Antibinding of atomic electrons in strong inhomogeneous magnetic fields

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The ground-state energy of heavy one-electron ions in an inhomogeneous locally bounded magnetic field is estimated by the variational principle. The ions are described by means of the pseudorelativistic Herbst-Chandrasekhar operator. Two classes of magnetic fields are considered which model a field-free region around the central charge. It is shown that for a certain size of this region the ground-state energy becomes positive and increases strongly with the magnetic field strength. This behavior is in contrast to the two-dimensional case where electrons can be bound by such a field-free region.

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I. INTRODUCTION

The interest in electrons subject to inhomogeneous magnetic fields was revived by the preparation of graphene monolayers which give rise to a purely two-dimensional electronic motion. It was suggested by Egger and coworkers to apply a static magnetic field, oriented perpendicular to the monolayer, which is constant outside a cylinder of radius r_0 and zero inside (Fig. 1(a)). In a rigorous theoretical approach, based on the two-dimensional Dirac-Weyl equation, it was shown that an electron gets bound in such a field-free disk, the number of bound states increasing with r_0 [1,2]. In accordance with the experimental spectrum, the electron mass is thereby set equal to zero [1]. Also a mathematical analysis of the two-dimensional confinement by this magnetic field was provided for the case of interacting massless multifermions [3].

In the three-dimensional atomic case where the confinement in the x_3 direction (the field direction) is achieved by a fixed central Coulomb potential, a massless particle can be simulated by an appropriate magnetic field of very large strength. A magnetic field which shows this feature was introduced in [4] and is of asymptotic growth but has also a depleted interior region (Fig. 1(b)). In the presence of such a field the Herbst operator, used to model relativistic atomic systems [5], exhibits a scaling property which reduces the mass term, the more so, the larger the field strength B.

In the present work the question is addressed whether, for magnetic fields of the type discussed above, the binding of the electron increases with the size of the depleted region as in the two-dimensional case. Taken into consideration that the influence of magnetic fields in two and three dimensions is often quite different (e.g., the ground-state binding of the atomic electron in a *homogeneous* magnetic field increases with B; see, e.g., the review by Lai [6]), the answer is not easily predictable.

Rather than progressing with a fully relativistic approach we estimate the ground-state energy of the electron by means of a more transparent variational calculation. A trial function which is suitable in a wide range of magnetic fields was introduced by Rau and coworkers [7] in the context of Schrödinger operators. It was shown for homogeneous magnetic fields that this trial function not only provides the correct limits for $B \to 0$ and $B \to \infty$, but that also for intermediate field strengths it is able to reproduce the binding energies from accurate numerical calculations [8]. Slightly modified trial functions were used in the context of the pseudorelativistic Brown-Ravenhall operator [9,10] and the Herbst operator [4]. However, restriction was made to the presence of very strong magnetic fields.

The paper is organized as follows. For the two types of magnetic fields discussed above the ground-state energy of the Herbst operator is estimated in Secs. II A and III B, respectively (using the trial function from [7]), and its dependence on the field parameters is investigated for the fixed central charge $Z = 80$. In Secs. III and IV the stability of these results is tested by choosing different types of trial functions, including such which mimic relativistic effects. A short conclusion is given in Sec. V.

II. VARIATIONAL PRINCIPLE FOR THE HERBST OPERATOR

Relativistic one-electron ions are conventionally described by the Dirac operator H [11]. In the presence of a Coulomb field V and a magnetic field $\mathbf{B}_A$ generated by a vector potential $\mathbf{A}$, this operator is given by (in relativistic units, $\hbar = c = 1$)

$$H = D_A + V, \quad D_A = \boldsymbol{\alpha} \cdot (\mathbf{p} - e\mathbf{A}) + \beta\, m, \qquad V = -\frac{\gamma}{x}. \tag{2.1}$$

In this expression $\boldsymbol{\alpha}$ and β are the Dirac matrices, $\mathbf{p} = -i\nabla$ is the momentum operator, $x = |\mathbf{x}|$, and $\gamma = Ze^2$ is the electric potential strength (Z is the charge of the point-like nucleus which is fixed at the origin and $e^2 \approx 1/137.036$ is the fine structure constant).

One way to avoid dealing with the negative continuum, which, in contrast to the nonrelativistic case, causes the Dirac operator to be unbounded from below, is the introduction of semibounded pseudorelativistic operators such as the Herbst operator [5]. This operator was originally put forth by Chandrasekhar (see, e.g., [12]) and acts in the Hilbert space $L_2(\mathbb{R}^3) \otimes \mathbb{C}^2$,

$$h^H = E_A + V, \qquad E_A = |D_A| = \sqrt{[\boldsymbol{\sigma} \cdot (\mathbf{p} - e\mathbf{A})]^2 + m^2}, \tag{2.2}$$

where $\boldsymbol{\sigma}$ is the vector of Pauli spin matrices. For $\mathbf{A} \in L_{2,\mathrm{loc}}(\mathbb{R}^3)$ the form domain of E_A is the Sobolev space $H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2$.

