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Two-dimensional magnetoexcitons: a shifted 1/N approach

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Abstract. The energy spectrum of two-dimensional magnetoexcitons has been calculated using the shifted 1/N expansion method (N the space dimension). It is found that even in the leading-term approximation this approach provides remarkably accurate and simple analytic expressions for the magnetoexciton energies for any magnetic field strength and electron-hole mass ratio. For the infinite-hole-mass exciton (hydrogenic impurity) our results show an excellent agreement with previously reported numerical data in the whole magnetic field range. Higher terms in the expansion which allow a systematic improvement of low-energy values are also considered.

1. Introduction

The linear and nonlinear optical properties of direct band gap semiconductor quantum wells near the fundamental absorption edge are dominated by excitons. It is now well established that confinement of excitons on length scales smaller than the bulk Bohr radius leads to an enhanced resonant optical response. In view of the potential applications of low-dimensional structures, the study of exciton states found in these systems, with and without external fields, is an issue of technical as well as scientific importance. There are several good reasons to consider the 2D exciton problem in a magnetic field, putting aside effects of finite well width, finite barrier height and valence band mixing. First, the 2D exciton problem is exactly solvable in the absence of magnetic fields providing a good starting point to consider magnetic field effects. Second, magnetoexcitons in quasi-two-dimensional semiconductor systems have been studied extensively, both experimentally and theoretically: both numerical calculations and empirical fit formulas for the energies are available [1, 2, 3]. Nevertheless, the accuracy of numerical methods is best checked if simple analytic, or, in their absence, semi-analytic, solutions can be obtained.

From a theoretical point of view, studies of excitons in low-dimensional systems have often utilized either variational approaches, based on the prescription of trial wave functions, or perturbative expansions from known results in the weak- and strong-magnetic-field limits. It is important to elaborate on new forms to attack this problem. A semi-classical approach might give, in several cases, useful insights about the physics of these systems without the necessity of performing highly time consuming calculations. In this paper we present one such alternative which besides its great level of accuracy is simple enough to guarantee flexibility in the study of the physics of hydrogen-like systems in low-dimensional systems. The method we use provides direct interpretation in terms of semiclassical results allowing for systematic quantum corrections. The 1/N method (N is the space dimension), which we consider here, has been widely used in studying few-particle systems in atomic and molecular physics [4], nuclear physics [5] and quark physics [6, 7]. Application of this method to few-electron systems confined in an optical trap has also been considered.

The shifted 1/N approach has been devised to consider exactly two problems of great physical interest: the Coulomb and harmonic potentials [9, 10]. For these two potentials, taken independently one of the other, the method gives the exact result for the energy spectrum at first order, i.e. N^{-1} ; higher-order terms turn out to cancel exactly. With this result at hand it is interesting to investigate the reliability of the method for a problem where these two potentials appear simultaneously as is the case for a two-dimensional exciton in a magnetic field. It is worth noting that the Coulomb problem in a magnetic field has been already treated by the unshifted 1/N method by Bender et al [11] where higherorder corrections are shown to cause oscillations in the energy values as the magnetic field increases as a consequence of lacking the appropriate very-strong-magnetic-field limit (harmonic oscillator limit). The shifted 1/N method has been employed by Mustafa [12] in the study of the 2D donor impurity in the presence of an arbitrary magnetic field. In this last work comparison with numerical Padé approximants results [13, 14] has been performed showing an adequate agreement at intermediate magnetic fields but a completely wrong convergence of the energy levels to the B = 0 limit. This is fully unacceptable due to the fact that this method has been explicitly conceived to manage exactly the Coulomb problem. Therefore, a careful re-examination of the method as applied to hydrogen-like systems in 2D semiconductor heterostructures in the presence of a magnetic field must be accomplished.

