K}=\bigoplus_{(L,S)\in\mathscr{M}}\mathscr{K}_{L,S} \tag{9.3}$$

into subspaces $\mathscr{K}_{L,S}$ of definite total orbital angular momentum L and spin angular momentum S. This "typical" situation should be borne in mind in looking at the next theorem.

Theorem 9.1. *Let L_0 be the largest L appearing in the decomposition* (9.3) *and suppose there is a unique S_0 with $(L_0,S_0)\in\mathscr{M}$ and that $\dim\mathscr{K}_{L^0,S^0}=(2L_0+1)(2S_0+1)$. Let $H_m(B)=H(B)\restriction_{L_z=m}$. Then for any $m\geqq L_0+1$ there is a $b(m)>0$ so that for $0<B<b(m)$, $H_m(B)$ has an eigenvalue $E_m(B)$ satisfying*

$$E_m(B)<\Sigma(B)-c_mB^3 \tag{9.4}$$

with $\Sigma(B)$ the bottom of the continuum of $H(B)$ and $c_m>0$.

Theorem 9.2. *Fix $B>0$. Let $H(B)$, $H_m(B)$ and $\Sigma(B)$ be as in Theorem* 9.1. *Then there is an integer $M(B)>0$ so that for all $m\geqq M(B)$, $H_m(B)$ has an eigenvalue $E_m(B)$ satisfying*

$$E_m(B)<\Sigma(B)-c(B)m^{-3} \tag{9.5}$$

for some $c(B)>0$.

Remarks. 1) We believe that the m^{-3} behavior in (9.5) is optimal. If the ion with $B=0$ is not bound and $L_0=0$ we also believe that the B^3 behavior in (9.4) is optimal.

2) The addition of a term $-2\mathbf{B}\cdot\mathbf{S}$ to $H(B)$ reflecting the interaction of the electron spins with the magnetic field should not change the results (9.4) or (9.5).

3) Note that Theorem 9.2 says that *every* once negatively charged ion has an infinite number of bound states below the physical continuum if $B>0$.

Proof of Theorem 9.1. By the extension of Theorem 7.1 remarked upon in Sect. 7, $H^{n-1}(B)$ has exactly $q=\dim\mathscr{K}$ eigenvalues (counting multiplicity) near $E(0)$ for small B and at least one of these equals

$$E(B)=\inf\sigma(H^{n-1}(B)).$$

Let $\mathscr{K}(B)$ be the subspace of these q eigenvectors of $H^{n-1}(B)$. Since $H^{n-1}(B)=H^{n-1}(0)-BL_z+1/4B^2\sum_{j=1}^{n-1}\varrho_j^2$, first order perturbation theory [51, p. 443] shows that if $e(B)$ is one of these q eigenvalues with eigenvector belonging to a subspace with $L_z=\lambda$, then $e(B)=E(0)-B\lambda+O(B^2)$ so that for small $B>0$, $E(B)$

occurs on the subspace of highest L_z which intersects $\mathscr{K}(B)$. Since the highest L_z occuring in $\mathscr{K}$ is L_0, and since the orthogonal projection $P(B)$ onto $\mathscr{K}(B)$ converges in norm to the corresponding projection $P(0)$ onto $\mathscr{K}$, for $B>0$ $E(B)$ will occur on the subspace with $L_z=L_0$.

Let P_1 project on $\{\psi:L_z\psi=L_0\psi\}$ and similarity let P_2 projection $\{\psi:S_z\psi=S_0\psi\}$ where S_z is the total z-component of spin of the $n-1$ electrons. By assumption $P_1P_2P(0)$ is one dimensional so that for small $B>0$, $P_1P_2P(B)$ is one dimensional. Let

$$P_1P_2P(0)=(\eta(0),\cdot)\eta(0)$$

and define

$$\eta(B)=P(B)\eta(0)/\|P(B)\eta(0)\|.$$

Then for small $B>0$ we have

$$(H^{n-1}(B)-E(B))\eta(B)=0, \quad (L_z-L_0)\eta(B)=0. \tag{9.6}$$

We will need additional properties of $\eta(B)$ for small B. Let

$$P(B,\gamma)=U(\gamma)P(B)U(-\gamma)$$

with $U(\gamma)$ multiplication by $\exp(-i\gamma\sqrt{r_1^2+\ldots+r_{n-1}^2+1})$. By arguments of Combes and Thomas [15] combined with the stability arguments of Sect. 7, $P(B,\gamma)$ is analytic in γ in a disk of radius $2\delta_0>0$ independent of B for B small and as $B\to 0$, $P(B,\gamma)\xrightarrow{\|\cdot\|}P(0,\gamma)$ $(|\gamma|<2\delta_0)$. Thus as $B\to 0$

$$P(B,i\gamma)\eta(0)=U(i\gamma)\eta(B)(\eta(B),U(-i\gamma)\eta(0))\to U(i\gamma)\eta(0)(\eta(0),U(-i\gamma)\eta(0));\quad 0<\gamma<2\delta_0.$$

Dividing by $(\eta(B),U(-i\gamma)\eta(0))$ we obtain (for $0<\gamma<2\delta_0$)

$$\lim_{B\to 0}\|U(i\gamma)(\eta(B)-\eta(0))\|=0 \tag{9.7}$$

and by a simple argument

$$\lim_{B\to 0}\left\|U(i\gamma)\left(\sum_{j=1}^{n-1}\Delta_j\right)(\eta(B)-\eta(0)\right\|=0. \tag{9.8}$$

In particular for B small

$$\left\|U(i\delta_0)\left(\sum_{j=1}^{n-1}\Delta_j\right)\eta(B)\right\|+\|U(i\delta_0)\eta(B)\|\leqq\text{constant}. \tag{9.9}$$

