

Semiclassical self-consistent-field perturbation theory for the hydrogen atom in a magnetic field

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Abstract

A recently developed perturbation theory for solving self-consistent-field equations is applied to the hydrogen atom in a strong magnetic field. This system has been extensively studied using other methods and is therefore a good test case for the new method. The perturbation theory yields summable large-order expansions. The accuracy of the self-consistent-field approximation varies according to field strength and quantum state, but is often higher than the accuracy from adiabatic approximations. A new derivation is presented for the asymptotic adiabatic approximation, the most useful of the adiabatic approaches. This derivation uses semiclassical perturbation theory without invoking an adiabatic hypothesis.

[**Key words:** self-consistent-field theory, semiclassical perturbation theory, dimensional perturbation theory, adiabatic approximations, hydrogen atom in magnetic field]

I. INTRODUCTION

Large-order perturbation theory has been widely used to solve the Schrödinger equation for systems with only 1 or 2 degrees of freedom, and occasionally for 3-coordinate problems [1–4], but rarely for larger systems because it becomes increasingly difficult to compute expansion coefficients to sufficiently high order. A recently developed self-consistent-field (SCF) perturbation theory [5,6] reduces the computational cost by introducing a separability assumption. Here we apply this method to a simple 2-coordinate test case—the hydrogen atom in an external magnetic field.

We will use this system, which has been extensively studied with a wide variety of methods [7], to examine the accuracy of the separability assumption. In particular, we will compare the accuracy of the SCF approximation to that of adiabatic approximations. Our method is based on a semiclassical perturbation theory [8–13]. At first order in this perturbation expansion the Schrödinger equation becomes exactly separable in terms of a set of normal coordinates. These coordinates are a natural choice for a separability approximation. For a one-electron atom in a magnetic field the normal coordinates are the cylindrical coordinates (ρ, z) , with z along the field direction. It is well known that in the limit of infinite field strength the exact wavefunction is a separable product in these coordinates and that the z motion is much slower than the ρ motion [14]. This is the rationale behind adiabatic approximations [14–21], in which a solution for the ρ motion is obtained with z treated as a fixed parameter. These approximations simplify the computation of energies and provide a qualitative understanding of the energy level patterns [7,21]. Approximate methods are not as important for this problem as they used to be, now that increases in computer power have made exact calculations feasible for any field strength [7,22]. However, the asymptotic adiabatic approximation of Rösner *et al.* [21] is still useful for calculating quantities such as partition functions that require the computation of many energy levels.

Adiabatic approximations and the SCF theory are similar in that, in principle, they both become exact in the infinite-field limit. They differ in that the SCF method includes no assumption about fast and slow coordinates and uses a separable wavefunction at all values of field strength. They differ also in that the SCF perturbation theory becomes exact not just in the limit of infinite field strength but also in the limit of infinite magnetic quantum number m . Thus, the error from the SCF separability assumption can in principle remain small at field strengths at which the adiabatic hypothesis breaks down. We find in fact that the SCF results for energies are accurate even at small values of m and at relatively smaller field strengths.

Sections II and III describe our calculation method and Section IV shows representative results. In Section V we compare the accuracy of the SCF theory with that of the primitive adiabatic approximation of Schiff and Snyder [15], the true adiabatic approximation of Baldereschi and Bassani [19], and the asymptotic adiabatic approximation of Rösner *et al.* [21]. The asymptotic method was originally derived as an approximation to the primitive adiabatic method, yet it tends to be the more accurate of these two approaches. We show that the asymptotic method can be derived as a second-order semiclassical perturbation expansion, without assuming an adiabatic separation of variables. In Section VI we discuss our results and describe some potential advantages of the SCF theory.