In this paper we show explicitly that the shifted 1/N method accounts precisely for the magnetoexciton spectrum for any magnetic field strength. Convergence of higher-order terms is shown to be appropriate by calculating energy levels up to order N^{-3} in the whole range of magnetic fields. In particular, we investigate the accuracy of this method by comparing the magnetic field dependence of the exciton energy spectrum in the infinitehole-mass limit (hydrogen-like impurity) with the results reported in [13, 14] and [15] and (numerical exact results). We found an excellent quantitative agreement with these results for weak, intermediate and strong magnetic fields. This is in contrast with Mustafa's results [12] for the weak-magnetic-field limit. For a finite-hole-mass exciton we limit ourselves to the case of zero total linear momentum. The evolution of the lowest energy levels as a function of magnetic field and exciton reduced mass is considered.

In the following section, we present the theoretical model. In section 3, we present and discuss the results of our calculations. Our conclusions are given in section 4.

2. The theoretical approach

We consider the exciton problem in the effective mass approximation. The Hamiltonian of a hydrogen-like system in a homogeneous magnetic field is

$$H = \frac{1}{2m_e} (-i\hbar\nabla_1 + eA_1)^2 + \frac{1}{2m_h} (-i\hbar\nabla_2 - eA_2)^2 - \frac{q^2}{|r_1 - r_2|}$$
(1)

where m_e is the effective electron mass, m_h the effective hole mass, $q^2 = e^2/4\pi\epsilon_0\epsilon$ and ϵ is the dielectric constant (SI units are used). Without loss of generality we choose the symmetric gauge

$$A = \frac{1}{2}B \times r. \tag{2}$$

Following Lerner and Lozovik [16] we separate the motion of the centre of mass of the electron-hole pair in the magnetic field by taking for the exciton wave function the expression

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \exp[i\hbar(\mathbf{P} + e\mathbf{B} \times \mathbf{r}) \cdot \mathbf{R}]\Phi(\mathbf{r})$$
(3)

where R and r are the centre of mass and relative coordinate respectively. P denotes the eigenvalue of the exciton linear momentum operator. The Schrödinger equation for the magnetoexciton turns out to be

$$\left\{\frac{P^2}{2M} - \frac{\hbar^2}{2\mu}\nabla^2 + \frac{\mu\omega_c^2}{8}r^2 - \frac{\omega_c\beta}{2}L_z - \frac{\mu}{M}\omega_c(P_xy - P_yx) - \frac{q^2}{r}\right\}\Phi(r) = E\Phi(r)$$
(4)

where $M = m_e + m_h$ and $\mu^{-1} = m_e^{-1} + m_h^{-1}$ denote the total and reduced electron-hole mass respectively. L_z is the relative perpendicular angular momentum, the cyclotron frequency is $\omega_c = eB/\mu$ and $\beta = (m_e - m_h)/M$ is a measure of the electron-hole mass asymmetry. In this paper we limit ourselves to consider the two following situations: (i) Infinite-holemass limit (hydrogen-like impurity), where $M \to \infty$ and $\beta = -1$; (ii) finite-hole-mass magnetoexcitons with linear momentum P = 0. Solutions of (4) have been previously obtained by perturbation methods [16], numerical integration [15] and Padé approximants [13, 14] based on perturbation expansions about the weak- and strong-field limits. Here we transform (4) to an equation suitable to be solved by the shifted 1/N method.

For either of the two cases of interest in this work, (4) reduces to an equation where the cylindrical symmetry allows us to take for the wave function an expression such as $\Phi(r) = \xi(r) \exp(il\phi)$ where r and ϕ are the radial and azimuthal polar coordinates respectively and l denotes the angular momentum quantum number. The effective radial equation in N dimensions takes the form

$$\begin{cases} -l_B^2 \frac{d^2}{dr^2} + (k-\delta)(k-\delta+1)\left(\frac{l_B}{r}\right)^2 + \frac{1}{4}\left(\frac{r}{l_B}\right)^2 - 2\frac{l_B}{r}\frac{(q^2/l_B)}{\hbar\omega_c} \end{cases} u(r) \\ = \left(\frac{2E}{\hbar\omega_c} + \beta l\right)u(r) \tag{5}$$

