Variational ground state for relativistic ions in strong magnetic fields

D. H. Jakubassa-Amundsen*

Mathematics Institute, University of Munich, Theresienstrasse 39, 80333 Munich, Germany

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The lowest bound state of a one-electron ion in a constant magnetic field **B** is calculated from the pseudorelativistic no-pair Brown-Ravenhall operator. The variational wave function is chosen as the product of a Landau function (in the transverse direction) and a hydrogenic state (in the longitudinal direction). The dependence of the ground-state energy on the nuclear charge Z as well as on the magnetic field strength is investigated, and a scaling with B/Z^2 is observed. Relativistic effects are shown to be important both for large B and large Z. When $B\to\infty$, a decrease of the ground-state energy with $\sqrt{B}$ is found in contrast to the $\ln B$ behavior of the Pauli operator.

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I. INTRODUCTION

A relativistic atomic electron of mass m in a magnetic field $\mathbf{B}=\nabla\times\mathbf{A}$ resulting from a vector potential $\mathbf{A}$ is described by the Dirac operator H,

$$H = D_A + V, \quad D_A = \boldsymbol{\alpha}\cdot(\mathbf{p}-e\mathbf{A}) + \beta m, \tag{1.1}$$

where $\boldsymbol{\alpha},\beta$ are Dirac matrices and $V=-\frac{\gamma}{x}$ is the Coulomb field generated by a point nucleus of charge Z fixed at the origin. The coordinate and momentum of the electron are denoted, respectively, by $\mathbf{x}$ and $\mathbf{p}$ (with $x=|\mathbf{x}|=\sqrt{x_1^2+x_2^2+x_3^2}$), and the field strength is $\gamma=Ze^2$. Relativistic units ($\hbar=c=1$) are used in the formulas, with $e^2\approx 1/137.04$ being the fine structure constant.

The unboundedness of H from below (which is due to the presence of the positron states) is usually remedied by approximating H with semibounded pseudorelativistic operators if pair creation plays no role. A widely used pseudorelativistic operator which nevertheless accounts for the spin degrees of freedom is the Brown-Ravenhall operator h^{BR}. It can be obtained from a projection of H onto the positive spectral subspace of the electron at $V=0$ [1] (see also [2] for its mathematical analysis). Equivalently, h^{BR} is the first-order term (in γ) of the Douglas-Kroll series which results from a unitary transformation scheme [3] applied to H in order to decouple the positive and negative spectral subspaces.

Our motivation to study the lowest bound state of the single-particle Brown-Ravenhall operator is the fact that it provides the bottom of the essential spectrum of the respective two-particle operator [4]. In the absence of magnetic fields the ground-state energy of h^{BR} was first calculated by Hardekopf and Sucher [5] by solving numerically the corresponding eigenvalue equation in momentum space. These authors also showed that the difference from the exact Dirac eigenvalue, $E_g^D=m\sqrt{1-\gamma^2}$, is of the order of γ^5 (which amounts to an error of 4% for $Z=80$).

The convergence of the Douglas-Kroll series was investigated numerically (up to the 14th order in γ) by Hess and co-workers [6,7] for the ground state of one-electron and multielectron ions and atoms. They performed linearly combined atomic orbital (LCAO) calculations within a large Gaussian basis set (in coordinate space), which they transformed into a basis that diagonalizes the kinetic energy operator entering into all potential terms [8]. A rigorous mathematical proof of the series convergence was given only recently [9].

There is also an early study on the transformed Dirac operator which allows for a magnetic field [10]. In that work relativistic effects were estimated in perturbation theory by making an expansion in $1/c$ rather than invoking the Douglas-Kroll series. Such an expansion is, however, ill-defined [11], and it led to a serious overprediction of the relativistic effects.

Indeed, investigations carried out for small nuclear charges ($Z\leqslant 20$) on the Dirac operator itself showed that relativistic effects on its ground-state energy are very small in the considered range of magnetic field strengths [12,13]. In one method the wave function was expanded in terms of Landau levels and the resulting coupled differential equations were solved in an approximate way [12]. Another method used a trial function in a variational calculation which consisted of a superposition of products of a Landau function and a relativistic hydrogenic function [13].

In the general case where the trial function is not closely related to the true ground state, a minimax principle must be used to obtain the lowest bound state of the Dirac operator [14]. If, however, an operator is bounded from below, the much simpler minimum principle in a variational calculation is sufficient. Then, on one hand, a large basis of trial functions can be taken in order to obtain accurate results. On the other hand, appropriately chosen simple variational functions reduce the numerical effort considerably while retaining the important features. Such an approach was used by Rau and co-workers [15] to describe atoms and one-electron ions in intense magnetic fields. Neglecting relativistic and spin effects, they employed the Schrödinger operator $H_S=\frac{1}{2m}(\mathbf{p}-e\mathbf{A})^2+V$. If spin is considered (in a nonrelativistic way), the Schrödinger operator turns into the Pauli operator $H_P=H_S-\frac{1}{2m}e\boldsymbol{\sigma}\cdot\mathbf{B}$. Its ground state differs from that of H_S by simply a shift of $-\frac{1}{2m}eB$ (see, e.g., [16,15]), so that spin effects can easily be included.

The variational ground-state wave function in [15] for a one-electron ion is taken as a product state consisting of a

*dj@mathematik.uni-muenchen.de

hydrogenlike 1s function (to an effective charge which serves as variational parameter) and a ground-state Landau function (for the transverse degrees of freedom). The so determined ground-state energy has the correct behavior at $B=0$ by construction. For $B\to\infty$, with $\frac{eB}{2m}$ subtracted, it also shows the correct $(\ln B)^2$ behavior. Note that it is rigorously proven that the ground-state energy of the Pauli operator decreases according to $(\ln B)^2$ as $B\to\infty$, the error being of the order of $\ln B \ln(\ln B)$ [17].

It can be shown that for large magnetic fields where the magnetic length $\frac{1}{\sqrt{eB}}$ is much smaller than the scaled Bohr radius a_0/Z, the electron occupies the lowest Landau band [18]. Then the ground-state function is no longer dominated by a spherical hydrogenic state, but this state degenerates to a one-dimensional function in the direction of $\mathbf{B}$ (while the transverse degrees of freedom are confined by the magnetic field). In fact, this longitudinal function becomes an eigenstate to a δ-type potential when $B\to\infty$ [19].

In the present work we extend the Rau *et al.* method to the pseudorelativistic operators. As a matter of fact, a magnetic field can easily be incorporated into the Douglas-Kroll series [20,21]. The Brown-Ravenhall operator is well defined in the form sense for $\gamma<\gamma_c$ [the bound $\gamma_c=\frac{2}{\pi}$, corresponding to $Z=87$ and valid for $\mathbf{A}\in L_{2,\mathrm{loc}}(\mathbb{R}^3)$ and $\mathbf{B}$ bounded or in $L_2(\mathbb{R}^3)$ has recently [24] been increased to $2/(\frac{\pi}{2}+\frac{2}{\pi})$ for locally bounded $\mathbf{A}$]. However, for the higher-order terms of the Douglas-Kroll series, this bound on γ decreases with the magnetic field strength and goes to zero as $B\to\infty$ [21]. Therefore, the higher-order terms are inferior to the first-order term for very large magnetic fields (despite their better approximation of E_g^D at $B=0$).

