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Bound-state spectrum of the hydrogen atom in strong magnetic fields

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Energies of the bound states of the hydrogen atom in a uniform magnetic field are calculated for field strengths greater or equal to $B_0 \approx 2.35\times 10^9$ G. The convergent behavior of the quantum excesses (negative quantum defects) makes it possible to determine completely the bound-state spectrum for given values of the field strength B and the azimuthal quantum number m. For $|m|=0,1$, and 2 results are presented which determine to a uniform relative accuracy of at least 0.1% the energies of all bound states for arbitrary field strengths from $B/B_0=1$ to $B/B_0=500$ or higher, beyond which the adiabatic approximation is of comparable accuracy.

I. INTRODUCTION

The hydrogen atom in a strong uniform magnetic field[1] $\vec{B}=(0,0,B)$ is accurately described over a large range of field strengths B by the simple nonrelativistic single-particle Hamiltonian

$$H=\frac{p^2}{2\mu}-\frac{e^2}{r}+\omega l_z+\tfrac{1}{2}\mu\omega^2(x^2+y^2)\ , \tag{1}$$

where μ is the reduced mass of electron and proton and the oscillator frequency ω is half the cyclotron frequency

$$\omega=\tfrac{1}{2}\omega_c=eB/(2\mu c)\ .$$

At a field strength of

$$B=B_0=\mu^2e^3c/\hbar^3\approx 2.35\times 10^9\ \text{G}$$

the oscillator energy $\hbar\omega$ becomes equal to the Rydberg energy

$$R=\tfrac{1}{2}\mu e^4/\hbar^2\approx 13.6\ \text{eV}\ .$$

In terms of the dimensionless field-strength parameter

$$\gamma=B/B_0=\hbar\omega/R\ ,$$

relativistic corrections[2,3] to the simple model (1) are negligible for fields with $\gamma<10^4$. On the other hand, the effects of spin-orbit coupling[1] can be neglected for fields with $\gamma>10^{-4}$. The effect of the nonseparability of the two-body problem in the presence of an external magnetic field has been investigated by several authors.[3–5] For fields with $\gamma\gtrsim 100$, this effect is not negligible, but for a hydrogen atom at rest it can be accounted for accurately[5] by a constant energy shift which depends only on γ and the azimuthal quantum number m. For finite momenta of the hydrogen atom, simple scaling laws can be used[5] to reduce the two-body problem to the one-body problem described by (1).

For magnetic fields in the region $\gamma\approx 1$ and $\gamma>1$, which may be important in astrophysical situations,[6] the solutions of the Schrödinger equation governed by the Hamiltonian (1) are still fragmentary. This is true in spite of the formal simplicity of the problem and the large amount of attention it has received.[1–16] In the region $\gamma\geq 1$, accurate calculations of energy levels exist only for a few discrete field strengths and only for the lowest few eigenstates for a given azimuthal quantum number m. The reason for this is that, although axial symmetry and conservation of parity π reduce the problem to a two-dimensional Schrödinger equation in each m^π subspace of full Hilbert space, no further reduction to one-dimensional problems has been possible except in the adiabatic approximation,[12] which is accurate in the region $\gamma\gg 1$.

The present investigation is based on an expansion of the wave function of relative motion of electron and proton in Landau orbitals, which has already been used as an appropriate expansion for the high-field case by Simola and Virtamo.[8] In contrast to all previous investigations, the present calculation (which is described in Sec. II and in the Appendix) is accurate not only for low-lying states but also for highly excited states. This makes it possible to study the convergent behavior of the *quantum excesses* (negative quantum defects) in each m^π subspace and thus to completely determine the energies of *all bound states* for given values of the field-strength parameter γ and the azimuthal quantum number m. In Sec. III, results are presented for $|m|=0$, 1, and 2 which completely determine to a uniform *relative accuracy* better than 0.1% the energies of *all bound states* for *arbitrary field strengths* ranging from $\gamma=1$ to $\gamma=500$ or higher, beyond which the adiabatic approximation is of comparable accuracy.

II. METHOD

For a given azimuthal quantum number m, the wave function $\psi(\rho,z)$ $[\rho=(x^2+y^2)^{1/2}]$ can be expanded in Landau states $\varphi_{N,m}(\rho)$ which are eigenstates of the two-dimensional harmonic-oscillator Hamiltonian[17] with radial quantum number N and oscillator energy $(2N+|m|+1)\hbar\omega$:

$$\psi(\rho,z)=\sum_{N\geq 0}\varphi_{N,m}(\rho)\varphi_N(z) \ . \tag{2}$$

It is convenient to subtract from the Hamiltonian (1) the normal Zeeman shift $m\hbar\omega$ and the zero-point energy $(|m|+1)\hbar\omega$ of the lowest Landau state ($N=0$), so that the Hamiltonian no longer depends on the sign of m, and the ionization threshold lies at $E=0$ in each azimuthal subspace. Inserting the expansion (2) into the time-independent Schrödinger equation then leads to a set of coupled equations for the wave functions $\varphi_N(z)$:

$$\left[\frac{p_z^2}{2\mu}+V_{NN}(z)+2N\hbar\omega\right]\varphi_N(z) + \sum_{N'\neq N}V_{NN'}(z)\varphi_{N'}(z)=E\varphi_N(z) \ . \tag{3}$$

The diagonal potentials V_{NN} and the coupling potentials $V_{NN'}$, $N\neq N'$, are given by

$$V_{NN'}(z)=\int_0^\infty \rho\, d\rho\, \varphi_{N,m}(\rho)\frac{(-e^2)}{(\rho^2+z^2)^{1/2}}\varphi_{N',m}(\rho) \ . \tag{4}$$

Asymptotically ($|z|\rightarrow\infty$), the diagonal potentials approach the one-dimensional pure Coulomb potential whereas the coupling potentials vanish:

$$V_{NN'}(z)\sim -\delta_{N,N'}e^2/|z| \tag{5}$$

for $|z|\rightarrow\infty$. The deviation of the potentials (4) from the asymptotic form (5) is appreciable over a range of the order of the oscillator width $b=\sqrt{\hbar/\mu\omega}$ which is related to the field-strength parameter γ by

$$b=a_0\sqrt{2/\gamma} \ , \tag{6}$$

$a_0\approx 0.53$ Å being the Bohr radius.