where $u(r) = r^{\frac{N-1}{2}}\xi(r)$, $l_B = \sqrt{\hbar/\mu\omega_c}$ denotes the magnetic length and $k = |l| + (N-3)/2 + \delta$. δ is a suitable shift to be discussed below. The parameter 1/k is to be taken as an expansion parameter which amounts to considering the space dimension N or the angular momentum quantum number l as effectively large. By changing to a scaled variable such as $x = k^{-1/2}r$ the radial equation transforms to

$$\begin{cases} -\frac{l_B^2}{k^2} \frac{d^2}{dx^2} + \left(1 - \frac{\delta}{k}\right) \left(1 - \frac{\delta - 1}{k}\right) \left(\frac{l_B}{x}\right)^2 + \frac{1}{4} \left(\frac{x}{l_B}\right)^2 - \frac{2}{k^{3/2}} \frac{l_B}{x} \frac{(q^2/l_B)}{\hbar\omega_c} \right\} u(x) \\ = \frac{1}{k} \left(\frac{2E}{\hbar\omega_c} + \beta l\right) u(x). \tag{6}$$

This last equation is the starting point of the shifted 1/N method. The eigenvalues of (6) can be expanded in powers of 1/k as

$$\frac{1}{k}\left(\frac{2E}{\hbar\omega_c} + \beta l\right) = \sum_{j=0}^{\infty} \frac{\epsilon_{j/2}}{k^{j/2}}.$$
(7)

The leading approximation to the energy (or semiclassical limit) corresponds to the minimum of the effective potential for $k \to \infty$. Higher-order corrections are evaluated as fluctuations around this minimum. This corresponds to the minimum of the effective classical potential. The equation which determines this minimum is

$$\frac{1}{4} \left(\frac{x_0}{l_B}\right)^4 + \frac{1}{k^{3/2}} \left(\frac{x_0}{a_B^*}\right) = 1$$
(8)

where $a_B^* = \hbar^2 / \mu q^2$ denotes the effective Bohr radius. The leading term is therefore given by

$$E_0(n,l) = \frac{\hbar\omega_c}{2} \left[k \left(\frac{3}{4} \left(\frac{x_0}{l_B} \right)^2 - \left(\frac{l_B}{x_0} \right)^2 \right) - \beta l \right].$$
(9)

By expanding the effective potential in (6) around this minimum, i.e. x_0 , higher-order terms can be evaluated in a straightforward way (see the appendix for details). The first correction to the energy different from zero (of order k^{-1} , i.e. $E_1(n, l)$) is obtained by solving a one-dimensional effective harmonic oscillator equation. δ is fixed by imposing the vanishing of this last term which gives

$$\delta = \frac{1}{2} + (n + \frac{1}{2})\Omega \tag{10}$$

where

$$\Omega = \sqrt{1 + \frac{3}{4} \left(\frac{x_0}{l_B}\right)^4} \tag{11}$$

and $n = 0, 1, 2, \ldots$ It is worth noting that Ω depends on both quantum numbers, *n* and *l*, through its dependence on x_0 . It is interesting to verify that the leading-order term given by (9) is exact in the zero-magnetic-field (Coulomb problem) and very-highmagnetic-field (Landau problem) limits. If B = 0 then $x_0 = k^{3/2} a_B^*$, $\Omega = 1$ and $E_0(n, l) = -R^*/2(|l| + n + 1/2)^2$, where $R^* = \hbar^2/\mu a_B^{*2}$ is the effective Rydberg. On the other hand, if $B \to \infty$ then $x_0 = 2^{1/2} l_B$, $\Omega = 2$ and $E_0(n, l) = \hbar \omega_c [n + (|l| - \beta l + 1)/2]$. The next contribution different from zero turns out to be of order k^{-2} given by (for details see the appendix)

$$E_2(n,l) = R^* \left(\frac{a_B^*}{x_0}\right)^2 \frac{1}{k} \left[\frac{f_1(n)}{\Omega^4} + \frac{f_2(n)}{\Omega^2} + f_3(n) + f_4(n)\Omega^2\right]$$
(12)

where

$$f_1(n) = -\frac{1}{9}(30n^2 + 30n + 11) \tag{13}$$

$$f_2(n) = \frac{7}{36}(42n^2 + 42n + 13) \tag{14}$$

$$f_3(n) = -\frac{7}{18}(15n^2 + 15n + 4) \tag{15}$$

$$f_4(n) = (n + \frac{1}{2})^2.$$
(16)

