Rapidly Converging Bounds for the Ground-State Energy of Hydrogenic Atoms in Superstrong Magnetic Fields

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The calculation of rapidly converging lower and upper bounds to the ground-state energy, E_g, of hydrogenic atoms in superstrong magnetic fields ($B \gtrsim 10^9$ G) has been an important theoretical problem for the past twenty-five years. Much effort has gone into reconciling the many different estimates for E_g predicted by an assortment of techniques. On the basis of recently developed eigenvalue moment methods, a precise solution involving rapidly converging bounds to E_g, for arbitrary superstrong magnetic field strengths, is now possible.

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In earlier works Handy and Bessis[1] defined a *moment method* for generating rapidly converging lower and upper bounds to the eigenvalues of strongly coupled, singular quantum mechanical systems. In succeeding works[2,3] the general moment method was made more flexible through a reformulation in terms of the theory of linear programming.[4] In this paper we apply these techniques to one of the more important theoretical quantum physics problems of the past quarter century: the quadratic Zeeman effect for superstrong magnetic fields ($B \gtrsim 10^9$ G).[5] Our analysis is relevant because prior results have been unsatisfactory in defining a convincing theory. Indeed, an assortment of approximate techniques have been used including variational methods,[6] Padé resummation analysis,[7] numerical integration,[8] order-dependent conformal transformations,[9] and virial-theorem Hellman-Feynman analysis.[10] Despite these efforts, the significant variation in ground-state-energy estimates, as cited in Table I, led to little confidence in ascertaining the correct theory. The very nature of the eigenvalue moment method will permit us to solve this problem precisely!

The importance of our obtaining accurate eigenenergy estimates through narrow bounds is motivated by the results of Avron, Herbst, and Simon[11,12] which establish the logarithmic relation for the "binding energy," ϵ, in terms of the magnetic field, B (atomic units are used throughout; note that then $B=1$ corresponds to 2.35×10^9 G):

$$\epsilon = B/2 - E(Z=1,B) \tag{1}$$

$$\cong \tfrac{1}{2}[\ln(B/4)]^2. \tag{2}$$

Clearly, very good precision in the energy, E, is required in order to attain satisfactory precision in the measurement of large magnetic fields. This is an immediate concern in astrophysics[5] and solid-state research.[13,14]

In atomic units, the relevant Schrödinger equation for spinless hydrogenic atoms (atomic charge Z) in a uni-

TABLE I. Moment-method bounds for the ground-state binding energy, $\epsilon = B/2 - E$, of the quadratic Zeeman effect for hydrogenic atoms.

B	Lower bound for ϵ	Upper bound for ϵ	M	D_M	Variation in literature (Ref. 9)	Estimate[a] from Ref. 9
2	1.0222138	1.0222142	11	75	$0.61105 < \epsilon < 1.0224$	1.0222139(±6)
20	2.215325	2.215450	11	70	$2.051 < \epsilon < 2.2153$	2.2153(±11)
200	4.710	4.740	10	66	$4.28 < \epsilon < 4.72904$	4.725(±25)
300	5.34	5.39	10	66	$5.04 < \epsilon < 5.355$	5.355(±35)
1000	7.55	7.85	9	55	$6.11585 < \epsilon < 7.64$	7.64(±8)

[a]Figures in parentheses (±) refer to accuracy estimates on the last digits.

form magnetic field B is

$$[-\tfrac{1}{2}\Delta+\tfrac{1}{8}B^2(x^2+y^2)-Z/r-E]\Psi=0. \quad (3)$$

Because of the scaling relation $E(Z,B)=Z^2E(1,B/Z^2)$, it will suffice to only consider the case $Z=1$.

In keeping with the theory developed in Ref. 1 we first need to obtain a *moments equation* for the system in Eq. (3). Afterwards we will make use of the fundamental facts: The bosonic ground state must be nonnegative[15] and have finite moments.[16] Throughout this work, "nonnegative" refers to a function which is positive on a subset of nonzero measure and zero elsewhere.

The realization of a moments equation combined with the nonnegative character of the desired solution will define a true moment problem. As is well known, the traditional moment problem is concerned with the necessary and sufficient constraints that a set of moments must satisfy in order that they correspond to a nonnegative function.[17] By utilizing these constraints in a manner mandated by the "missing-moment" character[1-3] of the moment equation (to be explained) we can define a hierarchy of relations which will rapidly bound the physical energy value.

One convenient representation within which to obtain a moments equation is afforded by the parabolic coordinate space transformation

$$\xi=r-z>0, \quad \eta=r+z>0. \quad (4)$$

In addition, it will be more convenient to work in terms of the function $\rho(\xi,\eta)=\Psi(\xi,\eta)\exp(-B\xi\eta/4)$. Function transformations such as these are not arbitrary. They must preserve nonnegativity and insure that the transformed physical solutions correspond to uniquely bounded configurations.[1] To achieve this, minimal knowledge of the asymptotics of the wave function is essential. For the present case we have

$$\Psi(r,z)\cong\exp[-\tfrac{1}{4}B(r^2-z^2)-(2\epsilon)^{1/2}|z|].$$

Implementing the parabolic coordinate transformation we get

$$\partial_\xi(\xi\partial_\xi\rho)+\partial_\eta(\eta\partial_\eta\rho)+\tfrac{1}{2}B\xi\eta(\partial_\xi\rho+\partial_\eta\rho)+\rho[\tfrac{1}{2}(E+\tfrac{1}{2}B)(\xi+\eta)+Z]=0. \quad (5)$$

Note that the reflection symmetry for the ground state[11] $\Psi(r,z)=\Psi(r,-z)$ becomes an exchange symmetry $\rho(\xi,\eta)=\rho(\eta,\xi)$.