For each value of the azimuthal quantum number m and the parity π (with respect to reflection at the x-y plane) Eqs. (3) constitute a set of coupled-channels equations, the channels being defined by the radial quantum numbers N of the various Landau excitations perpendicular to the direction of the magnetic field. Neglecting the coupling potentials in (3) leads to a set of uncoupled ordinary differential equations for the wave functions $\varphi_N(z)$. This is the "adiabatic approximation" which has recently been studied in considerable detail by Wunner, Ruder, and Herold.[5,12] It becomes increasingly accurate as γ increases, and in the asymptotic limit $\gamma\rightarrow\infty$ it reduces to the problem of the one-dimensional free hydrogen atom which has been discussed by Loudon.[18]

By directly solving the coupled equations (3) including up to eight channels in the expansion (2), Simola and Virtamo[8] calculated the binding energy of the ground state in the subspace $m^\pi=0^+$ for fields with $\gamma=2,20\cdots 2\times 10^4$. Aldrich and Greene[9] have used a matrix-diagonalization procedure based on expanding the functions $\psi(\rho,z)$ in a basis of Gaussians of varying widths and have calculated up to six eigenvalues in a given m^π subspace for $\gamma=1$, 2, 5, and 10 and for some values $\gamma<1$. Except for the work of Wunner *et al.*,[12] who use the adiabatic approximation, Ref. 9 was up to now the only calculation which went beyond the lowest two or three eigenstates in a given m^π subspace for fields with $\gamma>1$.

The present calculation is based on diagonalizing the Hamiltonian matrix in a nonorthogonal basis obtained by expanding the wave functions $\varphi_N(z)$ in (2) and (3) in a basis of displaced Gaussians:

$$\varphi_i(z)=(\sqrt{\pi}b_i)^{-1/2}\exp[-(z-z_i)^2/2b_i^2] \ , \tag{7}$$

out of which components of positive or negative parity are projected according to the sign of π;

$$\varphi_i^\pm(z)=\tfrac{1}{2}[\varphi_i(z)\pm\varphi_i(-z)] \ . \tag{8}$$

The basis defined by Eqs. (7) and (8) is complete if reasonable (e.g., constant) width parameters b_i and a sufficiently dense mesh of displacements z_i are used.[19] In the present physical situation it turned out to be most effective to choose the spacing between neighboring mesh points and the corresponding width parameters to be proportional to the square root of the distance from the origin $z=0$, which for hydrogenlike states near the ionization threshold means proportional to the de Broglie wavelength. This is achieved by a basis

$$z_i = ca_0 i^2, \quad b_i = aca_0 i, \quad i=1,2,\ldots \tag{9}$$

defined by two dimensionless parameters: c which determines the density of the mesh and a which determines the overlap of neighboring Gaussians. For positive parity subspaces an additional Gaussian of width $b_0 = aca_0/2$ and centered at $z_0=0$ is included in the basis.

Since the basis (9) allows for tight mesh spacing near the origin, where the wave functions have the most short-range structure and is more widely spaced at large distances, it is well adapted to the description of highly excited hydrogenlike states. Tests on the negative parity states of the exactly soluble free one-dimensional hydrogen atom and in the framework of the adiabatic approximation showed that a uniform accuracy of about six significant figures can be obtained for the lowest n eigenvalues (in a given m^π subspace) if $5\times n$ to $10\times n$ Gaussians are included in the basis. Within the adiabatic approximation the present method reproduces virtually exactly the calculation of Wunner and Ruder [12(a)] for $\gamma=100$. In fact, for the 17 eigenvalues calculated by Wunner and Ruder for each azimuthal quantum number $|m|=0$, 1, and 2, the only deviation in the significant figures given is for the $m=0$ ground state, where the present calculation gives a binding energy 7.4937 Ry as opposed to the value 7.4940 Ry given in Ref. 12(a).

In the present calculation, up to 100 Gaussians were used to represent each wave function $\varphi_N(z)$ and up to 25 channels were included in the expansion (2). However, the convergence properties of the energy eigenvalues or rather of the associated quantum excesses (see Sec. III) made it possible to restrict the total dimensions (number of channels multiplied by the number of Gaussians) of the matrices to be diagonalized to 200 or less. Further details of the numerical calculation are given in the Appendix.

III. RESULTS

The ground-state binding energies obtained in the present calculation are shown (in units of rydbergs) in Table I and compared with the results of Simola and Virtamo[8] and Aldrich and Greene,[9] with the finite-elements calculation of Kaschiev, Vinitsky, and Vukajlović,[11] with the perturbative calculation of Pavlov-Verevkin and Zhilinskii,[13] and with the variational calculation of Praddaude,[7] who was one of the first authors to accurately calculate the lowest few eigenvalues in the region $\gamma\approx 1$. The results of the adiabatic approximation are also shown.

The present results agree to within at least 0.1% with most previous calculations. Whenever there is a noticeable disagreement between the results of Ref. 13 and those of Ref. 8, both of which claim high accuracy for very strong fields, the present results tend to agree more accurately with Ref. 8. In fact, the values presented by Pavlov-Verevkin and Zhilinskii[13] cannot be accurate to all significant figures given, because at $\gamma=2000$ their calculation gives less binding than the adiabatic approximation. Binding energies of a few excited states obtained for $\gamma=2$ are shown in Table II and compared with the results of Refs. 7, 9, and 13, as well as with the adiabatic approximation.

In Table II and throughout this paper, the bound states in each m^π subspace are labeled by the quantum number n which determines the energy of the state in the asymptotic limit $\gamma\to\infty$, where the spectrum becomes that of the one-dimensional hydrogen atom[18]

$$\lim_{\gamma\to\infty} E_n = -R/n^2 \tag{10}$$

for all m^π. In each m^π subspace there is one hydrogenlike state for each value of $n=1,2,3,\ldots$. In each positive parity subspace there is an additional "tightly bound state" which corresponds to $n=0$ and becomes infinitely bound in the limit $\gamma\to\infty$. In the region $\gamma\geq 1$, one quantum number n is sufficient to label all the bound states in each m^π subspace. States which in the adiabatic approximation correspond to higher Landau excitations $N=1,2,3,\ldots$ [see Eq. (2)], are separated from this lowest set of states by an energy of roughly $2N\hbar\omega=2\gamma R$ [see Eq. (3)], and all lie above the ionization threshold at $E=0$. Owing to the coupling between the various N channels, these states are unstable against decay of the Landau excitations.