It is straightforward to verify that $E_2(n, l) = 0$ for the two limits above considered: zero magnetic field, i.e. $\Omega = 1$, and infinite magnetic field, i.e. $\Omega = 2$. In order to test the convergence of the results at any magnetic field strength we push the calculation up to the next different-from-zero term which turns out to be of order k^{-3} . It is (for details see the appendix)

$$E_{3}(n,l) = R^{*} \left(\frac{a_{B}^{*}}{x_{0}}\right)^{2} \frac{1}{k^{2}} \left[\frac{g_{1}(n)}{\Omega^{9}} + \frac{g_{2}(n)}{\Omega^{7}} + \frac{g_{3}(n)}{\Omega^{5}} + \frac{g_{4}(n)}{\Omega^{3}} + \frac{g_{5}(n)}{\Omega} + g_{6}(n)\Omega\right]$$
(17)

where

$$g_1(n) = -\frac{5}{27}(94n^3 + 141n^2 + 109n + 31)$$
(18)

$$g_2(n) = \frac{5}{54}(830n^3 + 1245n^2 + 857n + 221)$$
(19)

$$g_3(n) = -\frac{5}{144}(3770n^3 + 5655n^2 + 3503n + 809)$$
(20)

$$g_4(n) = \frac{5}{216} (4574n^3 + 6861n^2 + 3875n + 794)$$
(21)

$$g_5(n) = -\frac{5}{432}(3406n^3 + 5109n^2 + 2677n + 487)$$
(22)

$$g_6(n) = 5(n + \frac{1}{2})^3.$$
⁽²³⁾

It is straightforward to verify that $E_3(n, l) = 0$ in the zero magnetic field limit and in the high-magnetic-field limit.

3. Results and discussion

For B = 0 the pure hydrogenic spectrum is composed of discrete (bound state) and continuous (scattering state) parts. For $B \neq 0$, the spectrum is always discrete because the effective potential (Coulomb plus diamagnetic or harmonic term) is infinitely high. From this it follows that all $B \neq 0$ electron-hole pair states must extrapolate to bound electron-hole pair states at B = 0. In what follows we take as the energy unit the effective Rydberg, i.e. $R^* = \mu_I q^4 / 2\hbar^2$ and the magnetic field will be expressed by the dimensionless quantity $\gamma = \hbar \omega_c / 2R^*$. In order to fix units we take $\mu_I = m_e$, i.e. the hydrogen-like impurity reduced mass value. We shall label the eigenstates with the standard spectroscopic notation s, p, d and f corresponding to |l| = 0, 1, 2 and 3 respectively, and + or - depending on the *l* sign. The label *n* corresponds to the Landau principal number. Therefore, states such as 1s, $2p^-$, $3d^-$ and $4f^-$ correspond to the same n = 0 value and will converge in the high-field limit to the lowest Landau level.



Figure 1. Minimum of the effective potential, x_0 in units of $2^{1/2}l_B$, as a function of the dimensionless magnetic field (see text) for the 1s, 2s and $2p^-$ states for two electron-hole mass ratios. Solid lines, impurity case, i.e. $\mu = \mu_I = m_e$; dashed lines, symmetrical case of equal electron and hole masses, i.e. $\mu = \mu_I / 2 = m_e/2$.

As can be inferred from equations (9), (12) and (17) the energy levels are determined by the position x_0 of the minimum of the classical effective potential in the $k \to \infty$ limit. In figure 1 we show the low-energy-levels variation of x_0 normalized to its strong-field limit value, i.e. $2^{1/2}l_B$, for two electron-hole mass ratios: the impurity limit (solid lines) and the symmetrical case of identical electron and hole masses (dashed lines). The magnetic field scale has been taken as $\gamma/(\gamma + 1)$ covering magnetic field strengths from zero to infinity. Note that x_0 is strongly dependent on the quantum numbers n and l. We observe that the lighter the exciton the larger is x_0 for each one of the states considered. The convergence



Figure 2. Convergence of the 1/N-method energy level results (in units of R^*) as a function of the dimensionless magnetic field strength: (a) ground state 1s energy level, (b) 3d⁻ level and (c) 4s level. Solid line: numerical calculation of [13]; dotted line: leading term E_0 ; dashed-dotted line: $E_0 + E_2$; dashed line: $E_0 + E_2 + E_3$.

to the strong-field limit value (magnetic length) is faster for the excited states than for the ground state as is to be expected.

