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Coulomb-Zeeman-Stark problem in two dimensions

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Coulomb-bound systems in reduced dimensions are sensitive probes of increased confinement. For example, the ground-state binding energy of hydrogen atoms increases by a factor of 4 when passing from three to two dimensions. Recently, quasi–two-dimensional hydrogen has been realized experimentally in the form of low-dimensional excitons. Their sensitivity to external electric and magnetic perturbations is reduced by the confinement. To quantify the reduction, we consider in the present work two-dimensional hydrogen in crossed electric and magnetic fields. We compare analytical, numerical, and variational results for the binding energy and dipole polarizability in arbitrary magnetic fields. Our analytical expressions for both weak and strong magnetic fields are supplemented by accurate variational and hypergeometric resummation results, thereby covering arbitrary magnetic fields.

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I. INTRODUCTION

Two-dimensional (2D) hydrogen is a useful model system for studies of the impact of dimensionality on Coulomb-bound systems [1–12]. In addition, 2D hydrogen has received significant attention as a model of excitons in 2D semiconductors and quantum wells [13–25]. Experimentally, the properties of 2D excitons have been probed using a wide range of techniques including optical, electric, and magnetic fields [20–25]. Such experiments provide important information about the exciton state itself when combined with accurate models. In a solid-state medium, the Coulomb potential is modified by dielectric screening. In atomically thin semiconductors, nonlocal screening implies a modified Coulomb interaction [26–28]. However, the pure r^{-1} potential characteristic of local screening is a useful approximation if screening by dielectric surroundings (rather than the 2D semiconductor itself) dominates [19]. The eigenstates of this 2D hydrogen model have previously been studied in detail and analytical bound and continuum states are known [1–12]. In turn, this makes the system highly suitable for applications of perturbation theory. Thus, low-order energy corrections due to either electric or magnetic fields have previously been obtained [1–8,15–17]. In fact, exact solutions for the Coulomb-Zeeman problem can be found for special values of the magnetic field [9,10], albeit not for the ground state. In a few cases, even relativistic effects in 2D hydrogen have been included [11,12].

Strong magnetic fields are frequently applied to characterize Coulomb-bound states in two dimensions [22,23]. The diamagnetic shift $E_{\rm dia} \propto \langle r^2\rangle \mathcal{B}^2$ in a perpendicular magnetic field $\mathcal{B}$ provides a measure of rms spread $\langle r^2\rangle$ of the wave function. Thereby, the impact of dielectric screening on localization can be deduced [22,23]. Similarly, Stark shifts $E_{\rm Stark} = -\frac{1}{2}\alpha\mathcal{E}^2$ in electric fields $\mathcal{E}$ measure the polarizability α; see Refs. [24,25]. In turn, α itself is another sensitive measure of localization. Very recently, simultaneous perturbations by crossed electric and magnetic fields have been applied in experiments on high-quality encapsulated samples [29]. In these experiments, a strong in-plane electric field lowers the exciton energy through the Stark shift. Thus, applying an inhomogeneous electric field over a narrow spatial region leads to center-of-mass localization and observable discrete states. By adding a perpendicular magnetic field, pronounced changes in the relative motion are revealed. Modeling of such systems under simultaneous electric and magnetic perturbations consequently poses an important theoretical challenge.

In the present work, we study the Coulomb-Zeeman-Stark problem of a 2D hydrogen atom perturbed simultaneously by crossed magnetic and electric fields. We analyze this double-perturbation problem using Dalgarno-Lewis perturbation theory [6,17,30–33]. Following conventional terminology, the term "Dalgarno-Lewis perturbation theory" is taken to mean solving sequences of inhomogeneous perturbation problems order by order. This approach is an alternative to traditional sum-over-states methods that express corrections in terms of contributions from individual unperturbed states. Such sums-over-states become integrals-over-states if unperturbed continuum states exist and, therefore, are difficult to evaluate with high accuracy. Dalgarno-Lewis perturbation theory provides an appealing alternative, in which exact corrections are found from solutions of inhomogeneous perturbation problems [6,17,30–33]. Thus, the problem of summing over continua is completely bypassed.

The geometry of the 2D Coulomb-Zeeman-Stark problem is shown in the inset of Fig. 1. The model consists of a Coulomb-bound electron subjected to in-plane electric fields and out-of-plane magnetic fields. In polar coordinates, the position of the electron is defined by radial coordinate r and angle θ measured relative to the direction of the electric field. Throughout, we use "exciton" units, which generalize atomic units to problems with dielectric constant ε

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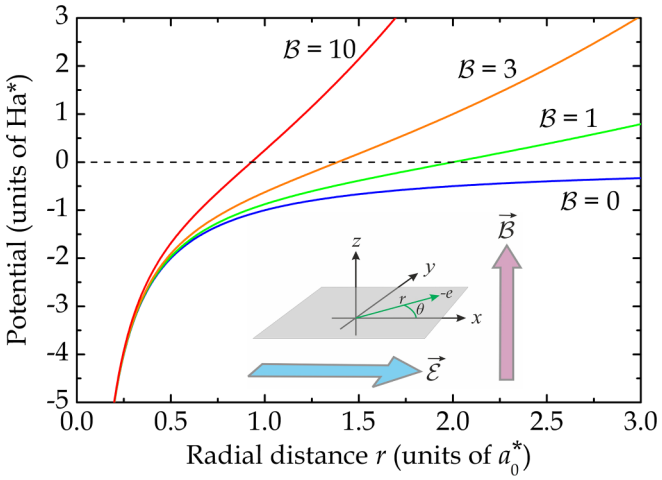

FIG. 1. Effective potential including Coulomb and magnetic terms. Inset illustrates the geometry of the 2D Coulomb-Zeeman-Stark problem.

and reduced mass $m_e m_h/(m_e+m_h) \equiv \mu m_0$, where $m_{e/h}$ are effective electron-hole masses and m_0 is the free-electron mass. Thus, we measure distances and energies in units of effective Bohr radii $a_0^* = (\varepsilon/\mu)a_0$ and effective hartrees $\mathrm{Ha}^* = \mu/\varepsilon^2\mathrm{Ha}$, where a_0 and Ha are the usual atomic quantities. These units correspond to measuring magnetic and electric fields in units of $\mathcal{B}_0 = \hbar/ea_0^{*2} = (\mu/\varepsilon)^2 235\mathrm{kT}$ and $\mathcal{E}_0 = \mathrm{Ha}^*/ea_0^* = (\mu^2/\varepsilon^3)5.1\times10^{11}\mathrm{V/m}$, respectively, while polarizabilities are in units of $\alpha_0^* = e^2a_0^{*2}/\mathrm{Ha}^*$. This allows us to write the 2D Coulomb-Zeeman-Stark Hamiltonian as

