Two methods for solving the Dirac equation without variational collapse

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Two special variational techniques, the Lehmann-Maehly (LM) method and the Kato method, recently proposed for solving the one-electron Dirac equation without variational collapse are investigated here in detail. Both methods represent significant progress compared to the traditional variational techniques because each of them provides rigorous upper and lower bounds to relativistic binding energies. A careful theoretical examination, however, reveals that only the LM method can be regarded as a radical solution of all the problems related to variational collapse. A numerical application to the Dirac equation for the hydrogen atom in a uniform magnetic field confirms this conclusion and shows as well that the LM method is also capable of yielding extremely accurate results and that the Kato method, in spite of a few limitations, represents in any case a useful approach. [S1050-2947(97)08107-9]

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I. INTRODUCTION

The Rayleigh-Ritz (RR) method represents a powerful tool for determining approximations to the eigenvalues and the eigenvectors of a given self-adjoint operator H. In addition to the self-adjointness, the application of the method, however, requires [1,2] precise conditions on the spectrum of H. First of all, this spectrum has to be at least semibounded (semibounded operators) either from below (bounded below operators) or from above (bounded above operators). Moreover, in the case of bounded below (above) operators, the lower (upper) part of the spectrum has to be purely discrete, i.e., made up only of finitely or infinitely many isolated eigenvalues of finite multiplicity. When all these conditions are satisfied, the RR method has remarkable properties. In the case of a bounded below operator H, these properties are the following.

(a) The eigenvalue problem for H is equivalent to certain minimum problems for the RR quotient $R(x)=\langle x|Hx\rangle/\langle x|x\rangle, x\neq 0,\ x\in D(H)\subset\mathcal{H}$, where $\mathcal{H}$ is a Hilbert space, $D(H)$ is the domain of H, and $\langle|\rangle$ is the scalar product of $\mathcal{H}$.

(b) If $\lambda_0\leqslant\lambda_1\leqslant\cdots$ are the eigenvalues of H and $\lambda_0^N\leqslant\lambda_1^N\leqslant\cdots$ are the eigenvalues of H_N [the matrix representation of H in an N-dimensional subspace $\mathcal{H}^N\subset D(H)$], then

$$\lambda_0\leqslant\lambda_0^N,\quad \lambda_1\leqslant\lambda_1^N,\ \ldots,\lambda_N\leqslant\lambda_N^N$$

(Poincaré's theorem).

(c) If $\mathcal{H}^N\subset\mathcal{H}^{N'}$, then

$$\lambda_i^{N'}\leqslant\lambda_i^N,\quad i=1,\ldots,N.$$

(d) Precise conditions for the analytical convergence as $N\to\infty$ of the eigenvalues λ_i^N and the associated eigenvectors ψ_i^N, $i=1,2,\ldots$, respectively, to the exact eigenvalues and eigenvectors of H can be established.

By virtue of these properties [3], the RR method (the traditional variational method) represents the most powerful and reliable tool for determining bound-state energies and corresponding eigenfunctions in nonrelativistic quantum mechanics. In this case, in fact, the application of the RR method is legitimate because Schrödinger operators have exactly the spectral properties specified above. However, the situation completely changes if one considers a Dirac operator D because, as is well known, Dirac operators are not semibounded. The application of the RR method for solving Dirac equations thus has no mathematical foundation and gives rise, as a consequence, to enormous difficulties. In the specialized literature [4], these difficulties are named ''variational collapse.'' This term makes reference to the fact that any positive-energy eigenvalue of D_N (the matrix representation of D in an N-dimensional subspace) may decrease without limit as the size of the basis is enlarged. This, however, is only the aspect of the variational collapse commonly referred to; its essence instead is that properties (a)–(d) do not hold anymore. Thus, in particular, no direct-minimization method, such as that described in [5], can be applied to find approximations to exact eigenvalues and eigenvectors of Dirac operators; the eigenvalues of D_N cannot be improved by a minimization procedure with respect to possible nonlinear parameters in the basis set; no monotonic improvement (or even no improvement at all) is guaranteed as N increases and the possibility of estimating the relative accuracy of two calculations employing two different basis sets is lost. The appearance then of unphysical positive eigenvalues of D_N (spurious states), mixed with the physical ones, contributes to complicate even more things. In the past ten years, a great many approaches (see Refs. [4,6–8] and references therein) have been proposed for avoiding the variational collapse. According to Ref. [4], these approaches can be classified into essentially three categories.

(i) The problem is not faced at the root, but some of its main difficulties are circumvented by means of special techniques. Very satisfactory results have been obtained [7] within this framework by choosing the basis set carefully.

(ii) The wrong nonrelativistic limit of Dirac operators is considered to be the main cause of variational collapse. Various techniques have been put forth to make calculations that admit the correct Schrödinger limit. Among these techniques the most promising one [4] consists in transforming the given Dirac operator by a Foldy-Wouthuysen transformation and then applying the RR method. From a general point of view, this approach is undoubtedly more satisfactory than (i); however, its mathematical foundation is somewhat obscure. Thus, in particular, one cannot state [4] whether it is actually sufficient to avoid all the diseases of variational collapse.

(iii) The fact that Dirac operators are not semibounded is considered to be at the origin of all the difficulties of the variational collapse. The given Dirac operator D is thus replaced by a certain function such that the resulting operator $f(D)$ is self-adjoint, bounded from below, and has the spectral properties required by the RR method. This method is then applied to $f(D)$.

