

# Analytical solutions for two electrons in an oscillator potential and a magnetic field

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Two electrons subject to the Coulomb interaction and confined by an anisotropic harmonic potential can be viewed in two ways. One is the ‘‘Hooke’s atom,’’ much used in density functional theory (DFT), but with the addition of an external magnetic field. The other is as a heliumlike three-dimensional quantum dot. Though some results on the systems are known in both the DFT and quantum dot literature, exact analytical solutions have been lacking for nonzero anisotropy (nonzero  $B$ ). For certain specific confinement strengths, we develop such solutions in closed form, hence include electron exchange and correlation exactly. As with the zero-field Hooke’s atom, those solutions can be the ground or excited states.

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## I. INTRODUCTION

In density functional theory (DFT), the need for accurate approximations to the electronic exchange-correlation energy  $E_{XC}$  has motivated many studies of a model system often called Hooke’s atom (HA) in the DFT literature. The basic HA is two electrons interacting by the Coulomb potential but confined by a harmonic potential rather than nuclear-electron attraction. This system is significant for DFT because, for certain values of the confining coupling constant, exact analytical solutions for various states of the HA are known [1–4]. Because the DFT universal functional is *independent* of the external potential and the HA differs from atomic He *only* by that potential, exact solutions of the HA allow construction of the exact  $E_{XC}$  functional and comparative tests of approximate functionals. Because much less is known about the approximate functionals in current density functional theory [5] than ordinary DFT, it would be of considerable value to the advancement of CDFT to have corresponding solutions for the HA in an external magnetic field.

When the HA is placed in an external magnetic field, its lateral confinement can exceed its vertical confinement. Taut [6] gave analytical solutions for a two-dimensional (2D) HA in a perpendicular  $B$  field. It is well known that the magnetic field can greatly complicate the motion of a Coulomb system. Even for the one-electron system (H atom), substantial effort is required to get highly accurate results in a  $B$  field [7–9]. Only recently have calculations on the He atom in a high field been pushed beyond the Hartree-Fock approximation [10]. When the nuclear attraction in the He atom is replaced by a harmonic potential, exact analytical results can serve as a stringent check on the accuracy of those correlated calculations.

The 2D HA in an external  $B$  field studied by Taut [6] can equally well be viewed as a model 2D quantum dot (QD). The ability to fabricate and probe such confined, few-electron systems (examples include Refs. [11,12]) has stimulated numerous theoretical studies on these ‘‘artificial atoms.’’ Reference [13] is a recent review. However, even the simplest nontrivial system, QD He, poses a significant challenge to theorists. Extensive numerical calculations have been done on the 2D He QD at different levels of approximation for the correlation energy [14–16]. To obtain a better quan-

titative description, especially for a small dot [17], allowance for electron motion in the third dimension is necessary. By considering such three-dimensional (3D) systems, Bruce and Maksym [18] obtained confinement energies consistent with the experimental data of Tarucha *et al.* [12]. Without the 3D contributions the results are off by 50%. Numerical studies of 3D QD He continue, for example, the recent coupled-channel calculation by Lin and Jiang [19].

Though highly accurate numerical solutions for QD He can be obtained readily, nevertheless analytical results are still sought, because the physical picture they provide is more illuminating than sheer numerics alone. The main obstacle to obtaining analytic solutions is the two-electron Coulomb repulsion term in the Hamiltonian, especially in the absence of what otherwise would be spherical symmetry (central field model). Thus the QD literature has several treatments in which the interaction is altered (sometimes quite drastically) to enable extraction of approximate analytical solutions for a 2D QD. See, for example, Refs. [20,21]. For the 3D He QD in a magnetic field, Nazmitdinov *et al.* [22] concluded that the ‘‘...problem is in general nonintegrable’’ [22(b)], discussed the circular 2D and spherical 3D cases as integrable, then treated the case of a 3D dot strongly localized in  $z$  with a classical decoupling of the  $z$  and  $x$ - $y$  followed by WKB quantization. They also found that, for some special cases, the problem is separable in a parabolic coordinate system [22] and provided numerical results [22(c)] but not closed analytical forms. Here we develop exact analytical solutions for some confinement frequencies in a nonzero field without altering the interaction.