To prove (9.4) we will use a trial vector $\Psi(B)$ constructed as follows:

$$\Psi(B)=P_a\Phi(B), \tag{9.10}$$

where $\Phi(B)\in\mathscr{H}=\bigotimes_{j=1}^{n}(L^2(\mathbb{R}^3)\otimes\mathbb{C}^2)$ and P_a projects onto $\mathscr{H}_a=\wedge^n(L^2(\mathbb{R}^3)\otimes\mathbb{C}^2)$. The vector $\Phi(B)$ is given by

$$\Phi(B)(\mathbf{r}_1,s_1;\ldots,\mathbf{r}_n,s_n)=\eta(B)(\mathbf{r}_1,s_1;\ldots,\mathbf{r}_{n-1},s_{n-1})f_m(\mathbf{r}_n)\left(1+\left(\sum_{j=1}^{n-1}z_j\right)g(\mathbf{r}_n)\right)\zeta(s_n), \tag{9.11}$$

where s_j is the spin coordinate of the j^{th} electron, $\zeta(s)$ is an arbitrary normalized spin wave function for the n^{th} electron, and

$$f_m(\mathbf{r}) = \phi_m(B, \boldsymbol{\varrho})\alpha^{1/2}e^{-\alpha|z|}, \tag{9.12}$$

where ϕ_m is the normalized ground state of

$$-\partial_x^2 - \partial_y^2 + 1/4 B^2\varrho^2 - B\ell_z$$

with energy B and $\ell_z\phi_m = m\phi_m$. Here of course $\ell_z = (\mathbf{r} \times (-i\nabla))\cdot\hat{\mathbf{z}}$. The function g is given by

$$g(\mathbf{r}) = -\beta\gamma(z)\,\mathrm{sgn}\,z(1+|\mathbf{r}|^2)^{-1}, \tag{9.13}$$

where $\gamma(z)$ is an even C^∞ function, 1 in a neighborhood of ∞ and 0 in a neighborhood of 0 with $0 \leqq \gamma \leqq 1$. The parameters α and β will be chosen so that β is positive with order of magnitude 1 while α is a constant times $B^{3/2}$. They are specified precisely in Eq. (9.48).

In (9.11), the $\eta f \zeta$ factor arises because we are putting the extra electron into a Landau orbit in the magnetic field in the xy plane and a weak coupling state in the z-direction. The factor $(1 + (\sum z_j)g)$ represents an ad-hoc modification of η to give η a dipole moment.

We will make use of the explicit form of $\phi_m(B, \boldsymbol{\varrho})$:

$$\phi_m(B, \boldsymbol{\varrho}) = e^{im\phi}(\pi m!)^{-1/2}(B/2)^{(m+1)/2}\varrho^m e^{-B\varrho^2/4} \tag{9.14}$$

which leads to the estimate

$$\begin{aligned} \int |\phi_m(B, \boldsymbol{\varrho})|^2(1+\varrho^2)^{-k}d^2\varrho &\geqq \text{const}\, B^{\min(m+1,k)}, \qquad k \neq m+1 \\ &\leqq \text{const}\, B^k \ln B^{-1}, \qquad k = m+1. \end{aligned} \tag{9.15}$$

We also have

$$\int |\phi_m(B, \boldsymbol{\varrho})|^2 \varrho^{-k} d^2\varrho = O(B^{k/2}), \qquad k < 2m+2. \tag{9.16}$$

We note for future reference that

$$\Sigma(B) \equiv \inf \sigma_{\text{ess}}(H(B)) = E(B) + B \tag{9.17}$$

and that

$$L_z\Psi(B) = (L_0 + m)\Psi(B). \tag{9.18}$$

We will always take $m \geqq 1$. We first calculate $\|\Psi(B)\|^2$. We denote by S_n the group of permutations of $\{1, \ldots, n\}$ and by T_Q the obvious permutation operator on

$$\mathscr{H} = \bigotimes_{j=1}^{n} (L^2(\mathbb{R}^3) \otimes \mathbb{C}^2)$$

corresponding to $Q \in S_n$. We have

$$\begin{aligned} P_a\Phi(B) &= (n!)^{-1/2} \sum_{Q \in S_n} (-1)^Q T_Q \Phi(B) \\ &= n^{-1/2}\Phi(B) + (n!)^{-1/2} \sum_{\substack{Q \in S_n \\ Q(n) \neq n}} (-1)^Q T_Q \Phi(B) \end{aligned}$$

so that

$$\|\Psi(B)\|^2=(\Phi(B),P_a\Phi(B))=n^{-1/2}\|\Phi(B)\|^2+(n!)^{-1/2}\sum_{\substack{Q\in S_n\\ Q(n)\neq n}}(-1)^Q(\Phi(B),T_Q\Phi(B)).$$

We claim that if $Q(n)\neq n$

$$(\Phi(B),T_Q\Phi(B))=O(\alpha B^{m+1})=O(B^{5/2+m})=O(B^{7/2}),$$

where we are using $m\geqq 1$ and $\alpha=(\text{const})B^{3/2}$. To see this we look at a typical term:

$$\left|\int \overline{\eta(B)(\mathbf{r}_1,s_1;\ldots;\mathbf{r}_{n-1},s_{n-1})\zeta(s_n)f_m(\mathbf{r}_n)}\eta(B)(\mathbf{r}_1,s_1;\ldots;\mathbf{r}_{n-2},s_{n-2};\mathbf{r}_n,s_n)\zeta(s_{n-1})f_m(\mathbf{r}_{n-1})\right.$$
$$dr_1\ldots dr_n \tag{9.19}$$
$$\leqq \text{const}\,\alpha B^{m+1}\int|\eta(B)(\mathbf{r}_1,s_1;\ldots;\mathbf{r}_{n-1},s_{n-1})\varrho_{n-1}^m|\,|\eta(B)(\mathbf{r}_1,s_1;\ldots;\mathbf{r}_{n-2},s_{n-2};\mathbf{r}_n,s_n)\varrho_n^m|$$
$$\cdot dr_1\ldots dr_n, \tag{9.20}$$

where we have used (9.14). Using the Schwarz inequality we have

$$\begin{aligned}(9.20)=&(\text{const})\alpha B^{m+1}\int|\eta(B)(\mathbf{r}_1,s_1;\ldots;\mathbf{r}_{n-1},s_{n-1})\varrho_{n-1}^m e^{-\delta_0|\mathbf{r}_n|/2}e^{\delta_0|\mathbf{r}_{n-1}|/2}\\ &\cdot|\eta(B)(\mathbf{r}_1,s_1;\ldots;\mathbf{r}_{n-2},s_{n-2};\mathbf{r}_n,s_n)\varrho_n^m e^{-\delta_0|\mathbf{r}_{n-1}|/2}e^{\delta_0|\mathbf{r}_n|/2}|dr_1\ldots dr_n\\ \leqq&(\text{const})\alpha B^{m+1}\|e^{1/2\delta_0|\mathbf{r}_{n-1}|}\varrho_{n-1}^m\eta(B)\|^2\int e^{-\delta_0|\mathbf{r}|}d^3r\\ \leqq&(\text{const})\alpha B^{m+1}.\end{aligned}$$