Table II shows that the present results agree with the calculations of Refs. 7 and 13 to within at least 0.1%, with the exception of the $n=0$ and $n=2$

TABLE I. Binding energies in units of rydbergs for the tightly bound state in the subspace $m^{\pi}=0^{+}$. Present results are compared with the adiabatic approximation and with the results of Praddaude,[a] Aldrich and Greene (A and G),[b] Kaschiev, Vinitsky, and Vukajlović (KVV),[c] Simola and Virtamo (S and V),[d] and Pavlov-Verevkin and Zhilinskii (P and Z).[e]

γ	1	2	20	200	2000
Adiabatic	1.363 21	1.799 55	4.298 60	9.383 4	18.574
Praddaude	1.662 33	2.044 42			
A and G	1.662 0	2.043 9			
KVV	1.662 28	2.044 43	4.407 3		
S and V		2.044	4.430 6	9.454 0	18.609 4
P and Z		2.028 64	4.428 92	9.458 08	18.548 10
Present	1.661	2.044	4.430 3	9.454	18.608

[a] Reference 7.
[b] Reference 9.
[c] Reference 11.
[d] Reference 8.
[e] Reference 13.

TABLE II. Binding energies in units of rydbergs of some levels for $\gamma=2$. Present results are compared with the adiabatic approximation and with the results of Praddaude,[a] P and Z,[b] and A and G[c] (see Table I for reference symbols).

n	Adiabatic	Praddaude	P and Z	A and G	Present
$m^{\pi}=0^{+}$					
0	1.799 54	2.044 42	2.028 64	2.0439	2.044
1	0.332 68	0.348 06	0.348 16	0.3473	0.348 0
2	0.134 66	0.138 84		0.1383	0.138 6
3	0.072 189			0.0736	0.073 73
4	0.044 878			0.0445	0.045 63
5	0.030 567			0.0265	0.030 99
$m^{\pi}=0^{-}$					
1	0.587 52	0.595 39	0.595 00	0.5950	0.595 41
2	0.192 23	0.193 88	0.193 64	0.1921	0.193 71
3	0.093 296			0.0910	0.093 795
4	0.054 816			0.0505	0.055 042
$m^{\pi}=1^{+}$					
0	1.154 32	1.199 17	1.198 56	1.1978	1.199 21
1	0.281 07	0.285 08	0.284 94	0.2826	0.284 90
2	0.121 38			0.1191	0.122 44
3	0.066 969			0.0628	0.067 498
$m^{\pi}=1^{-}$					
1	0.486 92	0.490 53	0.490 42	0.4893	0.490 48
2	0.173 82		0.174 56	0.1718	0.174 58
$m^{\pi}=2^{+}$					
0	0.924 21	0.942 43	0.942 24	0.9414	0.942 34
1	0.255 57		0.257 36	0.2562	0.257 35
$m^{\pi}=2^{-}$					
1	0.432 84		0.434 88	0.4321	0.434 91
2	0.162 86		0.163 32		0.163 32

[a] Reference 7.
[b] Reference 13.
[c] Reference 9.

states in the subspace $m^{\pi}=0^{+}$. However, if we look beyond the first two or three states in each m^{π} subspace, the present calculation is obviously a substantial improvement over the only previous calculation by Aldrich and Greene.[9] The binding energies of the excited states given in Ref. 9 are noticeably smaller than in the present calculation and, for larger values of n, even become smaller than the binding energies in the adiabatic approximation. This indicates that in Ref. 9 the subspace in which the Hamiltonian is diagonalized is too small to describe the more highly excited states. Enlarging the subspace leads to lower energy eigenvalues (higher binding energies) of *all* bound states.[20]

When dealing with hydrogenlike spectra as in the present case, it is convenient to study not the energy eigenvalues E_n themselves, but rather their deviations from a pure hydrogen spectrum as expressed in the *quantum excesses* δ_n:

$$E_n=-R/(n+\delta_n)^2 \ . \qquad (11)$$

Each *effective quantum number* $n+\delta_n$ defined by Eq. (11) will be larger than the corresponding quantum number n, because the true potential in Eq. (3) is less attractive at short distances than the potential of the free (one-dimensional) hydrogen atom. Thus, the quantum excesses δ_n are all positive and, according to Eq. (10), converge to zero in the asymptotic limit. Except for the plus sign in Eq. (11) the quantum excesses correspond to the "quantum defects" which are used to characterize the spectra of alkali-metal atoms, where the potential seen by the valence electron is that of a free hydrogen atom at large distances, but becomes more attractive at short distances.[21]

The quantum excesses δ_n are plotted in Fig. 1 against $1/n$ for $\gamma=2$ and for the m^{π} subspaces with $m=0,1,2$. The corresponding numbers deduced from the energy values of Aldrich and Greene[9] are shown for comparison.

As is expected[21] for a potential which differs from a pure Coulomb potential only at short distances, the quantum excesses in each m^{π} subspace converge to a finite limit as $n\rightarrow\infty$. In addition, Fig. 1 shows that within each m^{π} subspace, the dependence of the quantum excesses δ_n on n is very weak and is very similar in the adiabatic approximation and in the full calculation, especially if we look only at states with $n\geq 1$ and do not include the $n=0$ tightly bound state in the positive parity subspaces.