In order to test the reliability of the 1/N method we have plotted the energy levels (in units of the effective Rydberg, R^*) for the 1s, $3d^-$ and 4s states in figure 2 as the expansion in inverse powers of k in equation (7) is stopped at different orders. We consider the hydrogen-like impurity limit. Unlike results presented in [12], our results show a correct limit when the magnetic field goes to zero, as it should be. Our results are also compared with the numerical Padé approximants expressions obtained by MacDonald *et al* [13] for the same states (solid lines) (the two forms of Padé approximants in [13] and [14] give the same results in the energy scale we are interested in). It is worth noting that these numerical interpolations have also been proved numerically using the method of exact series expansion by Zhu *et al* [15] finding an excellent quantitative agreement with results in [13]. We observe that for the 1s state the leading-term approximation crosses from below to above the numerical result in the intermediate-field region (figure 2(a)); inclusion of higher-order term makes possible an excellent agreement with the numerical data. A similar comparison for the $3d^-$ state shows that the leading term is always higher in energy than the numerical ones but a quick convergence is obtained when higher-order terms are included (figure 2(b)). The situation is not so good for the highly excited 4s state where the leading term is always higher in energy than the numerical result and higher-order term corrections do not show a quick convergence (figure 2(c)). This feature associated with excited s states has also been previously noted and reported in the literature in connection with other types of central potential [17].



Figure 3. Hydrogen-like impurity limit results $(E_0 + E_2 + E_3)$ for ground and lowest excited states as obtained by the 1/N method (solid lines) as compared with numerical results from [13] (dashed lines). (a) s states; (b) p states; (c) d states; (d) two lowest f states. Note that the energy scale is compressed by the factor $1/(\gamma + 1)$.

A more extensive comparison between our analytic results and the Padé approximant calculations of [13] is now considered. In figure 3(a) we show the first four s states where we remark that the agreement between our results and the numerical ones is excellent for the ground state (1s) for magnetic fields of any strength. The agreement is not so good in the intermediate-field region for excited s states being less acceptable the higher in energy is the state. In figure 3(b) the lowest six p energy levels are depicted. We observe that the agreement between our results and the numerical ones is much better than for the s states case even for excited states. In figures 3(c) and (d) the lowest four d states and two f states, respectively, are plotted. We observe that in the scale of the figure our results and

the numerical ones agree perfectly for any magnetic field strength. It is worth pointing out that in the compressed energy scale used in figure 3 the energy values at $\gamma/(\gamma + 1) = 1$, i.e. infinite magnetic field, correspond exactly to the Landau values, as it should be. In summary, we found that for fixed *n*, the magnetoexciton energies for arbitrary magnetic field become more accurate as *l* increases. This is expected since the expansion parameter k^{-1} becomes smaller as *l* becomes larger. We conclude that the shifted 1/N method is an excellent alternative to calculate the energy spectrum of heavy excitons for arbitrary magnetic field strength.

Recently, El-Said [18] has applied this method to the study of the energy spectrum of an exciton in a harmonic quantum dot where the three lowest s state energy levels have been studied as a function of the harmonic confinement (the equivalent of the diamagnetic term in our work). However, our calculation shows (figure 3(a)) that his results are not reliable for excited s states where the larger difference is to be expected with the exact numerical data.



Figure 4. From bottom to top, energy levels of 1s, $2p^-$, $3d^-$ and $4f^-$ states as a function of the dimensionless magnetic field strength. Terms up to E_3 have been included, for two electronhole mass ratios: solid lines, light exciton $m_h/m_e = 1$; dashed lines, heavy exciton $m_h/m_e = 5$. Same energy scale compression as in figure 3.