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \frac{\gamma}{2}\mathcal{B}\hat{l}_z + \frac{1}{8}\mathcal{B}^2r^2 + \mathcal{E}r\cos\theta. \qquad (1)$$

Here, $\gamma = (m_h - m_e)/(m_h + m_e)$ depends on the effective mass ratio and $\hat{l}_z = -i\partial/\partial\theta$ is the angular momentum. In typical 2D semiconductors [34], $m_h \approx m_e$ and, therefore, $|\gamma| \ll 1$, implying a relatively unimportant linear Zeeman term. Of course, if $\mathcal{E} = 0$, the linear Zeeman term simply adds a constant $\frac{l}{2}\gamma\mathcal{B}$ to the energy of states with angular momentum l. The polarizability, however, is affected by γ even for s states. Thus, in the present work, we retain a finite γ to illustrate the influence on the polarizability. Generally, a finite γ only appears in the magnetic corrections to the polarizability and we demonstrate that the effect is small even in the extreme case $|\gamma| \sim 1$.

In Fig. 1, we illustrate the effects of increasing magnetic fields on the confinement of the electron as expressed via the Coulomb-Zeeman potential $V(r) = -1/r + \mathcal{B}^2r^2/8$. It is clear that strong magnetic fields $\mathcal{B} > 1$ lead to a significant localization. The electric field counteracts localization by displacing the electron horizontally. The combined effect of both fields is captured by the $\mathcal{B}$- dependent polarizability $\alpha(\mathcal{B})$ that is expected to be reduced as $\mathcal{B}$ increases. As mentioned above, the polarizability follows from the second-order Stark shift $E_{\mathrm{Stark}} = -\frac{1}{2}\alpha(\mathcal{B})\mathcal{E}^2$. The explicit form of $\alpha(\mathcal{B})$ is the primary target of the present work. In relatively weak fields, an expansion $\alpha(\mathcal{B}) = \alpha_0 + \alpha_1\mathcal{B}^2 + \cdots$ applies while, as demonstrated below, $\alpha(\mathcal{B}) = \tilde{\alpha}_0/\mathcal{B}^2 + \tilde{\alpha}_1/\mathcal{B}^{5/2} + \cdots$ applies in very strong fields $\mathcal{B} \gg 1$. In the present work, explicit three- and two-term expansions are derived for weak- and strong fields, respectively. Only the ground $1s$ state is considered but the developed methods are applicable to excited states as well.

II. WEAK-FIELD DALGARNO-LEWIS PERTURBATION THEORY

We begin by briefly outlining our Dalgarno-Lewis approach as applied to weak magnetic fields. In general, an eigenstate may be expanded in powers of the electric field $\varphi(\vec{r}) = \sum_p \varphi_p(\vec{r})\mathcal{E}^p$. Since the geometry of the present problem is inversion symmetric in the absence of the electric field, only even-order energy corrections $\Delta E = -\frac{1}{2}\alpha(\mathcal{B})\mathcal{E}^2 - \frac{1}{4}\beta(\mathcal{B})\mathcal{E}^4 + \ldots$ to nondegenerate eigenstates exist, among which the Stark shift is the lowest one. Provided φ_0 and φ_1 are known, the Stark shift is [6,17,30–33] $E_{\mathrm{Stark}} = \langle\varphi_0|r\cos\theta|\varphi_1\rangle\mathcal{E}^2$. This is the approach we follow in the weak-$\mathcal{B}$ limit since a perturbation series for φ_0 and φ_1 in powers of $\mathcal{B}$ can be found. We write radial parts in the form $R^{(n,m)}(r)$ with n and m indicating orders of $\mathcal{E}$ and $\mathcal{B}$, respectively. Thus, for s states with

$$\varphi_0(\vec{r}) = (2\pi)^{-1/2}\sum_{p=0}^{\infty} R^{(0,2p)}(r)\mathcal{B}^{2p},$$

$$\varphi_1(\vec{r}) = (2\pi)^{-1/2}\sum_{p=0}^{\infty}[R^{(1,2p)}(r)\mathcal{B}^{2p}\cos\theta + iR^{(1,2p+1)}(r)\mathcal{B}^{2p+1}\sin\theta], \qquad (2)$$

we get

$$E_{\mathrm{Stark}}(B) = \tfrac{1}{2}\{\langle R^{(0,0)}|r|R^{(1,0)}\rangle + \langle R^{(0,2)}|r|R^{(1,0)}\rangle\mathcal{B}^2 + \langle R^{(0,0)}|r|R^{(1,2)}\rangle\mathcal{B}^2 + \cdots\}\mathcal{E}^2. \qquad (3)$$

Hence, writing $E_{\mathrm{Stark}}(\mathcal{B}) = \sum_p E^{(2,2p)}\mathcal{B}^{2p}\mathcal{E}^2$, we identify $E^{(2,0)} = \frac{1}{2}\langle R^{(0,0)}|r|R^{(1,0)}\rangle$ and $E^{(2,2)} = \frac{1}{2}\langle R^{(0,2)}|r|R^{(1,0)}\rangle + \frac{1}{2}\langle R^{(0,0)}|r|R^{(1,2)}\rangle$ for the first two terms in the Stark series. Note that brackets involving only radial functions are understood to imply radial integration alone, i.e., $\langle R^{(n,m)}|V(r)|R^{(p,q)}\rangle \equiv \int_0^\infty R^{(n,m)*}(r)V(r)R^{(p,q)}(r)rdr$. The starting point for the inhomogeneous perturbation sequence is the unperturbed Coulomb ground state $R^{(0,0)}(r) = 4e^{-2r}$ with energy -2. In absence of an electric field, the energy is written $E_0(\mathcal{B}) = \sum_p E^{(0,2p)}\mathcal{B}^{2p}$ such that $E^{(0,0)} = -2$. Collecting terms of identical power of $\mathcal{B}$, we get

$$\left\{-\frac{1}{2}\nabla_r^2 - \frac{1}{r}\right\}R^{(0,2n)}(r) + \frac{1}{8}r^2R^{(0,2n-2)}(r) - \sum_{m=0}^{n} E^{(0,2n-2m)}R^{(0,2m)}(r) = 0. \qquad (4)$$

TABLE I. Coefficients of energy and Stark series to order $\mathcal{B}^{10}$.