In the last inequality we have used (9.9). In addition

$$\|\Phi(B)\|^2=1+\left\|\left(\sum_{j=1}^{n-1}z_j\right)\eta(B)\right\|^2\|f_m g\|^2 \tag{9.21}$$

with

$$\begin{aligned}\|f_m g\|^2&\leqq\alpha\beta^2\int|\phi_m(B,\boldsymbol{\varrho})|^2(1+|\mathbf{r}|^2)^{-2}d^2\varrho\,dz\\ &=\alpha\beta^2\int|\phi_m(B,\boldsymbol{\varrho})|^2(1+\varrho^2)^{-3/2}d^2\varrho(\text{const})\\ &=\alpha\beta^2O(B^{3/2}),\end{aligned} \tag{9.22}$$

where we have used (9.15) with $m\geqq 1$. We thus have

$$\|\Psi(B)\|^2=n^{-1/2}+O(B^3). \tag{9.23}$$

A similar analysis of the exchange terms in $(\Psi(B),(H(B)-E(B)-B)\Psi(B))$ using (9.9) yields

$$(\Psi(B),(H(B)-B-E(B))\Psi(B))=n^{-1/2}(\Phi(B),(H(B)-B-E(B))\Phi(B))+O(B^{7/2}), \tag{9.24}$$

where on the right hand side of (9.24) $H(B)$ is considered as an operator in $\mathscr{H}$. Thus combining (9.23) and (9.24) we see that it suffices to show that

$$(\Phi(B),(H(B)-B-E(B))\Phi(B))<-d_mB^3 \tag{9.25}$$

for some $d_m>0$ and $B>0$ and sufficiently small. We calculate the left hand side of (9.25) using the operator relation

$$-f\Delta f=-\tfrac{1}{2}(\Delta f^2+f^2\Delta)+(\nabla f)^2$$

with $f=1+\left(\sum_{j=1}^{n-1} z_j\right) g(\mathbf{r}_n)$ and where the Laplacian and gradient include all variables except z_n. We obtain

$$(\Phi(B),(H(B)-B-E(B))\Phi(B))=\left\|\frac{d}{dz_n}\Phi(B)\right\|^2+(n-1)\|f_m g\|^2 + \left\|\eta(B)\sum_{j=1}^{n-1} z_j\right\|^2 \|f_m \nabla_\perp g\|^2+(\Phi(B), W\Phi(B)),\tag{9.26}$$

where we have used

$$H(B)=H_{n-1}(B)-\Delta_n+\tfrac{1}{4}B^2\varrho_n^2-B\ell_{z_n}+W$$

with

$$W(\mathbf{r}_1,\ldots,\mathbf{r}_n)=\sum_{j=1}^{n-1}\left(\frac{1}{|\mathbf{r}_j-\mathbf{r}_n|}-\frac{1}{|\mathbf{r}_n|}\right).$$

We calculate

$$\left\|\frac{d}{dz_n}\Phi(B)\right\|^2=\alpha^2\left(1+\left\|\left(\sum_{j=1}^{n-1} z_j\right)\eta(B)\right\|^2\|f_m g\|^2\right) + \left\|\left(\sum_{j=1}^{n-1} z_j\right)\eta(B)\right\|^2\left\|f_m\frac{dg}{dz_n}\right\|^2.\tag{9.27}$$

We have already estimated $\|f_m g\|^2$ in (9.22)

$$(n-1)\|f_m g\|^2\leqq \alpha\beta^2 B^{3/2}\gamma_m.\tag{9.28}$$

Using (9.15) with $m\geqq 1$ and $\alpha=O(B^{3/2})$ we have

$$\left\|f_m\frac{d}{dz_n}g\right\|^2=O(B^{7/2}\ln B^{-1}),\tag{9.29}$$

$$\|f_m\nabla_\perp g\|^2=O(B^{7/2}),\tag{9.30}$$

and thus

$$(\Phi(B),(H(B)-E(B)-B)\Phi(B))=\alpha^2+\alpha\beta^2B^{3/2}\gamma_m+(\Phi(B), W\Phi(B)) + O(B^{7/2}\ln B^{-1}).\tag{9.31}$$

We now estimate $(\Phi(B), W\Phi(B))$:

$$(\Phi(B), W\Phi(B))=I_1(B,m)+I_2(B,m)+I_3(B,m),\tag{9.32}$$

where

$$I_1(B,m)=\int dr_1\ldots dr_{n-1}\,dr|\eta(B)(\mathbf{r}_1,\ldots,\mathbf{r}_{n-1})|^2 W(\mathbf{r}_1,\ldots,\mathbf{r}_{n-1},\mathbf{r})|f_m(\mathbf{r})|^2 = \alpha(n-1)\int dr_1\,dr\,\lambda_B(\mathbf{r}_1)(|\mathbf{r}_1-\mathbf{r}|^{-1}-|\mathbf{r}|^{-1})|\phi_m(B,\mathbf{\varrho})|^2 e^{-2\alpha|z|}.\tag{9.33}$$

Here $|\eta(B)(\mathbf{r}_1,\ldots,\mathbf{r}_{n-1})|$ indicates the norm in the spin variables and

$$\lambda_B(\mathbf{r}_{n-1})=\int dr_1\ldots dr_{n-2}|\eta(B)(\mathbf{r}_1,\ldots,\mathbf{r}_{n-1})|^2.$$

$$I_2(B,m)=\alpha(n-1)\beta^2\int dr_1\,dr\,\tilde{\lambda}_B(\mathbf{r}_1)(|\mathbf{r}_1-\mathbf{r}|^{-1}-|\mathbf{r}|^{-1})|\phi_m(B,\mathbf{\varrho})|^2 e^{-2\alpha|z|}\gamma(z)^2(1+|\mathbf{r}|^2)^{-2},\tag{9.34}$$

where

$$\tilde{\lambda}_B(\mathbf{r}_{n-1}) = \int dr_1 \ldots dr_{n-2} \left| \left(\sum_{j=1}^{n-1} z_j \right) \eta(B)(\mathbf{r}_1, \ldots, \mathbf{r}_{n-1}) \right|^2 .$$