The γ dependence of the quantum excesses δ_0 and δ_1 is shown in Figs. 2 and 3, respectively, for m^{π} subspaces with $m=0,1,2$ and for $1\leq\gamma\leq 500$. For

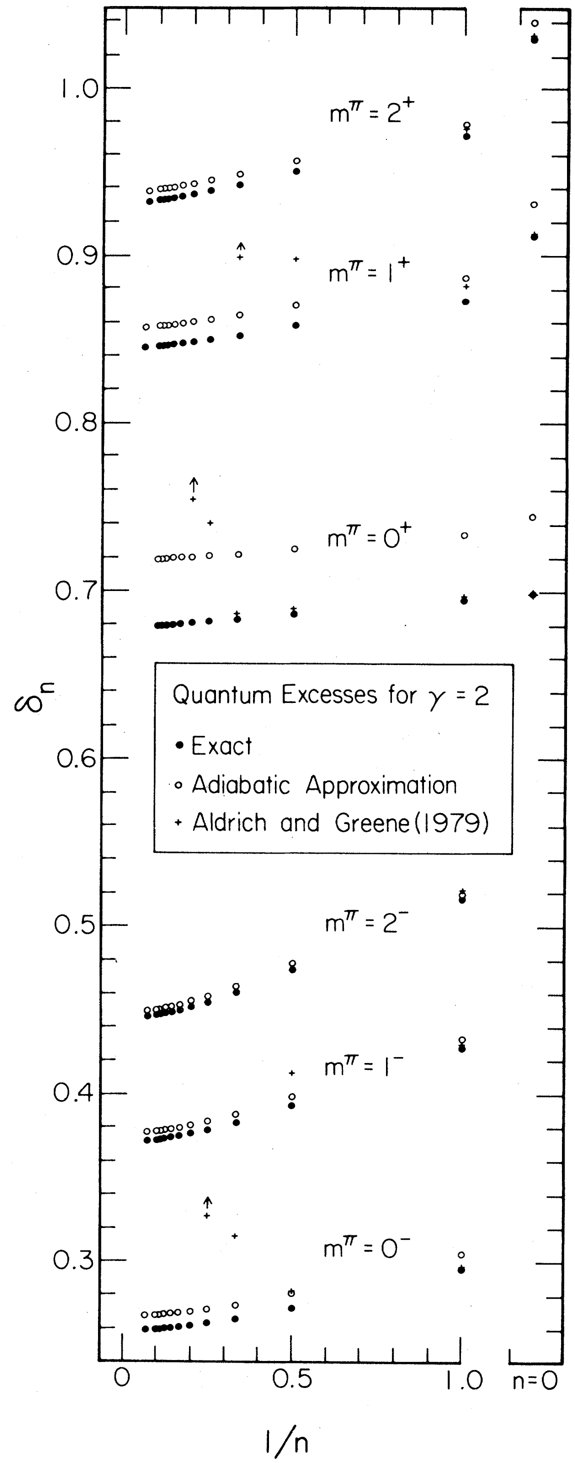

FIG. 1. Quantum excesses δ_n for $\gamma=2$ in the m^{π} subspaces with $m=0$, 1, and 2. Present results (solid dots) are compared with the adiabatic approximation (open circles) and with the results of Aldrich and Greene, Ref. 9 (crosses).

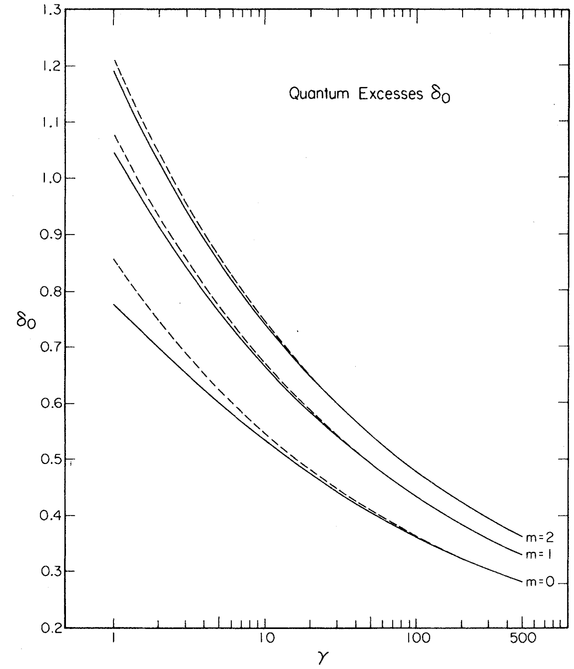

FIG. 2. Quantum excesses δ_0 corresponding to the tightly bound states for azimuthal quantum numbers $m=0$, 1, and 2. Dashed lines show the results of the adiabatic approximation.

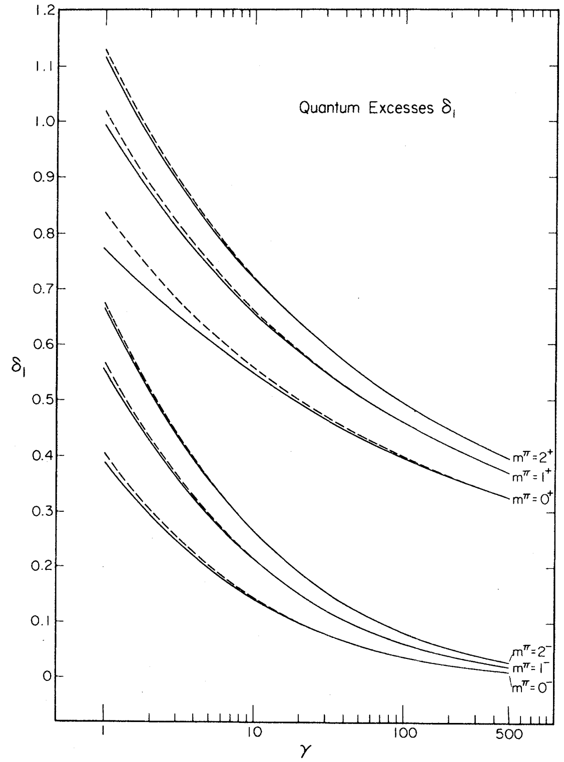

FIG. 3. Quantum excesses δ_1 in the m^π subspaces with $m=0$, 1, and 2. Dashed lines show the results of the adiabatic approximation.

reasons discussed by Loudon,[18] the asymptotic ($\gamma \to \infty$) convergence to zero is much slower in the positive parity subspaces than in the negative parity subspaces. For a given value of the azimuthal quantum number m, the values of δ_0 and δ_1 (for both values of π) converge to $|m|+1$ in the low field limit $\gamma \to 0$.