In our variational ansatz a one-dimensional hydrogenic function (together with the Landau function) is used for the ground state of the Brown-Ravenhall operator, valid if B is sufficiently large. The model is described in Sec. II and the asymptotic B-dependence is extracted in Sec. III. Section IV provides variational results for the $B=0$ case, including a comparison with the accurate ground-state energy. The B dependence of the ground-state energy (for $B/Z^2\lesssim 10^{13}$ G) is discussed in Sec. V with particular emphasis on a scaling property, as well as on the onset of relativistic effects. The conclusion is drawn in Sec. VI.

II. VARIATIONAL MODEL

The Brown-Ravenhall operator in a magnetic field is given by [22,21]

$$h^{\mathrm{BR}} = E_A + V_1 + V_2, \tag{2.1}$$

$$V_1 = -\gamma A_E \frac{1}{x} A_E, \quad V_2 = -\gamma A_E \frac{\boldsymbol{\sigma}\cdot\mathbf{p}_A}{E_A+m}\frac{1}{x}\frac{\boldsymbol{\sigma}\cdot\mathbf{p}_A}{E_A+m}A_E,$$

where $E_A=|D_A|$ is the kinetic energy operator,

$$E_A = \sqrt{p_A^2 - e\boldsymbol{\sigma}\cdot\mathbf{B}+m^2}, \quad A_E = \sqrt{\frac{E_A+m}{2E_A}} \tag{2.2}$$

and $\mathbf{p}_A=\mathbf{p}-e\mathbf{A}$. $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ is the vector of Pauli spin matrices. In the following we take $\mathbf{B}=B\mathbf{e}_3$ to be a constant magnetic field along the $\mathbf{e}_3$ axis, generated by

$$\mathbf{A}(\mathbf{x}) = \frac{B}{2}(-x_2,x_1,0) \tag{2.3}$$

which obeys $\boldsymbol{\nabla}\cdot\mathbf{A}=0$. h^{BR} acts in the Hilbert space $L_2(\mathbb{R}^3)\otimes\mathbb{C}^2$ and extends to a self-adjoint operator for $\gamma<\gamma_c$. Its form domain is $H_{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^2$ where $H_{1/2}$ denotes a Sobolev space.

Let us first switch off the scalar potentials V_1 and V_2. Then we can profit from the fact that $E_A^2=2mH_P(V=0)+m^2$ so that E_A^2 (and thus E_A) is diagonalized by the eigenstates of the Pauli operator.

The ground state is characterized by a spin-up state, $\psi_{0\uparrow}=\psi_{0k}\binom{1}{0}$, resulting in $-e\boldsymbol{\sigma}\cdot\mathbf{B}\psi_{0\uparrow}=-e\sigma_3 B\psi_{0\uparrow}=-eB\psi_{0\uparrow}$. Taking the normalized lowest Landau function [16,15] and allowing for a free electronic motion in the x_3 direction, we have

$$\psi_{0k}(\varrho,x_3) = N_0 e^{-eB\varrho^2/4}e^{ikx_3}, \quad N_0=\sqrt{\frac{eB}{2\pi}},$$

and

$$E_A^2\psi_{0\uparrow} = [(eB+k^2)-eB+m^2]\psi_{0\uparrow} = (k^2+m^2)\psi_{0\uparrow}, \tag{2.4}$$

where $\varrho=\sqrt{x_1^2+x_2^2}$ is the radial coordinate perpendicular to $\mathbf{B}$. Thus the corresponding eigenvalue of E_A is given, independently of B, by the energy $\sqrt{k^2+m^2}$ of a free relativistic electron of momentum k.

The presence of the Coulomb field restricts the motion in the x_3 direction and we choose for our variational wave function a superposition of momentum states, $\psi_g=\psi_0\binom{1}{0}$, normalized to unity, with

$$\psi_0(\mathbf{x}) = \tilde{N}_0 e^{-eB\varrho^2/4}\int_{-\infty}^{\infty}dk\tilde{f}(k)e^{ikx_3}, \tag{2.5}$$

$$\tilde{f}(k) = \frac{aZ'}{\pi\sqrt{Z'^2+k^2}}K_1(a\sqrt{Z'^2+k^2}), \quad \tilde{N}_0=\left(\frac{eB}{4\pi a K_1(2aZ')}\right)^{1/2},$$

where K_1 is a modified Bessel function and

$$a = 1/\sqrt{eB} \tag{2.6}$$

the magnetic length. The function $\tilde{f}$ is taken as the Fourier transform of a one-dimensional hydrogenic ground-state function to a parameter $Z'=Z_{\mathrm{eff}}/a_0$ [where Z_{eff} is an effective charge—our variational parameter—and $a_0=\hbar^2/(me^2)$ the Bohr radius] [[23] (3.914)],

$$\int_{-\infty}^{\infty}dk\tilde{f}(k)e^{ikx_3} = e^{-Z'\sqrt{a^2+x_3^2}}. \tag{2.7}$$

The idea behind the choice (2.7) is the confinement of the electronic motion in the (x_1,x_2) direction by the magnetic length, valid if $a\ll a_0/Z$ or equivalently, $B\gg Z^2m^2e^3$ (in conventional units, $1m^2e^3c/\hbar^3=2.35\times10^9$ G). Its advantage compared to the ansatz used in [15], where $\exp(-Z'x)$ is taken instead of $\exp(-Z'\sqrt{a^2+x_3^2})$, is the exact diagonalization of the kinetic energy E_A because the Fourier transform (2.7) does not affect the transverse degrees of freedom. We note in passing that in [15] the cyclotron radius $r_c=\sqrt{2}a$ is taken as the magnetic scale. This leads to the condition $B \geqslant 2Z^2m^2e^3$.

Let us now determine the expectation value of $h^{BR}-m$ (where the electron's rest energy mc^2 is subtracted) with respect to the function ψ_g. For the kinetic energy we obtain, using Eq. (2.7) for the inverse Fourier transformation,

$$\begin{aligned}(\psi_g,(E_A-m)\psi_g) &= \tilde{N}_0\int_{-\infty}^{\infty} dk\tilde{f}(k)\int_{\mathbb{R}^3} d\mathbf{x}\bar{\psi}_g(\mathbf{x})(\sqrt{k^2+m^2}-m)e^{-eB\varrho^2/4}e^{ikx_3}\\ &= \frac{2aZ'^2}{\pi K_1(2aZ')}\int_0^{\infty} dk\frac{1}{Z'^2+k^2}K_1^2(a\sqrt{Z'^2+k^2})\\ &\quad\times(\sqrt{k^2+m^2}-m).\end{aligned} \tag{2.8}$$

In order to evaluate the potential terms, also $\bar{\psi}_g$ must be taken in its momentum representation (2.5) because in V_1 and V_2, E_A enters on both sides of the Coulomb potential $-\gamma/x$. As $\tilde{f}$ and A_E are even functions of k we obtain

$$(\psi_g,V_1\psi_g) = -4\gamma\tilde{N}_0^2\int_{-\infty}^{\infty} dx_3F^2(x_3)2\pi\int_0^{\infty}\varrho d\varrho \times e^{-eB\varrho^2/2}\frac{1}{\sqrt{\varrho^2+x_3^2}},$$

$$F(x_3) = \int_0^{\infty} dk\tilde{f}(k)A_E\cos kx_3. \tag{2.9}$$

We have [[23] (3.468)]

$$2\int_0^{\infty}\varrho d\varrho e^{-eB\varrho^2/2}\frac{1}{\sqrt{\varrho^2+x_3^2}} = \sqrt{\frac{2\pi}{eB}}e^{eBx_3^2/2}\left[1-\phi\left(|x_3|\sqrt{\frac{eB}{2}}\right)\right]. \tag{2.10}$$