And

$$I_3(B,m) = -2\beta\alpha \int dr_1 \ldots dr_{n-1} dr |\eta(B)(\mathbf{r}_1, \ldots, \mathbf{r}_{n-1})|^2 \left(\sum_{j=1}^{n-1} z_j \right) W(\mathbf{r}_1, \ldots, \mathbf{r}_{n-1}, \mathbf{r}) \cdot e^{-2\alpha|z|} \gamma(z) \operatorname{sgn} z (1+|\mathbf{r}|^2)^{-1} |\phi_m(B, \varrho)|^2 . \tag{9.35}$$

We want to show that I_1 and I_2 are negligible. Since $\| |\mathbf{r}_1 - \mathbf{r}|^{-1}(-\Delta_1 + 1)^{-1} \| \leqq \text{const}$, the integral

$$\alpha(n-1) \int_{|\mathbf{r}| \leqq 1} dr_1 dr \lambda_B(\mathbf{r}_1)(|\mathbf{r}_1 - \mathbf{r}|^{-1} - |\mathbf{r}|^{-1}) |\phi_m(B, \varrho)|^2 e^{-2\alpha|z|} \tag{9.36}$$

is less than

$$(\text{const})\alpha \int_{|r| \leqq 1} dr |\mathbf{r}|^{-1} |\phi_m(B, \varrho)|^2 = \alpha O(B^{m+1}) = O(B^{7/2}) \tag{9.37}$$

so that in (9.33) we need only consider the region $|\mathbf{r}| \geqq 1$. Similarly

$$\alpha(n-1) \int_{\substack{|\mathbf{r}| \geqq 1 \\ |\mathbf{r}_1| > 1/2|\mathbf{r}|}} dr_1 dr \lambda_B(\mathbf{r}_1)(|\mathbf{r}_1 - \mathbf{r}|^{-1} + |\mathbf{r}|^{-1}) |\phi_m(B, \varrho)|^2 e^{-2\alpha|z|}$$

$$\leqq \alpha(n-1) \int_{\substack{|\mathbf{r}| \geqq 1 \\ |\mathbf{r}_1| > 1/2|\mathbf{r}|}} dr_1 \ldots dr_{n-1} dr \langle \eta(B)(\mathbf{r}_1, \ldots, \mathbf{r}_{n-1}), (|\mathbf{r}_1 - \mathbf{r}|^{-1} + |\mathbf{r}|^{-1}) \eta(B)(\mathbf{r}_1, \ldots, \mathbf{r}_{n-1}) \rangle |\phi_m(B, \varrho)|^2$$

$$\leqq \alpha(n-1) \int_{|r| \geqq 1} dr_1 \ldots dr_{n-1} dr e^{-\delta_0|\mathbf{r}|/2} (\| |\mathbf{r}_1 - \mathbf{r}|^{-1}(-\Delta_1 + 1)^{-1} \| + 1) \cdot e^{\delta_0 |\mathbf{r}_1|} |(-\Delta_1 + 1) \eta(B)(\mathbf{r}_1, \ldots, \mathbf{r}_{n-1})|^2 |\phi_m(B, \varrho)|^2$$

$$\leqq (\text{const})\alpha \int dr e^{-\delta_0|\mathbf{r}|/2} |\phi_m(B, \varrho)|^2 = O(\alpha B^{m+1}) = O(B^{7/2}) . \tag{9.38}$$

In the second line above $\langle \; , \; \rangle$ indicates inner product in the spin variables. Thus in (9.33) we need only consider the region $|\mathbf{r}| \geqq 1$, $|\mathbf{r}_1| \leqq \frac{1}{2}|\mathbf{r}|$. In this region we use a multipole expansion of $|\mathbf{r}_1 - \mathbf{r}|^{-1} - |\mathbf{r}|^{-1}$:

$$|\mathbf{r}_1 - \mathbf{r}|^{-1} - |\mathbf{r}|^{-1} = \sum_{\ell=1}^{k} \frac{4\pi}{2\ell+1} \sum_{\lambda=-\ell}^{\ell} \overline{Y_\ell^\lambda}(\theta_1, \phi_1) Y_\ell^\lambda(\theta, \phi) |\mathbf{r}_1|^\ell |\mathbf{r}|^{-\ell-1} + O(|\mathbf{r}_1|^{k+1}/|\mathbf{r}|^{k+2}) . \tag{9.39}$$

An important fact is that for $l > 0$ (and $l < 2m+2$ so that the integral converges)

$$\int |\phi_m(B, \varrho)|^2 Y_\ell^\lambda(\theta, \phi) |\mathbf{r}|^{-\ell-1} dr = 0 . \tag{9.40}$$

This follows from $\int P_\ell(\cos\theta) |\mathbf{r}|^{-\ell-1} dz = 0$ which in turn can be seen from the fact that a) by a change of variable $\int P_\ell(\cos\theta) |\mathbf{r}|^{-\ell-1} dz = c\varrho^{-\ell}$ and

b) $(\partial_x^2 + \partial_y^2) \int P_\ell(\cos\theta) |\mathbf{r}|^{-\ell-1} dz = \int \Delta(P_\ell(\cos\theta) |\mathbf{r}|^{-\ell-1}) dz = 0$.

Thus $(\partial_x^2+\partial_y^2)c\varrho^{-\ell}=0$ which implies $c=0$ or $\ell=0$. We use (9.39) with $k=3$. Noting that the dipole term vanishes we have:

$$I_1 \leqq \alpha(n-1)\sum_{\ell=2}^{3}\frac{4\pi}{2\ell+1}\sum_{\lambda=-\ell}^{\ell}\int_{\substack{|\mathbf{r}|\geqq 1\\ |\mathbf{r}_1|<1/2|\mathbf{r}|}}$$

$$\cdot dr dr_1 \lambda_B(\mathbf{r}_1)\bar{Y}_\ell^\lambda(\theta_1,\phi_1)Y_\ell^\lambda(\theta,\phi)|\mathbf{r}_1|^\ell|\phi_m(B,\varrho)|^2 e^{-2\alpha|z|}|\mathbf{r}|^{-\ell-1}$$

$$+(\text{const})\alpha\int_{\substack{|\mathbf{r}|\geqq 1\\ |\mathbf{r}_1|<1/2|\mathbf{r}|}} dr dr_1\lambda_B(\mathbf{r}_1)|\mathbf{r}_1|^4|\phi_m(B,\varrho)|^2|\mathbf{r}|^{-5}+O(B^{7/2}). \tag{9.41}$$