## II. EXACT ANALYTICAL SOLUTIONS

The system Hamiltonian for the case of a magnetic field  $B$  along the  $z$  direction reads

$$H = \sum_{i=1}^2 \left[ \frac{1}{2m_e^*} \left( \vec{p}_i + \frac{e}{c} \vec{A}(\vec{r}_i) \right)^2 + \frac{m_e^*}{2} [\omega_{\perp}^2 (x_i^2 + y_i^2) + \omega_{\parallel}^2 z_i^2] \right] + \frac{e^2}{\epsilon |\vec{r}_1 - \vec{r}_2|} + H_{\text{spin}}. \quad (1)$$

Here  $H_{\text{spin}} = -g^* \mu_B (\vec{s}_1 + \vec{s}_2) \cdot \vec{B}$ . In the case of the He 3D QD,

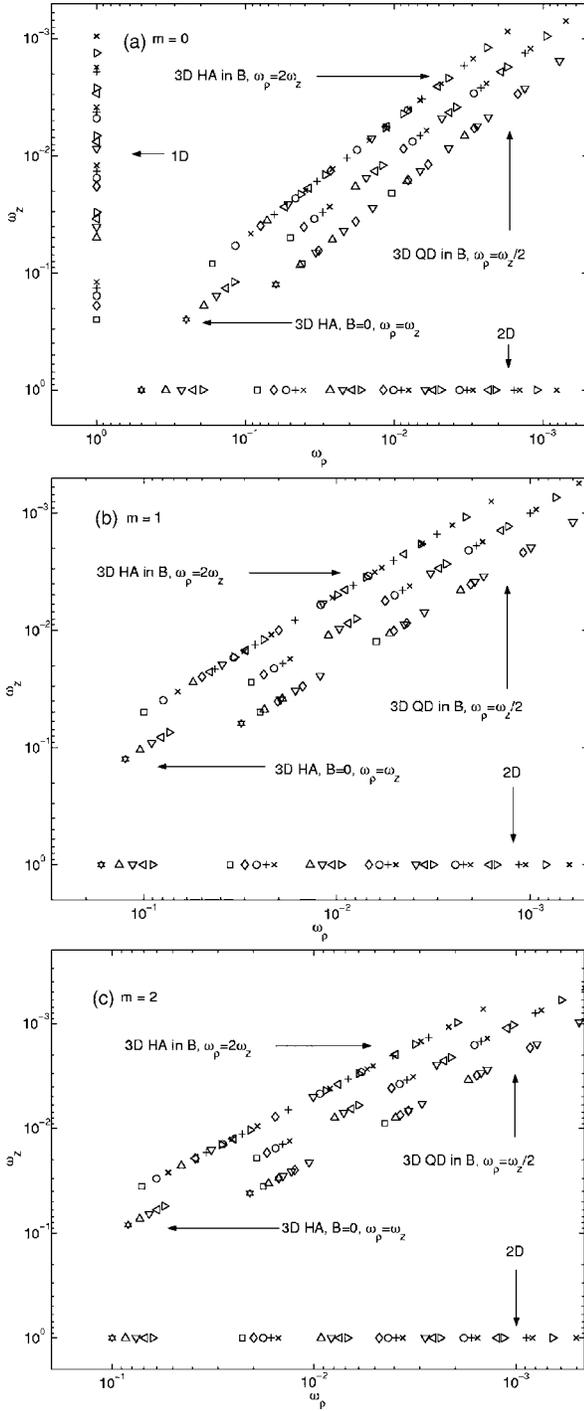


FIG. 1. Confinement strengths amenable to analytical solution of Eq. (2). Panels (a)–(c) are for  $m=0, 1, 2$ , respectively. The 10 symbols (hexagon, square, up triangle, diamond, down triangle, circle, left triangle, plus sign, right triangle, and x mark) correspond to integers 1, 2, ..., 10 that are the highest order of the polynomial factor of the relative motion wave functions in  $z$  for 1D, in  $\rho$  for 2D, in  $r$  for the 3D HA ( $B=0$ ), and in  $t$  for the QD. For the 3D HA in  $B \neq 0$ , those symbols stand for the values of  $(N_z + \pi_z)$  in, for example, Eq. (12). For the spherical HA, only  $\pi_z=0$  is included; notice that its odd parity ( $\pi_z=1, m$ ) and even parity ( $\pi_z=0, m+1$ ) states are degenerate. For the 2D case,  $\omega_z=\infty$  has been shifted to  $\omega_z=1$ . For the 1D case,  $\omega_\rho=\infty$  has been shifted to  $\omega_\rho=1$ .

$m_e^*$  is the effective electron mass,  $\varepsilon$  the effective dielectric constant of the material,  $g^*$  the effective Landé factor, and  $\omega_\perp$  and  $\omega_\parallel$  are the confinement frequencies perpendicular and parallel to the  $B$  field. Using the vector potential in the symmetrical gauge  $\vec{A}(\vec{r}) = \frac{1}{2}\vec{B} \times \vec{r}$  for the  $B$  field, the appropriate effective atomic units are  $\hbar = m_e^* = e = 4\pi\varepsilon = 1$ . (Notice that this choice would give “scaled Hartree units,” not a problem here.) As usual, we introduce center-of-mass (CM) and relative coordinates  $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ ,  $\vec{r} = \vec{r}_1 - \vec{r}_2$ , respectively. The Hamiltonian Eq. (1) separates into CM and relative-motion parts  $H = H_{\text{CM}} + H_{\text{rel}} + H_{\text{spin}}$ . The solution to the CM part,  $H_{\text{CM}} = \frac{1}{4}[(\nabla_{\vec{R}}/i) + 2\vec{A}(\vec{R})]^2 + \omega^2 R^2$ , is well known, so we focus on the relative motion

$$H_{\text{rel}} = -\nabla^2 + \omega_\rho^2 \rho^2 + \omega_z^2 z^2 + \frac{1}{r} + \frac{m}{2} \omega_c. \quad (2)$$

Here  $\rho = \sqrt{x^2 + y^2}$ ,  $\omega_\rho = \sqrt{(\omega_\perp^2/4) + (\omega_c^2/16)}$ ,  $\omega_z = \omega_\parallel/2$ , and  $\omega_c = eB/m_e^*c$  is the cyclotron frequency.

The HA problem in a  $B$  field is recovered by setting  $m_e^*$  to the bare electron mass  $m_e$ ,  $\varepsilon = \varepsilon_0$ ,  $g^* = g$ , and letting  $\omega_\perp = \omega_\parallel = \omega$  in Eq. (1). The corresponding atomic units are the familiar  $\hbar = m_e = e = 4\pi\varepsilon_0 = 1$  (Hartree atomic units). In what follows we designate the case  $\omega_\perp \neq \omega_\parallel$  as the quantum dot or QD and  $\omega_\perp = \omega_\parallel = \omega$  as the Hooke’s atom or HA. For both we use bare Hartree units, i.e.,  $m_e^* = m_e$ ,  $\varepsilon = \varepsilon_0$ ,  $g^* = g$ .

The relative motion eigenvalue problem from Eq. (2) generally cannot be solved analytically in either spherical or cylindrical coordinates. A special case is  $\omega_\rho = \omega_z$  which restores rotational symmetry. For the QD, this case corresponds to an external magnetic field  $B = (2m_e^*c/e)\sqrt{\omega_\parallel^2 - \omega_\perp^2}$  [22]. For the HA, it corresponds to vanishing  $B$  field [3].