For the numerical evaluation of the probability function ϕ we use an integral representation (for $0 \leqslant y \lesssim 50$) and, respectively, the asymptotic expansion [[23] (8.254)] (for $y>50$),

$$\begin{aligned}E(y) &:= \sqrt{\pi}e^{y^2}[1-\phi(y)]\\ &= \int_0^{\infty} d\tau\frac{e^{-\tau}}{\sqrt{\tau+y^2}} = \frac{1}{y}\left[1-\frac{1}{2y^2}+\frac{3}{4y^4}-\frac{15}{8y^6}+O\left(\frac{1}{y^8}\right)\right].\end{aligned} \tag{2.11}$$

Concerning the potential term V_2 we must evaluate $\boldsymbol{\sigma}\cdot\mathbf{p}_A\frac{1}{x}\boldsymbol{\sigma}\cdot\mathbf{p}_A$ on a spin-up eigenstate of type (2.4). With the vector potential $\mathbf{A}$ from Eq. (2.3) and $\mathbf{p}=-i\boldsymbol{\nabla}$, we obtain

$$(\mathbf{p}-e\mathbf{A})\psi_{0k} = \begin{pmatrix}\frac{eB}{2}(ix_1+x_2)\\ \frac{eB}{2}(ix_2-x_1)\\ k\end{pmatrix}\psi_{0k} \tag{2.12}$$

so that, with $\psi_{0\uparrow}(k)=\psi_{0k}\binom{1}{0}$,

$$\begin{aligned}&\left(\psi_{0\uparrow}(k'),\boldsymbol{\sigma}\cdot\mathbf{p}_A\frac{1}{x}\boldsymbol{\sigma}\cdot\mathbf{p}_A\psi_{0\uparrow}(k)\right)\\ &\quad=\left(\psi_{0\uparrow}(k'),\left(\mathbf{p}_A\frac{1}{x}\mathbf{p}_A+i\boldsymbol{\sigma}\cdot\mathbf{p}_A\cdot\frac{1}{x}\mathbf{p}_A\right)\psi_{0\uparrow}(k)\right)\\ &\quad=\left(\psi_{0\uparrow}(k'),\frac{kk'}{x}\psi_{0\uparrow}(k)\right).\end{aligned} \tag{2.13}$$

Hence, the restriction of this operator to $\psi_{0\uparrow}$ is independent of B. Therefore,

$$(\psi_g,V_2\psi_g) = -4\gamma\tilde{N}_0^2\int_{-\infty}^{\infty} dx_3G^2(x_3)2\pi\int_0^{\infty}\varrho d\varrho \times e^{-eB\varrho^2/2}\frac{1}{\sqrt{\varrho^2+x_3^2}},$$

$$G(x_3) = \int_0^{\infty} dk\tilde{f}(k)A_E\frac{1}{E_A+m}k\sin kx_3. \tag{2.14}$$

Note that the integrands in Eqs. (2.9) and (2.14) are even functions of x_3, simplifying the respective integration region to $[0,\infty)$.

For the numerical evaluation of the integrals it is convenient to shift variables from x_3 to y by means of $y=\sqrt{\frac{eB}{2}}x_3$ in order to get rid of the B dependence in the function E from Eq. (2.11). In turn, we measure the magnetic field in units of Z^2, i.e., $B=\lambda Z^2[m^2e^3]$, $\lambda \geqslant 2$, and introduce the scaled variables

$$\tilde{a} = a\sqrt{\frac{eB}{2}} = \frac{1}{\sqrt{2}},\quad \mu = m/\sqrt{\frac{eB}{2}} = \frac{\sqrt{2}}{\sqrt{\lambda}Ze^2},$$

$$\tilde{Z} = Z'/\sqrt{\frac{eB}{2}} = \frac{Z_{\text{eff}}\sqrt{2}}{\sqrt{\lambda}Z},\quad \kappa = k/\sqrt{\frac{eB}{2}}. \tag{2.15}$$

Then we obtain for the energy functional $E_0[Z_{\text{eff}}]$,

$$\begin{aligned}(\psi_g,(h^{BR}-m)\psi_g) &= c_0\int_0^{\infty} d\kappa\frac{1}{\tilde{Z}^2+\kappa^2}\\ &\quad\times K_1^2(\tilde{a}\sqrt{\tilde{Z}^2+\kappa^2})(\sqrt{\kappa^2+\mu^2}-\mu)\\ &\quad-\frac{Ze^2c_0}{\pi}\int_0^{\infty} dyE(y)(I_1^2+I_2^2) =: E_0[Z_{\text{eff}}],\end{aligned} \tag{2.16}$$

where

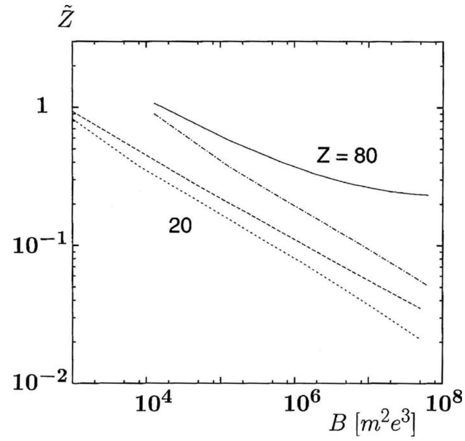

FIG. 1. $\tilde{Z}=Z_{\mathrm{eff}}\sqrt{2}/(Z\sqrt{\lambda})$ as a function of the magnetic field strength B (in units 2.35×10^9 G) for $Z=20$ (– – –) and $Z=80$ (—). Results are also shown for the nonrelativistic model of Rau and co-workers [15]: $Z=20$ (---) and $Z=80$ (-·-·-).

$$c_0 = \frac{\sqrt{2\lambda}Z\tilde{a}\tilde{Z}^2}{\pi K_1(2\tilde{a}\tilde{Z})}me^2,$$

$$I_1 = \int_0^\infty d\kappa \frac{1}{\sqrt{\tilde{Z}^2+\kappa^2}}K_1(\tilde{a}\sqrt{\tilde{Z}^2+\kappa^2}) \times\left(\frac{\sqrt{\kappa^2+\mu^2}+\mu}{\sqrt{\kappa^2+\mu^2}}\right)^{1/2}\cos(\kappa y),$$

$$I_2 = \int_0^\infty d\kappa \frac{\kappa}{\sqrt{\kappa^2+\mu^2}+\mu}\frac{1}{\sqrt{\tilde{Z}^2+\kappa^2}}K_1(\tilde{a}\sqrt{\tilde{Z}^2+\kappa^2}) \times\left(\frac{\sqrt{\kappa^2+\mu^2}+\mu}{\sqrt{\kappa^2+\mu^2}}\right)^{1/2}\sin(\kappa y). \tag{2.17}$$

Finally we determine Z_{eff} from the variational principle

$$\delta E_0[Z_{\mathrm{eff}}] = 0. \tag{2.18}$$

Equivalently, the ground-state energy of the Brown-Ravenhall operator is estimated from above by $E_g^{\mathrm{BR}} = \min_{Z_{\mathrm{eff}}>0} E_0[Z_{\mathrm{eff}}]$.

III. ASYMPTOTIC B-DEPENDENCE

In this section we will show that E_g^{BR} decreases according to $\sqrt{B}$ for $B\to\infty$. This is done by considering the behavior of the scaled variational parameter $\tilde{Z}$ which solves Eq. (2.18). Figure 1 shows $\tilde{Z}$ as a function of B for $Z=20$ and 80. Whereas $\tilde{Z}$ decreases for $Z=20$ according to a power law ($\sim B^{-0.3}$) even for the highest fields considered, there is a distinct flattening of $\tilde{Z}$ with increasing B in the relativistic case $Z=80$. These numerical results suggest that for relativistic ions the optimized scaled variational parameter tends to a strictly positive constant as $B\to\infty$, a conjecture which is proven below.