In the $\ell=2,3$ terms we first add back in the regions $|\mathbf{r}|<1$, $|\mathbf{r}_1|<\frac{1}{2}|\mathbf{r}|$ and $|\mathbf{r}_1|>\frac{1}{2}|\mathbf{r}|$. This contributes $O(B^{7/2})$ as in (9.37) and (9.38). Then we use (9.40) to replace $e^{-2\alpha|z|}$ by $e^{-2\alpha|z|}-1$. The estimate $|e^{-2\alpha|z|}-1\leqq 2\alpha|z|$ then gives

$$I_1\leqq(\text{const})\alpha^2\sum_{\ell=2}^{3}\int dr dr_1\lambda_B(\mathbf{r}_1)|\mathbf{r}_1|^\ell|\phi_m(B,\varrho)|^2|z|\,|\mathbf{r}|^{-\ell-1}$$

$$+(\text{const})\alpha\int_{|\mathbf{r}|\geqq 1} dr|\phi_m(B,\varrho)|^2|\mathbf{r}|^{-5}+O(B^{7/2}). \tag{9.42}$$

Using (9.15) and (9.16) we find

$$I_1=O(\alpha^2B^{1/2})+O(\alpha B^2\ln B^{-1})=O(B^{7/2}\ln B^{-1}). \tag{9.43}$$

A similar but simpler analysis of I_2 gives $I_2=O(B^{7/2})$ so that

$$(\Phi(B),W\Phi(B))=I_3(B,m)+O(B^{7/2}\ln B^{-1}). \tag{9.44}$$

We now estimate I_3, given by (9.35). As above in the term corresponding to $|\mathbf{r}_j-\mathbf{r}|^{-1}-|\mathbf{r}|^{-1}$ the contribution from $|\mathbf{r}_j|>\frac{1}{2}|\mathbf{r}|$ is $O(B^{7/2})$. In the region $|\mathbf{r}_j|<\frac{1}{2}|\mathbf{r}|$ we use

$$|\mathbf{r}_j-\mathbf{r}|^{-1}-|\mathbf{r}|^{-1}=\mathbf{r}_j\cdot\mathbf{r}/|\mathbf{r}|^3+O(|\mathbf{r}_j|^2/|\mathbf{r}|^3).$$

The estimates (9.15) and (9.16) show that $|\mathbf{r}_j|^2/|\mathbf{r}|^3$ contributes $O(B^{7/2}\ln B^{-1})$. We are thus left with $\mathbf{r}_j\cdot\mathbf{r}/|\mathbf{r}|^3$ in the region $|\mathbf{r}_j|<\frac{1}{2}|\mathbf{r}|$. Adding back in the region $|\mathbf{r}_j|>\frac{1}{2}|\mathbf{r}|$ again contributes $O(B^{7/2})$. For the same reason we can replace $\gamma(z)$ by 1 so that

$$I_3=-2\beta\alpha\int dr_1\dots dr_{n-1}dr|\eta(B)(\mathbf{r}_1,\dots,\mathbf{r}_{n-1})|^2\left(\sum_{j=1}^{n-1}z_j\right)\sum_{j=1}^{n-1}(\mathbf{r}_j\cdot\mathbf{r}/|\mathbf{r}|^3)$$

$$\cdot e^{-2\alpha|z|}\operatorname{sgn}z(1+|\mathbf{r}|^2)^{-1}|\phi_m(B,\varrho)|^2+O(B^{7/2}\ln B^{-1})$$

$$=-2\beta\alpha\left\|\left(\sum_{j=1}^{n-1}z_j\right)\eta(B)\right\|^2\int|z|(1+|\mathbf{r}|^2)^{-1}|\mathbf{r}|^{-3}|\phi_m(B,\varrho)|^2d^2\varrho dz+O(B^{7/2}\ln B^{-1}). \tag{9.45}$$

Using $\alpha\leqq\text{const}\,B^{3/2}$ and $m\geqq 1$ it is easy to show that

$$\lim_{B\downarrow 0}B^{-3/2}\int|z|(1+|\mathbf{r}|^2)^{-1}|\mathbf{r}|^{-3}|\phi_m(B,\varrho)|^2d^2\varrho dz=4\tilde{\lambda}_m>0,$$

where $\tilde{\lambda}_m$ depends only on m. In addition, by (9.7)

$$\left\|\left(\sum_{j=1}^{n-1}z_j\right)\eta(B)\right\|\to\left\|\left(\sum_{j=1}^{n-1}z_j\right)\eta(0)\right\|\quad\text{and thus for small}\quad B>0$$

$$(\Phi(B),W\Phi(B))<-4\beta\alpha B^{3/2}\lambda_m, \tag{9.46}$$

where $\lambda_m = \left\| \left(\sum_{j=1}^{n-1} z_j \right) \eta(0) \right\|^2 \tilde{\lambda}_m$. (9.46) and (9.31) imply that for small $B>0$

$$(\Phi(B), (H(B) - E(B) - B)\Phi(B)) \leqq \alpha^2 + \alpha\beta^2 B^{3/2}\gamma_m - 2\beta\alpha B^{3/2}\lambda_m . \tag{9.47}$$

We now choose

$$\begin{aligned} \beta &= \lambda_m/\gamma_m \\ \alpha &= (\lambda_m^2/2\gamma_m)B^{3/2} . \end{aligned} \tag{9.48}$$

The result is

$$(\Phi(B), (H(B) - E(B) - B)\Phi(B)) \leqq -(\lambda_m^2/2\gamma_m)^2 B^3 \tag{9.49}$$

which is (9.25). This completes the proof. □

Remark. We have not really exploited the freedom of the choice of spinor function ζ in (9.11) or the choice of total S_z^{n-1} of the $n-1$ electron wave function. If $S_0 \neq 0$ we can obtain (by taking suitable linear combinations of states with $S_z^{n-1} = S_0$ and ζ spin down and $S_z^{n-1} = S_0 - 1$ and ζ spin up) bound states with total $S = S_0 \pm \frac{1}{2}$ and so *two* bound states for each value of L_z in the regimes where we found one. In particular if $S_0 = \frac{1}{2}$ (e.g. hydrogen) we get both triplet ($S=1$) and singlet states.