Since the effective potential in Eq. (2)  $V(r) = \omega_\rho^2 \rho^2 + \omega_z^2 z^2 + (1/r)$  is expressed as a combination of cylindrical coordinate variables  $(\rho, z)$  and the spherical coordinate variable  $r$ , it proves convenient also to express the relative-motion wave function in those combined, redundant variables  $\psi(\vec{r}) = \psi(\rho, z, r(\rho, z), \varphi)$ . In part motivated by asymptotics, we choose the form

$$\psi(\vec{r}) = e^{-(\omega_z/2)z^2 - (\omega_\rho/2)\rho^2} |m|_z \pi_z u(r, z) e^{im\varphi}, \quad (3)$$

where  $\pi_z = 0$  for even  $z$  parity, 1 for odd  $z$  parity. Then  $(H_{\text{rel}} - E_{\text{rel}})\psi(\vec{r}) = 0$  yields

$$\left[ -\frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial z^2} - \frac{2z}{r} \frac{\partial^2}{\partial z \partial r} - \frac{2}{r} [1 + \pi_z + |m| + (\omega_\rho - \omega_z)z^2 - \omega_\rho r^2] \frac{\partial}{\partial r} + 2 \left( \omega_z z - \frac{\pi_z}{z} \right) \frac{\partial}{\partial z} + \frac{1}{r} - \tilde{E} \right] u(r, z) = 0, \quad (4)$$

where  $\tilde{E} = E_{\text{rel}} - (m/2)\omega_c - (2\pi_z + 1)\omega_z - 2(|m| + 1)\omega_\rho$ . For the QD, it is useful to absorb  $z^{\pi_z}$  to be in  $u(r, z)$  or, equivalently, require that  $u(r, z)$  admit both positive and negative  $z$  parity. For the HA, explicit parity is more useful. With the change of variables,  $\xi = \frac{1}{2}(r+z)$ ,  $\eta = \frac{1}{2}(r-z)$ , Eq. (4) becomes

TABLE I. Confinement frequencies  $\omega_z$  which have analytical solutions to Eq. (2) [ $\omega_\rho = \omega_z/2$ , see Eq. (9) for their eigenvalues].

$n$	$\pi_z^a$	State <sup>b</sup>	$m=0^c$	$m=1$	$m=2$
1	+	$g$	0.1250000 (1)	0.0625000	0.0416667
2	+	$g$	0.0208333 (2)	0.0125000	0.0089286
2	+/-	$e/g$	0.0833333 (3)	0.0500000	0.0357143
3	+	$g$	0.0067407 (4)	0.0045672	0.0034455
3	+/-	$e/g$	0.0164515 (6)	0.0106450	0.0079067
3	+/-	$e$	0.0520416 (7)	0.0383746	0.0298292
3	+	$e$	0.0858519 (5)	0.0475162	0.0335915
4	+	$g$	0.0029597	0.0021683	0.0017053
4	+/-	$e/g$	0.0057990	0.0040530	0.0031256
5	+	$g$	0.0015504	0.0011973	0.0009720
5	+/-	$e/g$	0.0026546	0.0019752	0.0015740

<sup>a</sup>+ = even  $z$  parity, - = odd  $z$  parity.

<sup>b</sup> $g$  = ground state,  $e$  = excited state.

<sup>c</sup>Numbers in parentheses are the listing number in Table II.

$$\left[ -\xi \frac{\partial^2}{\partial \xi^2} - \eta \frac{\partial^2}{\partial \eta^2} - [1 + |m| + 2\xi\eta(\omega_z - 2\omega_\rho)] \left( \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta} \right) + 2\omega_z \left( \xi^2 \frac{\partial}{\partial \xi} + \eta^2 \frac{\partial}{\partial \eta} \right) - \tilde{E}(\xi + \eta) + 1 \right] u(\xi, \eta) = 0. \quad (5)$$