Order p	$E^{(0,2p)}$	$E^{(2,2p)}$
0	-2	$-21/256$
1	$3/64$	$5\,439/262\,144$
2	$-159/65\,536$	$-1\,314\,225/134\,217\,728$
3	$17\,967/33\,554\,432$	$1\,907\,054\,535/274\,877\,906\,944$
4	$-15\,522\,195/68\,719\,476\,736$	$-953\,987\,914\,203/140\,737\,488\,355\,328$
5	$5\,189\,052\,801/35\,184\,372\,088\,832$	$1\,257\,601\,415\,564\,403/144\,115\,188\,075\,855\,872$

Here, $\nabla_r^2 = \partial^2/\partial r^2 + r^{-1}\partial/\partial r$ is the radial 2D Laplacian. The particular solutions are readily found to be polynomials in r times the ground state. Also, at each order, a homogeneous solution is added in order to maintain unity normalization of φ_0, that is, $\langle R^{(0,0)}|R^{(0,2)}\rangle = 0$ and $\langle R^{(0,0)}|R^{(0,4)}\rangle + \langle R^{(0,4)}|R^{(0,0)}\rangle + \langle R^{(0,2)}|R^{(0,2)}\rangle = 0$, etc. Explicitly, for the first two corrections, we then find

$$R^{(0,2)}(r) = \left(\frac{17}{256} - \frac{3r^2}{32} - \frac{r^3}{12}\right)e^{-2r},$$
$$R^{(0,4)}(r) = \left(-\frac{4983}{524\,288} + \frac{27r^2}{8192} + \frac{3r^3}{1024} + \frac{31r^4}{8192} + \frac{7r^5}{2560} + \frac{r^6}{1152}\right)e^{-2r}. \quad (5)$$

Also, after elementary integrations, the perturbation series for the energy becomes

$$E_0(\mathcal{B}) = -2 + \frac{3}{64}\mathcal{B}^2 - \frac{159}{65\,536}\mathcal{B}^4 + O(\mathcal{B}^6). \quad (6)$$

This series agrees with known results [1,2,7,8]. In Table I, coefficients up to order $\mathcal{B}^{10}$ are provided.

We may then proceed to computing the electric-field correction. Collecting first-order terms in $\mathcal{E}\sin\theta$ and $\mathcal{E}\cos\theta$ yields the coupled problems

$$\left\{-\frac{1}{2}\nabla_r^2 - \frac{1}{r} + \frac{1}{2r^2} + \frac{1}{8}\mathcal{B}^2r^2 - E_0(\mathcal{B})\right\}\sum_p R^{(1,2p+1)}(r)\mathcal{B}^{2p+1} + \frac{\gamma}{2}\sum_p R^{(1,2p)}(r)\mathcal{B}^{2p+1} = 0, \quad (7)$$

and

$$\left\{-\frac{1}{2}\nabla_r^2 - \frac{1}{r} + \frac{1}{2r^2} + \frac{1}{8}\mathcal{B}^2r^2 - E_0(\mathcal{B})\right\}\sum_p R^{(1,2p)}(r)\mathcal{B}^{2p} + \frac{\gamma}{2}\sum_p R^{(1,2p+1)}(r)\mathcal{B}^{2p+2} + r\sum_p R^{(0,2p)}(r)\mathcal{B}^{2p} = 0 \quad (8)$$

We solve these order by order. Hence, collecting $\mathcal{B}^{2p}$ terms with $p = 0, 1, 2$:

$$\left\{-\frac{1}{2}\nabla_r^2 - \frac{1}{r} + \frac{1}{2r^2} - E^{(0,0)}\right\}R^{(1,0)}(r) + rR^{(0,0)}(r) = 0,$$
$$\left\{-\frac{1}{2}\nabla_r^2 - \frac{1}{r} + \frac{1}{2r^2} - E^{(0,0)}\right\}R^{(1,1)}(r) + \frac{\gamma}{2}R^{(1,0)}(r) = 0,$$
$$\left\{-\frac{1}{2}\nabla_r^2 - \frac{1}{r} + \frac{1}{2r^2} - E^{(0,0)}\right\}R^{(1,2)}(r) + \left\{\frac{1}{8}r^2 - E^{(0,2)}\right\}R^{(1,0)}(r) + rR^{(0,2)}(r) = 0. \quad (9)$$

Solving from the top eventually demonstrates that

$$R^{(1,0)}(r) = -\left(\frac{3}{4} + r\right)re^{-2r},$$
$$R^{(1,1)}(r) = \gamma\left(\frac{17}{128} + \frac{17r}{96} + \frac{r^2}{12}\right)re^{-2r},$$
$$R^{(1,2)}(r) = \left\{\left(\frac{27}{1024} + \frac{9r}{256} + \frac{31r^2}{512} + \frac{7r^3}{128} + \frac{r^4}{48}\right) - \gamma^2\left(\frac{349}{12\,288} + \frac{349r}{9216} + \frac{49r^2}{2304} + \frac{r^3}{192}\right)\right\}re^{-2r}. \quad (10)$$

Higher corrections of even order are expressed as polynomials of degree $3p/2 + 2$ times the exponential and rapidly become very complicated. The first term $R^{(1,0)}$ agrees with known results [6,16,31,32]. It is relatively straightforward to compute the Stark shift:

$$E_{\text{Stark}}(\mathcal{B}) = \left\{-\frac{21}{256} + \frac{5439 - 1261\gamma^2}{262\,144}\mathcal{B}^2 - \frac{23\,656\,050 - 7\,721\,145\gamma^2 + 773\,869\gamma^4}{2\,415\,919\,104}\mathcal{B}^4 + O(\mathcal{B}^6)\right\}\mathcal{E}^2 \quad (11)$$