II. SEMICLASSICAL PERTURBATION THEORY

Mlodinow's semiclassical perturbation expansion [8] is an example of a class of perturbation theories in which a discrete dimensionality parameter is treated as a continuous variable [23]. These "dimensional" perturbation theories are being applied to an increasingly wide variety of problems in condensed-matter physics, statistical mechanics, particle physics, polymer physics, and chemical physics [24]. In the case of the Schrödinger equation the perturbation expansion parameter is asymptotically proportional to $1/D$, where D is the dimensionality of coordinate space. This expansion can often be computed to very large order and accurately summed at $D = 3$ [11–13,25–29].

The nonrelativistic energy levels, in atomic units, of a hydrogen atom in a uniform magnetic field \mathbf{B} are $E + mB/2$, where m is the magnetic quantum number and E is an eigenvalue of the operator $H = T + V$,

$$T = -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{(2|m| + D - 2)(2|m| + D - 4)}{8\rho^2} \quad (2.1)$$

and

$$V = -(\rho^2 + z^2)^{-1/2} + \frac{1}{8}B^2\rho^2. \quad (2.2)$$

In these units $B = 1$ corresponds to a field strength of $m_e^2 c e^3 / \hbar^3$, which is approximately 2.35×10^5 T. The kinetic energy operator, Eq. (2.1), is expressed in a form valid for arbitrary D [30]. The coordinates (ρ, z) are cylindrical coordinates with the z axis oriented in the direction of \mathbf{B} .

Let

$$\delta = [|m| + a + (D - 3)/2]^{-1}, \quad (2.3)$$

where a is an arbitrary constant. We will use δ as the expansion parameter for the perturbation theory [31]. The main purpose of the shift constant a is to preserve δ as a finite parameter at $m = 0$. The dimensional scalings

$$\rho = \delta^{-2}\tilde{\rho}, \quad z = \delta^{-2}\tilde{z}, \quad E = \delta^2\tilde{E}, \quad B = \delta^3\tilde{B}, \quad (2.4)$$

of the units of distance, energy, and field strength, respectively, yield the eigenvalue equation

$$\left[-\frac{1}{2}\delta^2 \left(\frac{\partial^2}{\partial \tilde{\rho}^2} + \frac{\partial^2}{\partial \tilde{z}^2} \right) + \frac{1 - 2a\delta + (a^2 - 1/4)\delta^2}{2\tilde{\rho}^2} - (\tilde{\rho}^2 + \tilde{z}^2)^{-1/2} + \frac{1}{8}\tilde{B}^2\tilde{\rho}^2 - \tilde{E} \right] \Psi = 0. \quad (2.5)$$

Note that the only D dependence in Eq. (2.5) is in the parameter δ . Therefore, we can set

$$\delta = 1/(|m| + a) \quad (2.6)$$

and consider $\delta \rightarrow 0$ as equivalent to the limit of large $|m|$.

In the limit of small δ the factor of δ^2 plays the role of \hbar^2 in the Schrödinger equation for a particle of unit mass subject to an effective potential

$$V_{\text{eff}}(\tilde{\rho}, \tilde{z}) = \frac{1}{2}\tilde{\rho}^{-2} - (\tilde{\rho}^2 + \tilde{z}^2)^{-1/2} + \frac{1}{8}\tilde{B}^2\tilde{\rho}^2. \quad (2.7)$$

In the limit $\delta \rightarrow 0$ all of the eigenvalues collapse to the value $\tilde{E}_0 = V_{\text{eff}}(\tilde{\rho}_{\text{min}}, \tilde{z}_{\text{min}})$, where $(\tilde{\rho}_{\text{min}}, \tilde{z}_{\text{min}})$ is the minimum of the effective potential. This minimum corresponds to $\tilde{z}_{\text{min}} = 0$ with $\tilde{\rho}_{\text{min}}$ equal to a positive root of the equation $\tilde{B}^2\tilde{\rho}_{\text{min}}^4 = 4(1 - \tilde{\rho}_{\text{min}})$.