Proof of Theorem 9.2. Let us first assume that $H^{n-1}(B)$ has a ground state which as before we call $\eta(B)$. We use the same trial wave function (9.10) as in the proof of Theorem 9.1. Again the parameters α and β will be chosen so that β is a positive constant and α is a constant times $m^{-3/2}$. They are specified precisely in Eq. (9.70). The analysis of

$$(\Psi(B), (H(B) - B - E(B))\Psi(B))/(\Psi(B), \Psi(B))$$

is based in part on the estimates (m large, $k>0$, $\lambda>0$)

$$\int \varrho^{-k} |\phi_m(B, \mathbf{\varrho})|^2 d^2\varrho \leqq c_k m^{-k/2} , \tag{9.50}$$

$$\int e^{-\lambda\varrho^2} |\phi_m(B, \mathbf{\varrho})|^2 d^2\varrho \leqq c(\lambda) e^{-\gamma(\lambda)m} ; \quad \gamma(\lambda) > 0 \tag{9.51}$$

which replace (9.15) and (9.16). To understand (9.50) and (9.51) consider the measure

$$|\phi_m(B, \mathbf{\varrho})|^2 d^2\varrho = \varrho |\phi_m(B, \mathbf{\varrho})|^2 d\varrho d\phi .$$

Writing $\varrho^{2m+1} e^{-B\varrho^2/2} = e^{-h(\varrho)}$ we see that h has a minimum when $\varrho = \varrho_m$,

$$\varrho_m = \sqrt{(2m+1)/B} . \tag{9.52}$$

If we use the approximation $h(\varrho) \cong h(\varrho_m) + \frac{1}{2}h''(\varrho_m)(\varrho - \varrho_m)^2$ and Stirling's formula, we find

$$|\phi_m(B, \mathbf{\varrho})|^2 d^2\varrho \cong \frac{d\phi}{2\pi} \frac{B}{\pi} e^{-B(\varrho - \varrho_m)^2} d\varrho .$$

For our purposes the estimate

$$\begin{aligned} h(\varrho) &\geqq h(\varrho_m) + \tfrac{1}{2}(\varrho - \varrho_m)^2 (\inf_{x \geqq 0} h''(x)) \\ &= h(\varrho_m) + \tfrac{1}{2}B(\varrho - \varrho_m)^2 \end{aligned}$$

is sufficient. It leads to

$$\varrho|\phi_m(B,\boldsymbol{\varrho})|^2 \leqq (\text{const})\, e^{-B(\varrho-\varrho_m)^2/2}\,.$$

This and the simple estimate $\int\limits_{\varrho\leqq 1} \varrho^{-k}|\phi_m(B,\boldsymbol{\varrho})|^2 d^2\varrho \leqq (\text{const})^m/m!$ for large m suffice to establish (9.50) and (9.51).

We now estimate each of the terms encountered in the proof of Theorem 9.1. When convenient we will use $\beta=O(1)$, $\alpha=O(m^{-3/2})$. The exchange terms typified by (9.19) are small because of the falloff of $\eta(B)$ proved in Theorem 8.1. In fact because of (9.51)

$$(9.19)=O(\alpha\exp(-m(\text{const}))\,.$$

From (9.50) it follows that

$$\|f_m g\|^2 = O(\alpha m^{-3/2}\beta^2)\,, \tag{9.53}$$

$$\|f_m \nabla_\perp g\|^2 = O(\alpha m^{-5/2}\beta^2)\,, \tag{9.54}$$

$$\left\|f_m \frac{d}{dz_n} g\right\|^2 = O(\alpha m^{-2}\beta^2)\,, \tag{9.55}$$

and thus

$$\|\Phi(B)\|^2 = 1 + \left\|\sum_{j=1}^{n-1} z_j\eta(B)\right\|^2 \|f_m g\|^2 = 1 + O(\alpha m^{-3/2})\,. \tag{9.56}$$

It is clear from (9.56) and the exponential decrease of the exchange terms that it suffices to show

$$(\Phi(B),(H(B)-E(B)-B)\Phi(B)) \leqq -d_1 m^{-3} \tag{9.57}$$

for some $d_1>0$. From (9.53) and (9.55) we have

$$\begin{aligned}\left\|\frac{d}{dz_n}\Phi(B)\right\|^2 &= \alpha^2(1+O(\alpha m^{-3/2})) + O(\alpha m^{-2})\\ &= \alpha^2 + O(m^{-7/2})\end{aligned} \tag{9.58}$$

and thus looking at (9.26) and using (9.53) and (9.54)

$$(\Phi(B),(H(B)-B-E(B))\Phi(B)) \leqq \alpha^2 + \beta^2\alpha m^{-3/2}c_1 + (\Phi(B), W\Phi(B)) + O(m^{-7/2})\,. \tag{9.59}$$

In estimating the contributions of $I_1(B,m)$ and $I_2(B,m)$ we use the same technique as in Theorem 9.1. The contribution from $|\mathbf{r}_1|>1/2|\mathbf{r}|$ is $O(e^{-m(\text{const})})$ because of the $e^{-\text{const}\,\varrho^2}$ decrease of $\eta(B)$. We find

$$\begin{aligned} I_1 \leqq\; & \alpha(n-1)\sum_{\ell=2}^{3}\frac{4\pi}{2\ell+1}\sum_{\lambda=-\ell}^{\ell}\int dr_1 dr\lambda_B(\mathbf{r}_1)|\mathbf{r}_1|^\ell |Y_\ell^\lambda(\theta_1,\phi_1)\,Y_\ell^\lambda(\theta,\phi)||\phi_m(B,\boldsymbol{\varrho})|^2\\ & \cdot |\mathbf{r}|^{-\ell-1}2\alpha|z|\\ & + (\text{const})\alpha\int dr_1 dr\lambda_B(\mathbf{r}_1)|\mathbf{r}_1|^4|\phi_m(B,\boldsymbol{\varrho})|^2|\mathbf{r}|^{-5} + O(\alpha e^{-m(\text{const})})\\ =\; & O(\alpha^2 m^{-1/2}) + O(\alpha m^{-2})\\ =\; & O(m^{-7/2})\,.\end{aligned} \tag{9.60}$$

Similarly we have

$$I_2 = O(\beta^2 \alpha m^{-3}) = O(m^{-9/2}). \tag{9.61}$$

The dipole contribution to I_3 is

$$D(m) = -2\beta a \left\| \eta(B) \left(\sum_{j=1}^{n-1} z_j \right) \right\|^2 \int \gamma(z)|z|(1+|\mathbf{r}/^2)^{-1}|\mathbf{r}|^{-3}|\phi_m(B,\boldsymbol{\varrho})|^2 e^{-2\alpha|z|} dr \tag{9.62}$$

and an easy estimate gives

$$|I_3 - D| \leqq (\text{const})\alpha \int (1+|\mathbf{r}|^2)^{-1}|\mathbf{r}|^{-3}|\phi_m(B,\boldsymbol{\varrho})|^2 dr + O(e^{-m(\text{const})}) = O(m^{-7/2}). \tag{9.63}$$