This latter approach is clear because the self-adjointness of Dirac operators can be proved [9] for a large class of potentials; the prescription for defining $f(D)$ is given by spectral theory [10] and the application of the RR method is perfectly legitimate. Compared to approaches (i) and (ii), it is also much simpler and gets, in our opinion, to the main root of the problem, i.e., to the fact that Dirac operators are not semibounded. Indeed, as we shall see in detail later, approach (iii) sets up again properties (a)–(d) above. Obviously, its effective usefulness depends on the existence of a suitable function $f(D)$. Hill and Krauthauser have shown recently [8] that a choice for $f(D)$ particularly advantageous is the function $(D-\rho)^{-1}$, where ρ is a real number not belonging to the spectrum of D. In Ref. [8] one can find an investigation of approach (iii) employing such a function as well as a preliminary numerical test on the Dirac hydrogen atom. Among the advantages of choosing the function $(D-\rho)^{-1}$, Hill and Krauthauser point out and illustrate [Eq. (9) in [8]] the remarkable possibility of determining, in addition to upper bounds to the eigenvalues of D, lower bounds as well. A comment is now in order. The idea of employing approach (iii) with the choice $f(D)=(D-\rho)^{-1}$ as a technique for avoiding variational collapse appears in Ref. [8]. However, it is nothing but a special application of the Lehmann-Maehly (LM) method, i.e., the method that Lehmann and Maehly [11] introduced as a general procedure for determining rigorous upper and lower bounds to the eigenvalues of a given self-adjoint operator not necessarily semibounded. Thus, for matters of a historical nature, we shall keep on calling here ''LM method'' approach (iii) with the choice $f(D)=(D-\rho)^{-1}$. It should be observed that another method for avoiding the variational collapse has been recently proposed as well [12]. This second method is nothing but the application of certain formulas, shown by Kato [13] almost half a century ago, for determining rigorous upper and lower bounds to the eigenvalues of a given operator satisfying once more the hypothesis of being self-adjoint but not necessarily semibounded. In the present paper, we shall call ''Kato method'' both Kato's formulas [13] as well as their employment for avoiding the variational collapse. Although the Kato method, as we shall see, presents close connections with the LM method, it has different properties and cannot be classified in any of the three categories above. In particular, contrary to the LM method, it does not set up again the previously mentioned properties (a)–(d). More important is that the Kato method is capable of yielding rigorous upper bounds to relativistic energies, thereby overcoming the worst disease of variational collapse. The possibility then of the Kato method providing lower bounds as well is an element of further interest. These considerations as well as the encouraging preliminary investigations in Refs. [8,12] have motivated the present paper, whose main aim is a further investigation of both the LM method and the Kato method as techniques for avoiding variational collapse. The paper is organized as follows: In Sec. II we describe the mathematical foundation of the two methods, in Sec. III we present a numerical application of each of them to the Dirac equation for the hydrogen atom in uniform magnetic fields, and in Sec. IV we compare their performances and discuss the numerical results obtained.

II. METHODS

As we said, the LM method and the Kato method are two techniques for determining rigorous upper and lower bounds to the eigenvalues of a given self-adjoint operator not necessarily semibounded. In the present section we show concisely and without any proof the mathematical foundation of the two methods. Proofs and a more detailed description can be found in [2] and in references therein.

A. The Lehmann-Maehly method

Let $\mathcal{H}$ be a complex separable Hilbert space, with scalar product and norm denoted by $\langle|\rangle$ and $\|\cdot\|$, respectively. Let H be a self-adjoint operator in $\mathcal{H}$, satisfying the only hypothesis that at least a part of its spectrum is purely discrete. This part of spectrum is thus made up only of finitely or infinitely many eigenvalues

$$\cdots\leqslant E_{-n-1}\leqslant E_{-n}\leqslant\cdots\leqslant E_{-1}\leqslant E_0\leqslant E_1\leqslant\cdots\leqslant E_n\leqslant E_{n+1}\leqslant\cdots, \tag{1}$$

each of finite multiplicity.

Consider the operator $(H-\rho)^{-1}$, where

$$E_k<\rho<E_{k+1},\quad k=0,\pm1,\ldots. \tag{2}$$

This operator [10] is bounded, self-adjoint, and, in correspondence with the eigenvalues (1), presents the purely discrete spectrum

$$\lambda_k\leqslant\lambda_{k-1}\leqslant\cdots<0<\cdots\leqslant\lambda_{k+2}\leqslant\lambda_{k+1}, \tag{3}$$

where

$$\lambda_i=(E_i-\rho)^{-1},\quad i=k,k-1,\ldots,k+2,k+1. \tag{4}$$

The application of the RR method to the operator $(H-\rho)^{-1}$ is thus perfectly legitimate. Henceforth, we shall denote the corresponding RR eigenvalues by $\lambda_i^N, i=k,k-1,\ldots,k+2,k+1$, where N is the dimension

of the subspace employed. Owing to the spectrum (3) and if N is big enough, one finds (counting multiplicity) r^N negative RR eigenvalues

$$\lambda_k^N \leqslant \lambda_{k-1}^N \leqslant \cdots \leqslant \lambda_{k-r^N+1}^N < 0 \tag{5}$$

and s^N positive RR eigenvalues

$$0 < \lambda_{k+s^N}^N \leqslant \cdots \leqslant \lambda_{k+2}^N \leqslant \lambda_{k+1}^N. \tag{6}$$