In order to have a formulation suitable for the entire range of field strengths, we introduce a further scaling of distance and energy with the substitutions

$$\xi = \tilde{\rho}/\tilde{\rho}_{\text{min}}, \quad \eta = \tilde{z}/\tilde{\rho}_{\text{min}}, \quad (2.8)$$

which yields the effective potential

$$W(\xi, \eta) = \frac{1}{2\xi^2} - \frac{1-g}{(\xi^2 + \eta^2)^{1/2}} + \frac{1}{2}g\xi^2, \quad (2.9)$$

where

$$g = 1 - \tilde{\rho}_{\text{min}} = \tilde{B}^2\tilde{\rho}_{\text{min}}^4/4. \quad (2.10)$$

Variation of g from 0 to 1 corresponds to variation of \tilde{B} from zero to infinity, according to the relation

$$\tilde{B} = 2g^{1/2}(1-g)^{-2}. \quad (2.11)$$

Higher orders in the perturbation theory are obtained by introducing displacement coordinates q_1 and q_2 , defined by $\xi = 1 + \delta^{1/2}q_1$, $\eta = \delta^{1/2}q_2$, and then expanding W in powers of $\delta^{1/2}$, and collecting terms of given order. At order $(\delta^{1/2})^2$ we have a Schrödinger equation for a harmonic oscillator. In general, the next step in the analysis would be to diagonalize the harmonic Hamiltonian with a normal-mode transformation. However, in this case there is no coupling between q_1 and q_2 at this order. Therefore, q_1 and q_2 are themselves the normal coordinates. The Schrödinger equation is

$$\left[-\frac{\delta}{2} \left(\frac{\partial^2}{\partial q_1^2} + \frac{\partial^2}{\partial q_2^2} \right) + W - \tilde{\rho}_{\text{min}}^2 \tilde{E} \right] \Psi = 0 \quad (2.12)$$

and the perturbation expansions for the effective potential, the wavefunction, and the scaled eigenvalues, respectively, have the forms

$$W = \tilde{\rho}_{\text{min}}^2 \tilde{E}_0 + \delta \left[\frac{1}{2}\omega_1^2 q_1^2 + \frac{1}{2}\omega_2^2 q_2^2 - a + v(q_1, q_2) \right], \quad (2.13)$$

$$v(q_1, q_2) = \sum_{k=1}^{\infty} \delta^{k/2} v_k(q_1, q_2), \quad (2.14)$$

$$\Psi(q_1, q_2) = \sum_{k=0}^{\infty} \delta^{k/2} \Psi_k(q_1, q_2), \quad (2.15)$$

$$\epsilon \equiv \tilde{\rho}_{\text{min}}^2 (\tilde{E} - \tilde{E}_0) / \delta = \sum_{k=0}^{\infty} \delta^{k/2} \epsilon_k. \quad (2.16)$$

The v_k in Eq. (2.14) are polynomials of degree $k + 2$, and $\epsilon_k = 0$ for odd k .

At first order in δ the expansion coefficient for the eigenvalue is

$$\epsilon_0 = \epsilon_0^{(1)} + \epsilon_0^{(2)} - a, \quad (2.17)$$

in terms of the harmonic eigenvalues

$$\epsilon_0^{(i)} = (n_i + \frac{1}{2})\omega_i \quad (2.18)$$

with harmonic frequencies

$$\omega_1 = (1 + 3g)^{1/2}, \quad \omega_2 = (1 - g)^{1/2}. \quad (2.19)$$

III. SELF-CONSISTENT-FIELD THEORY

Let us express the wavefunction as a separable product in terms of the normal coordinates,

$$\Psi(q_1, q_2) = \psi^{(1)}(q_1)\psi^{(2)}(q_2). \quad (3.1)$$

The SCF equations are

$$\left[-\frac{1}{2} \frac{d^2}{dq_i^2} + \frac{1}{2} \omega_i^2 q_i^2 + \bar{v}^{(i)}(q_i) - \epsilon^{(i)} \right] \psi_i(q_i) = 0, \quad (3.2)$$