TABLE I. $\tilde{Z}$ and the corresponding scaled ground-state energy $\tilde{E}(0,\tilde{Z}(0))=E_g^{\mathrm{BR}}/(Z\sqrt{\lambda})$ in atomic units at $\mu=0$ (corresponding to $B=\infty$) for nuclear charges Z ranging from 20 to 80.

Z	$\tilde{Z}(0)$	$E_g^{\mathrm{BR}}/\sqrt{B}$
20	0.0074	−0.0718
40	0.054	−1.425
60	0.137	−4.777
80	0.239	−9.868

In order to derive the asymptotic B dependence of the ground-state energy we define $\tilde{E}(\mu,\tilde{Z}) = (\psi_g,(h^{\mathrm{BR}}-m)\psi_g)/\sqrt{B}$ according to Eq. (2.16). At $B=\infty$ we have $\mu=0$ where the right-hand side (rhs) of Eq. (2.16) divided by $\sqrt{B}$ is independent of B and so is the variational solution $\tilde{Z}(0)$. Table I gives the numerical results for $\tilde{Z}(0)$ and $\tilde{E}(0,\tilde{Z}(0))$ for various nuclear charges Z. Thus a finite $\tilde{Z}(0)>0$ guarantees not only that $|\tilde{E}(0,\tilde{Z}(0))|<\infty$ (as the respective integrals are convergent), but also that $\tilde{E}(0,\tilde{Z}(0))<0$.

The existence of the limit $\lim_{\mu\to0}\tilde{Z}(\mu)=\tilde{Z}(0)$ implies the existence of $\lim_{\mu\to0}\tilde{E}(\mu,\tilde{Z}(\mu))=\tilde{E}(0,\tilde{Z}(0))=-\tilde{c}$ as discussed near the end of this section. As a result,

$$E_g^{\mathrm{BR}} \sim -\tilde{c}B^{1/2} \quad \text{as } B\to\infty. \tag{3.1}$$

In order to prove the above conjecture we start by showing that there are constants a_0,b_0 so that as $B\to\infty$ the optimized $\tilde{Z}$ obeys $0<a_0\leq\tilde{Z}\leq b_0<\infty$. In other words we prove by contradiction that (i) $\tilde{Z}$ does not tend to zero and (ii) $\tilde{Z}<\infty$ as $B\to\infty$.

(i) Let us assume first that $\tilde{Z}\to0$ as $B\to\infty$, as in the nonrelativistic case. In the unscaled variables this corresponds to $\tilde{a}\tilde{Z}=aZ'\to0$. Since $a\to0$ like $B^{-1/2}$ we thus assume that Z' increases more weakly than $B^{1/2}$ as $B\to\infty$. This property holds for all effective charges in a neighborhood of the solution to the variational principle. Therefore, we will calculate the kinetic and potential energy as a function of the effective charge and only subsequently consider the variational principle.

From the behavior of the modified Bessel function near zero, $K_1(z)\sim\frac{1}{z}$ as $z\to0$, we obtain for the kinetic energy (2.8),

$$(\psi_g,E_A\psi_g) \sim \tilde{c}Z'^3\int_0^\infty dk\frac{1}{(Z'^2+k^2)^2}\sqrt{k^2+m^2}, \tag{3.2}$$

independent of a. With $k=Z'\zeta$ and $Z'\to\infty$ with $B\to\infty$,

$$Z'^3\int_0^\infty dk\frac{\sqrt{k^2+m^2}}{(Z'^2+k^2)^2} = Z'\int_0^\infty d\zeta\frac{\sqrt{\zeta^2+(m/Z')^2}}{(1+\zeta^2)^2} \sim \tilde{c}Z', \tag{3.3}$$

where $\tilde{c}>0$, so that the kinetic energy becomes linear in Z'. We note that the step from Eqs. (2.8) to (3.2) implies an interchange of limits $B\to\infty$ and $k\to\infty$. This relies on Eq. (3.2) being a convergent majorant since K_1 is monotonically decreasing.

For the potential energy we use Eq. (2.17) with the substitution $\kappa=\tilde{Z}\eta$ [[23], (3.723)],

$$I_1 \sim \frac{1}{\tilde{a}\tilde{Z}}\int_0^\infty d\eta \frac{\cos(\tilde{Z}y\eta)}{1+\eta^2} = \frac{\pi}{2\tilde{a}\tilde{Z}}e^{-\tilde{Z}y}. \tag{3.4}$$

Further, from Eq. (2.11) with $M=50$,

$$\int_0^\infty dy E(y)e^{-2\tilde{Z}y} = \int_0^M dy E(y) e^{-2\tilde{Z}y} + \int_M^\infty dy\left[\frac{1}{y}+O\left(\frac{1}{y^3}\right)\right]e^{-2\tilde{Z}y}$$
$$= c(\tilde{Z}) - \mathrm{Ei}(-2\tilde{Z}M) \to \tilde{c} - \ln(\tilde{Z}) \quad (\tilde{Z}\to 0), \tag{3.5}$$

since the first integral as well as the higher-order terms (in $\frac{1}{y}$) of the second integral lead to a finite result which is independent of $\tilde{Z}$ as $\tilde{Z}\to 0$. We have also used the near-zero expansion of the exponential integral Ei [[23] (3.352), (8.214)].

For the second contribution I_2 we have [[23], (3.723)],

$$I_2 \sim \frac{1}{\tilde{a}\tilde{Z}}\int_0^\infty d\eta \frac{\sin(\tilde{Z}y\eta)}{1+\eta^2} = \frac{1}{2\tilde{a}\tilde{Z}}[e^{-\tilde{Z}y}\,\mathrm{Ei}(\tilde{Z}y) - e^{\tilde{Z}y}\,\mathrm{Ei}(-\tilde{Z}y)]. \tag{3.6}$$

Dividing again the integration region of $\int_0^\infty dy E(y) I_2^2$ into the intervals $[0,M]\cup[M,\infty)$ and using that $|\int_0^\infty d\eta \sin(\tilde{Z}y\eta)/(1+\eta^2)|\leq\frac{\pi}{2}$, the integral over $[0,M]$ is finite irrespective of $\tilde{Z}$ [if the prefactor $(\tilde{a}\tilde{Z})^{-1}$ is ignored]. The boundedness of the integral in Eq. (3.6) also assures the convergence concerning the higher-order terms (in $\frac{1}{y}$) in the integral over $[M,\infty)$. In order to show that the remaining integral is bounded we substitute $\tilde{Z}y=\zeta$ and obtain from Eq. (3.6),

$$\int_M^\infty dy \frac{1}{y} I_2^2 \sim \frac{1}{(2\tilde{a}\tilde{Z})^2}\int_0^\infty \frac{d\zeta}{\zeta}[e^{-\zeta}\,\mathrm{Ei}(\zeta) - e^{\zeta}\,\mathrm{Ei}(-\zeta)]^2 \tag{3.7}$$

as $\tilde{Z}\to 0$. With $e^{-\zeta}\,\mathrm{Ei}(\zeta)-e^{\zeta}\,\mathrm{Ei}(-\zeta)\sim -2\zeta\ln\zeta$ as $\zeta\to 0$ the integral converges near zero.