From now on we limit ourselves to consider n = 0 states, i.e. those states that in the independent particle picture should tend to the lowest Landau level at very high magnetic fields. Figure 4 shows the evolution of the energy levels of states 1s, $2p^-$, $3d^-$ and $4f^-$ for two values of the reduced mass ratio: $\mu_I/\mu = 1.2$ (a typical value for a heavy exciton in GaAs, dashed lines) and $\mu_I/\mu = 2$ (as appropriate for simulating a light exciton in GaAs, solid lines). It is clear that the energy levels of the light exciton present more drastic variation with the magnetic field compared with the heavy exciton case. It should be noticed that the limit at infinite magnetic field is consistent with what we can expect from a consideration of the Landau level ordering of a particle of reduced mass μ . In particular, it is to be noted that for the case of a symmetrical mass exciton the paramagnetic term disappears, breaking completely the high degeneracy of the Landau levels.



Figure 5. From bottom to top, energy levels of 1s, $2p^-$, $3d^-$ and $4f^-$ states (up to term E_3) as a function of the dimensionless electron-hole reduced mass for two magnetic field strengths: dashed lines, low magnetic field $\gamma = 0.25$ (B = 1.58 T for GaAs); solid lines, high-magnetic-field case $\gamma = 4$ (B = 25.3 T for GaAs). Note that $\mu_I/\mu = 1$ corresponds to the hydrogen-like impurity case and $\mu_I/\mu = 2$ corresponds to the symmetrical electron-hole mass exciton.

Finally, it is interesting to obtain from our analytic results trends in the magnetoexciton spectrum as the electron-hole mass ratio is changed. From figure 5 it is obvious that the energy levels for the high-magnetic-field case present the most sensitive variation with the electron-hole mass ratio, approaching the linear variation as predicted by a simple independent particle calculation. It is also interesting to note that in the weak-magnetic-field case, a typical heavy exciton, corresponding to $\mu_1/\mu = 1.2$ in GaAs, should present in the low-energy part of its spectrum roughly the same energy levels as for the hydrogen-like impurity ($\mu_1/\mu = 1$).

4. Conclusions

We have presented a detailed study of the energy spectrum of two-dimensional magnetoexcitons as obtained by the shifted 1/N method. We have found excellent quantitative agreement with previously reported numerical results for the hydrogen-like impurity or heavy-exciton case. The energy spectrum as a function of the electron-hole mass ratio indicates a more sensitive variation in the strong-magnetic-field limit than in the weak-field limit. We conclude that the shifted 1/N method is an excellent choice to calculate the energy spectrum of excitons for arbitrary magnetic field strength.

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Appendix

In this appendix we collect the main results to calculate higher-order terms to the energy levels. The Hamiltonian H, the eigenvalues ϵ and the eigenstates $|\chi\rangle$ are expanded in powers of $k^{-1/2}$. The first terms of the Hamiltonian series read

$$H_0 = \frac{3}{4} \left(\frac{x_0}{l_B}\right)^2 - \left(\frac{l_B}{x_0}\right)^2 = \epsilon_0 \tag{A1}$$

$$H_{1/2} = 0$$
 (A2)

$$H_1 = -l_B^2 \frac{d^2}{du^2} - (2\delta - 1)\left(\frac{l_B}{x_0}\right)^2 + \frac{u^2}{x_0^2}\left(\left(\frac{l_B}{x_0}\right)^2 + \left(\frac{x_0}{l_B}\right)^2\right)$$
(A3)

$$H_{3/2} = u \frac{2(2\delta - 1)l_B^2}{x_0^3} - \frac{u^3}{x_0 l_B^2}$$
(A4)

$$H_2 = \delta(\delta - 1)\frac{l_B}{x_0}^2 - u^2 \frac{3(2\delta - 1)l_B^2}{x_0^4} + \frac{u^4}{x_0^4} \left(3\left(\frac{l_B}{x_0}\right)^2 + \frac{1}{2}\left(\frac{x_0}{l_B}\right)^2\right)$$
(A5)