where $i = 1$ or 2 , and

$$\bar{v}^{(i)}(q_i) = \langle \psi^{(j)}(q_j) | v(q_1, q_2) | \psi^{(j)}(q_j) \rangle_{q_j}, \quad (3.3)$$

with $(i, j) = (1, 2)$ or $(2, 1)$. Eq. (3.2) yields the “best” solutions for the $\psi^{(i)}$ according to the variational principle for the energy. The SCF approximation for the total energy can be calculated as

$$\epsilon = \epsilon^{(1)} + \epsilon^{(2)} - \langle \psi^{(2)}(q_2) | \bar{v}^{(2)}(q_2) | \psi^{(2)}(q_2) \rangle_{q_2}. \quad (3.4)$$

Let

$$\psi^{(i)}(q_i) = \sum_{k=0}^{\infty} \delta^{k/2} \psi_k^{(i)}(q_i) \quad (3.5)$$

and

$$\epsilon^{(i)} = \sum_{k=0}^{\infty} \delta^{k/2} \epsilon_k^{(i)}. \quad (3.6)$$

Substituting these expansions into the two SCF equations and collecting terms by order in $\delta^{1/2}$ yields two sets of perturbation equations that are coupled implicitly through the dependence of $\bar{v}^{(i)}$ on $\psi^{(j)}$.

Consider the expansion of $\bar{v}^{(i)}(q_i)$ at some arbitrary order $\delta^{k/2}$. Substituting Eq. (2.14) for v and Eq. (3.5) for $\psi^{(j)}$ into Eq. (3.3) yields a sum of the terms $\langle \psi_{k_1}^{(j)} | v_{k_2} | \psi_{k_3}^{(j)} \rangle$ such that $k_1 + k_2 + k_3 = k$. However, the smallest possible value of k_2 is 1, which implies that the largest possible value for k_1 or k_3 is $k - 1$. Therefore, the equation that determines $\psi_k^{(i)}$ depends on the $\psi_{k'}^{(j)}$ only for $k' < k$. Thus, perturbation theory uncouples the SCF equations order by order. Detailed derivations of the perturbation equations are presented in Refs. [5] and [6].

By assuming separability in terms of the normal coordinates, we ensure that the SCF theory will be exact to order δ in the energy expansion. The error due to the separability assumption will be of order δ^2 .

IV. RESULTS

The SCF energy levels can be uniquely labeled by the magnetic quantum number m and by the harmonic quantum numbers (n_1, n_2) . The expression for the eigenvalue E is

$$E = (|m| + a)^{-2} \tilde{E}_0 + (|m| + a)^{-3} \tilde{\rho}_{\min}^{-2} \epsilon, \quad (4.1)$$

where a is the arbitrary shift parameter. ϵ is calculated as an asymptotic expansion. In general, we choose

$$a = n_1 + n_2 + 1, \quad (4.2)$$

so that in the limit $B \rightarrow 0$ the zeroth-order term in Eq. (4.1) yields the exact hydrogenic energy.

For the exact nonseparable problem, (n_1, n_2) are true quantum numbers only in the limit $\tilde{B} \rightarrow \infty$. As \tilde{B} is decreased, all but the $(0, 0)$ and $(1, 0)$ states will undergo avoided crossings, which occur at \tilde{B} values for which the harmonic frequencies are in integer ratios. At very high field strengths the avoided crossings are sharp and well defined while at lower field strengths they can be broad and complicated [32,33].