For investigating $\zeta\to\infty$ we make a partial integration of the left-hand side (lhs) of Eq. (3.6). Then

$$\int_M^\infty dy \frac{1}{y} I_2^2 \sim \frac{1}{(\tilde{a}\tilde{Z})^2}\int_0^\infty \frac{d\zeta}{\zeta}\left(\frac{1}{\zeta} - \frac{2}{\zeta}\int_0^\infty d\eta \frac{\eta\cos\zeta\eta}{(1+\eta^2)^2}\right)^2. \tag{3.8}$$

Since $|\cos\zeta\eta|\leq 1$, the η-integral is finite for all ζ so that the ζ-integral converges for $\zeta\to\infty$.

Collecting results,

$$(\psi_g,(V_1+V_2)\psi_g) \sim \tilde{c}\sqrt{\lambda}\tilde{Z}^3\frac{1}{\tilde{Z}^2}\ln(\tilde{Z}) \sim -c_2 Z'\ln B \tag{3.9}$$

as $B\to\infty$ where $c_2>0$ is some constant. The variational functional becomes

$$E_0[Z_{\text{eff}}] \sim (\tilde{c} - c_2\ln B)Z_{\text{eff}}/a_0 \quad (B\to\infty) \tag{3.10}$$

and it is obvious that $\delta E_0[Z_{\text{eff}}]=0$ has no solution.

(ii) Let us now assume that $aZ'\to\infty$ as $B\to\infty$. As a consequence, $Z'\sim B^{1/2}w(B)$ with $w(B)\to\infty$ as $B\to\infty$. Using the asymptotic behavior of the modified Bessel function, $K_1(z)\sim\sqrt{\frac{\pi}{2}}e^{-z}/\sqrt{z}$ as $z\to\infty$, we have from Eq. (2.8),

$$(\psi_g,E_A\psi_g) \sim \tilde{c}Z'\sqrt{aZ'}\int_0^\infty d\zeta \frac{\zeta}{(1+\zeta^2)^{3/2}}e^{-2aZ'(\sqrt{1+\zeta^2}-1)}. \tag{3.11}$$

We make further the substitution $x=2aZ'(\sqrt{1+\zeta^2}-1)$. This leads to

$$(\psi_g,E_A\psi_g) \sim \frac{\tilde{c}}{2}\sqrt{\frac{Z'}{a}}\int_0^\infty \frac{dx}{(1+x/2aZ')^2}e^{-x}. \tag{3.12}$$

The integral converges to a finite (nonzero) limit as $aZ'\to\infty$. In order to show this we use a sandwich estimate,

$$\int_0^{2aZ'}\frac{dx}{4}e^{-x} \leq \int_0^\infty \frac{dx}{(1+x/2aZ')^2}e^{-x} \leq \int_0^\infty dx e^{-x}. \tag{3.13}$$

For $aZ'\to\infty$ the lower bound tends to $\frac{1}{4}$, and the upper bound is 1. Thus, the kinetic energy behaves like $\sqrt{Z'/a}\sim B^{1/2}\sqrt{w(B)}$. As a consequence, the potential energy must decrease at least like $B^{1/2}\sqrt{w(B)}$ in order to produce a bound state. It is rigorously established that such a bound ground state of h^{BR} exists for arbitrarily large B if $\gamma<\frac{2}{\pi}$ [24,4,25].

On the other hand, the ground-state energy can decrease at most like $\sqrt{B}$. This is due to the relative form boundedness of V_1+V_2 with respect to E_A. Indeed, following [2,26] we can write $(\psi,(V_1+V_2)\psi)=(\tilde{\psi},\tilde{\beta}U_0VU_0^{-1}\tilde{\beta}\tilde{\psi})$ for $\psi\in H_{1/2}(\mathbb{R}^3)\otimes\mathbb{C}^2$ and $\tilde{\psi}=\binom{\psi}{0}$. Here, $\tilde{\beta}=\frac{1+\beta}{2}$ projects onto the upper components of a Dirac four-spinor and U_0 is the unitary Foldy-Wouthuysen transformation which commutes with E_A. Then one gets from the diamagnetic inequality and the Kato inequality [26]

$$|(\psi,(V_1+V_2)\psi)| = |(\psi_0,V\psi_0)| \leq \gamma\frac{\pi}{2}(\psi_0,\sqrt{E_A^2+e\boldsymbol{\sigma}\cdot\mathbf{B}}\psi_0)$$
$$\leq \gamma\frac{\pi}{2}(\psi,E_A\psi) + \gamma\frac{\pi}{2}\sqrt{eB}\|\psi\|^2, \tag{3.14}$$

where we have introduced $\psi_0=U_0^{-1}\tilde{\beta}\tilde{\psi}=U_0^{-1}\tilde{\psi}$. This leads to the inequality,

$$(\psi,h^{\rm BR}\psi) \geq \left(1-\gamma\frac{\pi}{2}\right)(\psi,E_A\psi) - \gamma\frac{\pi}{2}\sqrt{eB}\|\psi\|^2. \tag{3.15}$$

For $\gamma<\frac{2}{\pi}$ the rhs of Eq. (3.15) is thus a lower bound for the ground-state energy, allowing at most a decrease according to $B^{1/2}$. This contradicts $aZ'\to\infty$.

Finally we prove that $\tilde{Z}$ as a function of the inverse magnetic field converges to its limiting value at $B=\infty$ (allowing for the choice $a_0=b_0$) and so does $\tilde{E}(\mu,\tilde{Z}(\mu))$. Since for $B\to\infty$ we have $\tilde{Z}\neq 0$ at the energy minimum we can assume $B\geq B_0$ sufficiently large so that $\tilde{Z}$ can be restricted to a positive interval $\tilde{I}$. Then the integrands in Eqs. (2.16) and (2.17) are continuous in κ and μ in the interval $[0,\infty)\times[0,\mu_0]$ with $\mu_0=m/\sqrt{eB_0/2}$ except possibly in the point $(\kappa,\mu)=(0,0)$, and they are also continuous and continuously differentiable with respect to $\tilde{Z}$ for $\tilde{Z}\in\tilde{I}$. Since all integrals are convergent, $\tilde{E}$ is a continuous function of μ and $\tilde{Z}$, and so is the derivative $\partial\tilde{E}/d\tilde{Z}$. The existence of a numerical solution $\tilde{Z}(\mu_0)$ satisfying $\frac{\partial\tilde{E}}{\partial\tilde{Z}}(\mu_0,\tilde{Z}(\mu_0))=0$ together with the existence of a ground state for any $\mu<\mu_0$ guarantees that there is a continuous solution $\tilde{Z}(\mu)$ to $\frac{\partial\tilde{E}}{\partial\tilde{Z}}(\mu,\tilde{Z}(\mu))=0$ for $0\leq\mu\leq\mu_0$, whence also $\tilde{E}(\mu,\tilde{Z}(\mu))$ is continuous. This assures the convergence of $\tilde{E}(\mu,\tilde{Z}(\mu))\to\tilde{E}(0,\tilde{Z}(0))$ as $\mu\to 0$. Thus our result (3.1) is established.

We note that in the nonrelativistic case, the operator $\sqrt{k^2+m^2}-m$ must be replaced by $\frac{k^2}{2m}$ in Eq. (3.2) so that the kinetic energy behaves like Z'^2 instead of Z' as $B\to\infty$. This gives [15] $E_0^{nr}[Z_{\rm eff}]\sim\tilde{c}_1Z_{\rm eff}^2-\tilde{c}_2Z_{\rm eff}\ln B$ and hence

$$\delta E_0^{nr}[Z_{\rm eff}]=0 \Leftrightarrow Z_{\rm eff}=\frac{\tilde{c}_2}{2\tilde{c}_1}\ln B, \tag{3.16}$$

which leads to $E_g^{nr}\sim-\tilde{c}(\ln B)^2$ as $B\to\infty$, where $\tilde{c}$ is a generic constant.