More-precise values of the quantum excesses δ_0 and δ_1 are tabulated in Table III together with the results δ_0^{ad} and δ_1^{ad} of the adiabatic approximation. The mesh of field-strength parameters γ is so dense that quadratic interpolation of the quantum excesses as functions of $\log\gamma$ gives values of δ_0 and δ_1 at intermediate values of γ to within 10^{-4}, except in the region near $\gamma=1$, where the maximum error is approximately 2×10^{-4}.

Once δ_1 is known for any given value of γ, m, and π, the energies of the higher-lying bound states can be obtained via Eq. (11) from the *quantum excess differences*

$$\epsilon_n=\delta_n-\delta_1,\quad n=2,3,4,\ldots \tag{12}$$

For reasons discussed above in connection with Fig. 1, the quantum excess differences ϵ_n are very small, converge to a finite limit as $n \to \infty$, and do not change strongly when going from the adiabatic approximation to the full calculation. In fact, the values of ϵ_n converge much more rapidly as functions of the numbers of channels included in the expansion (2) than the corresponding quantum excesses. This makes the accurate calculation of the energies of highly excited states possible without diagonalizing immense matrices (see the Appendix). For $\gamma \geq 10$, the values of ϵ_n are already given to within less than 10^{-4} if the adiabatic approximation is used for both δ_n and δ_1 in Eq. (12).

The quantum excess differences ϵ_n are shown in Fig. 4 as functions of γ for m^π subspaces with $m=0$, 1, and 2. The limiting values of ϵ_n as $n \to \infty$ are given in Table IV for various values of γ.

In the negative parity subspaces, the quantum excess differences converge uniformly to zero with increasing γ at roughly the same rate as the corresponding quantum excesses. The signs of ϵ_n are all negative and for a given value of γ the magnitudes increase monotonically with increasing n to a limit which is roughly one power of ten smaller than the corresponding value of δ_1.

In each positive parity subspace there is a value of the field-strength parameter γ near which all quantum excess differences change sign. For each value of m, the zeros of $\epsilon_2, \epsilon_3, \epsilon_4, \ldots$ form a monotonically increasing sequence of numbers

TABLE III. Quantum excesses δ_0 and δ_1 for the m^π subspaces with $m=0$, 1, and 2. δ_0^{ad} and δ_1^{ad} are the results of the adiabatic approximation.

	Positive parity				Negative parity	
γ	δ_0	δ_0^{ad}	δ_1	δ_1^{ad}	δ_1	δ_1^{ad}
$m=0$						
1	0.7758±2	0.85648	0.7651±2	0.83611	0.38673	0.40456
2	0.6995	0.74545	0.6952	0.73374	0.29595	0.30463
5	0.6020	0.62375	0.6066	0.62446	0.19932	0.20257
10	0.53492	0.54740	0.54694	0.55733	0.14310	0.14461
20	0.47512	0.48232	0.49460	0.50068	0.09979	0.10047
50	0.40705	0.41058	0.43536	0.43843	0.05918	0.05941
100	0.36323	0.36530	0.39704	0.39888	0.03850	0.03859
200	0.32523	0.32645	0.36344	0.36454	0.02433	0.02437
500	0.28270	0.28330	0.32511	0.32567	0.01274	0.01275
1000	0.25545	0.25582				
2000	0.23182	0.23203				
5000	0.20521	0.20532				
$m=1$						
1	1.04645	1.07737	0.99620	1.01831	0.55580	0.56618
1.5	0.96643	0.98864	0.92207	0.93803	0.47809	0.48504
2	0.91317	0.93076	0.87350	0.88623	0.42787	0.43308
3	0.84302	0.85570	0.81045	0.81977	0.36372	0.36717
5	0.76257	0.77099	0.73939	0.74571	0.29327	0.29531
10	0.66654	0.67139	0.65612	0.65988	0.21454	0.21552
20	0.58411	0.58692	0.58566	0.58790	0.15298	0.15344
50	0.49304	0.49442	0.50832	0.50947	0.09373	0.09389
100	0.43563	0.43643	0.45942	0.46011	0.06254	0.06261
200	0.38650	0.38697	0.41716	0.41758	0.04051	0.04054
500	0.33218	0.33242	0.36963	0.36985	0.02185	0.02185
1000	0.29779	0.29793				
$m=2$						
1	1.19005	1.20760	1.11718	1.12880	0.66680	0.67387
1.5	1.09359	1.10626	1.02867	1.03718	0.57535	0.58014
2	1.03014	1.04020	0.97124	0.97810	0.51636	0.51997
3	0.94732	0.95460	0.89728	0.90235	0.44099	0.44342
5	0.85323	0.85809	0.81458	0.81806	0.35810	0.35955
10	0.74198	0.74478	0.71853	0.72062	0.26500	0.26571
20	0.64722	0.64885	0.63794	0.63921	0.19150	0.19184
50	0.54323	0.54403	0.55028	0.55093	0.11969	0.11982
100	0.47802	0.47849	0.49527	0.49566	0.08115	0.08120
200	0.42242	0.42270	0.44801	0.44825	0.05341	0.05344
500	0.36120	0.36134	0.39516	0.39528	0.02938	0.02939

$\gamma_2, \gamma_3, \gamma_4, \ldots$, which are restricted to a small range $\Delta\gamma$ and converge to a limit γ_c. Numerical values of $(\gamma_c, \Delta\gamma)$ are (18, 0.5) for $m=0$, (41, 1.5) for $m=1$, and (64, 3) for $m=2$. In the region $\gamma<\gamma_c-\Delta\gamma$, the behavior of the quantum excess differences ϵ_n is similar to the behavior in the negative parity subspaces. In the region $\gamma_c-\Delta\gamma\leq\gamma\leq\gamma_c$ all values of ϵ_n are very small, viz., smaller than approximately 10^{-4}. This means that in each positive parity subspace there exists a small range of field-strength parameters for which all quantum excesses δ_n with the exception of the quantum excess δ_0 associated with the tightly bound state, are equal to within approximately 10^{-4}. In the region $\gamma>\gamma_c$, the quantum excess differences in the positive parity subspaces are positive; their magnitudes remain rather small and depend very weakly on γ.