The polarizability is therefore

$$\alpha(\mathcal{B}) = \frac{21}{128}\left(1 - \frac{5439 - 1261\gamma^2}{21\,504}\mathcal{B}^2 + \frac{23\,656\,050 - 7\,721\,145\gamma^2 + 773\,869\gamma^4}{198\,180\,864}\mathcal{B}^4\right) + O(\mathcal{B}^6). \tag{12}$$

This expression is the most significant result of the present work. In the special case $\gamma = 0$,

$$\alpha_{\gamma=0}(\mathcal{B}) = \frac{21}{128}\left(1 - \frac{259}{1024}\mathcal{B}^2 + \frac{438\,075}{3\,670\,016}\mathcal{B}^4\right) + O(\mathcal{B}^6). \tag{13}$$

The first term is in perfect agreement with previous results obtained without considering magnetic fields [3,6,16,17,32,33]. As shown below, the three-term expansion remains accurate up to $\mathcal{B} \approx 1$. We note that the quadratic correction to the Stark shift varies as $(5439-1261\gamma^2)/262\,144$. Hence, even extremely mass-imbalanced cases with $|\gamma| \sim 1$ are insensitive to the linear Zeeman correction. As shown in the Appendix, the polarizability of three-dimensional hydrogen to order $\mathcal{B}^2$ is $\alpha_{3D}(\mathcal{B}) = \frac{9}{2}\{1 - (1116-319\gamma^2)\mathcal{B}^2/432\}$. The structure of this expression is similar to the 2D result with the γ term reducing the magnetic correction. The unperturbed polarizability in 2D (21/128) is much smaller than the 3D value (9/2) as a result of confinement. Similarly, the relative importance of the 2D magnetic correction is much smaller than in 3D (259/1024 vs 1116/432), testifying further to the influence of confinement.

Remarkably, all linear Zeeman corrections, i.e., terms of order $(\gamma\mathcal{B})^m$, can be obtained in closed form for arbitrary dimension and order m. To understand how, we disregard the quadratic Zeeman term as well as the Stark term in Eq. (1) and consider an eigenstate $|nl(\gamma)\rangle$ with eigenvalue $E_{nl}(\gamma)$. Using a traditional sum-over-states approach, the polarizability is then

$$\alpha(\gamma) = \sum_{n=2}^{\infty}\sum_{l=\pm1}\frac{|\langle 1s(\gamma)|x|nl(\gamma)\rangle|^2}{E_{nl}(\gamma) - E_{1s}(\gamma)}. \tag{14}$$

This is an exact expression (in the absence of quadratic Zeeman corrections) requiring only $\mathcal{E} = 0$ information. Now, because $|nl(\gamma)\rangle = |np(0)\rangle$ and $E_{nl}(\gamma) = E_{np}(0) + \frac{l}{2}\gamma\mathcal{B}$, this simplifies to

$$\alpha(\gamma) = 2\sum_{n=2}^{\infty}|\langle 1s(0)|x|np(0)\rangle|^2\frac{E_{np}(0) - E_{1s}(0)}{[E_{np}(0) - E_{1s}(0)]^2 - \left(\frac{1}{2}\gamma\mathcal{B}\right)^2}. \tag{15}$$

Mathematically, this is *exactly* identical to the expression for the frequency-dependent dynamic polarizability $\alpha(\omega)$ with the identification $\omega = \frac{1}{2}\gamma\mathcal{B}$. A closed-form formula for $\alpha(\omega)$ in the absence of magnetic fields but valid for arbitrary frequency and dimension D was derived in Ref. [35]. The result is essentially an algebraic factor multiplying a single ${}_2F_1$ hypergeometric function and, in the present context, immediately provides the linear Zeeman correction to all orders. The low-frequency expansion

$$\alpha(\omega) = \frac{(D-1)^4(D+1)(2D+3)}{128} + \frac{(D-1)^8(D+1)(137+220D+123D^2+24D^3)}{98304}\omega^2 + \frac{(D-1)^{12}(D+1)(26\,873+61\,434D+58\,800D^2+29\,554D^3+7803D^4+864D^5)}{226\,492\,416}\omega^4 + O(\omega^6) \tag{16}$$

evaluates to

$$\alpha_{D=2}(\gamma) = \frac{21}{128} + \frac{1261}{131\,072}\gamma^2\mathcal{B}^2 + \frac{773\,869}{1\,207\,959\,552}\gamma^4\mathcal{B}^4 + O(\gamma^6\mathcal{B}^6),$$
$$\alpha_{D=3}(\gamma) = \frac{9}{2} + \frac{319}{48}\gamma^2\mathcal{B}^2 + \frac{297\,541}{27\,648}\gamma^4\mathcal{B}^4 + O(\gamma^6\mathcal{B}^6), \tag{17}$$

in 2 and 3 dimensions, respectively. These are obviously in full agreement with Eqs. (12) and (A3). Moreover, the universal high-frequency behavior $\alpha(\omega) \approx -1/\omega^2$ means that the polarizability in strong fields must contain a $-4/(\gamma\mathcal{B})^2$ term, as is confirmed below. This remarkable connection between $(\mathcal{B} \neq 0,\ \omega = 0)$ and $(\mathcal{B} = 0,\ \omega \neq 0)$ results unfortunately does not apply when the quadratic Zeeman term is included, as the full dynamic polarizability is unknown in this case.

In Table I, more coefficients of the Stark series $E_{\text{Stark}}(\mathcal{B}) = \sum_p E^{(2,2p)}\mathcal{B}^{2p}\mathcal{E}^2$ for $\gamma = 0$ are provided. Investigating the coefficients of both series to even higher order reveals that their absolute magnitude starts to increase beyond a certain order. This is a sign that the perturbation series are, in fact, divergent as would be expected, since the substitution $\mathcal{B} \to i\mathcal{B}$ clearly implies a divergence even for arbitrarily small $\mathcal{B}$, i.e., a vanishing radius of convergence. Thus, both series should really be considered asymptotic rather than Taylor series.