The nonrelativistic results according to [15], described in Sec. V, are also included in Fig. 1. They show a power law decrease of $\tilde{Z}$ with B for both values of Z. Note the deviations from the Brown-Ravenhall result even in the nonrelativistic case ($Z=20$), which become larger when B increases.

Although not shown in the figure we have tested the convergence of $\tilde{Z}(\mu)$ for $Z=80$ up to $\lambda=10^{13}$. Actually $\tilde{Z}(\mu)$ is not monotonically decreasing towards $\tilde{Z}(0)$, but has a shallow minimum near $\lambda=10^5$ (caused by the spin-dependent potential V_2).

IV. FIELD-FREE CASE

In this section we compare the ground-state energy of the Brown-Ravenhall operator for $B=0$, obtained from a variational model, with the accurate LCAO results from [7]. In order to study the dependence of this ground-state energy on the variational wave function we have used two types, a spherical hydrogenic wave function,

$$\tilde{\psi}_0(\mathbf{x})=\frac{Z'^{3/2}}{\sqrt{\pi}}e^{-Z'x}=\int_{\mathbb{R}^3}d\mathbf{k}\tilde{f}_0(k)e^{i\mathbf{k}\cdot\mathbf{x}},$$

$$\tilde{f}_0(k)=\frac{1}{\pi^{5/2}}\frac{Z'^{5/2}}{(k^2+Z'^2)^2}, \tag{4.1}$$

and a relativistic function,

$$\psi_{\rm rel}(\mathbf{x})=N_0x^{\tilde{\gamma}}e^{-Z'x}=\int_{\mathbb{R}^3}d\mathbf{k}\tilde{f}_{\rm rel}(k)e^{i\mathbf{k}\cdot\mathbf{x}},$$

$$\tilde{f}_{\rm rel}(k)=N_0\frac{\Gamma(2+\tilde{\gamma})}{2\pi^2k}\frac{1}{(Z'^2+k^2)^{1+\tilde{\gamma}/2}}\sin\left((2+\tilde{\gamma})\arctan\frac{k}{Z'}\right),$$

$$N_0=\frac{(2Z')^{3/2+\tilde{\gamma}}}{\sqrt{4\pi\Gamma(3+2\tilde{\gamma})}},\qquad \tilde{\gamma}=\sqrt{1-(Z'e^2)^2}-1, \tag{4.2}$$

which is (apart from a constant) identical to the large component of the Dirac ground-state wave function. Their Fourier representations [[23] (3.944)] are required because $e^{i\mathbf{kx}}$ is an eigenfunction to $E_p=E_A(B=0)$ with eigenvalue $\sqrt{k^2+m^2}$.

Using the nonrelativistic spin-up state, $\tilde{\psi}_{0\uparrow}=\tilde{\psi}_0\binom{1}{0}$, we obtain for the expectation value of the kinetic energy,

$$(\tilde{\psi}_{0\uparrow},E_p\tilde{\psi}_{0\uparrow})=\frac{Z'^{3/2}}{\sqrt{\pi}}\int_{\mathbb{R}^3}d\mathbf{k}\tilde{f}_0(k)\sqrt{k^2+m^2}\int_{\mathbb{R}^3}d\mathbf{x}e^{-Z'x}e^{i\mathbf{k}\cdot\mathbf{x}}$$
$$=\frac{32Z'^5}{\pi}\int_0^\infty k^2dk\frac{\sqrt{k^2+m^2}}{(k^2+Z'^2)^4}. \tag{4.3}$$

This integral can be evaluated analytically in terms of a hypergeometric function ${}_2F_1$ [[23], (3.259)] so that

$$(\tilde{\psi}_{0\uparrow},(E_p-m)\tilde{\psi}_{0\uparrow})=m\left[\frac{64}{15\pi}{}_2F_1\left(-\frac{1}{2},\frac{3}{2},\frac{7}{2},1-\left(\frac{Z'}{m}\right)^2\right)-1\right]. \tag{4.4}$$

Denoting $E_k=\sqrt{k^2+m^2}$ and $A_k=[(E_k+m)/E_k]^{1/2}$ we obtain for the first potential term,

$$(\tilde{\psi}_{0\uparrow},V_1\tilde{\psi}_{0\uparrow})$$
$$=-\frac{\gamma}{2}\int_{\mathbb{R}^3}d\mathbf{x}\int_{\mathbb{R}^6}d\mathbf{k}'d\mathbf{k}\tilde{f}_0(k')e^{-i\mathbf{k}'\cdot\mathbf{x}}A_{k'}\frac{1}{x}\tilde{f}_0(k)e^{i\mathbf{k}\cdot\mathbf{x}}A_k$$
$$=-\frac{32\gamma Z'^5}{\pi^2}\int_0^\infty\frac{dx}{x}\left(\int_0^\infty kdk\frac{1}{(k^2+Z'^2)^2}A_k\sin kx\right)^2. \tag{4.5}$$

Concerning V_2 we note that due to the symmetry of the integration intervals the expectation value of $\boldsymbol{\sigma}\cdot\mathbf{p}\frac{1}{x}\boldsymbol{\sigma}\mathbf{p}$ is just $\frac{1}{x}\mathbf{k}'\cdot\mathbf{k}$ (since E_k, A_k, and $\tilde{f}_0$ are even functions). We write the angular integral of $d\mathbf{k}$ in the following way:

$$\begin{aligned}\int_{S^2} d\Omega_k \mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} &= -i\nabla_{\mathbf{x}} \int_{S^2} d\Omega_k e^{i\mathbf{k}\cdot\mathbf{x}} \\ &= -i\nabla_{\mathbf{x}} \frac{4\pi \sin kx}{kx} \\ &= 4\pi i \mathbf{x} \frac{k}{x} j_1(kx),\end{aligned} \tag{4.6}$$

where j_1 is a spherical Bessel function. Then

$$\begin{aligned}(\tilde{\psi}_{0\uparrow}, V_2 \tilde{\psi}_{0\uparrow}) &= -\frac{\gamma}{2}\int_{\mathbb{R}^3} d\mathbf{x} \int_{\mathbb{R}^6} d\mathbf{k}' d\mathbf{k} \tilde{f}_0(k') \\ &\quad \times e^{-i\mathbf{k}'\cdot\mathbf{x}} \frac{1}{E_{k'}+m} A_{k'} \frac{1}{x} \mathbf{k}' \cdot \mathbf{k} \frac{1}{E_k+m} A_k \tilde{f}_0(k) e^{i\mathbf{k}\cdot\mathbf{x}} \\ &= -\frac{32\gamma Z'^5}{\pi^2}\int_0^\infty x dx \\ &\quad \times \left(\int_0^\infty k^3 dk \frac{1}{(k^2+Z'^2)^2} \frac{1}{E_k+m} A_k j_1(kx) \right)^2.\end{aligned} \tag{4.7}$$

We note that Eq. (4.7) is subordinate to Eq. (4.5) by approximately a factor of $(\frac{k}{E_k+m})^2 \sim (\frac{Z'}{2m})^2 = (\frac{Z_{\text{eff}}}{2\times 137.04})^2$ if $k \ll m$, respectively, $Z' \ll m$. However, V_2 gains importance at relativistic charges.