For any field-strength parameter γ between unity and 500, the numerical values of the quantum excess differences can easily be read off from Fig. 4 to

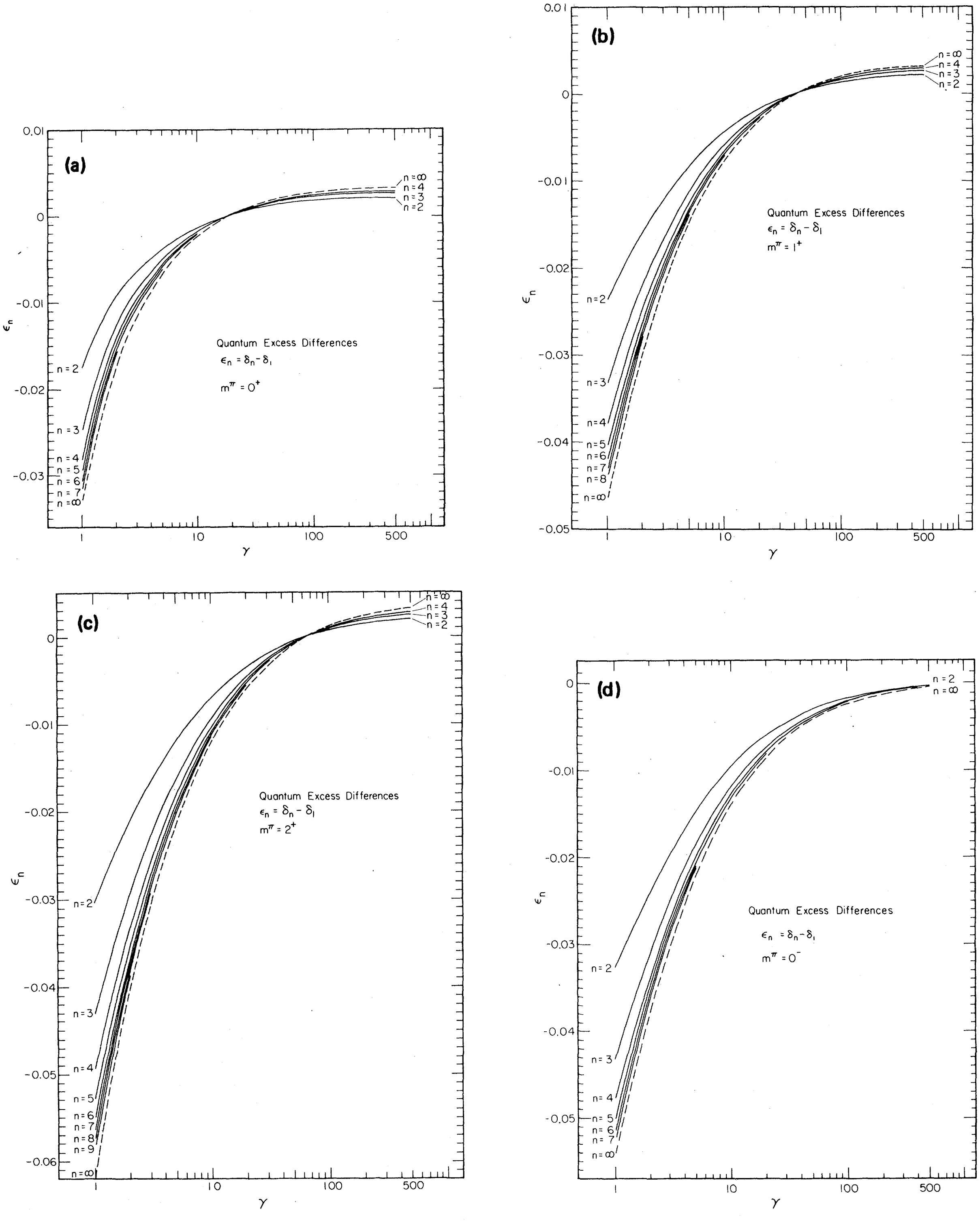

FIG. 4. Quantum excess differences $\epsilon_n = \delta_n - \delta_1$ in the subspaces (a) $m^\pi = 0^+$, (b) $m^\pi = 1^+$, (c) $m^\pi = 2^+$, (d) $m^\pi = 0^-$, (e) $m^\pi = 1^-$, and (f) $m^\pi = 2^-$.