III. STRONG-FIELD DALGARNO-LEWIS PERTURBATION THEORY

Next, we turn to the case of strong magnetic fields, in which the Coulomb attraction is the perturbation. To obtain a formal perturbation series we therefore write the Coulomb potential as $-e^2/r$ even if $e = 1$ in our units. Accordingly, we write radial parts in the form $\tilde{R}^{(n,m)}(r)$ with n and m indicating

orders of $\mathcal{E}$ and e^2, respectively. Thus, we now have

$$\varphi_0(\vec{r}) = (2\pi)^{-1/2}\sum_{p=0}^{\infty}\tilde{R}^{(0,p)}(r)e^{2p},$$
$$\varphi_1(\vec{r}) = (2\pi)^{-1/2}\sum_{p=0}^{\infty}\{\tilde{R}_+^{(1,p)}(r)e^{i\theta} + \tilde{R}_-^{(1,p)}(r)e^{-i\theta}\}e^{2p}, \quad (18)$$

in complete analogy with the weak-$\mathcal{B}$ case. Also, we now write the energy as $E_0(\mathcal{B}) = \sum_p \tilde{E}^{(0,p)}e^{2p}$. If the magnetic field is completely dominating, the ground state is the Gaussian $\tilde{R}^{(0,0)}(r) = \sqrt{\mathcal{B}}e^{-\mathcal{B}r^2/4}$ with energy $\tilde{E}^{(0,0)} = \mathcal{B}/2$ and first-order correction $\tilde{E}^{(0,1)} = -\langle\tilde{R}^{(0,0)}|r^{-1}|\tilde{R}^{(0,0)}\rangle = -\sqrt{\pi\mathcal{B}/2}$. Again, we construct the perturbation sequence but now by collecting powers of e^2. Hence,

$$\left\{-\frac{1}{2}\nabla_r^2 + \frac{1}{8}\mathcal{B}^2r^2 - \frac{\mathcal{B}}{2}\right\}\tilde{R}^{(0,1)}(r) + \left\{\sqrt{\frac{\pi\mathcal{B}}{2}} - \frac{1}{r}\right\}\tilde{R}^{(0,0)}(r) = 0. \quad (19)$$

Writing the unknown as an integral $\tilde{R}^{(0,1)}(r) = \tilde{R}^{(0,0)}(r)\int_0^{r\sqrt{\mathcal{B}/2}}F(x)dx$, it is readily found that $F(x)$ satisfies a simple first-order differential equation with particular solution

$$F(x) = \sqrt{\frac{2\pi}{\mathcal{B}}}\frac{e^{x^2}\Phi_C(x) - 1}{x}, \quad (20)$$

where Φ_C is the complementary error function. The homogeneous part is again found by normalization to power e^2, i.e., by requiring $\langle\tilde{R}^{(0,0)}|\tilde{R}^{(0,1)}\rangle = 0$. In fact, a closed-form expression for the first Coulomb correction $\tilde{R}^{(0,1)}(r)$ can be found upon evaluating the integral of $F(x)$. Unfortunately, the result is rather complicated involving the exponential integral Ei and hypergeometric function ${}_2F_2$:

$$\tilde{R}^{(0,1)}(r) = \sqrt{\frac{\pi}{2}}e^{-\mathcal{B}r^2/4}\left\{\mathrm{Ei}\left(\frac{\mathcal{B}r^2}{2}\right) - \ln\left(\frac{\mathcal{B}r^2}{8}\right) - 2r\sqrt{\frac{2\mathcal{B}}{\pi}}{}_2F_2\left[\frac{1}{2}, 1, \frac{3}{2}, \frac{3}{2}, \frac{1}{2}\mathcal{B}r^2\right] - \gamma_E\right\}. \quad (21)$$

Here, γ_E in the last term is Euler's constant. However, using integration by parts in the integral form provides a simple expression for the second-order energy correction:

$$\begin{aligned}\tilde{E}^{(0,2)} &= -\langle\tilde{R}^{(0,0)}|r^{-1}|\tilde{R}^{(0,1)}\rangle \\ &= -\sqrt{\frac{\pi\mathcal{B}}{2}}\int_0^{\infty}\Phi_C(x)F(x)dx - \pi\ln 2 \\ &= 4C - 2\pi\ln 2, \end{aligned} \quad (22)$$

where C is Catalan's constant. This allows us to find the energy to order $\mathcal{B}^0$ (in the absence of electric fields):

$$E_0(\mathcal{B}) = \frac{\mathcal{B}}{2} - \sqrt{\frac{\pi\mathcal{B}}{2}} + 4C - 2\pi\ln 2 + O(\mathcal{B}^{-1/2}). \quad (23)$$

The analytical form of the constant term, which apparently has not been obtained previously, agrees with the numerical value reported by MacDonald and Ritchie [1] and Adams [2].

We then turn to the perturbation by electric fields. At order e^0, the Stark corrections $\tilde{R}_\pm^{(1,0)}(r)$ obey

$$\left\{-\frac{1}{2}\nabla_r^2 + \frac{1}{2r^2} \pm \frac{\gamma\mathcal{B}}{2} + \frac{1}{8}\mathcal{B}^2r^2 - \frac{\mathcal{B}}{2}\right\}\tilde{R}_\pm^{(1,0)}(r) + \frac{1}{2}r\tilde{R}^{(0,0)}(r) = 0, \quad (24)$$

with a straightforward solution $\tilde{R}_\pm^{(1,0)}(r) = -re^{-\mathcal{B}r^2/4}/[\sqrt{\mathcal{B}}(1\pm\gamma)]$ and Stark shift $\tilde{E}^{(2,0)} = -2/[\mathcal{B}^2(1-\gamma^2)]$. A similar problem is readily set up for $\tilde{R}_\pm^{(1,1)}(r)$. However, because $\tilde{R}^{(0,1)}$ is complicated, it is advantageous to interchange the role of perturbations. Hence, we choose to find wave-function corrections of order $\mathcal{E}^2e^0$ rather than $\mathcal{E}^1e^2$. The former is of the form $\varphi_2(\vec{r}) = (2\pi)^{-1/2}[\tilde{R}_0^{(2,0)}(r) + \tilde{R}_+^{(2,0)}(r)e^{2i\theta} + \tilde{R}_-^{(2,0)}(r)e^{-2i\theta}]$ and only the first term in the square brackets contributes to the Stark shift. This part obeys

$$\left\{-\frac{1}{2}\nabla_r^2 + \frac{1}{8}\mathcal{B}^2r^2 - \frac{\mathcal{B}}{2}\right\}\tilde{R}_0^{(2,0)}(r) + \frac{1}{2}r[\tilde{R}_+^{(1,0)}(r) + \tilde{R}_-^{(1,0)}(r)] + \frac{2}{\mathcal{B}^2(1-\gamma^2)}\tilde{R}^{(0,0)}(r) = 0, \quad (25)$$