$$H_{5/2} = -u \frac{2\delta(\delta - 1)l_B^2}{x_0^3} + u^3 \frac{4(2\delta - 1)l_B^2}{x_0^5} - 2\frac{u^5}{x_0^5} \left(2\left(\frac{l_B}{x_0}\right)^2 + \frac{1}{2}\left(\frac{x_0}{l_B}\right)^2\right)$$
(A6)

$$H_3 = u^2 \frac{3\delta(\delta - 1)l_B^2}{x_0^4} - u^4 \frac{5(2\delta - 1)l_B^2}{x_0^6} + \frac{u^6}{x_0^6} \left(5\left(\frac{l_B}{x_0}\right)^2 + \left(\frac{x_0}{l_B}\right)^2\right)$$
(A7)

where a shift of the origin of coordinates has been introduced by $u = k^{1/2}(x - x_0)$. Note that H_0 is nothing but the minimum of the effective classical potential. The Hamiltonian H_1 describes a one-dimensional harmonic oscillator problem. The eigenfunctions of this Hamiltonian, which we label $|n\rangle$, are taken as the basis set in terms of which we calculate the perturbations of higher orders in the energy and wave functions. The energy term of order k^{-2} , i.e. ϵ_2 in (7), yields to the first correction of the leading term. It is therefore

$$E_2(n,l) = R^* \left(\frac{a_B^*}{x_0}\right)^2 \frac{1}{k} \Big[\langle n | H_{3/2} | \chi_{1/2}(n) \rangle + \langle n | H_2 | n \rangle \Big].$$
(A8)

In a similar way we obtain the energy term of order k^{-3} , i.e. ϵ_3 in (7), which yields to

$$E_{3}(n, l) = R^{*} \left(\frac{a_{B}^{*}}{x_{0}}\right)^{2} \frac{1}{k^{2}} \Big[\langle n | H_{3/2} | \chi_{3/2}(n) \rangle + \langle n | H_{2} | \chi_{1}(n) \rangle \\ + \langle n | H_{5/2} | \chi_{1/2}(n) \rangle + \langle n | H_{3} | n \rangle \Big].$$
(A9)

The corrections to the wave functions are given by

$$|\chi_{1/2}(n)\rangle = \frac{1}{2\Omega} \sum_{m \neq n} \frac{\langle m | H_{3/2} | n \rangle}{n - m} | m \rangle \tag{A10}$$

$$|\chi_{1}(n)\rangle = \frac{1}{2\Omega} \sum_{m \neq n} \frac{1}{n - m} \Big[\frac{1}{2\Omega} \sum_{m' \neq n} \frac{\langle m | H_{3/2} | m' \rangle \langle m' | H_{3/2} | n \rangle}{n - m'} + \langle m | H_{2} | n \rangle \Big] |m\rangle$$
(A11)

$$\begin{aligned} |\chi_{3/2}(n)\rangle &= \frac{1}{2\Omega} \sum_{m \neq n} \frac{1}{n - m} \left[-\frac{\epsilon_2(n)}{2\Omega} \frac{\langle m | H_{3/2} | n \rangle}{n - m} \right. \\ &+ \frac{1}{2\Omega} \sum_{m' \neq n} \frac{\langle m | H_{3/2} | m' \rangle \langle m' | H_2 | n \rangle + \langle m | H_2 | m' \rangle \langle m' | H_{3/2} | n \rangle}{n - m'} \\ &+ \frac{1}{(2\Omega)^2} \sum_{m' \neq n} \sum_{m' \neq n} \frac{\langle m | H_{3/2} | m' \rangle \langle m' | H_{3/2} | m'' \rangle \langle m'' | H_{3/2} | n \rangle}{(n - m')(n - m'')} \\ &+ \langle m | H_{5/2} | n \rangle \right] | m \rangle. \end{aligned}$$
(A12)

By a straightforward application of the raising and lowering operators of the harmonic oscillator problem to expressions (A8) and (A9) with expressions (A10), (A11) and (A12), the higher-order terms given in equations (12) and (17) are obtained.

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