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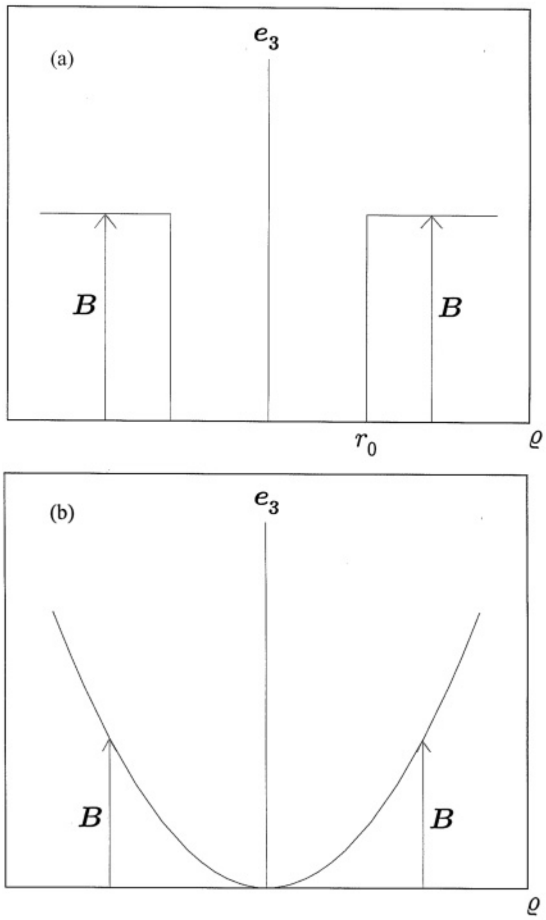

FIG. 1. (a) Cylindrically symmetric Egger-type magnetic field, $\varrho = \sqrt{x_1^2 + x_2^2}$. (b) Magnetic field with asymptotic growth in the special case of cylindrical symmetry ($\tau = 2$).

It was shown in [4] that h^H is bounded from below if $\gamma < \frac{2}{\pi}$ ($Z \leqslant 87$) and if $\mathbf{B}_A$ is locally bounded. Under these conditions h^H can be extended to a self-adjoint operator.

In the following we assume that the field $\mathbf{B}_A$ is generated by a two-dimensional vector potential $\mathbf{A} = (A_1, A_2, 0)$ taken to be independent of x_3 and obeying $\nabla \cdot \mathbf{A} = 0$. Then the kinetic energy can be decomposed in the following way:

$$E_A^2 = E_{xy}^2 + \left(p_3^2 + m^2\right), \qquad E_{xy}^2 = \sum_{k=1}^{2} (p_k - eA_k)^2 - e\sigma_3 B_A. \tag{2.3}$$

For a given trial function $\psi_t \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2$, normalized to unity, we have by the Schwarz inequality the estimate for the ground-state energy E_g of the Herbst operator,

$$E_g \leqslant (\psi_t, h^H \psi_t) \leqslant \sqrt{\left(\psi_t, E_A^2\, \psi_t\right)} + (\psi_t, V\, \psi_t) =: E^H[\psi_t]. \tag{2.4}$$

We wish to discuss the Herbst operator for two classes of locally bounded magnetic fields $\mathbf{B}_A$, the first being of asymptotic growth,

$$\mathbf{B}_{A_1}(\mathbf{x}) = B\, \frac{1+\tau}{2}\, (0, 0, |x_1|^\tau + |x_2|^\tau), \tag{2.5}$$

characterized by the parameters B and $\tau \geqslant 0$, where $\tau = 0$ corresponds to a constant magnetic field of strength B in the direction of the x_3 axis. For this class of fields it was proven (for $0.1 \lesssim \gamma < \frac{2}{\pi}$ and large B) that a bound ground state exists when τ is subcritical, $\tau < \tau_c$, where τ_c depends on Z as well as on B [4].

The suppression of the magnetic force around the origin (being the stronger the larger τ) can also be described by the (simpler) second class of magnetic fields. This class was introduced by Egger and coworkers in the context of the two-dimensional electronic motion [1],

$$\mathbf{B}_{A_2}(\mathbf{x}) = B\, \theta(\varrho - r_0)\, \mathbf{e}_3, \quad \varrho = \sqrt{x_1^2 + x_2^2}, \tag{2.6}$$

where θ is Heaviside's step function. It is parametrized by the field strength B and the radius r_0 of the field-free region. The constant magnetic field is included in the class (2.6) for $r_0 = 0$. The energy functionals pertaining to the fields (2.5) and (2.6) will be denoted by $E^{H1}[\psi_t]$ and $E^{H2}[\psi_t]$, respectively.

As trial function we take, following Rau *et al.* [7],

$$\psi_t(\mathbf{x}) = N_t\, e^{-\nu^2 \varrho^2/2}\, e^{-Z'x} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad N_t = \left[\frac{\nu^4}{Z'\pi}\, \frac{1}{\psi(2,2,Z'^2/\nu^2)} \right]^{\frac{1}{2}}, \tag{2.7}$$

where the spin direction is taken parallel to $\mathbf{B}_A$. In the normalization constant N_t, $\psi(n,k,\xi)$ is the irregular confluent hypergeometric function which is readily expressed in terms of the integral representation ([13], p. 1058),

$$\psi(n,k,\xi) = \frac{1}{\Gamma(n)} \int_0^\infty dt\, e^{-\xi t}\, \frac{t^{n-1}}{(1+t)^{n+1-k}}. \tag{2.8}$$

In (2.7), $\nu = \sqrt{2s}(eB)^{d/2}$ measures the inverse extension of the electron orbit perpendicular to $\mathbf{B}_A$, where $d > 0$ is a field-specific constant. Besides the effective charge Z' we have introduced s as a second variational parameter ($s = \frac{1}{4}$ for constant magnetic fields). Thus the trial function mimics an eigenstate for the lowest Landau level (in the case of vanishing scalar potential and constant magnetic field) as well as the hydrogenic ground state (in the case of zero magnetic field).