with solution $\tilde{R}_0^{(2,0)}(r) = [\mathcal{B}(1-\gamma^2)r^2 - 4]e^{-\mathcal{B}r^2/4}/[\mathcal{B}^{5/2}(1-\gamma^2)^2]$. In turn, the $\mathcal{E}^2e^2$ energy correction is $\tilde{E}^{(2,1)} = -\langle\varphi_1|r^{-1}|\varphi_1\rangle - \langle\varphi_0|r^{-1}|\varphi_2\rangle - \langle\varphi_2|r^{-1}|\varphi_0\rangle$ with φ_p restricted to order e^0. We then find the full Stark shift from

$$E_{\mathrm{Stark}}(\mathcal{B}) = \left\{\sum_{l=\pm}\left[\langle\tilde{R}^{(0,0)}|r|\tilde{R}_l^{(1,0)}\rangle - \langle\tilde{R}_l^{(1,0)}|r^{-1}|\tilde{R}_l^{(1,0)}\rangle e^2\right] - 2\langle\tilde{R}^{(0,0)}|r^{-1}|\tilde{R}_0^{(2,0)}\rangle e^2 + \cdots\right\}\mathcal{E}^2. \quad (26)$$

This finally leads to the polarizability:

$$\alpha(\mathcal{B}) \approx \frac{4}{\mathcal{B}^2(1-\gamma^2)}\left(1 - \frac{e^2}{1-\gamma^2}\sqrt{\frac{2\pi}{\mathcal{B}}}\right) + O(\mathcal{B}^{-3}). \quad (27)$$

This result clearly breaks down if $|\gamma| = 1$. Retaining a finite mass ratio, this limit is never actually encountered. However, a significant enhancement of the polarizability is expected as $|\gamma| \sim 1$ is approached. We also note that $\alpha(\mathcal{B}) \approx -4/(\mathcal{B}\gamma)^2$ in the limit $\mathcal{B}\gamma \to \infty$ as required by the high-frequency limit of the dynamic polarizability. In fact, the usual dynamic polarizability of a harmonic oscillator $\alpha(\omega) = 1/(\omega_0^2 - \omega^2)$ with oscillator frequency ω_0 immediately yields the first term in Eq. (27) since $\omega_0 = \mathcal{B}/2$ for Landau levels. The result, Eq. (27), is presumably only the first two terms in an expansion that is finite even if $|\gamma| = 1$. Although no rigorous proof has been found, it is tempting to conjecture that the full strong-field result is

$$\alpha(\mathcal{B}) \approx \frac{4}{\mathcal{B}^2[1 - \gamma^2 + e^2\sqrt{2\pi/\mathcal{B}}]}. \quad (28)$$

This form follows directly from Eq. (15) if first-order Coulomb perturbed wave functions are used. Hence, it is straightforward to show that only $1s \to 2p$ transitions con-

tribute at order e^2 and that

$$2|\langle 1s|x|2p\rangle|^2[E_{2p}-E_{1s}]=1+O(e^4),$$
$$[E_{2p}-E_{1s}]^2-\left(\frac{1}{2}\gamma\mathcal{B}\right)^2=\frac{\mathcal{B}^2[1-\gamma^2+e^2\sqrt{2\pi/\mathcal{B}}]}{4}+O(e^4) \tag{29}$$

Thus, combining the two *without expanding the ratio* produces Eq. (28). As we demonstrate below, the conjectured form, Eq. (28), is in excellent agreement with numerical results spanning the entire range $0\leqslant\gamma\leqslant 1$. Moreover, we demonstrate that the $\alpha(\mathcal{B})\approx\tilde{\alpha}_0/\mathcal{B}^2+\tilde{\alpha}_1/\mathcal{B}^{5/2}$ dependence in strong fields can be applied to design a highly accurate hypergeometric approximant covering both strong- and weak-field cases.

IV. ANALYTICAL AND NUMERICAL RESULTS

In order to validate and assess the range of validity of the analytical expressions obtained above, we compare to numerical diagonalization results. To this end, we apply a Gaussian basis of the form $\exp(-\beta_i r^2)$ with $\beta_i=10^{-3}\times 2^i$ and $i=0\ldots 60$ for all radial functions. The polarizability is found from the numerical Stark shift in a small electric field, $\mathcal{E}=10^{-3}$. In very large magnetic fields, numerical stability requires a more localized basis $\beta_i=10^{-1}\times 2^i$ and a stronger electric field and we consequently multiply $\mathcal{E}$ by a factor $\mathcal{B}/\mathcal{B}_0$. Furthermore, for the important case $\gamma=0$, we construct an accurate variational ansatz that successfully reproduces exact results. Thus, taking inspiration from Eq. (5), we try the ansatz $\varphi_0(r)=Ne^{-2r}e^{-\beta r^2/4}$, where N is a normalization constant and β an adjustable parameter found by minimizing the energy

$$E(\beta)=\frac{1}{8}\left\{3\beta+\frac{16+3\beta}{\beta^2}\mathcal{B}^2-\frac{\mathcal{B}^2+\beta^2}{\beta-2e^{8/\beta}\sqrt{2\pi\beta}\Phi_C\left(\sqrt{\frac{8}{\beta}}\right)}\right\}. \tag{30}$$

For small and large $\mathcal{B}$, we find approximately $\beta\approx 56\mathcal{B}^2/(256+69\mathcal{B}^2)$ and $\beta\approx\mathcal{B}-(\pi\mathcal{B}/2)^{1/2}$, respectively. In an electric field, a correction $(ar+br^2)\varphi_0(r)\cos\theta$ is added to $\varphi_0(r)$, where a and b are additional variational parameters. Minimization with respect to a and b is done analytically [under the assumption that $\varphi_0(r)$ solves the unperturbed problem] but leads to a rather cumbersome expression, which is omitted here. The chosen form ensures agreement with the exact result in both vanishing and very strong magnetic fields. In fact, it can be shown that the leading two terms in both E_0 and α are reproduced exactly for both small and large $\mathcal{B}$.