One can expect that the major qualitative difference between the SCF eigenvalues and the exact eigenvalues will be the behavior at avoided crossings. The separability assumption ensures that for the SCF results (n_1, n_2) will be good quantum numbers for all values of \tilde{B} . Thus, the SCF eigenvalues will cross diabatically. Figure 1 compares exact and SCF results as functions of the parameter g for a manifold of states with $|m| = 30$. ($g = 0$ corresponds to $\tilde{B} = 0$ and $g = 1$ corresponds to $\tilde{B} = \infty$, according to Eq. (2.10).) This Figure gives the energy as the scaled quantity

$$\epsilon' = |m|^3 [E - |m|^{-2} \tilde{E}_0(a = 0)], \quad (4.3)$$

which is simply the value of ϵ that corresponds to $a = 0$. The advantage of ϵ' is that it omits the uninteresting but strongly field dependent zero-point energy and, in contrast to ϵ , it uses the same scaling factor for all values of n_1 and n_2 . We obtain convergent SCF results for ϵ' over almost the full range of g using Padé summation. It can be seen that the SCF results are very close to the exact results except in the vicinity of broad avoided crossings.

Figure 2 shows the accuracy of the SCF approximation for the binding energy (the difference between the total energy and the energy of a free electron in the magnetic field) in

unscaled units as a function of B and m for the “circular” states, $(n_1, n_2) = (0, 0)$. For given value of B the accuracy increases significantly with increasing $|m|$. This is consistent with the fact that the underlying separability assumption is exact within first-order perturbation theory in $\delta \sim |m|^{-1}$.

For given $|m|$, the error from the SCF approximation at first holds steady at the field-free value as B increases. Note that the field-free H atom is not separable in the coordinates ρ and z . Then at a critical value of B , the accuracy begins to improve, with the error diminishing approximately as $B^{-1/2}$. The increase in accuracy begins when the field-dependent term $\tilde{B}^2 \tilde{\rho}^2/8$ starts to dominate the coupling term $-(\tilde{\rho}^2 + \tilde{z}^2)^{-1/2}$ in Eq. (2.5). The critical value is smaller at large $|m|$, since $B = (|m| + a)^{-3} \tilde{B}$. At this critical field strength the magnetic field and the Coulomb field on the electron are of the same magnitude, since the radius of the electron orbit increases with $|m|$ as $(|m| + a)^2$.

We have used Padé approximants to sum the perturbation expansions. For the results from which Fig. 2 was prepared, the approximants converge with a precision that is greater than the accuracy of the underlying separability assumption. The rate of convergence slows as B increases. This appears to be due to the fact that $\tilde{\rho}_{\min}$ approaches zero in the large- B limit, which causes the expansion of the Coulomb term in Eq. (2.7) to diverge.

V. COMPARISON WITH ADIABATIC APPROXIMATIONS

There are three different computational techniques that have been referred to in the literature as “adiabatic approximations” for the one-electron atom in a magnetic field. The earliest is the method developed by Schiff and Snyder [15], which we will call the “primitive” adiabatic approximation. That approach is based on the approximation

$$\Psi(\rho, z) = f_{n_1, n_2, m}(z) \Phi_{n_1, m}^{(\text{Landau})}(\rho), \quad (5.1)$$

where the $\Phi_{n_1, m}^{(\text{Landau})}$ are the well-known Landau functions [14], which result from solving the Schrödinger equation without the Coulomb potential. The Landau quantum number n_1 is equivalent to our harmonic quantum number for ρ motion in the limit $\delta \rightarrow 0$, while the quantum number n_2 , which is equal to the number of longitudinal nodes, is equivalent to our harmonic quantum number for z motion. The longitudinal functions f are determined by solving Schrödinger equations with effective potentials

$$V_{n_1, m}^{(\text{Landau})}(z) = -\langle \Phi_{n_1, m}^{(\text{Landau})} | (\rho^2 + z^2)^{-1/2} | \Phi_{n_1, m}^{(\text{Landau})} \rangle. \quad (5.2)$$

The second approach [19,20], which we call the “true” adiabatic approximation, uses an expression of the form

$$\Psi(\rho, z) = G_{n_1, n_2, m}(z) F_{n_1, m}(z; \rho). \quad (5.3)$$

In the function F , the z dependence is treated parametrically, in a manner analogous to the Born-Oppenheimer approximation in molecular physics. The function $G_{n_1, n_2, m}(z)$ is an eigenfunction of a Hamiltonian in which the potential is a function $W_{n_1, m}^{(\text{adiab})}(z)$ that is calculated at each point as the eigenvalue of the ρ equation.