The ground-state energy is estimated by the infimum of the energy functional $E^H[\psi_t]$,

$$E_g^H := \inf_{Z'>0, s>0} E^H[\psi_t]. \tag{2.9}$$

It is easy to show that for vanishing magnetic field E_g^H agrees with the exact Dirac ground-state energy. Since for $B_A = 0$ the trial function reduces to $\psi_t(\mathbf{x}) = (Z'^{3/2}/\pi^{\frac{1}{2}})\, e^{-Z'x} \binom{1}{0}$, we get

$$E^H[\psi_t] = \sqrt{(\psi_t, (p^2 + m^2)\, \psi_t)} - \gamma \left(\psi_t, \frac{1}{x}\, \psi_t \right) = \sqrt{Z'^2 + m^2} - \gamma Z'. \tag{2.10}$$

From $\partial E^H / \partial Z' = 0$ we obtain $Z' = m\gamma/\sqrt{1-\gamma^2}$ and thus

$$E_g^H(B_A = 0) = \inf_{Z'>0} E^H[\psi_t](B_A = 0) = m\sqrt{1-\gamma^2}, \tag{2.11}$$

which is equal to the exact Dirac energy.

TABLE I. Ground-state energy (rest energy subtracted, in atomic units) for $Z = 20$ as a function of $\lambda = B/Z^2$ for a constant magnetic field of strength B. The second column gives the results from the present calculation, the third column comprises the exact results [14,15]. E_{g-}^{exs} is obtained from the Schrödinger scaling of the exact result for $Z = 5$ at $\lambda = 10$ [16] and for $Z = 1$ when $\lambda \geqslant 20$ [14]. B is given in units of $B_0 = 2.35 \times 10^9$ G.

λ	E_{g-}^{H}	E_{g-}^{ex}	E_{g-}^{exs}
0.025	−205.90	−205.98	
0.25	−244.61	−244.95	
2	−407.65	−409.55	
10	−690.89		−699.16
20	−871.44		−886.16
200	−1841.75		−1890.85
500	−2436.99		−2502.81
2000	−3635.26		−3721.84

Moreover, the variationally determined ground-state energy for a constant magnetic field compares well with the available results for $Z > 10$ from elaborate relativistic calculations [14,15]. Thereby it is advantageous to subtract the rest energy of the electron, i.e., to consider $E_{g-}^{H} = E_{g}^{H} - m$. Table I gives the comparison for $Z = 20$. For $\lambda = B/Z^2 \geqslant 10$, the reference values are obtained from the Schrödinger scaling (see below) of the exact results.

There is one additional exact calculation for uranium ($E_{g-}^{\text{ex}} = -4861.61$ a.u.) [15] but for a very small field, $B = 1$ (relating to $\lambda = 1.182 \times 10^{-4}$), where the numerical inaccuracy of our result ($E_{g-}^{H} = -4860.05$ a.u.) is quite large (∼2 a.u.).

A. Magnetic fields with asymptotic growth

Magnetic fields of the class (2.5) are generated by the vector potentials

$$\mathbf{A}_1(\mathbf{x}) = \frac{B}{2}\,(-x_2|x_2|^\tau, x_1|x_1|^\tau, 0), \quad \tau \geqslant 0. \tag{2.12}$$

In the trial function (2.7) we take $d = \frac{2}{2+\tau}$. This choice preserves the scaling property of the Herbst operator [4]. We decompose

$$\left(\psi_t, E_A^2\, \psi_t\right) = M_{\text{an}} + M_{\text{num}}^{(1)}, \tag{2.13}$$

where M_{an} is the analytic part,

$$M_{\text{an}} = 2\nu^2 - Z'^2 + m^2 - \nu^4\,(\psi_t, \varrho^2\,\psi_t) - 2\nu^2 Z'\left(\psi_t, \frac{\varrho^2}{x}\,\psi_t\right) + 2Z'\left(\psi_t, \frac{1}{x}\,\psi_t\right), \tag{2.14}$$

while $M_{\text{num}}^{(1)}$ is the B-dependent part to be evaluated numerically,

$$M_{\text{num}}^{(1)} = \left(\frac{eB}{2}\right)^2 (\psi_t, (|x_1|^{2+2\tau} + |x_2|^{2+2\tau})\,\psi_t) - eB\,\frac{1+\tau}{2}\,(\psi_t, (\,|x_1|^\tau + |x_2|^\tau)\,\psi_t). \tag{2.15}$$

Using the cylindrical symmetry of ψ_t and spherical coordinates (x,ϑ,φ) we have

$$(\psi_t, |x_1|^\tau\,\psi_t) = (\psi_t, |x_2|^\tau\,\psi_t) = 2N_t^2 \int_0^\infty dx\; x^2\, e^{-2Z'x} \times \int_0^1 d(\cos\vartheta)\; e^{-\nu^2 x^2 \sin^2\vartheta}\; x^\tau\; (\sin\vartheta)^\tau \int_{-\pi}^{\pi} d\varphi\; |\cos\varphi|^\tau. \tag{2.16}$$

With the substitution $y = \sin^2\vartheta$ we obtain ([13], p. 318,369)

$$(\psi_t, (|x_1|^\tau + |x_2|^\tau)\,\psi_t) = 8\pi N_t^2\,\frac{1}{1+\tau}\int_0^\infty dx\, x^{2+\tau} e^{-2Z'x} e^{-\nu^2 x^2} \times {}_1F_1\left(\frac{1}{2}, \frac{3+\tau}{2}, \nu^2 x^2\right), \tag{2.17}$$

where ${}_1F_1(a,b,z)$ is the (regular) confluent hypergeometric function.