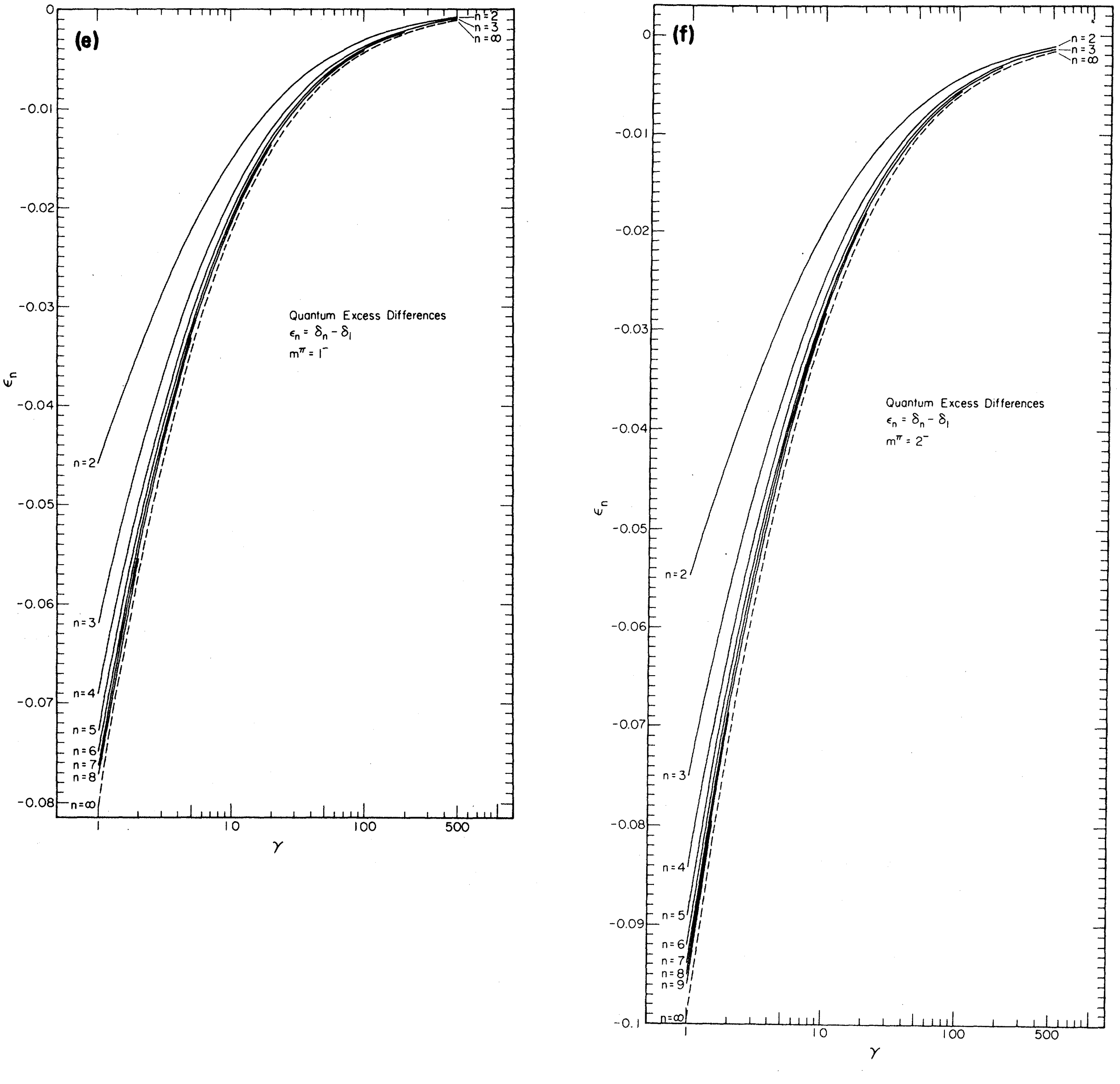

FIG. 4. (*Continued.*)

within an accuracy of less than 10^{-3}, except near $\gamma = 1$, where the error may be up to 3×10^{-3} for some states with $n \geq 8$. Together with the numbers in Table III, the curves in Fig. 4 give all effective quantum numbers $n+\delta_n$ to within a *relative accuracy* of less than 0.05%. Because of the convergent behavior of the quantum excesses δ_n, there is no upper limit on the value of n and the relative accuracy of the effective quantum numbers actually improves with increasing n.

Thus, Table III and Fig. 4 determine the energies (11) of *all bound states* in any m^π subspace with $|m| = 0$, 1, or 2 to a *relative accuracy* better than 0.1% for any value of γ in the range $\gamma = 1$ to 500. For fields stronger than $\gamma = 500$, the adiabatic approximation is valid to within this accuracy except for the energies of the tightly bound states in the subspaces $m^\pi = 0^+$ and $m^\pi = 1^+$. In order to bridge this gap to the region where energy eigenvalues in the adiabatic approximation are accurate to at least ca. 0.1%, the range of values of γ for which δ_0 was calculated was extended to $\gamma = 5000$ for $m = 0$ and to $\gamma = 1000$ for $m = 1$ (see Table III).

TABLE IV. Limiting values ϵ_∞ of the quantum excess differences $\epsilon_n=\delta_n-\delta_1$ in the m^π subspaces with $m=0$, 1, and 2.

m^π γ	0^+	1^+	2^+	0^-	1^-	2^-
1	−0.033	−0.0463	−0.0615	−0.054	−0.0803	−0.0995
2	−0.017	−0.0294	−0.0402	−0.0376	−0.0569	−0.0713
5	−0.0064	−0.0145	−0.0213	−0.0219	−0.0343	−0.0438
10	−0.0022	−0.0076	−0.0120	−0.0139	−0.0225	−0.0292
20	+0.0003	−0.0030	−0.0059	−0.0085	−0.0142	−0.0188
50	+0.0022	+0.0006	−0.0009	−0.0042	−0.0073	−0.0099
100	+0.0027	+0.0020	+0.0012	−0.0024	−0.0043	−0.0059
200	+0.0031	+0.0028	+0.0023	−0.0013	−0.0024	−0.0034
500	+0.0033	+0.0032	+0.0032	−0.0005	−0.0011	−0.0015

IV. SUMMARY

A straightforward matrix-diagonalization procedure has been used to calculate the energies of the bound states of a hydrogen atom in a uniform magnetic field of strength $B \geq B_0 \approx 2.35\times10^9$ G. At such strong fields the bound-state spectrum for a given azimuthal quantum number m is similar to the spectrum of the free one-dimensional hydrogen atom which it approaches in the asymptotic limit $\gamma=B/B_0\rightarrow\infty$.

For finite values of γ, the deviations of the spectrum from the asymptotic limit are appropriately described by the quantum excesses δ_n, defined by Eq. (11). For given values of γ, m, and the parity π (with respect to reflection at the x-y plane) the quantum excesses converge to a finite limit and this makes a complete determination of the bound-state spectrum possible. An interesting feature in m^π subspaces of positive parity is the existence of a field strength γ_c (depending on m) near which all quantum excesses δ_n, with the exception of the quantum excess δ_0 corresponding to the tightly bound state, are virtually equal.

For $|m|=0$, 1, and 2 the quantum excesses δ_0 and δ_1 can be determined from Table III with the help of quadratic interpolation for arbitrary field strengths in the range $\gamma=1$ to 500, going up to $\gamma=5000$ and 1000 for the δ_0 quantum excess in the subspaces $m^\pi=0^+$ and 1^+, respectively. For more highly excited states, the quantum excesses can be determined by reading the values of the corresponding quantum excess differences $\delta_n-\delta_1$ in Fig. 4. Table III and Fig. 4 together determine, to a relative accuracy of at least 0.05%, the effective quantum numbers $n+\delta_n$ of all bound states for arbitrary field strengths in the range $\gamma=1$ to 500 (to $\gamma=5000$ and 1000 for the tightly bound states in the subspaces $m^\pi=0^+$ and 1^+, respectively). The corresponding energies are determined to a uniform relative accuracy of at least 0.1% and the relative accuracy actually increases with increasing quantum number n. For higher fields, the adiabatic approximation, which reduces the Schrödinger equation to a set of uncoupled linear ordinary differential equations in one variable, is at least of comparable accuracy.