The two-dimensional Stieltjes moments are defined by

$$\mu(n,m)=\int_0^\infty d\xi\int_0^\infty d\eta\,\xi^n\eta^m\rho(\xi,\eta).$$

The application of $\xi^n\eta^m$ to both sides of Eq. (5) and the performance of the necessary integration by parts yields the moment equation

$$n^2\mu(n-1,m)+m^2\mu(n,m-1)-\tfrac{1}{2}[Bn+\epsilon]\mu(n,m+1)-\tfrac{1}{2}[Bm+\epsilon]\mu(n+1,m)+Z\mu(n,m)=0. \quad (6)$$

It is clear that a "star-nearest neighbor" relation is defined by Eq. (6). In addition, from the previously defined exchange symmetry one has $\mu(n,m)=\mu(m,n)$.

It is simple to show that once ϵ and the moments $\mu(0,0),\mu(1,1),\ldots,\mu(M,M)$ are specified, all the moments $\mu(n,m)$ satisfying $n+m\le 2M+1$ are determined. We designate all the diagonal moments $\{\mu(m,m)\,|\,0\le m<\infty\}$ as missing moments.

The finite-difference moment equation is linear and homogeneous. The latter allows us to choose the normalization

$$\sum_{k=0}^{M}\mu(k,k)=1, \quad (7)$$

which guarantees that the missing moments are bounded within the unit hypercube. The linear nature of Eq. (6) together with Eq. (7) immediately leads to a linear dependence on the unconstrained missing moments [$\mu(0,0)$ is eliminated],

$$\mu(n,m)=\hat{M}_E(n,m;0)+\sum_{k=1}^{M}\hat{M}_E(n,m;k)u(k), \quad (8)$$

where $u(k)=\mu(k,k)$, and the $\hat{M}_E$'s are energy-dependent coefficients readily obtainable from the moment equation. A fuller discussion of the relevant formalism is given in Ref. 3.

It has been proved elsewhere[3] that the necessary and sufficient conditions for $\rho(\xi,\eta)$ to be nonnegative on the quadrant $\xi,\eta\ge 0$ correspond to

$$\sum_{k=1}^{M}u(k)\left[(-)\sum_{p,q=1}^{D_M}C^{(l)}(i,j)_p\hat{M}_E(l+i_p+i_q,j_p+j_q;k)C^{(l)}(i,j)_q\right] < \sum\sum_{p,q=1}^{D_M}C^{(l)}(i,j)_p\hat{M}_E(l+i_p+i_q,j_p+j_q;0)C^{(l)}(i,j)_q, \quad (9)$$

where $D_M \le (M+1)(M+2)/2$, $l=0,1$, and the C's are arbitrary. The coordinate pair sequence $(i,j)_p=(i_p,j_p)$ is ordered in terms of increasing sum $i+j$, and increasing j: $(0,0)_1$, $(1,0)_2$, $(0,1)_3$, $(2,0)_4$, $(1,1)_5$, $(0,2)_6$, $(3,0)_7, \dots$. The dimensionality, D_M, insures that only those M_E's corresponding to the first M missing moments are considered.

The relations in Eq. (9) correspond to linear inequalities involving the missing moments $u(1-M)$ as independent variables. The structure of Eq. (9) is of the standard linear-programming form,[4] $\mathbf{Au} \le \mathbf{B}$, where the rectangular matrix, $\mathbf{A}$, and vector, $\mathbf{B}$, are generated by the arbitrary vector coefficients, C.

For fixed E and M, the preceding inequalities (uncountably infinite in number) will either have a missing-moment solution subset, $\mathcal{S}$, or not. In the former case, it can be shown that $\mathcal{S}$ must be bounded and convex, and correspond to intersecting nonlinear hypersurfaces.[4] Our objective is to partition an arbitrary energy interval (keeping M fixed) and determine at each energy point whether or not $\mathcal{S}$ exists, thereby also determining if the associated energy is physically possible or impossible, respectively. In this manner, converging lower and upper bounds to the true physical energy can be obtained.

The direct implementation of the previously described program is clearly impossible given the uncountably infinite number of linear-inequality constraints. However, it is intuitively clear that any nonlinear convex subset, such as $\mathcal{S}$, can be arbitrarily approximated within the circumscribing envelope of a finite number of appropriately chosen intersecting hyperplanes. Indeed, $\mathcal{S}$'s nonexistence would require finding a finite number of linear-inequality hyperplanes that satisfy Eq. (9) and yet do not envelop a common interior missing-moment subset. We now describe a procedure for achieving this.