The error made in replacing $\gamma(z)(1+|\mathbf{r}|^2)^{-1}e^{-2\alpha|z|}$ by $|\mathbf{r}|^{-2}$ in (9.62) can be estimated by (9.50) with the result

$$D(m) = d(m) + O(m^{-4}), \tag{9.64}$$

where

$$d(m) = -2\beta\alpha \left\| \eta(B) \sum_{j=1}^{n-1} z_j \right\|^2 \int |\mathbf{r}|^{-5}|z|\,|\phi_m(B,\boldsymbol{\varrho})|^2 dr \tag{9.65}$$

and combining (9.60) through (9.65) gives

$$(\Phi(B), W\Phi(B)) = d(m) + O(m^{-7/2}). \tag{9.66}$$

Now $\int |z|\,|\mathbf{r}/^{-5}|\phi_m(B,\boldsymbol{\varrho})|^2 dr = \tilde{c}\int \varrho^{-3}|\phi_m(B,\boldsymbol{\varrho})|^2 d^2\varrho$. Using the ideas leading to (9.50) and (9.51) it is easy to show

$$\lim_{m\to\infty} \varrho_m^3 \int \varrho^{-3}|\phi_m(B,\boldsymbol{\varrho})|^2 d^2\varrho = 1, \tag{9.67}$$

where $\varrho_m = \sqrt{(2m+1)/B}$. Thus for large enough m

$$d(m) < -2\beta\alpha\gamma_1 m^{-3/2},$$

where $\gamma_1 > 0$ and hence for large m

$$(\Phi(B), W\Phi(B)) \leqq -2\beta\alpha\gamma_1 m^{-3/2} + O(m^{-7/2}). \tag{9.68}$$

Combining (9.59) and (9.68) gives

$$(\Phi(B), (H(B) - B - E(B))\Phi(B)) = \alpha^2 + (\beta^2 c_1 - 2\beta\gamma_1)\alpha m^{-3/2} + O(m^{-7/2}). \tag{9.69}$$

We choose

$$\beta = \gamma_1/c_1$$
$$\alpha = (\gamma_1^2/2c_1)m^{-3/2} \tag{9.70}$$

and find

$$(\Phi(B), (H(B) - B - E(B))\Phi(B)) = -(\gamma_1^2/2c_1)^2 m^{-3} + O(m^{-7/2}). \tag{9.71}$$

This is (9.57) and thus the proof is complete except for the existence of a ground state $\eta(B)$ for $H^{n-1}(B)$. This existence can be shown by an induction argument: To show that the system with nuclear charge $n-1$ and 1 electron has a ground state we refer to [9]. Once it has been established that a system of nuclear charge $n-1$ and $k-1$ electrons (for some k with $1 < k < n-1$) has a ground state $\eta'(B)$ we use a trial wave function

$$P_a\eta'(B)(\mathbf{r}_1, s_1; \ldots; \mathbf{r}_{k-1}, s_{k-1}) f_m(\mathbf{r}_k)\zeta(s_k)$$

to show that the system of nuclear charge $n-1$ and k electrons has a ground state. As above we take m large, show exchange terms are exponentially small and find that the important contribution to the negative of the trial binding energy is

$$\begin{aligned}&\alpha^2 + \alpha \int dr dr_1 \ldots dr_{k-1} |\eta'(B)(\mathbf{r}_1, \ldots, \mathbf{r}_{k-1})|^2 \\ &\quad \cdot \left(\sum_{j=1}^{k-1} |\mathbf{r}_j - \mathbf{r}|^{-1} - (n-1)|\mathbf{r}|^{-1} \right) |\phi_m(B, \boldsymbol{\varrho})|^2 e^{-2\alpha|z|} \\ &\quad = \alpha^2 - \alpha(n-k) \int dr |\phi_m(B, \boldsymbol{\varrho})|^2 |\mathbf{r}|^{-1} e^{-2\alpha|z|} + O(\alpha m^{-1/2}). \end{aligned} \tag{9.72}$$

Here we have used $\|\eta'(B)\| = 1$. Using the structure of the measure $|\phi_m(B, \boldsymbol{\varrho})|^2 d^2\varrho$ it is easy to show

$$(9.72) = \alpha^2 - \alpha(n-k) \int e^{-2\alpha|z|} (\varrho_m^2 + z^2)^{-1/2} dz + O(\alpha m^{-1/2}). \tag{9.73}$$

We note that

$$\int e^{-2\alpha|z|} \frac{1}{\sqrt{\varrho_m^2 + z^2}} dz = \int e^{-2\alpha\varrho_m|z|} \frac{1}{\sqrt{1 + z^2}} dz. \tag{9.74}$$

For large $\alpha\varrho_m$

$$(9.74) = (\alpha\varrho_m)^{-1} + O((\alpha\varrho_m)^{-2})$$

so that by choosing $\alpha = (\text{const})\varrho_m^{-1/2}$, we find

$$(9.72) < -(\text{const})\varrho_m^{-1}.$$

This completes the proof. □

Remark. In [8] we remarked in a footnote that a crucial element in the proof that He^- has a bound state for $B > 0$ was the fact that He develops a quadrupole moment when $B > 0$ (and small). Although the existence of this quadrupole moment is proved in Appendix 1 our original calculations were in error and thus this quadrupole moment plays no role in our proof of binding.

Appendix 1

Quadrupole Moments[1]

In our preliminary work on negative ions, we considered quadrupole moments of atoms in magnetic fields. While these are no longer necessary for our arguments there, we feel one of our results on that subject is worth reporting:

Theorem A.1. *If the ground state of an atom in zero magnetic field has $L=0$, then for all small field the atom has a non-zero quadrupole moment, i.e., with $\varrho^2 = \Sigma\varrho_i^2$, $z^2 = \Sigma z_i^2$*

$$\langle(\varrho^2 - 2z^2)\rangle \neq 0.$$

Remarks. If $L \neq 0$, then modulo a miraculous cancellation, there is a quadrupole moment at $B=0$ and thus by continuity one for small B.