For the relativistic function (4.2) we proceed in a similar way and obtain the result, setting $\psi_{\text{rel}\uparrow} = \psi_{\text{rel}}\binom{1}{0}$,

$$\begin{aligned}(\psi_{\text{rel}\uparrow}, (E_p - m)\psi_{\text{rel}\uparrow}) &= c_{00}\int_0^\infty dk \frac{1}{(Z'^2+k^2)^{2+\tilde{\gamma}}} \\ &\quad \times \sin^2\left((2+\tilde{\gamma}) \arctan \frac{k}{Z'} \right) \\ &\quad \times (\sqrt{k^2+m^2} - m),\end{aligned}$$

$$c_{00} = \frac{16}{\pi} 2^{2\tilde{\gamma}} Z'^{3+2\tilde{\gamma}} \frac{\Gamma^2(2+\tilde{\gamma})}{\Gamma(3+2\tilde{\gamma})} \tag{4.8}$$

and

$$(\psi_{\text{rel}\uparrow}, (V_1+V_2)\psi_{\text{rel}\uparrow}) = -\frac{\gamma}{\pi} c_{00} \int_0^\infty x dx (I_{10}^2 + I_{20}^2),$$

$$I_{10} = \int_0^\infty k dk \frac{1}{(Z'^2+k^2)^{1+\tilde{\gamma}/2}} \sin\left((2+\tilde{\gamma}) \arctan \frac{k}{Z'} \right) A_k \frac{\sin kx}{kx}, \tag{4.9}$$

$$\begin{aligned}I_{20} &= \int_0^\infty k^2 dk \frac{1}{(Z'^2+k^2)^{1+\tilde{\gamma}/2}} \frac{1}{E_k+m} A_k \\ &\quad \times \sin\left((2+\tilde{\gamma}) \arctan \frac{k}{Z'} \right) j_1(kx).\end{aligned}$$

The decrease of these integrals with k is slightly weaker than for those in Eqs. (4.5) and (4.7). Again, the total energy is minimized with respect to the variational parameter $Z_{\text{eff}} = Z' a_0$.

Our results for the ground-state energy are given in atomic units ($a_0 = 1$). In order to convert relativistic units (r.u.) into atomic units (a.u.) we note that the energy unit is $E_0 = \frac{me^4}{\hbar^2} = 27.21$ eV $= 1$ a.u. and that the momentum unit is a_0^{-1} [16]. We write $\sqrt{k^2+m^2} = m\sqrt{1+(\frac{ka_0}{ma_0})^2} = m\sqrt{1+(ka_0)^2 e^4}$ and further, $m[\text{r.u.}] = \frac{m}{E_0}[\text{a.u.}] = \frac{1}{e^4}[\text{a.u.}]$ as well as $\gamma[\text{r.u.}] = \frac{\gamma}{E_0}[\text{a.u.}] = \frac{Z}{me^2}[\text{a.u.}]$. m occurs also in $Z'/m = Z_{\text{eff}} e^2$ which is dimensionless. In short, one must to replace Z' by Z_{eff}, γ by Z, the prefactor m in the kinetic energy [and in Eq. (2.17)] by $1/e^4$ but elsewhere m by $1/e^2$.

TABLE II. Ground-state energy at $B=0$ for $Z=20$, 40, 60, and 80. $E_g^D - m$, Dirac energy. E_g^{BR}, present results using the hydrogenic wave function (4.1). E_{rel}, present results with the relativistic trial function (4.2). E_g^{RW}, LCAO results taken from Reiher and Wolf [7]. All energies in atomic units.

Z	$E_g^D - m$	E_g^{BR}	E_{rel}	E_g^{RW}
20	−201.1	−201.1	−201.3	−201.3
40	−817.8	−817.6	−822.4	−823.9
60	−1896	−1893	−1928	−1934
80	−3532	−3513	−3647	−3686

Table II gives the ground state (with the rest energy subtracted) for one-electron ions with Z between 20 and 80. The third and fourth columns contain, respectively, the results for E_g^{BR} and E_{rel}. As a matter of fact, E_g^{BR} is quite close to the exact Dirac energy, with a difference not exceeding 0.5% even for $Z=80$. The relativistic trial function, on the other hand, reproduces the LCAO results within 1%. It is evident that the LCAO results for the Brown-Ravenhall operator fall below the Dirac energy, the more so, the higher Z. Detailed calculations [7] show that one must include (for $Z \sim 80$) all terms of the Douglas-Kroll series up to fifth order in the field strength γ to approach the Dirac energy within 0.01%. One is led to explain the reasonable agreement between E_g^{BR} and $E_g^D - m$ by the fact that although h^{BR} is exaggerating the relativistic effects, this is compensated for by forming the expectation value with a nonrelativistic function. This gives us confidence that also for $B \neq 0$ the Dirac results are well represented by our variational results obtained from nonrelativistic functions.

V. NUMERICAL RESULTS FOR $B \neq 0$

We have determined E_g^{BR} from the energy functional (2.16) for nuclear charges between 1 and 80 and for a large variety of magnetic fields B. Figure 2 shows the dependence of the ground-state energy on Z for fixed B. It is evident that E_g^{BR} decreases not only with B but also with Z. When approximated by $-E_g^{\text{BR}} \sim Z^s$ (which is fairly accurate for $Z \lesssim 80$) we have $s \approx 2.1$ when $B=0$, $s \approx 1.25$ when $B = 2.56 \times 10^4$ (in units of $m^2 e^3$) which increases to $s \approx 1.55$ for $B = 10^7$.

The competition between the magnetic length and the scaled Bohr radius suggests to consider B/Z^2 as the relevant

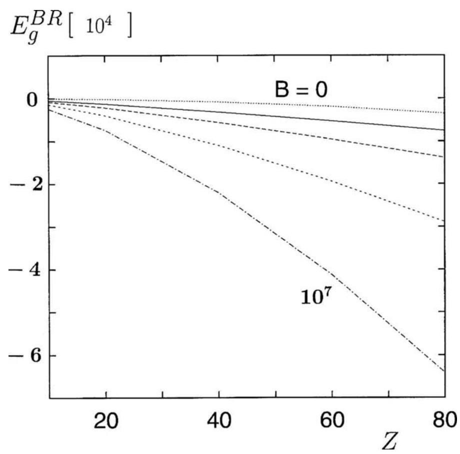

FIG. 2. Ground-state energy E_g^{BR} as a function of the nuclear charge for fixed magnetic field B. (⋯), $B=0$. (—), $B=2.56\times 10^4$ (in units 2.35×10^9 G). (– – –), $B=1.28\times 10^5$. (---), $B=10^6$. (-·-·-), $B=10^7$.

magnetic field parameter. In fact, when $B/Z^2=\lambda m^2 e^3$ is kept fixed but Z is varied, the ratio $E_g^{\mathrm{BR}}(Z,B)/E_g^{\mathrm{BR}}(Z,0)$ [where the latter is calculated with the spherical nonrelativistic trial function (4.1)] is approximately constant. This suggests the factorization

$$E_g^{\mathrm{BR}}(Z,B) \approx E_g^{\mathrm{BR}}(Z,0) f(B/Z^2) \tag{5.1}$$

with some function f only depending on λ. As seen from Fig. 3, the scaling (5.1) is well satisfied for $Z \lesssim 20$, but even for $Z=80$ the deviations from a universal function f are rather small. When $Z=80$, f may be approximated by a power law, $f \sim \lambda^s$ with $s\approx 0.35$, for $20 \lesssim \lambda \lesssim 10^4$. It follows from Table I that the scaling does no longer hold at $B=\infty$. Indeed (at $Z=80$), s increases for $\lambda \gtrsim 10^4$ to its asymptotic value $s=0.5$, valid for $\lambda \gtrsim 10^7$. The strong change in s near $\lambda=10^5$ may be related to the minimum in the variational parameter $\tilde{Z}$.