The matrix elements in (2.14) are evaluated in a similar way. With the help of $xe^{-2Z'x} = -\frac{1}{2}\frac{d}{dZ'}(e^{-2Z'x})$ we find ([13], p. 867; see also [7])

$$(\psi_t, \varrho^2\,\psi_t) = -\frac{Z'}{\nu^6}\,\pi N_t^2\,\psi'\left(2, 1, \frac{Z'^2}{\nu^2}\right),$$
$$\left(\psi_t, \frac{\varrho^2}{x}\,\psi_t\right) = \frac{1}{\nu^4}\,\pi N_t^2\,\psi\left(2, 1, \frac{Z'^2}{\nu^2}\right) \tag{2.18}$$

and

$$\left(\psi_t, \frac{1}{x}\,\psi_t\right) = \frac{\pi}{\nu^2}\,N_t^2\,\psi\left(1, 1, \frac{Z'^2}{\nu^2}\right) \tag{2.19}$$

which also determines the potential energy, $(\psi_t, -\frac{\gamma}{x}\,\psi_t)$. The derivative $\psi'(n,k,\xi)$ with respect to ξ is readily obtained from the integral representation (2.8).

For the discussion of the Z and B dependences of the variationally determined ground-state energy it is convenient to introduce the parameter $\lambda = B/Z^2$. In the case of a constant magnetic field λ provides the ratio between the magnetic and electric field strengths acting on the electron [7]. For Schrödinger operators there is an exact scaling which allows to express the ground-state energy divided by Z^2 just in terms of λ [14,17]. Also for relativistic systems this scaling is satisfied quite well up to $\lambda \sim 10^3$ [9]. Therefore the basic physics can be displayed with a single choice of Z.

Figure 2(a) shows the ground-state energy E_{g-}^{H1} for $Z = 80$ as a function of the asymptotic growth τ. Clearly, for a constant magnetic field ($\tau = 0$) E_{g-}^{H1} is decreasing with B. At large τ, on the other hand, the variational ground-state energy tends to the exact Dirac energy in the absence of a magnetic field [i.e., (2.11), with rest energy subtracted]. This can readily be explained by the fact that large τ correspond to a near-zero magnetic field in an extended region around the nucleus. Note that for small magnetic field strengths E_{g-}^{H1} approaches this asymptotic value from below, while at the higher B a maximum evolves, such that eventually the asymptotic energy is approached from above.

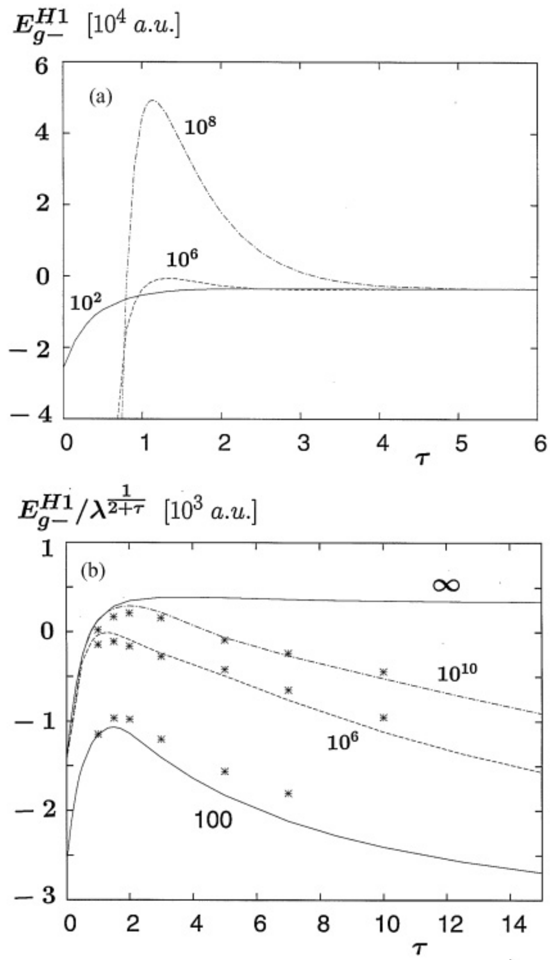

FIG. 2. Ground-state energy (without rest energy) for $Z = 80$ and the magnetic field (2.5) as a function of τ. The parameter λ labeling the curves relates to the field strength according to $B = \lambda Z^2$ (in units of $B_0 = 2.35 \times 10^9$ G). (a) Unscaled energy E_{g-}^{H1} (in atomic units) for $\lambda = 100$ (———), 10^6 (– – – – –), and 10^8 (– · – · –). The asymptotic value is the Dirac energy for $B = 0$, −3532.19 a.u. (b) Scaled energy $E_{g-}^{H1}/\lambda^{1/(2+\tau)}$ for $\lambda = 100$ (————), 10^6 (– – – –), 10^{10}(– · – · –), and ∞ (————, uppermost curve). Included are results using the energy functional $E^{H1}[\psi_t^{(1)}]$ (∗, see Sec. III).

When one introduces (for $B \neq 0$) the scaled parameters $\tilde{Z} = Z'/\nu$ and $\tilde{m}_s = m/\nu$ one can show that the energy functional $E^{H1}[\psi_t]$ scales with the field strength B according to $\nu \sim B^{d/2}$. In particular, with $d = \frac{2}{2+\tau}$, the variationally determined ground-state energy can be written in the following way:

$$E_{g-}^{H1} = E_g^{H1} - m = \nu\left(\tilde{E}_g^{H1} - \tilde{m}_s\right) \sim B^{\frac{1}{2+\tau}}\,\tilde{E}_{g-}^{H1}, \qquad (2.20)$$

where $\tilde{E}_{g-}^{H1}$ depends on B only through the scaled mass $\tilde{m}_s$. In turn, $\tilde{m}_s$ influences the optimized parameters $\tilde{Z}$ and s (which, since $\tilde{m}_s \to 0$ as $B \to \infty$, tend to constant values as $B \to \infty$). Based on the existence of a bound ground state (for small τ) it was proven in [4] that also the exact ground-state energy of h^H decreases with B according to $B^{\frac{1}{2+\tau}}$ when $B \to \infty$.