Applying now the Poincaré theorem [see property (b) in the Introduction and also Ref. [3]) and making use of Eq. (4) and inequalities (5) and (6), one gets immediately

$$E_k \geqslant \frac{1}{\lambda_k^N} + \rho, \quad E_{k-1} \geqslant \frac{1}{\lambda_{k-1}^N} + \rho, \ldots$$

$$E_{k-r^N+1} \geqslant \frac{1}{\lambda_{k-r^N+1}^N} + \rho \tag{7}$$

and

$$E_{k+1} \leqslant \frac{1}{\lambda_{k+1}^N} + \rho, \quad E_{k+2} \leqslant \frac{1}{\lambda_{k+2}^N} + \rho, \ldots$$

$$E_{k+s^N} \leqslant \frac{1}{\lambda_{k+s^N}^N} + \rho. \tag{8}$$

In other words, applying in a subspace suitably large the RR method to the operator $(H-\rho)^{-1}$, with a parameter ρ satisfying condition (2) with a given index k, we can get lower bounds for the r^N exact eigenvalues of H, $E_i < \rho$, $i = k, k-1, \ldots k-r^N+1$, and upper bounds for the s^N exact eigenvalues of H, $E_j > \rho$, $j = k+1, k+2, \ldots k+s^N$. Thus, with two choices of ρ, say ρ_1, ρ_2, each satisfying a condition (2) with a different value of the index k, we can obtain, if N is big enough, both upper and lower bounds for all the eigenvalues of H belonging to the interval (ρ_1, ρ_2).

The practical application of the LM method presents, however, two difficulties: calculating the matrix elements of the inverse of $(H-\rho)$ and choosing a suitable parameter ρ. A remedy for the first difficulty is employing [8,11] as basis set the vectors

$$\tilde{\phi}_i = (H-\rho)\phi_i, \quad i = 1,2, \ldots, N, \tag{9}$$

where $\{\phi_i\}_{i=1}^N$ are vectors of $D(H)$ linearly independent but not necessarily orthonormal. The original RR method for the operator $(H-\rho)^{-1}$ in fact becomes [2], in the basis (9), the generalized eigenvalue problem

$$(H-\rho)_N \psi^N = \lambda^N (H-\rho)_N^2 \psi^N, \tag{10}$$

where $(H-\rho)_N$ and $(H-\rho)_N^2$ are the $N \times N$ matrices $\{\langle \phi_i | (H-\rho)\phi_j \rangle\}_{i,j=1}^N$ and $\{\langle \phi_i | (H-\rho)^2 \phi_j \rangle\}_{i,j=1}^N$, respectively. Thus the presence of the operator $(H-\rho)^{-1}$ is avoided and we have to deal only with the more tractable operator $(H-\rho)^2$. The second difficulty, as we shall discuss in Sec. IV, can be serious in some situations. For the moment we observe that by varying ρ in a given interval (E_k, E_{k+1}), $k = 0, \pm 1, \ldots$, the lower bounds (7) improve as $\rho \to E_{k+1}$, whereas the upper bounds (8) improve as $\rho \to E_k$.

B. The Kato method

In comparison with the LM method, the Kato method follows a very different approach. It applies essentially elements of spectral theory to determine accurate intervals that contain points of the spectrum of a given self-adjoint operator H not necessarily semibounded. Given a vector $\psi \in D(H)$ $(\|\psi\| = 1)$, let us compute the quantities $\langle H \rangle = \langle \psi | H \psi \rangle$ and $\Delta = (\langle H^2 \rangle - \langle H \rangle^2)^{1/2}$. Then the half-closed interval

$$(\langle H \rangle - \Delta, \langle H \rangle + \Delta]$$

contains at least a point of the spectrum of H (Weinstein's formula). Now assume that we are able to determine an open interval (a,b) containing an eigenvalue (say E_k) as a unique point of the spectrum of H and consider the conditions

$$\langle H \rangle < b, \quad \xi \equiv \langle H \rangle - \frac{\Delta^2}{b - \langle H \rangle} > a \tag{11}$$

and

$$\langle H \rangle > a, \quad \zeta \equiv \langle H \rangle + \frac{\Delta^2}{\langle H \rangle - a} < b. \tag{12}$$

Then, if ψ satisfies condition (11) we have $\xi \leqslant E_k < b$, if ψ satisfies condition (12) we have $a < E_k \leqslant \zeta$, and if ψ satisfies both conditions (11) and (12) we get

$$\xi \leqslant E_k \leqslant \zeta \tag{13}$$

(Kato's formula). In other words, if one knows rough bounds to E_k, one can determine some others that are more accurate. Formula (13) turns out to be scarcely precise if the spectral region that one is interested in presents eigenvalues that are densely crowded. In this case, the following generalization of formula (13) can be shown [13]. Suppose that the interval (a,b) contains m eigenvalues, say $E_1 \leqslant E_2 \leqslant \cdots \leqslant E_m$, but no further point of the spectrum of H. Choose m orthonormal vectors $\tilde{\psi}_1, \tilde{\psi}_2, \ldots \tilde{\psi}_m$ such that the matrix $\langle \tilde{\psi}_i | H \tilde{\psi}_j \rangle$ is diagonal, i.e., $\langle \tilde{\psi}_i | H \tilde{\psi}_j \rangle = \langle H \rangle_{\tilde{\psi}_i} \delta_{ij}$, $i,j = 1,2, \ldots m$ and such that

$$a < \langle H \rangle_{\tilde{\psi}_1} \leqslant \langle H \rangle_{\tilde{\psi}_2} \leqslant \cdots \leqslant \langle H \rangle_{\tilde{\psi}_m} < b.$$