It is easy to see that, for the special case  $\omega_z = 2\omega_\rho$ , which can be realized in the QD ( $\omega_\perp \neq \omega_\parallel$ ) by imposing an external field  $B = (m_e^* c / e) \sqrt{\omega_\parallel^2 - 4\omega_\perp^2}$ , Eq. (5) can be separated into two parts  $u(\xi, \eta) = f_1(\xi)f_2(\eta)$ ,

$$\left( -t \frac{\partial^2}{\partial t^2} - (1 + |m|) \frac{\partial}{\partial t} + 2\omega_z t^2 \frac{\partial}{\partial t} - \tilde{E}t \right) f_i(t) = c_i f_i(t), \quad (6)$$

where  $i=1,2$  and  $c_1 + c_2 = -1$ . A power series expansion

$$f_i(t) = \sum_{j=0}^{\infty} B_{ij} t^j \quad (7)$$

yields the recurrence relation

$$(j+1)(j+1+|m|)B_{i,j+1} = [2\omega_z(j-1) - \tilde{E}]B_{i,j-1} - c_i B_{i,j}. \quad (8)$$

A sufficient condition for the summation in Eq. (7) to terminate after  $n+1$  terms is that  $B_{n+1} = 0$  and  $\tilde{E} = 2n\omega_z$ . Inversion

of  $B_{n+1}(n, |m|, \omega_z, c_i) = 0$  to get an expression of  $c_i$  and imposition of  $c_1 + c_2 = -1$  gives the values of  $\omega_z(n, |m|)$  required for a closed solution. Some examples are given in Table I. Then a back-substitution gives  $f_i(t)$ , hence  $\psi(\rho, z, r(\rho, z), \varphi)$ , with eigenvalue of

$$E_{\text{rel},n} = [2(n+1) + |m|]\omega_z + \frac{m}{2}\omega_c. \quad (9)$$

Some finite-term  $f_i(t)$  for  $m=0$  are given in Table II.

The foregoing procedure also applies for the noninteracting case by omission of the  $1/r$  term in Eq. (2). The separation constraint becomes  $c_1 + c_2 = 0$ , which always can be satisfied for arbitrary  $\omega_z$ , so the wave function always is separable into two parts as in Eq. (6). Comparing the interacting and noninteracting cases, one immediately realizes that, at those frequencies found already, the eigenvalue of the interacting system is degenerate with a higher excited state of the noninteracting system subject to the same confinement potentials.

Next we consider another special case,  $\omega_\rho = 2\omega_z = \omega$ . It corresponds to imposition of an external field  $B = 2\sqrt{3}\omega$  upon a HA ( $\omega_\perp = \omega_\parallel$ ) with intrinsic confinement strength  $\omega$ . For nonzero  $m$  values, Eq. (4) is not separable as previously discussed [22]. Instead, we make a direct, double power-series expansion

TABLE II. Some solutions to Eq. (6) for confinement potential  $\omega_\rho = \omega_z/2, m=0$ .

No.	$\omega_z$	$c$	$f(t)$
1	1/8	$c_1 = c_2 = -1/2$	$1 + t/2$
2	1/48	$c_1 = c_2 = -1/2$	$1 + t/2 + t^2/24$
3	1/12	$c_1 = 0, c_2 = -1$	$f_1(t) = 1 - t^2/12, f_2(t) = 1 + t + t^2/6$
4/5	$\frac{10 \mp \sqrt{73}}{216}$	$c_1 = c_2 = -1/2$	$f_1(t) = f_2(t) = 1 + t/2 - \frac{1 \mp \sqrt{73}}{144} t^2 - \frac{83 \mp 11\sqrt{73}}{7776} t^3$
6	$\frac{10 - 3\sqrt{3}}{292}$	$c_{1,2} = -\sqrt{(20 \pm 2\sqrt{73})\omega_z}$	$1 - c_{1,2}t + \left( \frac{39 - 19\sqrt{3}}{3504} \pm \frac{201 - 53\sqrt{3}}{3504\sqrt{73}} \right) t^2 (10 + 3\sqrt{3} \pm \sqrt{73} + t)$
7	$\frac{10 + 3\sqrt{3}}{292}$	$c_{1,2} = \mp \sqrt{(20 \pm 2\sqrt{73})\omega_z}$	$1 - c_{1,2}t + \left( \frac{39 + 19\sqrt{3}}{3504} \pm \frac{201 + 53\sqrt{3}}{3504\sqrt{73}} \right) t^2 (10 - 3\sqrt{3} \pm \sqrt{73} + t)$