Probably the most useful of the adiabatic approximations is the asymptotic approximation of Rösner, *et al.* [21]. Consider the case $n_1 = 0$. (These are the most important states, since eigenvalues for $n_1 > 0$ in strong fields lie above the ionization threshold.) The integrand in Eq. (5.2) contains the product

$$\Phi_{0,m}^{(\text{Landau})*} \Phi_{0,m}^{(\text{Landau})} \propto e^{-B\rho^2/2} \rho^{2|m|+1}, \quad (5.4)$$

which is a bell-shaped curve peaked at the point $\rho_0 = [(2|m| + 1)/B]^{1/2}$. Replacing $(\rho^2 + z^2)^{-1/2}$ in Eq. (5.2) with its asymptotic expansion about ρ_0 and then retaining only the leading term after evaluating the integral leads to the expression

$$V_p^{(\text{Landau})}(z) \sim V_p^{(\text{asympt})} = -2(1/p + z^2)^{-1/2}, \quad (5.5)$$

$$p = B/(2|m| + 1). \quad (5.6)$$

The striking feature of Eq. (5.5) is the fact that it no longer depends on B and m separately, but only on the quantity p . This reduction in the dimensionality of the manifold of eigenvalues greatly facilitates the calculation of quantities such as partition functions that require the computation of very large numbers of energy levels.

Figures 3 and 4 compare the accuracy of the SCF theory with that of the various adiabatic approximations for states with $(n_1, n_2) = (0, 0)$ and $(0, 2)$, respectively. For the $(0, 0)$ manifold, the SCF results are in general significantly more accurate than the primitive and asymptotic adiabatic results, especially at lower field strengths. For the $(0, 2)$ manifold the trends are less clear. The primitive adiabatic, asymptotic adiabatic, and SCF results are comparable in accuracy. The accuracy increases with $|m|$ for all three methods but the increase in general is greatest for the SCF method, especially at lower B .

True adiabatic results are available only for states with $|m| = 0$ or 1 [20]. Although the true adiabatic theory is in principle the most accurate (and laborious) of the adiabatic methods, it yields energies that are furthest from the exact results for $m = 0$.

It is interesting, also, that for states with $n_2 > 0$ the primitive adiabatic theory is generally *less* accurate than the asymptotic theory, despite the fact that the latter was derived as an approximation to the former. In fact, it is possible to derive the asymptotic theory from a semiclassical perturbation analysis, without invoking the adiabatic hypothesis. Let us make the substitutions

$$E = \delta^{-2} \tilde{E}, \quad B = \delta^{-1} \tilde{B}. \quad (5.7)$$

Note that these differ from the dimensional scalings in Eq. (2.4). The Schrödinger equation is now

$$\left[-\frac{1}{2}\delta^2 \left(\frac{\partial^2}{\partial \rho^2} + \frac{\partial^2}{\partial z^2} \right) + \frac{1 - 2a\delta + (a^2 - 1/4)\delta^2}{2\rho^2} - \delta^2(\rho^2 + z^2)^{-1/2} + \frac{1}{8}\tilde{B}^2\rho^2 - \tilde{E} \right] \Psi = 0, \quad (5.8)$$

instead of Eq. (2.5). In the $\delta \rightarrow 0$ limit the Coulombic potential drops out and Ψ concentrates along the cylinder defined by $\rho = \rho_{\min}$, with $\rho_{\min} = (2/\tilde{B})^{1/2}$. The scaled energy approaches

the value $\tilde{E}_0 = \tilde{B}/2$. If we introduce the displacement coordinate $q_1 = (\rho - \rho_{\min})/\delta^{1/2}$ and expand Eq. (5.8) in powers of $\delta^{1/2}$, keeping terms up to order δ^2 , we obtain the uncoupled equations