Then

$$\langle H \rangle_{\tilde{\psi}_k} - \sum_{i=k}^{m} \frac{\Delta_{\tilde{\psi}_i}^2}{b - \langle H \rangle_{\tilde{\psi}_i}} \leqslant E_k \leqslant \langle H \rangle_{\tilde{\psi}_k} + \sum_{i=1}^{k} \frac{\Delta_{\tilde{\psi}_i}^2}{\langle H \rangle_{\tilde{\psi}_i} - a},$$

$$k = 1,2, \ldots m, \tag{14}$$

where $\Delta_{\tilde{\psi}_i}^2 = (\langle H^2 \rangle_{\tilde{\psi}_i} - \langle H \rangle_{\tilde{\psi}_i}^2)$ (the generalized Kato formula). It should be observed that the quantity Δ^2 (mean-square energy deviation) permits also estimates of the error in the $\mathcal{H}$ norm of any approximate eigenvector ψ $(\|\psi\| = 1)$. Confining ourselves to the case where the interval (a,b) con-

tains the sole nondegenerate eigenvalue E_k as a unique point of the spectrum of H, denoting by ψ_k ($\|\psi_k\|=1$) the exact eigenvector associated with E_k, and supposing that ψ satisfies conditions (11) and (12), one can indeed show [2,13]

$$\|\psi-\psi_k\|\leqslant(2-2\sqrt{1-\sigma^2})^{1/2}\equiv\Sigma, \tag{15}$$

where

$$\sigma^2=\{[\langle H\rangle-(a+b)/2]^2+\Delta^2\}/[(b-a)/2]^2.$$

More accurate estimates (15) can be obtained if either $\zeta\leqslant(a+b)/2$ or $\xi\geqslant(a+b)/2$, in correspondence with the following values of σ^2:

$$\sigma^2=\begin{cases}\Delta^2/[(\langle H\rangle-a)^2+\Delta^2], & \zeta\leqslant(a+b)/2\\ \Delta^2/[(b-\langle H\rangle)^2+\Delta^2], & \xi\geqslant(a+b)/2.\end{cases}$$

Formulas (13) and (14) show that the application of the Kato method presents problems similar to those in the LM method, i.e., a preliminary rough knowledge of the spectrum that one is interested in and the evaluation of the matrix elements of H^2. Although the LM method and the Kato method seem at first sight to have nothing in common, a more accurate analysis reveals a close connection between them. To see that, we note first that points a and b in inequalities (11) and (12) do not belong to the spectrum of H; thus they can be also regarded as special points ρ satisfying conditions (2). Now, set in inequalities (11) and (12) $a=\rho_1$ and $b=\rho_2$. Denote by $\mathcal{H}^N_{\rho_2}$ the subspace spanned by the N vectors (9), with $\rho=\rho_2$, and suppose that there exists a vector $\psi\in\mathcal{H}^N_{\rho_2}$ satisfying inequalities (11), i.e., such that the Kato lower bound $\xi(\rho_2,\psi)$ to E_k exists. Then there exists also [2] a corresponding LM lower bound, which is the optimal value of $\xi(\rho_2,\psi)$ as ψ is varied on $\mathcal{H}^N_{\rho_2}$. Analogously, if there exists a vector $\psi\in\mathcal{H}^N_{\rho_1}$ satisfying inequalities (12), there exists consequently a LM upper bound to E_k, which represents the optimization of the Kato upper bound $\zeta(\rho_1,\psi)$ as ψ is varied on $\mathcal{H}^N_{\rho_1}$.

III. APPLICATION OF THE LEHMANN-MAEHLY AND KATO METHODS

In this section we describe the application of the LM method and the Kato method to the Dirac equation for the hydrogen atom in uniform magnetic fields. Such a choice has been motivated by the importance that the problem of the hydrogen atom in uniform magnetic fields has taken on in the past 25 years, as well as by the fact that this problem has been investigated so far mainly within a nonrelativistic framework. Accurate relativistic calculations have appeared indeed only a few years ago in a paper by Chen and Goldman [7].

The Dirac Hamiltonian (in atomic units) for a hydrogen atom, with a point nucleus fixed in the origin, placed in a uniform magnetic field $\vec{B}=B\hat{z}$ is

$$H^D=c\,\vec{\alpha}\cdot\left(\vec{p}+\frac{\vec{A}}{c}\right)+\beta c^2-\frac{1}{r}, \tag{16}$$

where $\vec{\alpha}$ and β are the usual 4×4 Dirac matrices and $\vec{A}=\frac{1}{2}B\hat{z}\times\vec{r}$. The magnetic field B is here measured in units of $(e/\hbar)^3m_e^2c\simeq2.35\times10^9$ G.

The Hamiltonian (16) is self-adjoint [9]; thus it satisfies the main property that both the LM method and the Kato method require. In order to apply these methods it is therefore enough to introduce a proper basis set $\{\phi_i\}_{i=0}^N$. Before we specify this set, it should be observed [see Eqs. (9) and (10)] that a basis set is necessary for the LM method, whereas it is not for the Kato method. The latter in fact needs an approximate eigenfunction ψ [formula (13)] or approximate eigenfunctions $\tilde{\psi}_1,\ldots\tilde{\psi}_m$ [formula (14)] as starting points, but it does not require that these approximations are of variational nature. In the present paper, however, we determine ψ and $\tilde{\psi}_1,\ldots,\tilde{\psi}_m$ in the Kato method variationally, i.e., by applying the RR method directly to H^D and choosing then as $\psi,\tilde{\psi}_1,\ldots,\tilde{\psi}_m$ certain eigenfunctions of H^D_N (the matrix representation of H^D in an N-dimensional subspace [14]). The basis set employed by us in the present paper is the same as the one in Refs. [7,12], i.e.,