TABLE III. Confinement frequencies  $\omega_z$  which have analytical solutions to Eq. (2) [ $\omega_z = \omega/2, B = 2\sqrt{3}\omega$ , see Eq. (12) for their eigenvalues].

$N_z$	$\pi_z^a$	State <sup>b</sup>	$m=0^c$	$m=1^c$	$m=2^c$
2	+	<i>g</i>	0.0833333(1)	0.0500000	0.0357143
2	-	<i>g</i>	0.0357143	0.0277778(2)	0.0227273(3)
4	+	<i>g</i>	0.0133800(5)	0.0100000	0.0077870
4	-	<i>g</i>	0.0070789	0.0059139	0.0050468
4	+	<i>e</i>	0.0395861	0.0250000(4)	0.0193869
4	-	<i>e</i>	0.0258158	0.0196437	0.0161673
6	+	<i>g</i>	0.0040457	0.0034301	0.0029164
6	-	<i>g</i>	0.0025458	0.0022352	0.0019779
8	+	<i>g</i>	0.0016991	0.0015158	0.0013556
8	-	<i>g</i>	0.0011904	0.0010780	0.0009796
10	+	<i>g</i>	0.0008658	0.0007924	0.0007270
10	-	<i>g</i>	0.0006492	0.0005995	0.0005548

<sup>a</sup>+ = even *z* parity, - = odd *z* parity.

<sup>b</sup>*g* = ground state, *e* = excited state.

<sup>c</sup>Numbers in parentheses are the listing number in Table IV.

$$u(r, z) = \sum_{n_r, n_z=0}^{\infty} A_{n_r, n_z} r^{n_r} z^{n_z} \quad (10)$$

to transform Eq. (4) into a recurrence relation,

$$\begin{aligned} & -2(n_r + 2)(\omega_\rho - \omega_z)A_{n_r+2, n_z-2} - (n_r + 2)[n_r + 3 + 2(|m| + \pi_z \\ & + n_z)]A_{n_r+2, n_z} + A_{n_r+1, n_z} + [2(n_r\omega_\rho + n_z\omega_z) - \tilde{E}]A_{n_r, n_z} \\ & - (n_z + \pi_z + 1)(n_z + \pi_z + 2)A_{n_r, n_z+2} = 0, \end{aligned} \quad (11)$$

where  $A_{i,j} = 0$  for  $i < 0$ , or  $j < 0$ , or  $j = 2k + 1$ . We seek values of  $\tilde{E}, \omega_\rho, \omega_z$  for which the right hand side of Eq. (10) terminates at finite order. Assume the highest power of  $z$  that appears is  $N_z$ , ( $A_{i,j > N_z} = 0$ ), where  $N_z$  is an even number. For  $N_z > 2$ , generally there is no solution to the set of equations that follow from Eq. (11). However, a judicious choice,  $\omega_\rho = 2\omega_z, \tilde{E} = 2N_z\omega_z$ , allows us to set  $A_{i,j} = 0$  for  $2i + j > N_z$ , since there are  $(N_z/2) + 1$  recurrence relations of Eq. (11) with  $2n_r + n_z = N_z$  that then are satisfied automatically. Now we find values of  $\omega_z$  that correspond to an analytical solution.