Figure 2(b) depicts the scaled ground-state energies $E_{g-}^{H1}/\lambda^{\frac{1}{2+\tau}}$ of Fig. 2(a), including the limiting case $\tilde{m}_s = 0$ (which corresponds to $B = \infty$). It can be strictly proven [4] and is verified in the figure that the scaled energy increases with B (i.e., decreases with $m/B^{1/(2+\tau)}$). All curves show a maximum near $\tau = 1.5$ which becomes positive when $\lambda > 10^6$ (corresponding to $B > 10^6\,Z^2 B_0$ with $B_0 = 2.35 \times 10^9$ G the unit field). For λ fixed and $\tau \to \infty$ the scaled energy approaches the Dirac energy too (since $\lim_{\tau\to\infty} E_{g-}^{H1}/\lambda^{\frac{1}{2+\tau}} = \lim_{\tau\to\infty} E_{g-}^{H1}$).

B. Egger-type magnetic fields

In this section we consider a magnetic field which is constant outside a cylinder of radius r_0 centered around the x_3 axis, and zero inside. This field, given by (2.6), is generated by the vector potential [3]

$$\mathbf{A}_2(\mathbf{x}) = \frac{B}{2}\left(1 - \frac{r_0^2}{\varrho^2}\right)\theta(\varrho - r_0)\,(-x_2,x_1,0). \qquad (2.21)$$

In order to preserve the scaling property we have to set $d = 1$ in the trial function (2.7) (corresponding to $\tau = 0$ in the field $\mathbf{A}_1$), such that $\nu = \sqrt{2s\,eB}$.

The field-dependent part of the energy functional $E^{H2}[\psi_t]$ is most readily evaluated when cylindrical coordinates (ϱ,φ,x_3) are used. With the help of the integral

$$\int_{-\infty}^{\infty} dx_3\; e^{-2Z'\sqrt{\varrho^2+x_3^2}} = 2\varrho\; K_1(2\varrho Z'), \qquad (2.22)$$

where K_1 is a modified Bessel function, we get

$$M_{\text{num}}^{(2)} = 4\pi N_t^2 \int_{r_0}^{\infty} d\varrho\; e^{-\nu^2\varrho^2}\; K_1(2\varrho Z') \times \left[\left(\frac{eB}{2}\right)^2 \left(\varrho^2 - r_0^2\right)^2 - eB\varrho^2\right]. \qquad (2.23)$$

Thus, with (2.4) and (2.13),

$$E^{H2}[\psi_t] = \sqrt{M_{\text{an}} + M_{\text{num}}^{(2)}} + (\psi_t, V\,\psi_t). \qquad (2.24)$$

In Fig. 3(a) the ground-state energy E_{g-}^{H2}, resulting from the infimum of (2.24) with respect to Z' and s, is plotted for fixed λ as a function of $\tilde{d} = r_0\sqrt{\lambda}$. In this representation the curves are very similar to those shown in Fig. 2(a). In particular, the maximum (which appears for sufficiently high field strengths) is also at a fixed position, $\tilde{d} \approx 3$. Again, the field-free Dirac energy is approached when $\tilde{d} \to \infty$.

When the scaling with ν is introduced, such that ϱ is replaced by $\tilde{\varrho} = \varrho\nu$, the hole radius r_0 changes into $r_0\nu$ which increases according to $B^{\frac{1}{2}}$. Thus $\tilde{d}$ from Fig. 3(a) can be interpreted as the scaled hole radius in units of the K-shell radius, $1/Z$. Figure 3(b) displays the scaled energy $E_{g-}^{H2}/\lambda^{\frac{1}{2}}$ for a wide range of λ as a function of $\tilde{d}$. Again, this r_0 dependence resembles the τ dependence of $E_{g-}^{H1}/\lambda^{\frac{1}{1+\tau}}$ from Fig. 2(b), with two minor exceptions: The maximum becomes positive for $\lambda > 48.9$ which is much lower than the corresponding value in Fig. 2(b) ($\lambda > 10^6$). Also, the behavior for $B \to \infty$ is different. While the curves for $\lambda = 10^8$ and $\lambda = \infty$ nearly coincide in Fig. 3(b), they differ considerably in Fig. 2(b). This is related to the additional B dependence of the abscissa in Fig. 3(b). The range $0 \leqslant \tilde{d} \leqslant 30$ corresponds to a nearly homogeneous field ($r_0 \approx 0$) for $\lambda \gtrsim 10^6$ such that the convergence with $\lambda \to \infty$ mimics the fast convergence of