$$\phi^{(h)}_{nl_h}(r,\theta,\varphi)=r^{\gamma-1+n}e^{-\lambda r-\mu r^2\sin^2\theta}\times(\cos\theta)^{l_h-|m_h|}(\sin\theta)^{|m_h|}e^{im_h\varphi}\omega_h, \tag{17}$$

$$n=0,1,2,\ldots,N_r,\quad h=1,2,3,4,$$

where r,θ,φ are spherical coordinates; $\gamma=\sqrt{\kappa^2-\alpha^2}$, with κ being the Dirac quantum number and α the fine-structure constant; $m_h=j_z-\nu_h/2$, with $\nu_1=\nu_3=1$, $\nu_2=\nu_4=-1$ and j_z being the eigenvalue of the z component J_z of the total angular momentum; λ and μ are nonlinear variational parameters, and ω_h is the four-component spin function. The quantity l_h takes on values greater than or equal to $|m_h|$, which are even numbers up to $2N_\theta$ for even- (odd-) parity states and $h=1,2$ ($h=3,4$) and odd numbers up to $2N_\theta+1$ for odd- (even-) parity states and $h=1,2$ ($h=3,4$). Thus the total number of the vectors employed, i.e., the dimension N of the subspace, is

$$N=(N_r+1)(4N_\theta+3). \tag{18}$$

The structure of the basis (17) corresponds chiefly to the following: Considering that H^D commutates with the operator J_z and with the parity operator, the basis (17) gives rise (with the rules above for the values taken on by m_h and l_h) to eigenfunctions of these two operators, it reproduces the exact solutions of the Dirac equation in the two extreme situations $Z=1$, $B=0$ and $Z=0$, $B>0$ (Z is the atomic number), and it satisfies the boundary condition at $r\to0$ and ∞ and has the correct nonrelativistic limit. As we said, a difficulty in applying both the LM method [see Eq. (10)] and the Kato method [see formulas (13) and (14)] is that in addition to the matrix elements of H^D one needs also those of $(H^D)^2$. In our case, however, the matrix elements of these two operators in the basis (17) can be expressed in terms of a general integral that can always be evaluated numerically. Details about that can be found in Refs. [7,12]. It should also be observed that the basis (17) is not orthonormal. Its orthonormalization, as we said [see Eq. (9)], is not strictly

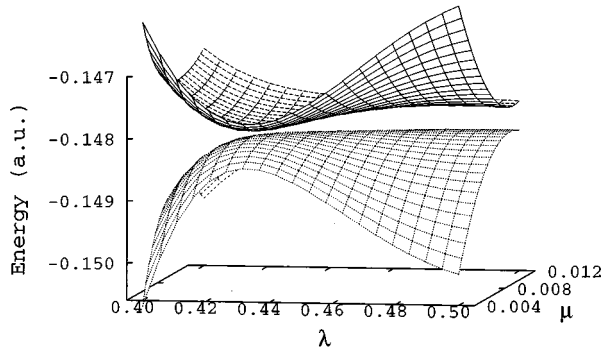

FIG. 1. LM upper bound and LM lower bound to the relativistic binding energy of the first excited state $j_z^P=\frac{1}{2}^+$ of the hydrogen atom in the uniform magnetic field $B=0.1$, plotted against the nonlinear parameters λ,μ in the basis (17). The dimension of the subspace employed is $N=28$, with [see Eq. (18)] $N_r=3$ and $N_\theta=1$.

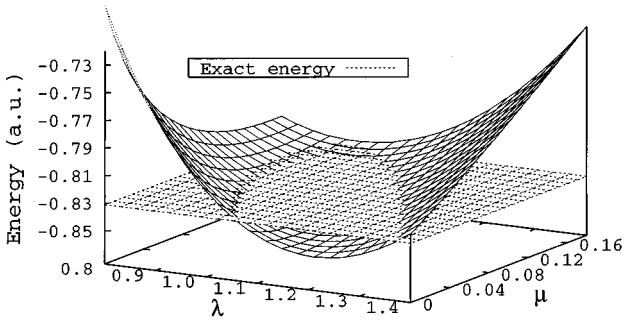

FIG. 3. Variational approximation for the relativistic ground-state binding energy of the hydrogen atom in the magnetic field $B=1$, plotted against the nonlinear parameters λ,μ. The dimension of the subspace employed is $N=3$, with $N_r=0$ and $N_\theta=0$. The reference horizontal plane represents the ''exact'' binding energy, i.e., that determined by LM bounds.

required by the LM method, but it turns out to be convenient in the Kato method. Thus, in practice, we first orthonormalize the set (17) and then we employ the orthonormalized vectors, say $\{\phi_i^{(h)\prime}\}$, as vectors $\{\phi_i\}$ in Eq. (9) to apply the LM method and as a basis set as well to apply the RR method to H^D, i.e., to apply the Kato method. The matrix elements of H^D and $(H^D)^2$ with respect to the vectors $\{\phi_i^{(h)\prime}\}$, which thus appear in Eq. (10), are then obtained from those in the basis (17) by linear transformations. A disadvantage of the basis (17) is that it presents problems of near linear dependence; thus, in practice, one cannot use a dimension N greater than ~ 280. This reduced dimension limits in some cases the precision of our results; however, it is quite sufficient to investigate the performance of the LM method and the Kato method as tools for avoiding variational collapse. This investigation is indeed the primary goal of the present paper.