Repeated application of Eq. (11) for each combination of  $-1 \leq n_r \leq (N_z/2) - 2, N_z - 2(n_r + 1) \geq n_z \geq 2$ , allows us to express all the coefficients  $A_{0 < i \leq (N_z/2), 0 \leq j \leq N_z - 2i}$  in terms of

$\{A_{0,0 \leq j \leq N_z}\}$ . Invoking Eq. (11) for  $n_z = 0, -1 \leq n_r \leq (N_z/2) - 1$ , gives  $(N_z/2) + 1$  homogenous linear equations involving  $\{A_{0,0 \leq j \leq N_z}\}$ . To have nontrivial solutions, the determinant of this set of equations must be zero, a requirement which reduces to finding the roots of a polynomial equation in  $\omega_z$ . Table III gives examples of roots that are frequencies that correspond to closed-form analytical solutions.

For each frequency found in the previous step, the corresponding eigenvector  $\{A_{0,0 \leq j \leq N_z}\}$  determines the vector of all the coefficients  $A_{0 < i \leq (N_z/2), 0 \leq j \leq N_z - 2i}$ . Substitution of them into Eq. (10) gives the wave function with the relative-motion energy of

$$E_{\text{rel}} = [(N_z + \pi_z + 2|m|) + \frac{5}{2} + \sqrt{3}m]\omega. \quad (12)$$

Table IV gives explicitly some of the solutions to Eq. (2).

One limiting case,  $\omega_z \rightarrow \infty$ , which reduces the system to a 2D problem, was discussed in Ref. [6]. Another limiting case,  $\omega_\rho \rightarrow \infty$ , reduces the system to a 1D problem that is quite easily solved. Together with the two cases treated in this paper, we have in total five families of analytical solutions for confinement frequencies falling into one of the following five categories: (i)  $\omega_z \rightarrow \infty$ ; (ii)  $\omega_z = 2\omega_\rho$ ; (iii)  $\omega_z = \omega_\rho$ ; (iv)  $\omega_z = \omega_\rho/2$ ; (v)  $\omega_\rho \rightarrow \infty$ . Within each category, there are

TABLE IV. Some solutions to Eq. (2) for confinement potential  $\omega = 2\omega_z, B = 2\sqrt{3}\omega$ .

No.	$\omega$	Relative motion wave function
1	1/6	$e^{-(z^2 + 2\rho^2)/24} (1 + r/2 + z^2/12)$
2	1/18	$e^{-(z^2 + 2\rho^2)/72} \rho z (1 + r/6 + z^2/108) e^{i\varphi}$
3	1/22	$e^{-(z^2 + 2\rho^2)/88} \rho^2 z (1 + r/8 + z^2/176) e^{2i\varphi}$
4	1/20	$e^{-(z^2 + 2\rho^2)/80} \rho (1 + r/4 - z^2/40 + \rho^2/80 - rz^2/160 - z^4/3200) e^{i\varphi}$
5	$\frac{25-3\sqrt{17}}{472}$	$e^{-\omega(z^2 + 2\rho^2)/4} (1 + \frac{r}{2} + \frac{1-22\omega}{48} rz^2 + \frac{1+2\omega}{24} r^2 + \frac{1-18\omega}{8} z^2 + \frac{11-314\omega}{11328} z^4)$

discrete, denumerable frequencies that have analytical solutions, which could be either the ground state or excited states. They are summarized in Fig 1.

### III. REMARKS

The *ansatz* we used, Eq. (3), appears to be closely related to the asymptotics that underpin the oscillator representation method [23] though we do not use that scheme. The solutions presented here provide the explicit completion, as far as we can tell, of the five integrable cases identified by Simonović and Nazmitdinov [22(c)]. As in the spherical case [6], one cannot guarantee *a priori* that a particular analytical so-

lution is a ground or excited state. However, careful numerical calculation of the eigenspectrum, tested for precision against the analytical solutions for a specified confinement potential and external field, can resolve that issue. Reference [22(c)] provides an example. We will discuss our numerical approach and inversion of exact and numerical results to obtain CDFT functionals for the HA elsewhere.

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