1 We thank M. Aizenman for contributing to the proof of Theorem A.1

Proof. For all small B, the ground state will have $L_z=0$. For $L_z=0$, we can write the Hamiltonian as $H(B^2, B^2)$ where

$$H(\lambda, \mu)=H(B=0)+\tfrac{1}{6}[\lambda r^2+\mu(1/2\varrho^2-z^2)].$$

For all small λ, μ, the ground state will have $L_z=0$. Thus for small B^2, we can think of turning on the perturbation in two steps: first take λ to B^2, and then μ to B^2. $H(B^2, 0)$ will still have an $L_z=0$ ground state so

$$\langle(\varrho^2-2z^2)\rangle_{\lambda=B^2, \mu=0}=0.$$

By concavity of the ground state energy in μ, with λ fixed,

$$\langle(\varrho^2-2z^2)\rangle_{\lambda,\mu}$$

is strictly monotone decreasing, i.e.

$$\langle(\varrho^2-2z^2)\rangle_{B^2,B^2}<0. \quad \square$$

Appendix 2

Quasimomentum Dependence in the $Q=0$ Sector

Consider a Hamiltonian of n-particles of charges e_j, $j=1, \ldots, n$ in a magnetic field:

$$H=\sum_{j=1}^{n}(2m_j)^{-1}(-i\nabla_j-e_j(1/2\mathbf{B}\times\mathbf{r}_j))^2+\sum_{i=j}V_{ij}(r_i-r_j).$$

In [10], we noted that H commutes with the *quasimomentum*

$$\mathbf{k}=\mathbf{p}_T+1/2\mathbf{B}\times\mathbf{R},$$

where $\mathbf{p}_T=\sum_j(-i\nabla_j)$ is the total "momentum" and

$$\mathbf{R}=\sum_{i=1}^{n}e_i\mathbf{r}_i$$

is the center of charge. We also noted that so long as the total charge $Q=\sum_{i=1}^{n}e_i$ was zero, the components of $\mathbf{k}$ commuted with each other, so diagonalizing $\mathbf{k}$ we obtain direct integral decompositions (on constant fibre, $\mathscr{H}$)

$$H=\int H(\mathbf{k})d^3k; \quad \mathbf{k}=\int \mathbf{k}d^3k.$$

Our purpose here is to note a very simple formula for the k dependence of $H(\mathbf{k})$.

Theorem A.2. $H(\mathbf{k})=H(0)+\dfrac{k^2}{2M}-\left(\dfrac{\mathbf{k}}{M}\times\mathbf{B}\right)\cdot\mathbf{R}$ *where* $M=\sum m_i$.

Remarks. 1) Since $x_i\equiv r_i-r_n(i=1, \ldots, n-1)$ commutes with $\mathbf{k}$, we can choose $\mathscr{H}$ to be functions of the x_i. Notice that since $Q=0$

$$R=\sum_{i=1}^{n-1}c_ix_i$$

so R is a function on $\mathscr{H}$.

2) Physically, if we think of moving from $\mathbf{k}=\mathbf{0}$ to $\mathbf{k}=\mathbf{k}_0$, as boosting to a velocity $\mathbf{V}=\mathbf{k}_0/M$, then the formula for $\mathbf{H}(\mathbf{k}_0)$ has a very pleasing interpretation: $k_0^2/2M=1/2MV^2$ is the CM kinetic energy and $-\sum e_i(\mathbf{V}\times\mathbf{B})\cdot\mathbf{r}_i$ is just the potential of an electric field $V\times B$ that the Lorentz force law says is the effect of adding a constant to the velocities. Despite this attractive picture, we caution the reader that $\mathbf{k}/M$ is *not* the center of mass velocity, i.e., if $\boldsymbol{\varrho}=\sum_{i=1}^{n} m_i\mathbf{r}_i/M$, then $i[H,\boldsymbol{\varrho}]$ is not a constant of the motion, and, in particular, it is not $\mathbf{k}/M$. (Neither is $\mathbf{k}/M$ the center of charge velocity.)

Proof. Let

$$\boldsymbol{\varrho}=M^{-1}\sum_{i=1}^{n} m_i\mathbf{r}_i.$$

Then $[\mathbf{k}_j,\boldsymbol{\varrho}_\ell]=-i\delta_{j\ell}$ and thus $e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}$ translates $\mathbf{k}$ by $\boldsymbol{\alpha}$, i.e.

$$e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}\mathbf{k}\,e^{-i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}=\mathbf{k}-\boldsymbol{\alpha}.$$

Thus, if $A(\mathbf{k})$ represents the fiber of A at $\mathbf{k}$:

$$(e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}He^{-i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}})(\mathbf{k})=H(\mathbf{k}-\boldsymbol{\alpha}). \tag{A.1}$$

But

$$e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}\mathbf{p}_i e^{-i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}=\mathbf{p}_i-\frac{m_i}{M}\boldsymbol{\alpha}.$$

Thus, if $\boldsymbol{\pi}_j=\mathbf{p}_j-e_j(1/2\mathbf{B}\times\mathbf{r}_j)$

$$\begin{aligned}e^{i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}He^{-i\boldsymbol{\alpha}\cdot\boldsymbol{\varrho}}&=H+\sum_{j=1}^{n}(2m_j)^{-1}\left\{\left(\boldsymbol{\pi}_j-\frac{m_j}{M}\boldsymbol{\alpha}\right)^2-\boldsymbol{\pi}_j^2\right\}\\&=H+(2M)^{-1}\boldsymbol{\alpha}^2-(M)^{-1}\boldsymbol{\alpha}\cdot\sum_{j=1}^{n}\boldsymbol{\pi}_j\\&=H+(2M)^{-1}\boldsymbol{\alpha}^2-(M)^{-1}\boldsymbol{\alpha}\cdot(\mathbf{k}-\mathbf{B}\times\mathbf{R}).\end{aligned}$$

Now take $\mathbf{k}=\mathbf{0}$ and $\boldsymbol{\alpha}=-\mathbf{k}_0$ in (A.1) and obtain

$H(\mathbf{k}_0)=H(0)+(2M)^{-1}\mathbf{k}_0^2-M^{-1}\mathbf{k}_0\cdot(\mathbf{B}\times\mathbf{R})$. □

Acknowledgements. It is a pleasure to thank M. Aizenman, J. Feldman, A. Grossman, M. Klaus, A. Martin, L. Rosen, E. and R. Seiler for valuable discussions and L. Glasser and J. Cizek for telling us of [47]. B. Simon would like to thank the Technion Physics Department for its hospitality during the completion of this work.

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Communicated by J. Ginibre

Received August 11, 1980