IV. RESULTS AND DISCUSSION

According to the analysis of Sec. II, we expect that both the LM method and the Kato method yield useful upper and lower bounds to the eigenvalues of the Dirac Hamiltonian (16). However, we should also expect that all the remarkable properties (a)–(d) of the RR method in the Introduction continue to hold in the LM method but they do not in the Kato method. The former, in fact, is nothing but the RR method applied to the bounded self-adjoint operator $(H^D-\rho)^{-1}$, whereas the latter is founded on spectral theory and thus it has nothing to do with the RR method. Figures 1, 2, and 3 illustrate the behavior of the LM bounds, the Kato bounds, and the variational approximations, respectively, as a function of the nonlinear parameters λ,μ in the basis (17). We can see that both LM bounds and Kato bounds always bracket the exact binding energy and moreover have extremum properties. These facts in particular give us a reliable and easy way to optimize the parameters λ and μ. The variational approximation, on the contrary, shows a minimum that has no physical meaning but, even worse, takes on values both bigger and smaller than the exact binding energy. Figures 4, 5, and 6 illustrate the behavior of the LM bounds, the Kato bounds, and the variational approximations, respectively, as a function of the total number N of the basis vectors employed. In particular, Fig. 4 shows the remarkable monotonic behavior of the LM bounds as a function of N [property (c) in the Introduction], whereas Figs. 5 and 6 show that this is not a property of either the Kato method

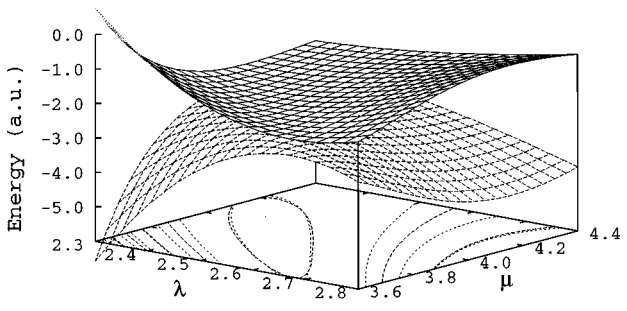

FIG. 2. Kato upper bound and Kato lower bound to the relativistic ground-state binding energy of the hydrogen atom in the magnetic field $B=20$, plotted against the nonlinear parameters λ,μ in the basis (17). The dimension of the subspace employed is $N=9$, with $N_r=2$ and $N_\theta=0$.

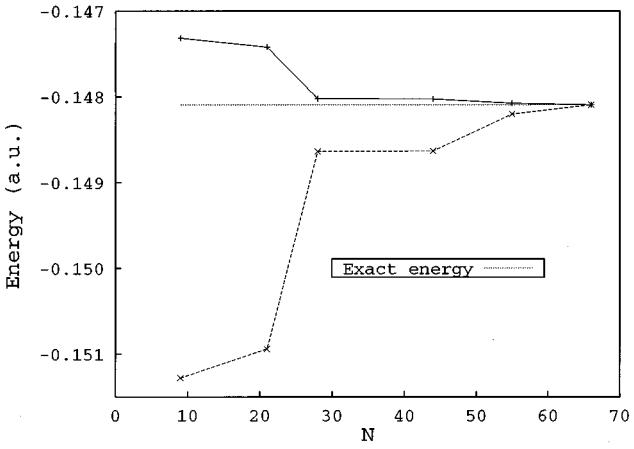

FIG. 4. LM upper bound and LM lower bound to the relativistic binding energy of the same state as in Fig. 1, as a function of the basis size N.

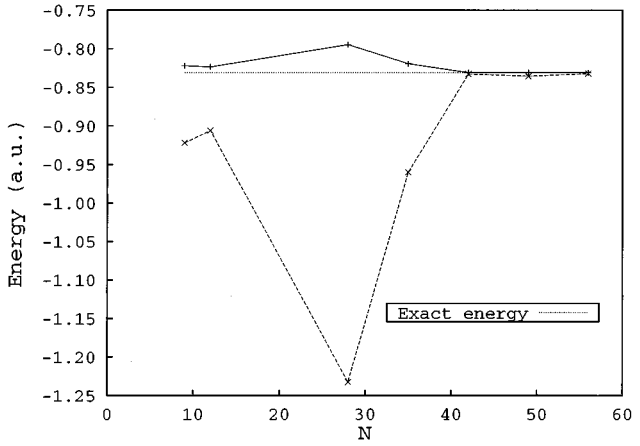

FIG. 5. Kato upper bound and Kato lower bound to the relativistic binding energy of the same state as in Fig. 3, as a function of the basis size N.

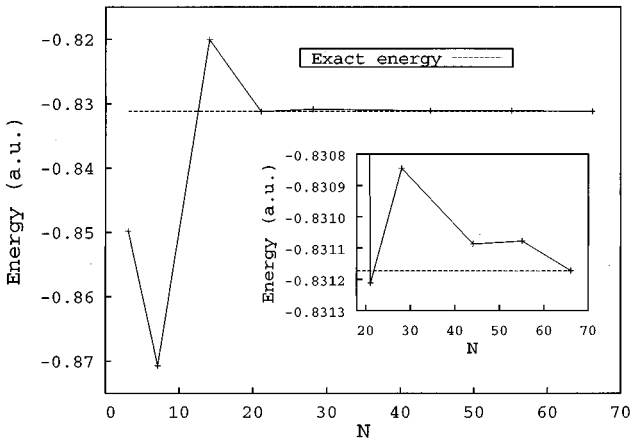

FIG. 6. Variational approximation for the relativistic binding energy of the same state as in Figs. 3 and 5, as a function of the basis size N.