Numerical, variational, and asymptotic results for $\gamma=0$ are compared in Fig. 2. Although the polarizability is our main concern in the present work, results for the energy E_0 are included as well. Focusing first on the energy in the upper panel, the variational energy, Eq. (30), is generally found to be in good agreement with numerically exact results. The asymptotic expansions Eqs. (6) and (23) are shown as green and blue curves, respectively. The weak-$\mathcal{B}$ expansion is seen to be reasonably precise in the range $0\leqslant\mathcal{B}<2$. In contrast, Eq. (23) entails an error of about $\sim 0.16\text{Ha}^*$ even for magnetic fields as large as $\mathcal{B}\approx 10$. This indicates that a significant $O(\mathcal{B}^{-1/2})$ correction is missing. By comparison to exact results, we estimate $\sim -0.45\mathcal{B}^{-1/2}$ for the correction.

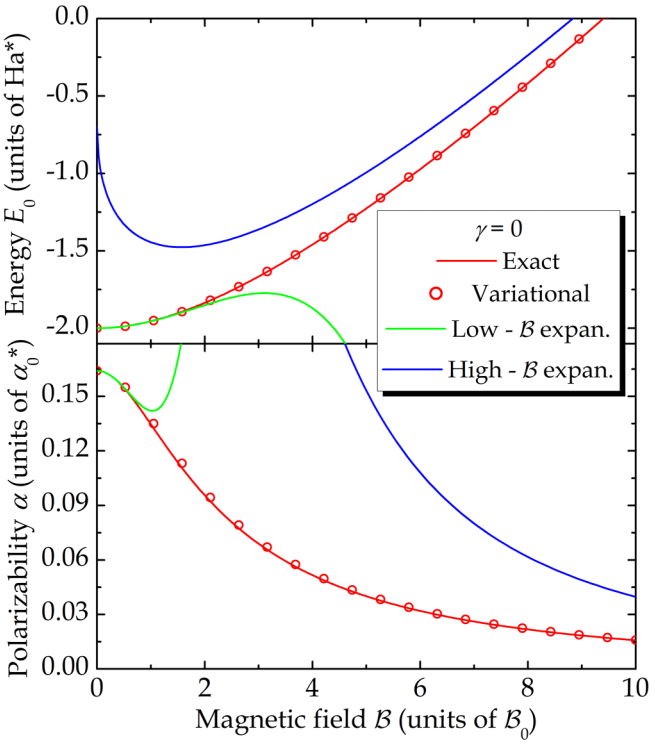

FIG. 2. Comparison of numerically exact results (red curves), variational results (circles), and asymptotic expansions (green and blue curves). Upper and lower panels show energy and polarizability (with $\gamma=0$) vs magnetic field, respectively.

The polarizability in the lower panel of Fig. 2 is seen to be monotonically decreasing with magnetic field as expected. Thus, a field of $\mathcal{B}\approx 2$ reduces $\alpha(\mathcal{B})$ to half the value of $\alpha(0)$. Again, the variational result is in excellent agreement with the exact one for arbitrary magnetic fields. The plot also includes the conjectured Eq. (28) as well as the low-$\mathcal{B}$ expansion, Eq. (12), that is seen to break down around $\mathcal{B}\approx 0.5$. The conjectured high-$\mathcal{B}$ expansion, Eq. (28), significantly overestimates the polarizability in the shown range, while Eq. (27) (not shown) underestimates the actual result and even changes sign near $\mathcal{B}\approx 6.4$ in clear contradiction with the correct behavior. Thus, even though Eqs. (27) and (28) are both correct for very large magnetic fields (if $|\gamma|<1$), neither provide reliable approximants in realistic fields.

As in the normal Stark case without magnetic fields [6,32], an accurate hypergeometric approximant for $\alpha(\mathcal{B})$ can be found covering the entire range of magnetic fields. Hence, we write

$$\alpha(\mathcal{B})\approx\alpha_0\times{}_2F_1[h_1,h_2,h_3,h_4\mathcal{B}^2]. \tag{31}$$

The constants $h_{1\ldots4}$ must be fixed by matching to asymptotic results. Requiring agreement with the series $\alpha(\mathcal{B})=\alpha_0+\alpha_1\mathcal{B}^2+\alpha_2\mathcal{B}^4+O(\mathcal{B}^6)$ given by Eq. (12) yields $h_4=2\alpha_1\alpha_2/[(1+h_1)(1+h_2)\alpha_1^2-2h_1h_2\alpha_0\alpha_2]$ and $h_3=h_1h_2h_4(\alpha_0/\alpha_1)$. For large $\mathcal{B}$, Eq. (31) has a power dependence ${}_2F_1[h_1,h_2,h_3,h_4\mathcal{B}^2]\approx c_1\mathcal{B}^{-2h_1}+c_2\mathcal{B}^{-2h_2}$. Thus, the correct leading powers of Eq. (27) are found if $h_1=1$ and $h_2=5/4$. However, an even better agreement is found if h_1 and h_2 are fitted to match the exact behavior in the range

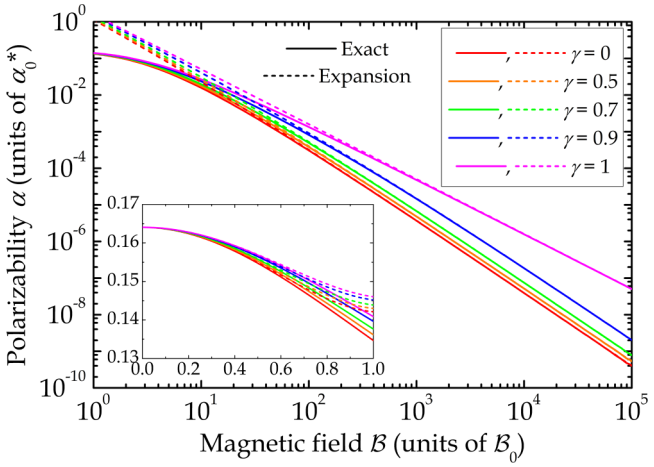

FIG. 3. Dependence on the mass factor γ in the linear Zeeman term. Numerically exact results (solid curves) are compared to asymptotic expansions (dashed curves). The main panel illustrates the strong-field case, while the inset shows weak-field numerics and three-term expansions. Note that the conjectured form, Eq. (28), is used in the main panel.