Assume that the number of missing moments, M, is fixed. Let E be also fixed at some arbitrary value. Consider the missing-moment normalization condition in Eq. (7). It defines for us the initialization inequalities

$$u(k)<1, \quad \text{for } 1 \le k \le M. \tag{10}$$

This is our starting polytope (i.e., a convex subset bounded by intersecting hyperplanes). Note that within the theory of linear programming it is usually assumed that the independent variables, $u(1-M)$, are positive.

We now define a fast "cutting" procedure by which to determine if there does not exist a nonlinear missing-moment subset, $\mathcal{S}$, satisfying all of Eq. (9), for fixed E and M. The procedure to be described is inductive. Assume that there exists a missing-moment polytope solution subset, $\mathcal{P}$, for the linear-inequality relations

$$\sum_{k=1}^{M} A(l,k)u(k) \le B(l), \quad l \le L, \tag{11}$$

which also include Eq. (10). From the theory of linear programming, the solution set must be convex.[4] It is assumed that each row of the rectangular matrix A is normalized as follows:

$$\sum_{k=1}^{M} A^2(l,k)=1. \tag{12}$$

We want to cut the polytope solution of Eq. (11) into a much smaller region that better approximates $\mathcal{S}$ (if it exists). To do so we first locate a "deep" interior point. Contrary to the prescription defined in Ref. 3 we will take as our deep interior point the center of the largest M-dimensional sphere that is inscribed within the polytope $\mathcal{P}$. To find this we add a "slack" variable, R, to the inequality relations in Eq. (11):

$$\sum_{k=1}^{M} A(l,k)u(k)+R \le B(l), \quad l \le L. \tag{13}$$

There are now $M+1$ independent variables [the $u(k)$'s and R]. We define R to be our "objective" function and use any standard linear-programming code to optimize the objective function. This will give us the location of the center of the maximum inscribed sphere, $\mathbf{u}_0$, and the associated radius, R_0. It is simple to prove that for a properly normalized A matrix (i.e., unit vectors for the rows) the optimal R value corresponds to the largest inscribed sphere.

Let us define the matrices

$$M_l^{(l)}(p,q)=\sum_{k=0}^{M} \hat{M}_E(l+i_p+i_q,j_p+j_q;k)u_0(k), \tag{14}$$

for $1 \le p,q \le D_M$, and $l=0,1$. Note that $u_0(0)=1$. For each l value determine as many as possible linearly independent vectors, $C_v^{(l)}$ [with components $C_v^{(l)}(i,j)_p$, $p=1,\dots,D_M$] satisfying

$$\langle C_v^{(l)} | M_l^{(l)} | C_v^{(l)} \rangle \le 0. \tag{15}$$

The index v is chosen sequentially and satisfies $v>L$ [Eq. (11)]. With the assumption that solutions to Eq. (15) exist, the coefficients

$$\tilde{A}(v,k)=-\sum_{p,q=1}^{D_M} C_v^{(l)}(i,j)_p \hat{M}_E(l+i_p+i_q,j_p+j_q;k)C_v^{(l)}(i,j)_q, \tag{16}$$

define inequalities that *violate* the moment-theorem constraints in Eq. (9), for missing-moment values in a neighborhood of $\mathbf{u}_0$:

$$\sum_{k=1}^{M} \tilde{A}(v,k)[u_0(k)+\delta u(k)] > \tilde{B}(v), \tag{17}$$

where $\tilde{B}(\nu) = -\tilde{A}(\nu,0)$.

The original polytope, $\mathcal{P}$, can be decomposed according to $\mathcal{P} = \mathcal{P}' \bigcup \mathcal{C}$, where the subset $\mathcal{C}$ satisfies Eq. (17) as well as Eq. (11). Supplementing the original L linear inequalities in Eq. (11) with the $A(\nu,k)$'s and $B(\nu)$'s $[A(\nu,k) = \tilde{A}(\nu,k)/\langle \tilde{A}_\nu | \tilde{A}_\nu \rangle$ and $B(\nu) = \tilde{B}(\nu)/\langle \tilde{A}_\nu | \tilde{A}_\nu \rangle]$, we obtain an updated set of linear inequalities that define the polytope $\mathcal{P}'$. The subset $\mathcal{C}$, containing the center point $\mathbf{u}_0$, is discarded by our cutting procedure.

The preceding inductive procedure is repeated until either no solution(s) to Eq. (15) can be found or the polytope is wiped out; thereby we conclude that the associated energy value is physically possible (up to order M) or impossible, respectively.

The results of our analysis are given in Table I. We also quote various estimates predicted by other methods. Our *rigorous* bounds confirm and improve, in an absolute manner, the estimates predicted by Le Guillou and Zinn-Justin.[9]

The moment method is a fundamentally simple and precise eigenvalue technique. Many problems have been solved, some of which have been cited here. Among these is the related problem of the spherically symmetric quadratic Zeeman potential discussed in great detail by Bessis, Vrscay, and Handy.[18] Bearing in mind that typical linear-programming problems in economics and operations research involve hundreds of independent variables (i.e., missing moments), we expect that the present methods will be relevant to the few-body problem.

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