or the variational approximations. Notice, however, that the Kato bounds remain in any case rigorous upper and lower bounds to the exact energy, while the value of the variational approximation oscillates around it. Tables I–III show the degree of accuracy that one can obtain by employing either the LM method or the Kato method. We can see that the LM results are in general much more accurate than the Kato ones. This different performance depends on the fact that the LM eigenfunctions calculated by us are much more precise than the variational ones, which we employ as trial wave functions in the Kato method [see error estimates $\Sigma_l^u(\mathrm{LM})$ and $\Sigma(\mathrm{K})$ in Tables I and II]. Although the RR method applied directly to H^D does not yield, in general, very accurate eigenfunctions and presents all the defects outlined in the

TABLE I. Relativistic ground-state binding energies [17] and error estimates of the associated eigenfunctions of the hydrogen atom in intense magnetic fields, in subspaces of given parity and projection of the total angular momentum J_z. Column B, values of the magnetic field; column P, parity; column N_r, N_θ, values of N_r and N_θ [see Eq. (18)]; column j_z, eigenvalues of J_z; column $-E_l^u(\mathrm{LM})$, upper bounds (upper rows) and lower bounds (lower rows) on the binding energies calculated by method; column $\Sigma_l^u(\mathrm{LM})$, error estimates [see Eq. (15)] of the eigenfunctions obtained by the LM method, where the upper (lower) rows are the estimates relative to the eigenfunctions corresponding to the upper (lower) bounds; column $-E_l^u(\mathrm{K})$, upper bounds (upper rows) and lower bounds (lower rows) on the binding energies calculated by the Kato method; column $\Sigma(\mathrm{K})$, error estimates of the variational eigenfunctions employed in the Kato method; column $-E^N$, variational approximations. Notice that coincident digits in a given pair of upper and lower bounds are not reported in the lower-bound row. Blank spaces in column $-E_l^u(\mathrm{K})$ mean that either no value for these quantities can be given or a value exists but it represents a bad estimate.

B	P	N_r, N_θ	j_z	$-E_l^u(\mathrm{LM})$	$\Sigma_l^u(\mathrm{LM})$	$-E_l^u(\mathrm{K})$	$\Sigma(\mathrm{K})$	$-E^N$
10	+	9,4	$-1/2$	1.747800687	3.8×10^{-5}	1.747800304	1.2×10^{-3}	1.747800687
				8	3.9×10^{-5}	2869		
20	+	11,5	$-1/2$	2.21540045	2.1×10^{-3}	2.21539	1.5×10^{-1}	2.21540091
				317	3.8×10^{-3}	6229		
500	+	9,4	$-1/2$	6.2570305	3.3×10^{-3}	6.22791	8.7×10^{-2}	6.2570326
				581	3.2×10^{-3}	7532		
10	−	9,4	$-3/2$	1.12542203	2.5×10^{-4}	1.12542119	5.2×10^{-3}	1.12542203
				4	6.7×10^{-4}	3626		
100	−	9,4	$-3/2$	2.63475382	1.4×10^{-3}	2.634414	2.4×10^{-2}	2.63475394
				584	1.1×10^{-3}	5981		
10	−	9,4	$-1/2$	0.38266318	1.7×10^{-3}		1.2	0.38266316
				38	1.2×10^{-3}			

TABLE II. Relativistic binding energies and eigenfunction error estimates for the first five states $j_z^P = -\frac{1}{2}^+$ of the hydrogen atom in the magnetic field $B=0.1$. Columns N_r, N_θ, $-E_l^u(\mathrm{LM})$, $\Sigma_l^u(\mathrm{LM})$, $-E_l^u(\mathrm{K})$, $\Sigma(\mathrm{K})$, and $-E^N$ are as in Table I. Column δE, relativistic corrections $\delta E=(E_R-E_{NR})/|E_{NR}|$, where E_R (relativistic energy) is determined by the LM bounds in this table, whereas E_{NR} (nonrelativistic energy) is determined by the Kato bounds according to Ref. [18]. Blank spaces in columns $-E_l^u(\mathrm{K})$, $\Sigma(\mathrm{K})$, and $\delta(E)$ have the same meaning as in Table I.

N_r N_θ	$-E_l^u(\mathrm{LM})$	$\Sigma_l^u(\mathrm{LM})$	$-E_l^u(\mathrm{K})$	$\Sigma(\mathrm{K})$	$-E^N$	δE
6,3	0.54753240833	9.8×10^{-6}	0.5475323991	8.4×10^{-4}	0.54753240834	-1.08×10^{-5}
	5	7.0×10^{-6}	6586			
9,4	0.1480917386	3.2×10^{-5}	0.0246		0.1480917386	-1.74×10^{-5}
	7	2.9×10^{-5}	0.7858			
9,4	0.074938688	1.5×10^{-5}	0.074624	4.3×10^{-1}	0.074938689	-8.75×10^{-6}
	99	9.7×10^{-4}	9189			
9,4	0.04356687	3.9×10^{-3}	0.02562		0.04356687	
	92	2.9×10^{-3}	7851			
8,4	0.0280747	9.4×10^{-2}			0.0280748	
	94	3.2×10^{-2}				