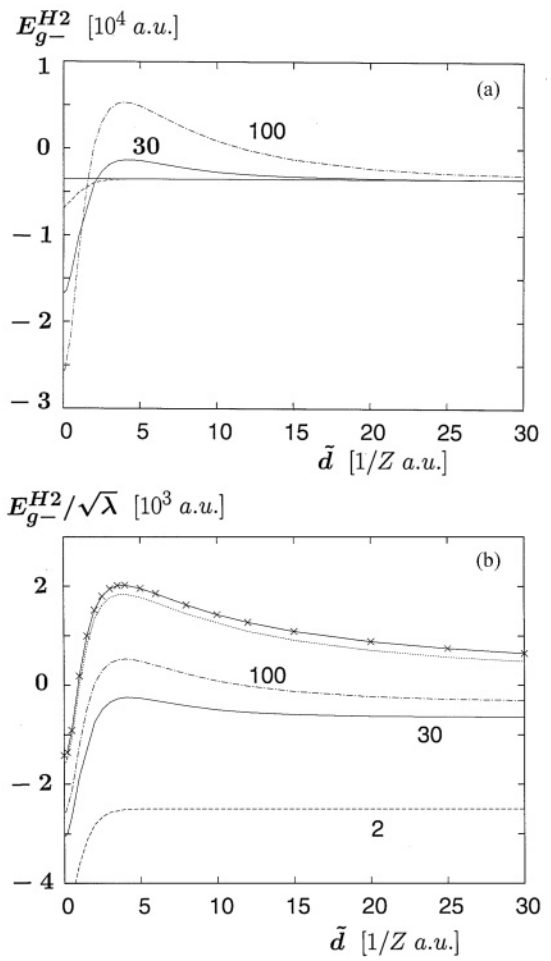

FIG. 3. Ground-state energy (without rest energy) for $Z = 80$ and the Egger field (2.6) as a function of the scaled hole radius $\tilde{d} = r_0\sqrt{\lambda}$ (in units of the K-shell radius, $1/Z$ a.u.). (a) Unscaled energy E_{g-}^{H2} (in atomic units) for $\lambda = 2$ (— — — — —), 30 (————), and 100 (— · — · —). The horizontal line marks the Dirac energy for $B = 0$, -3532.19 a.u. (b) Scaled energy $E_{g-}^{H2}/\lambda^{1/2}$ for $\lambda = 2$ (— — — — —), 30 (————), 100 (— · — · —), 10^4(· · · · · ·), and 10^8 (————, uppermost curve). Included are results for $\lambda = \infty$ (×).

the scaled ground-state energy with $\tilde{m}_s \to 0$ for $r_0 = 0$. The convergence proof from [4], based on the continuity of E_A as a function of m, holds for any $\tau > 0$. However, when the depleted region is large (Fig. 2(b)), the convergence with $\tilde{m}_s$ becomes slow. In this context we also note that the scaled energy $E_{g-}^{H2}/\lambda^{1/2}$ tends to a constant (for $r_0 \to \infty$) which, in contrast to $E_{g-}^{H1}/\lambda^{1/(2+\tau)}$ (for $\tau \to \infty$), decreases with λ.

III. COMPARISON WITH PREVIOUS RESULTS FOR $B \to \infty$

When the strength of a homogeneous magnetic field is very large ($\lambda \gg 1$), the confinement of the electron in the direction perpendicular to $\mathbf{B}_A$ is given by the cyclotron radius $a_0 = \sqrt{\frac{2}{eB}}$ (see, e.g., [7]). Assuming that this is also true for small τ we have in our earlier work [4] taken a separable trial function where in the hydrogenic part φ_z the coordinate ϱ is replaced by $a_0 = 1/\nu = \frac{1}{\sqrt{2s(eB)^{2/(2+\tau)}}}$,

$$\psi_t^{(1)}(\mathbf{x}) = \frac{\nu}{\sqrt{\pi}}\, e^{-\nu^2\varrho^2}\, \varphi_z(x_3) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{3.1}$$

$$\varphi_z(x_3) = [2a_0\, K_1(2a_0 Z')]^{-\frac{1}{2}}\, e^{-Z'\sqrt{a_0^2+x_3^2}}.$$

Consequently, a separable kinetic energy functional was taken, based on the inequality

$$(\psi, E_A\, \psi) \leqslant \sqrt{(\psi, E_{xy}^2\, \psi)} + \left(\psi, \sqrt{p_3^2 + m^2}\psi\right) =: E_{\rm sep}[\psi] \tag{3.2}$$

for any normalized $\psi \in H_{1/2}(\mathbb{R}^3) \otimes \mathbb{C}^2$. The estimate for the ground-state energy was obtained from minimizing the energy functional

$$E_{\rm sep}^{H1}\big[\psi_t^{(1)}\big] := E_{\rm sep}\big[\psi_t^{(1)}\big] + \left(\psi_t^{(1)}, V\, \psi_t^{(1)}\right) \tag{3.3}$$

relating to the field $\mathbf{B}_{A_1}$, with respect to Z' and s. For large τ this functional is expected to be inferior to $E^{H1}[\psi_t]$ from Sec. II, because $\mathbf{B}_{A_1}$ contains an extended depleted region where $\psi_t^{(1)}$ fails. This is confirmed for the limiting case $\tilde{m}_s = 0$ (i.e., $B = \infty$) in Fig. 4 where the scaled energies from the two functionals are compared for $\tau \lesssim 10$. The two curves cross near $\tau = 0.25$, and $E^{H1}[\psi_t]$ provides indeed the smaller energy estimate for all τ that exceed this value.

Since, however, two different functionals are used for the kinetic energy, both being upper bounds for $(\psi, E_A\, \psi)$, one may ask how the results will change when these functionals are interchanged while keeping the trial function fixed. Correspondingly, we define the two additional energy functionals $E_{\rm sep}^{H1}[\psi_t]$ with ψ_t from (2.7) as well as $E^{H1}[\psi_t^{(1)}]$ with the kinetic energy estimate from (2.4). The minimization of $E_{\rm sep}^{H1}[\psi_t]$ proves to be inferior at all τ investigated (see Fig. 4),