$$\left[-\frac{\delta}{2} \frac{d^2}{dx^2} + \frac{1 - 2a\delta + (a^2 - 1/4)\delta^2}{2(\rho_{\min} + \delta^{1/2}x)^2} + \frac{1}{8}\tilde{B}^2(\rho_{\min} + \delta^{1/2}x)^2 - \tilde{E}^{(1)} \right] \psi^{(1)}(x) = 0, \quad (5.9)$$

$$\left[-\frac{\delta^2}{2} \frac{d^2}{dz^2} - \delta^2(\rho_{\min} + z^2)^{-1/2} - \tilde{E}^{(2)} \right] \psi^{(2)}(z) = 0. \quad (5.10)$$

To solve Eq. (5.9) we remove all of the dimensional scalings. The result is simply the Landau equation, and

$$\begin{aligned} E^{(1)} &= \delta^{-2} \left[\frac{1}{2}\tilde{B} + \frac{1}{2}(2n_1 + 1 - a)\tilde{B}\delta \right] \\ &= (2n_1 + |m| + 1)(B/2) \end{aligned} \quad (5.11)$$

is the Landau energy. If the shift parameter a is chosen to be $1/2$, then $\tilde{B}/2 = p$ and the potential in Eq. (5.10) is identical to $V_p^{(\text{asympt})}$ in Eq. (5.5). In that case, $\psi^{(2)}$ is equivalent to the function $f_{0,n_2,m}$ as given by the asymptotic adiabatic approximation. Of course, the value of a is arbitrary in the perturbation theory. One can justify the choice $a = 1/2$ by requiring that the perturbation theory agree with the primitive adiabatic approximation in the limit of large B and $|m|$.

VI. DISCUSSION

In general the asymptotic adiabatic approximation and the SCF theory for this system appear to be complementary, in that the former is best for large values of the longitudinal quantum number n_2 and very large B while the SCF method is better for smaller n_2 and relatively smaller B . We have shown that the asymptotic method is in fact a type of second-order semiclassical perturbation theory, and does not depend on an adiabatic hypothesis for its validity. The advantage of the SCF approach is that it allows for very efficient computation of the perturbation expansion coefficients. This eliminates the error that arises from the need to truncate the asymptotic expansion at low order. However, it requires a separability approximation that is based on the assumption that the dynamics of the system is approximately harmonic. High excitation in the longitudinal or radial quantum numbers increases the importance of anharmonic effects. In contrast, the asymptotic approximation does not assume that the dynamics in the longitudinal coordinate is harmonic. For longitudinally excited states this advantage can outweigh the error from the second-order asymptotic truncation.

Our derivation of the asymptotic adiabatic approximation uses dimensional perturbation theory with an unconventional dimensional scaling. This illustrates the fact that the dimensional continuation of the Schrödinger equation is arbitrary as long as the Hamiltonian

is correct for $D = 3$. The standard dimensional continuation [3,4,34], which we described in Section II, is certainly the most widely used approach, but various other nonstandard definitions for the D -dimensional Hamiltonian have been suggested [26,35–38]. Our use of dimensional perturbation theory to explain the success of an adiabatic approximation is somewhat analogous to Goscinski and Mujica’s analysis of the hyperspherical adiabatic approximation for the two-electron atom [39]. It is possible that the particular approach we have used here, in which part of the problem (in this case the z dependence of the potential) is not expanded as a polynomial, will be useful in other contexts.

Both SCF and adiabatic approximations are widely used in molecular physics, and the general experience in that field is that SCF theory is easier to apply than adiabatic approximations and the computational effort grows less quickly as the number of degrees of freedom increases, but that an adiabatic calculation is more accurate than the corresponding SCF calculation [40]. Thus, our finding that the SCF theory is often the more accurate approach is notable.