Introduction, instead it yields in our case very accurate eigenvalues. Our variational approximations, in fact, have the same order of accuracy as the LM bounds. This, however, is not an advantage of the usual variational method in itself, but it depends only on the fact that we employ basis vectors carefully chosen [7] and with nonlinear parameters λ,μ optimized by minimizing $E^u(\mathrm{LM})$. As we said, the application of the two methods investigated here has a price: the calculation of matrix elements of $(H^D)^2$ and a preliminary rough knowledge of the spectrum that one is interested in. This price indeed is well rewarded because after all we can compute at the same time upper and lower bounds as well. It should be observed that the Kato method needs a more detailed preliminary knowledge of the spectrum. The Kato method, in fact, requires the determination of an interval (a,b) for each isolated eigenvalue or for each group of isolated eigenvalues; the LM method, on the contrary, requires only the determination of two parameters $\rho_1<\rho_2$, not belonging to the spectrum of H^D, for all the eigenvalues inside the interval (ρ_1,ρ_2). In the present paper we have chosen as ρ_1 suitable upper bounds to $-c^2$ and as ρ_2 a value lying in the interval $[E^u(\mathrm{LM}),E_l(\mathrm{LM})_{s+1}]$, where $E^u(\mathrm{LM})_s$ is a LM upper bound to a given eigenvalue E_s and $E_l(\mathrm{LM})_{s+1}$ is a LM lower bound to the eigenvalue E_{s+1}, whereas as a and b we have chosen two suitable LM bounds [15]. The choice above for ρ_2 reveals a difficulty of the LM method. When the distance of ρ_2 either from $E^u(\mathrm{LM})_s$ or from $E_l(\mathrm{LM})_{s+1}$ goes to zero, the matrix $(H^D-\rho_2)_N^2$, which appears in Eq. (10), becomes singular. Thus, as the density of eigenvalues increases, a higher and higher numerical accuracy is required to compute matrix elements of $(H^D-\rho_2)^2$ and the algorithm for solving Eq. (10) employed here, which needs the inversion of the matrix $(H^D-\rho_2)^2$, shows a decreasing performance. As a consequence, our LM upper bounds, which are determined by Eq. (10) with $\rho=\rho_1$ (ρ_1 is far from the spectrum), have a numerical accuracy of order two to three digits higher than our LM lower bounds, which are determined by Eq. (10) with $\rho=\rho_2$ (ρ_2 is close to the spectrum). This effect is evident in Table III, whose results are relative to densely crowded eigenvalues. In column $-E_l^u(\mathrm{LM})$, except for a few cases, we report in fact for each eigenvalue a single approximation, representing the numerically correct digits in the lower bound, which are thus always coincident with the corresponding digits of the more accurate upper bound. It is worthwhile observing that our results in Tables I–III have not only a demonstrative purpose, but are also interesting in themselves. In particular, the results in Table III, obtained by the LM method, represent an example of a rigorous computation of an extended series of relativistic excited states. A criticism of these results might be that we have confined ourselves to a weak magnetic field and to states not extremely excited. We believe that the LM method can be applied successfully also in these cases. The limits of our results, in fact, do not depend on the LM method in itself but rather on the particular basis employed. The basis (17) indeed is not very adaptable to increasing effective magnetic interactions in the case of excited states and presents, as we said, the problem of a near linear dependence. The conclusion of our investigation thus is that the LM method is in general a very satisfactory solution of all the diseases of the variational collapse. It indeed reestablishes all the familiar features of the nonrelativistic variational calculations.

(i) It does not give rise to any spurious states.

(ii) It provides rigorous upper and lower bounds to relativistic binding energies and very accurate approximate eigenfunctions as well.

(iii) The bounds have extremum properties with respect to

TABLE III. Specimen of relativistic binding energies from the first 42 states $j_z^P = -\frac{1}{2}^+$ of the hydrogen atom in the magnetic field $B = 2.5\times10^{-5}$. Column i, indices numbering the states according to decreasing binding energy, columns N_r, N_θ, $-E_l^u$(LM), $-E_l^u$(K), $-E^N$, and δE are as in Table II. A single value in columns $-E_l^u$(LM) and $-E_l^u$(K) means that the corresponding upper and lower bounds coincide within the accuracy of the digits given. Blank spaces in column $-E_l^u$(K) have the same meaning as in Table I.

i	N_r, N_θ	$-E_l^u$(LM)	$-E_l^u$(K)	$-E^N$	δE
1	1,0	0.50001915621	0.50001915621	0.50001915621	-1.33×10^{-5}
2	2,0	0.12501457794	0.12501457794	0.12501457794	-1.66×10^{-5}
3	3,1	0.05556878438 9	0.05556878 7363	0.05556878438	-1.31×10^{-5}
6	4,1	0.0312628049	0.031262801 8453	0.0312628049	-1.01×10^{-5}
9	5,2	0.0200126092	0.02001246 3420	0.0200126092	-6.34×10^{-6}
14	6,2	0.0139014009 10	0.0138995 9769	0.0139014009	-3.45×10^{-6}
19	7,3	0.010216549	0.010182 1187	0.010216549	-2.08×10^{-6}
26	8,3	0.007824929	0.00775 1053	0.007824929	-1.72×10^{-6}
33	9,4	0.006185229		0.006185229	-1.44×10^{-6}
42	10,5	0.005012340		0.005012340	-1.24×10^{-6}

the nonlinear variational parameters and monotonic behavior with respect to the linear ones [property (c) in the Introduction] and satisfy moreover the Poincaré theorem [property (b) in the Introduction].

(iv) Conditions for the analytical convergence of these bounds as well as of the corresponding eigenfunctions [property (d) in the Introduction] can also be established by a straightforward application of well-known results [16] about the convergence of the traditional RR method.

The Kato method shares with the LM method the advantage of providing rigorous upper and lower bounds to relativistic binding energies; however, these bounds do not vary monotonically as N increases, nor is it easy to establish conditions for their analytical convergence. A peculiarity of the Kato method is that it does not prescribe any procedure for determining the trial wave function ψ. In a certain sense, this fact makes the Kato method more general because it can be applied equally well in the case when one has at one's disposal an accurate approximate eigenfunction that, however, is not a variational one.

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