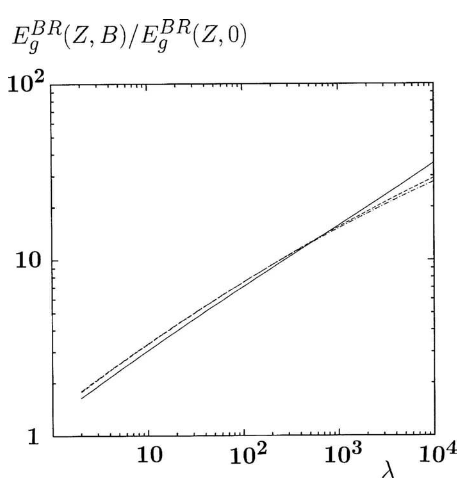

FIG. 3. Ratio between $E_g^{\mathrm{BR}}(Z,B)$ and the field-free ground-state energy $E_g^{\mathrm{BR}}(Z,0)$ as a function of the magnetic field parameter λ. Results for $Z=1$ (-·-·-), $Z=20$ (---), and $Z=80$ (—).

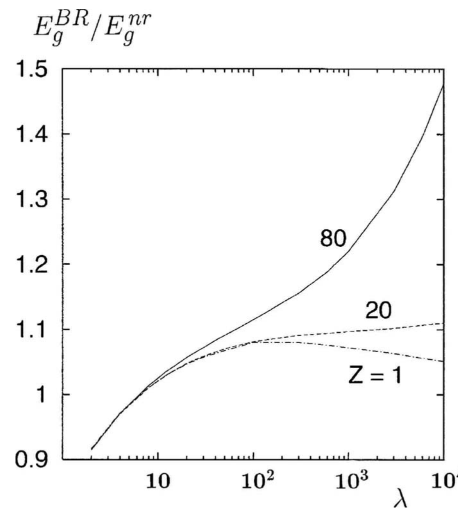

FIG. 4. Ratio between the relativistic ground-state energy E_g^{BR} and the results for E_g^{nr} from the nonrelativistic model of Rau and co-workers [15] as a function of λ. $Z=1$ (-·-·-), $Z=20$ (---), and $Z=80$ (—).

We have also compared our B-dependent ground-state energies to the nonrelativistic results from Rau *et al.* [15] who have derived an analytic formula for the energy functional of the one-electron ion (with the spin shift $\frac{eB}{2m}$ subtracted),

$$E_0^{nr}[Z_{\mathrm{eff}}] = \frac{me^4}{2}\left(Z_{\mathrm{eff}}^2 - 2ZZ_{\mathrm{eff}}\frac{U(1,1,\zeta)}{1-\zeta U(1,1,\zeta)}\right),$$

$$\zeta = \frac{2Z_{\mathrm{eff}}^2}{B} m^2 e^3. \tag{5.2}$$

In this equation U is the irregular degenerate hypergeometric function, and the relation $U(2,2,\zeta)=\zeta^{-1}-U(1,1,\zeta)$ was applied to the formula in [15]. For the numerical computation we have used the integral representation [[23], (9.211)]

$$U(1,1,\zeta) = \int_0^\infty dt e^{-\zeta t}\frac{1}{1+t}. \tag{5.3}$$

The nonrelativistic ground-state energy is obtained from $E_g^{nr}=\min_{Z_{\mathrm{eff}}>0} E_0^{nr}[Z_{\mathrm{eff}}]$. Figure 4 shows the ratio $E_g^{\mathrm{BR}}/E_g^{nr}$ as a function of the magnetic field parameter λ. The difference between the two theories in the nonrelativistic case ($Z=1$) at small λ is due to the choice of different variational wave functions. A spherical hydrogenic function gives results which deviate for $\lambda=2$ from the accurate ground-state energy (-1.022, calculated with the help of a large harmonic oscillator basis [27]) by only 4% and hence is superior to the one-dimensional function used in our model (which deviates by 13.5%). However, for very large λ the spherical wave function becomes effectively a one-dimensional one and indeed, the $Z=1$ ratio decreases towards unity for $\lambda \gtrsim 10^3$. Even more, the present result for $Z=1$ and $\lambda=5\times 10^3$ ($E_g^{\mathrm{BR}}=-11.67$) differs from an accurate relativistic calculation (-11.87 [13]) by only 1.7%. For $Z=20$, still considered to be nonrelativistic at $B=0$, the plotted ratio behaves very similar to the $Z=1$ case for $\lambda \lesssim 100$, but it continues to increase with λ for the higher magnetic fields. For $Z=80$, $|E_g^{\rm BR}|$ increases much faster with λ than $|E_g^{nr}|$, and the relativistic effects are large beyond $\lambda=100$. This feature may be explained by the fact that the larger B, the closer passes the electron by the nucleus. If, in addition, Z is high, the purely relativistic spin-dependent interaction term V_2 comes into play.

We recall that in the low-Z studies of the Dirac ground state [12,13] relativistic effects turned out to be negligibly small even for the highest B values considered. In fact, for $Z=1$ and $\lambda \leqslant 10^4$, relativistic effects were found to be below 0.01%. For $Z=20$ and $\lambda=2$ (where the accurate result, −409.6 [13] differs from $E_g^{nr}=-393.2$ again by only 4%), relativistic effects amount to 0.2%.

VI. CONCLUSION

We have calculated the ground-state energy of the pseudorelativistic Brown-Ravenhall operator for one-electron ions in strong magnetic fields up to $B=10^4Z^2[m^2e^3]$, using a simple variational wave function. For nonrelativistic systems ($Z \lesssim 20$) we have tested our results against the nonrelativistic variational theory of Rau and co-workers, and we have found that for moderate fields ($B \approx 10-20Z^2$ $[m^2e^3]$, large enough so that it is reasonable to use a one-dimensional hydrogenic trial function) $E_g^{\rm BR}$ differs from [15] by less than 5%. The influence of relativistic effects has been established for $Z \gtrsim 20$ and large magnetic fields, leading to a decrease of the ground-state energy relative to the nonrelativistic theory, the more so, the higher Z.

We have found that the ratio λ between the (square of the) scaled Bohr radius and the magnetic length should be considered as the relevant magnetic field parameter. In fact, the ground-state energy depends to a good approximation only on B/Z^2 rather than on B itself. This is in contrast to the scaling according to $B/Z^{4/3}$ and B/Z^3 for moderate and large B, respectively, derived from the Thomas-Fermi theory for multielectron atoms [28,18].

When B is increased to infinity, it is shown that the variational ground-state energy decreases like $-c_1B^{1/2}$, which is an upper bound to the true ground-state energy of the Brown-Ravenhall operator. On the other hand, a lower bound was derived earlier, $h^{\rm BR} \geqslant -c_2B^{1/2}$ (with c_1, c_2 constants). This leads to the conjecture that for the infimum of the spectrum of $h^{\rm BR}$ one has

$$\inf \sigma(h^{\rm BR}) \sim -\tilde{c}B^{1/2} \quad \text{as } B \to \infty. \tag{6.1}$$

This differs from the logarithmic B-dependence of the ground state of the one-electron Pauli operator. It is, however, consistent with a recent investigation of the Dirac operator where a scaling of the ground-state energy with $\sqrt{B}$ was derived in the asymptotic regime [29]. This confirms that relativistic effects indeed play an important role.

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