For azimuthal quantum numbers $|m|=0$, 1, and 2, Table III and Fig. 4 thus determine to a uniform relative accuracy of at least 0.1% the energies of all bound states of the hydrogen atom in uniform magnetic fields of any strength γ ranging from $\gamma=1$ to 500 or higher, beyond which the adiabatic approximation is at least of comparable accuracy.

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APPENDIX

For a given azimuthal quantum number $m\geq0$ and parity π let N_c be the number of channels included in the expansion (2) and n_z the number of Gaussians (7) used to represent each channel wave function $\varphi_N(z)$:

$$\psi(\rho,z)=\sum_{N=0}^{N_c-1}\sum_{i=1}^{n_z} C_{N,i}\varphi_{N,m}(\rho)\varphi_i^{\pi}(z)\,, \tag{A1}$$

where φ_i^π are the parity projected wave functions (8). The coupled-channel equations (3) then reduce to a discrete matrix-diagonalization problem

$$\sum_{M=0}^{N_c-1} \sum_{j=1}^{n_z} [H^\pi(N,i;M,j)-EA^\pi(N,i;M,j)]C_{M,j}=0 \tag{A2}$$

for all N,i. Because of the Gaussian nature of the basis functions, the Hamiltonian and overlap matrices are easy to calculate. In terms of the unprojected Gaussians (7),

$$A(N,i;M,j)=\delta_{N,M}\langle \varphi_i \mid \varphi_j \rangle \ , \tag{A3}$$

with

$$\langle \varphi_i \mid \varphi_j \rangle = \left[\frac{2b_i b_j}{(b_i^2+b_j^2)} \right]^{1/2} \exp \left[\frac{-\frac{1}{2}(z_i-z_j)^2}{(b_i^2+b_j^2)} \right] ,$$

and

$$H(N,i;M,j)=\langle \varphi_i \mid \varphi_j \rangle \left\{ \delta_{N,M} \left[2N\hbar\omega + \frac{\hbar^2}{2\mu(b_i^2+b_j^2)} \left[1-\frac{(z_i-z_j)^2}{b_i^2+b_j^2} \right] \right] \right.$$
$$\left. -e^2\frac{2}{\sqrt{\pi}}B \sum_{L=0}^{\min(N,M)} \frac{[N!M!(N+m)!(M+m)!]^{1/2}}{(N-L)!(M-L)!L!(m+L)!} I(N+M-2L,2L+m) \right\} \tag{A4}$$

with

$$I(N_1,N_2)= \int_0^1 \frac{(b^2x^2)^{N_1}[B^2(1-x^2)]^{N_2}}{[b^2x^2+B^2(1-x^2)]^{N_1+N_2+1}} \times \exp(-\Delta^2x^2/B^2)dx \ . \tag{A5}$$

In (A5), b is the oscillator width (6) associated with the magnetic-field-strength parameter γ and

$$B^2=2b_i^2b_j^2/(b_i^2+b_j^2) \ , \quad \Delta=\frac{1}{2}B^2 \left[\frac{z_i}{b_i^2}+\frac{z_j}{b_j^2} \right] . \tag{A6}$$

The parity projected matrix elements appearing in (A2) are given by, e.g.,

$$H^\pm(N,i;M,j)=\frac{1}{2}[H(N,i;M,j)\pm H(N,i;M,-j)] \ ,$$

where the minus sign in front of the symbol j means that z_j is to be replaced by $-z_j$ in the explicit expressions for the matrix elements (A3)–(A6). The integral (A5), which reduces to a simple beta function[22] if $b=B$ and $\Delta=0$, is calculated numerically. For $b \approx B$, an accuracy of roughly one in 10^6 was achieved with a mesh of 50 points. For $B \gg b$, the number of mesh points had to be increased by a factor of B/b in order to maintain this accuracy. This made the calculation of matrix elements rather time consuming for high values of γ.

The nonorthogonal basis (A3) was orthogonalized with the Schmidt orthogonalization procedure and the resulting Hamiltonian matrix was diagonalized with a standard package subroutine. The parameters c and a, which determine the Gaussian basis via Eq. (9), were determined by minimizing the energy of the first few states in a given m^π subspace for each value of γ. Typical values were $c \approx 0.1$ for $\gamma=1$ and $c \approx 0.015$ for $\gamma=500$. Values of a depended weakly on γ and ranged between 2.5 and 4.5.

Using the basis (9), the number of eigenvalues obtained to a given accuracy in a given m^π subspace depends linearly on the number of Gaussians used. In the region $\gamma \gtrsim 1$ the first n eigenstates were obtained to about six significant figures with $5\times n$ to $7\times n$ Gaussians. For higher fields, the mesh has to be denser and the number of Gaussians needed to maintain this accuracy increases and reaches $10\times n$ to $15\times n$ at $\gamma=500$.

The convergence of the energies (and the quantum excesses) as functions of the number of channels N_c is quite slow, especially in the $m^\pi=0^+$ subspace. The binding energies given in Table I for $\gamma=1$ and 2 are extrapolated to $N_c=\infty$ from values obtained with $N_c \leq 25$. The values actually calculated with $N_c=25$ are 1.655 Ry for $\gamma=1$ and 2.041 Ry for $\gamma=2$.

Despite the slow convergence of the energies and quantum excesses, the quantum excess differences ϵ_n defined by Eq. (12) converge very rapidly as functions of the number of channels N_c. Except for the region $\gamma<2$ in the $m^\pi=0^+$ subspace a three-channel calculation already gives the values of ϵ_n to within less than 3×10^{-4}. In all m^π subspaces the values of ϵ_n are already given to within less than 10^{-4} by the two-channel calculation for $\gamma \geq 5$ and by the one-channel calculation (adiabatic approximation) for $\gamma \geq 10$.

This rapid convergence of the quantum excess differences as functions of the number of channels makes it possible to determine the quantum excesses (and hence energies) of highly excited states without having to diagonalize huge matrices. In each m^{π} subspace, the low-lying levels are obtained from calculations using only a few Gaussians and large numbers (up to $N_c=25$) of channels. The more highly excited levels are obtained via the rapidly converging quantum excess differences with fewer channels but a large number (up to $n_z=100$) of Gaussians. The maximum total dimension $N_c \times n_z$ of the matrices diagonalized in the present calculation was 200.

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