$0 \leqslant \mathcal{B} \leqslant 10$, which leads to $h_1 \approx 0.925$ and $h_2 \approx 1.237$, respectively, reasonably close to analytical values based on leading powers. Adding the hypergeometric approximant to Fig. 2 leads to a curve that is practically indistinguishable from the exact one.

Turning to the dependence on the mass factor γ in the linear Zeeman term, Fig. 3 demonstrates that both low-field and high-field expansions are in good agreement with accurate numerical results in their appropriate limits. Importantly, the finite conjectured expression, Eq. (28), agrees with numerical $\gamma = 1$ results, while obviously Eq. (27) leads to a divergent polarizability. In particular, it is seen that the asymptotic slope in strong fields changes from -2 to $-3/2$ as $\gamma \to 1$. This lends strong support to the conjecture. The weak-field range, shown in the inset of Fig. 3, shows that Eq. (12) captures the leading γ dependence. We note that the polarizability increases monotonically with $|\gamma|$ irrespective of $\mathcal{B}$ field.

We finish by commenting on the applicability of the low-field expansion, Eqs. (12) and (13), in realistic experiments. Hence, we wish to establish whether the $\mathcal{B} \ll 1$ assumption is reliable is realistic cases. A noticeable magnetic correction to the dipole polarizability beyond the lowest $\mathcal{B}^2$ term requires magnetic fields of order $\mathcal{B}_0 = (\mu/\varepsilon)^2 235$ kT. Thus, materials featuring small reduced mass μ and large screening ε are candidates for observable higher-order corrections. In Ref. [19], an effective model of screening incorporating both the 2D semiconductor itself and the surrounding dielectric encapsulation was derived. For a semiconductor with nonlocal screening length r_0 and surrounding dielectric constant $\bar{\varepsilon}$, the authors of Ref. [19] find

$$\varepsilon \approx \frac{1}{2}\left(\bar{\varepsilon} + \sqrt{\bar{\varepsilon}^2 + \frac{16\mu r_0}{3a_0}}\right). \tag{32}$$

For WS_2 ($\mu = 0.22$ and $r_0 = 39.9$Å) and $MoSe_2$ ($\mu = 0.27$ and $r_0 = 51.2$Å), see Ref. [34], encapsulated by hBN ($\bar{\varepsilon} = 4.5$), we find $\mathcal{B}_0 \approx 204$ T and $\mathcal{B}_0 \approx 233$ T, respectively. Although very large fields around or even above 100 T are occasionally applied [23,36], it is clear that under most circumstances, measurements will be well within the perturbative regime. The characteristic field $\mathcal{B}_0$ could be lowered considerably if more efficiently screened samples were applied. In Ref. [37], MoS_2 deposited on Si ($\bar{\varepsilon} = 11.9$) and covered by various liquid dielectrics was investigated. A large enhancement of photoresponse was observed as a result of reduced exciton binding energies. In particular, deionized water (static dielectric constant ~ 80) increased photocurrent by nearly three orders of magnitude [37]. In the present context, encapsulating WS_2 in an $\bar{\varepsilon} = 11.9$ environment reduces the characteristic magnetic field to $\mathcal{B}_0 \approx 62$T. Thus, in this case, corrections beyond lowest order might become visible with available magnetic fields.

V. SUMMARY

In summary, we have studied 2D hydrogen atoms in crossed magnetic and electric fields. Such confined Coulomb-bound systems describe excitons confined to atomically thin semiconductors or quantum wells. Using exact perturbation theory, the electric dipole polarizability has been computed analytically in both weak and strong magnetic fields. Moreover, both variational and resummation approximants covering arbitrary fields have been devised. Compared to 3D hydrogen, the 2D polarizability is greatly reduced by confinement irrespective of magnetic-field strength. Thus, our findings show that magnetic corrections to the polarizability remain small for realistic magnetic fields. However, corrections beyond quadratic order could potentially be observable for excitons in highly screening dielectric surroundings.

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APPENDIX: THREE-DIMENSIONAL CASE

The three-dimensional (3D) case has previously been investigated using various versions of analytical perturbation theory [38,39]. The Hamiltonian is formally identical to Eq. (1) with the exception that the quadratic Zeeman term is $\mathcal{B}^2 r_\perp^2/8$, where $r_\perp$ denotes the component perpendicular to $\vec{\mathcal{B}}$. Hence, with standard polar and azimuthal angles θ and φ,

$$H_{3D} = -\frac{1}{2}\nabla^2 - \frac{1}{r} - i\frac{\gamma}{2}\mathcal{B}\frac{\partial}{\partial\varphi} + \frac{1}{8}\mathcal{B}^2 r^2 \sin^2\theta + \mathcal{E} r \sin\theta\cos\varphi. \tag{A1}$$

Quite analogous to the 2D case, the expansions of $\mathcal{E}^0$ and $\mathcal{E}^1$ states are then

$$\varphi_0(\vec{r}) = R^{(0,0)}(r) + R_0^{(0,2)}(r)\mathcal{B}^2 + R_2^{(0,2)}(r)\mathcal{B}^2\sin^2\theta + O(\mathcal{B}^4),$$
$$\varphi_1(\vec{r}) = \left\{R^{(1,0)}(r) + iR^{(1,1)}\mathcal{B}\tan\varphi + R_0^{(1,2)}(r)\mathcal{B}^2 + R_2^{(1,2)}(r)\mathcal{B}^2\sin^2\theta\right\}\sin\theta\cos\varphi + O(\mathcal{B}^3). \tag{A2}$$

The $R^{(0,n)}$ and $R^{(1,n)}$ functions are readily obtained applying the perturbation sequence as detailed in the main text. Finally,

in this case, the Stark shift becomes

$$E^{\mathrm{3D}}_{\mathrm{Stark}}(\mathcal{B}) = \left\{-\frac{9}{4} + \frac{1116 - 319\gamma^2}{96}\mathcal{B}^2 + O(\mathcal{B}^4)\right\}\mathcal{E}^2. \quad \text{(A3)}$$

The $\gamma = 0$ correction $93\mathcal{B}^2\mathcal{E}^2/8$ agrees with Refs. [38,39]. Moreover, for $\gamma = 1$, our value $797\mathcal{B}^2\mathcal{E}^2/96$ agrees with Manakov *et al.* [39], thus supporting their claim that the original value $731\mathcal{B}^2\mathcal{E}^2/96$ found by Turbiner [38] is, in fact, incorrect.

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