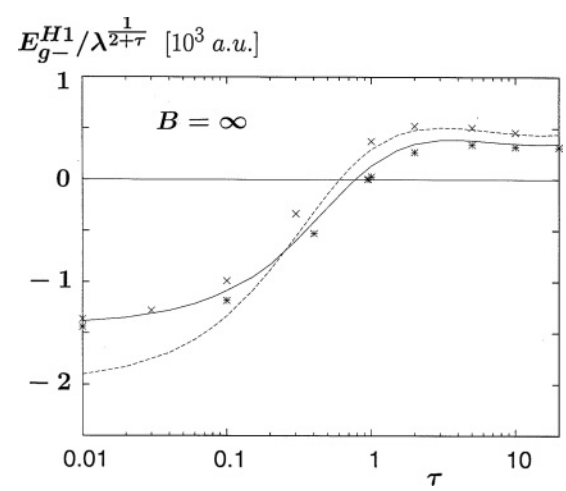

FIG. 4. Scaled ground-state energy $E_{g-}^{H1}/\lambda^{1/(2+\tau)}$ (without rest energy) for the magnetic field (2.5) of infinite strength ($B = \infty$) and $Z = 80$ as a function of τ. Results are shown for different trial functions and kinetic energy operators: ψ_t with (2.4), see also Fig. 2(b) (————); $\psi_t^{(1)}$ with (3.2) (— — — — —); ψ_t with (3.2) (×) and $\psi_t^{(1)}$ with (2.4) (∗).

whereas the use of a separable trial function together with the non-separable energy functional indeed provides the lowest energy estimate when $\tau > 0.2$. Thus a *separable* trial function (together with an appropriate energy functional) is the best choice at $B \to \infty$ for all values of τ. We note that this remains true for finite (but high) field strengths, provided τ is not too large (see Fig. 2(b)).

With the help of the functional $E^{H1}[\psi_t^{(1)}]$ the critical field growth τ_c below which the energy estimate is negative (hence guaranteeing the existence of a *bound* ground state) can be improved from $\tau_c = 0.602$ [4] to $\tau_c = 0.943$ (for $Z = 80$).

IV. STABILITY OF ANTIBINDING FOR MODIFIED TRIAL FUNCTIONS

The infimum E_g^H of the energy functional provides only an upper bound to the exact ground-state energy of the Herbst operator. In order to assure that the ground-state energy is indeed positive in a certain parameter range we apply trial functions of different type and study their influence on the variational energy in the case of the Egger-type field (2.6). Guided by the fact that for $B = 0$ the variationally determined ground-state energy of the related Brown-Ravenhall operator is lowered when the trial function accounts for the relativistic contraction [9], we consider the energy functional $E^H[\psi_t^{(2)}]$ from (2.4) with

$$\psi_t^{(2)}(\mathbf{x}) = N_2\, e^{-\nu^2\varrho^2/2}\, x^{\tilde\gamma}\, e^{-Z'x} \begin{pmatrix}1\\0\end{pmatrix}, \qquad \tilde\gamma = \sqrt{1-(Z'e^2)^2} - 1, \tag{4.1}$$

where $\nu = \sqrt{2s\, eB}$ as before. The normalization constant can be calculated along the lines of (2.16) and (2.17),

$$N_2 = \left[4\pi \int_0^\infty dx\, x^{2+2\tilde\gamma}\, e^{-2Z'x}\, e^{-\nu^2 x^2}\, {}_1F_1\left(\frac{1}{2},\frac{3}{2},\nu^2 x^2\right)\right]^{-\frac{1}{2}}. \tag{4.2}$$

As an alternative to $\tilde\gamma$ determined by Z', we have also considered $\tilde\gamma$ of the form $\tilde\gamma(\zeta) = \sqrt{1-(\zeta e^2)^2} - 1$, related to an independent variational parameter ζ (besides Z' and s).

Our results from the variation with respect to Z' and s are displayed in Fig. 5(a). We have plotted the scaled energies $E_{g-}^{H2}/\sqrt{\lambda}$, obtained from the functions ψ_t and $\psi_t^{(2)}$, respectively, versus the true hole radius $r_0 = \tilde d/\sqrt{\lambda}$. In this representation it becomes clear that the maximum of the energy shifts to smaller r_0 when the field strength increases. For the test cases $\lambda = 10^2$ and 10^4, relating to a positive maximum, the energy derived from the function (2.1) is always higher than the energy obtained in Sec. II B. This fact remains unchanged when ζ is introduced as a third variational parameter: Only for weak fields (such as $\lambda = 2$ and $\tilde d \gtrsim 3$) is the energy slightly lower when $\zeta > 0$ (the deviation from the $\zeta = 0$ results being below 1%).

When the field is switched off completely and correspondingly the factor $\exp(-\nu^2\varrho^2/2)$ omitted from the trial function (2.1) [such that the normalization constant reduces to $N_2 = (2Z')^{\frac{3}{2}+\tilde\gamma}/\sqrt{4\pi\Gamma(3+2\tilde\gamma)}$] the energy functional is given by

$$E_-^H[\psi_t^{(2)}] = \left(m^2 + \frac{Z'^2}{1+2\tilde\gamma}\right)^{\frac{1}{2}} - m - \gamma\, \frac{Z'}{1+\tilde\gamma}. \tag{4.3}$$

It turns out that its minimum is again *higher* than if $\tilde\gamma$ is set equal to zero (for $Z = 80$, one gets $E_{g-}^H = -3382.98$ a.u. as compared to -3532.19 a.u.). When ζ is treated as independent variational parameter, the minimum is obtained for $\tilde\gamma = 0$.