For the one-electron atom in an external field, approximate methods are not as important as they were previously, since various methods can now yield essentially exact numerical results on today’s computers [7,22]. However, such accurate calculations, with no approximations, are much more difficult for many-electron systems in strong fields. It is straightforward to apply SCF theory, with dimensional perturbation expansions, to systems with more than one electron [6] as long as a suitable definition for the dimensional continuation of the Hamiltonian is available. For a two-electron atom in a magnetic field, the standard dimensional continuation appears to be adequate. In Ref. [12] the exact dimensional expansions for H^- and He in a strong magnetic field were calculated to second order and found to agree reasonably well with variational results.

Furthermore, even for systems for which the exact energy can be accurately calculated, there is still a place for adiabatic and SCF calculations, which yield approximate results with relatively little computational effort. Suppose, for example, that one wanted to calculate the equilibrium constant for a chemical reaction involving simple atoms or molecules in very strong magnetic fields. Such a calculation could be of interest in the description of astrophysical phenomena. In principle, the equilibrium constant could be calculated from the partition functions obtained by summing over all quantum states of each of the reactants. In practice, this requires the computation of tremendous numbers of eigenvalues [41].

SCF calculations for an atom in a magnetic field can also be carried out using an iterative Hartree-Fock procedure [42,43]. Dimensional perturbation theory provides an efficient noniterative algorithm for solving SCF equations [6]. Furthermore, the normal coordinates implied by the large-dimension limit are an asymptotically optimal coordinate system for the separability assumption. For many-electron systems these coordinates yield a separable model that includes electron-correlation effects [44,45]. The error due to this separability assumption can be expected to be smaller than the error from an independent-electron separability assumption.

Some particular advantages of dimensional perturbation theory are becoming clear. It is in principle well suited to describing correlated electron dynamics [44–46] and provides a unified approach to bound states and resonances [11,12,27]. The method does not introduce approximations into the potential energy operator, and therefore is relatively insensitive to wide variations in physical parameters such as external field strengths. However, the com-

putational cost of calculating the expansion coefficients to sufficiently high order increases prohibitively with the number of coupled degrees of freedom. SCF approximations offer the possibility of bypassing these computational difficulties without a severe cost in accuracy.

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FIGURES

FIG. 1. Energies for even parity states (n_2 even), in scaled units, as function of field strength for $|m| = 30$. g is the field-strength parameter given by Eq. (2.11). The scaled energy, ϵ' , is given by Eq. (4.3). Each curve is labeled by the quantum numbers n_1 and n_2 .

FIG. 2. Accuracy of the SCF approximation for binding energies, as function of field strength for the manifold of circular states, $(n_1, n_2) = (0, 0)$. The ordinate is $-\log_{10} |(E_{\text{approx}} - E_{\text{exact}})/E_{\text{exact}}|$. The abscissa is the magnetic field strength in atomic units such that $B = 1$ corresponds to 2.35×10^5 T. The curves are labeled by the value of the magnetic quantum number.

FIG. 3. Accuracy of binding energies calculated by various methods, as function of field strength for the manifold of circular states, $(n_1, n_2) = (0, 0)$. The axes are labeled as in Fig. 2. The calculation methods are: SCF theory (solid curves); primitive adiabatic approximation [21] (dashed curves); asymptotic adiabatic approximation [21] (dash-dot curves); true adiabatic approximation [20] (\bullet). The panels are labeled by the value of the magnetic quantum number.

FIG. 4. Accuracy of binding energies calculated by various methods, as function of field strength for the manifold of states with $(n_1, n_2) = (0, 2)$. The axes are labeled as in Fig. 2. The calculation methods are: SCF theory (solid curves); primitive adiabatic approximation [21] (dashed curves); asymptotic adiabatic approximation [21] (dash-dot curves); true adiabatic approximation [20] (\bullet). The panels are labeled by the value of the magnetic quantum number.