We have also considered the case where a positive power of the radial coordinate is introduced into the trial function. In fact, when the scalar potential is absent ($Z = 0$) and the magnetic field homogeneous, the ground state of the electron is infinitely degenerate with eigenstates relating to different powers of ϱ [11]. When the magnetic field is kept homogeneous but the scalar potential is turned on the degeneracy is lifted, the energy increasing with increasing power of ϱ [6,7]. For the investigation in the case of inhomogeneous fields we

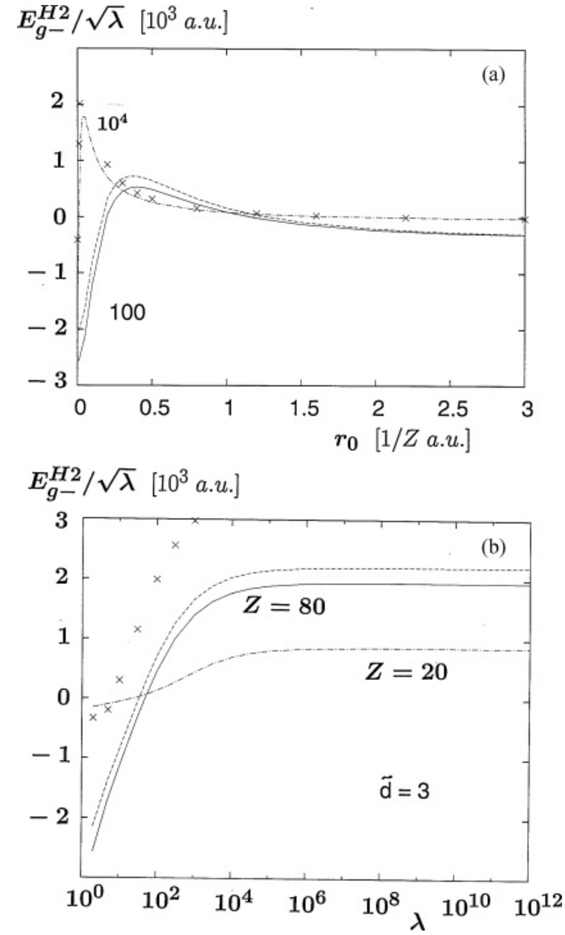

FIG. 5. Scaled ground-state energy $E_{g-}^{H2}/\lambda^{1/2}$ (without rest energy) for the Egger field (2.6) and the kinetic energy estimate from (2.4) with different trial functions. (a) for $Z = 80$ as a function of the hole radius r_0 (in units of the K-shell radius, $1/Z$ a.u.): ψ_t for $\lambda = 100$ (————) and $\lambda = 10^4$ (– · – · –); $\psi_t^{(2)}$ with $\tilde\gamma$ from (2.1) for $\lambda = 100$ (– – – – –) and $\lambda = 10^4$ (×). (b) for $\tilde d = 3$ as a function of λ for ψ_t and $Z = 80$ (————), $Z = 20$ (– · – · –), as well as for $\psi_t^{(3)}$ and $Z = 80$ for $l = 0.1$ (– – – – –) and $l = 1$ (×).

use the following trial function:

$$\psi_t^{(3)}(\mathbf{x}) = N_3\, e^{-\nu^2\varrho^2/2}\,(\varrho e^{i\varphi})^l\, e^{-Z'x} \begin{pmatrix}1\\0\end{pmatrix},$$

$$N_3 = \left[-\,\frac{\pi Z'\Gamma^2(l+1)}{\nu^{2l+4}}\,\psi'\left(l+1,1,\frac{Z'^2}{\nu^2}\right)\right]^{-\frac{1}{2}}, \tag{4.4}$$

where N_3 is the normalization constant, $\nu = \sqrt{2s\,eB}$ and ψ' the derivative of the irregular confluent hypergeometric function.

The B-independent part of the energy functional (2.4) can for $\psi_t^{(3)}$ still be evaluated analytically [7], whereas the B-dependent part is given by (2.23), modified by the additional factor ϱ^{2l} in the integrand, plus a nonvanishing contribution from the cross term,

$$\left(\psi_t^{(3)}, (-2eA_1p_1 - 2eA_2p_2)\,\psi_t^{(3)}\right)$$

$$= -4\pi\, l\, eBN_3^2 \int_{r_0}^{\infty} d\varrho\, \varrho^{2l} e^{-\nu^2\varrho^2}\left(\varrho^2 - r_0^2\right)K_1(2\varrho Z'). \tag{4.5}$$

If $l > 0$ is fixed, the minimum of this energy functional, $E^{H2}[\psi_t^{(3)}]$, is indeed higher than in the case of the variational function ψ_t from (2.7) and increases with l. The effect is particularly large when l is restricted to integers like in the degenerate $Z = r_0 = 0$ eigenstates. For $l = 0.1$ and 1 this is shown in Fig. 5(b) where the scaled energy near its maximum (at $\tilde{d} = 3$) is plotted as a function of the field strength. Included are the $l = 0$ results for $Z = 20$ to display the Z-dependent monotonous increase of the scaled energy with λ at fixed $\tilde{d}$ up to saturation for $\lambda \gtrsim 10^8$.

V. CONCLUSION

We have studied the ground-state energy of an atomic electron in an inhomogeneous magnetic field which is described by two parameters, the size of a field-free area around the nucleus and the field strength. Irrespective of the particular choice of the magnetic field the variational estimate of the ground-state energy of the Herbst operator, used to model the relativistic electron, becomes positive for a certain limited size of this field-free region if the field strength is larger than some critical value. The lowest energy estimate is obtained for a trial function which combines an eigenfunction of the lowest Landau level with a nonrelativistic hydrogenic function. The only exceptions are ultrastrong fields, including the limit $B \to \infty$, where a trial function, which is separable in the coordinates parallel and perpendicular to the magnetic field, is more appropriate.

Our conjecture that the antibinding of the electron in a particular parameter range is real and not an artefact due to an inappropriate choice of the trial function is supported by two facts. First, a positive maximum of the variational ground-state energy is obtained for all trial functions investigated. Second, this maximum increases with a positive power of the field strength. Thus we have established the possibility of static ionization of a heavy ion by means of an appropriately chosen strong inhomogeneous magnetic field.

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