

## Algebraic solution of a non-trivial oscillator problem

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**Abstract.** The energy spectrum of an electron confined to an anisotropic oscillator potential and moving in homogeneous crossed electric and magnetic fields is determined algebraically. The method is an instructive example of a non-invariance group approach. The result is useful for the computation of for example size effects on diamagnetic properties of non-spherical small metallic particles.

The aim of this paper is to solve the mathematical problem represented by equation (3). For pedagogical clarity, however, I shall start with a well defined physical problem.

Consider a non-relativistic electron of mass  $m$  and charge  $-e$  ( $e > 0$ ) moving in a homogeneous magnetic field  $\mathbf{B}$  and confined by an anisotropic oscillator potential. Its Hamiltonian is thus given by

$$\begin{aligned} H &\equiv H_0 + V \\ &= (\mathbf{p} + (e/c)\mathbf{A})^2/(2m) + \frac{1}{2}x^2\Omega_1^2m + \frac{1}{2}y^2\Omega_2^2m + \frac{1}{2}z^2\Omega_3^2m. \end{aligned} \quad (1)$$

What is the significance of this Hamiltonian? The oscillator potential may be interpreted as 'soft' walls confining the electron motion to a vessel defined by the equipotential lines  $V = \text{constant}$ . If all  $\Omega_i$  approach zero, the limit of an infinite system with a freely moving electron (apart from the magnetic field) is recovered. If (1) were used to describe a system of non-interacting electrons of fixed density  $n_e$  one would choose the  $\Omega_i$  size dependent (i.e. dependent on the dimensions of the actual box to which the electrons are confined, and which is to be simulated by the soft walls) such that in the thermodynamic limit the  $\Omega_i$  approach zero in such a way as to keep the density  $n_e$  fixed.

Thus, with finite  $\Omega_i$ , one can study, for example, size effects on the properties of metallic electrons confined to a small particle and subject to an external magnetic field. All one needs is the single particle spectrum of (1) because with it the density of states and all thermodynamic properties may be calculated.

In fact, Denton (1973) has carried out an extensive study of diamagnetic properties of small metallic particles on the basis of (1) with  $\Omega_3 = 0$ ,  $\Omega_1 = \Omega_2$  and the magnetic field pointing along the symmetry axis  $x_3$ . The level spectrum of this cylindrically symmetric case was determined earlier (Darwin 1930) analytically (i.e. by means of a power series expansion of wavefunctions). It is a simple exercise to derive the spectrum algebraically (i.e. by using only the canonical commutation relations between the dynamical variables  $\mathbf{r}$  and  $\mathbf{p}$ ), (Schuh 1973). Because of the symmetry, this problem is essentially a two-dimensional harmonic oscillator problem.

For the case  $\Omega_1 \neq \Omega_2$ , however, the problem appears much less trivial. Its solution, to which the rest of the paper is devoted, is meant to encourage the search for simple algebraic solutions in different but comparatively simple problems.

Note first that the dynamical variables corresponding to the symmetry axis of the ellipsoid along which the field points constitute no problem. For definiteness let  $\mathbf{B} = (0, 0, B)$ , then a gauge can be chosen in which  $A_z = 0$  and  $A_{x,y}$  will not depend on  $z$ . Thus the problem separates into the motion along the field axis and within the perpendicular plane:

$$H = p_z^2/2m + \frac{1}{2}z^2\Omega_3^2m + [p_\perp + (e/c)\mathbf{A}_\perp]^2/2m + \frac{1}{2}(\Omega_1^2x^2 + \Omega_2^2y^2)m \\ \equiv H_z + H_\perp.$$

Since  $[H_z, H_\perp] = 0$  the spectrum of  $H$  is known once that of  $H_\perp$  has been determined.

One may even include an in-plane homogeneous electric field  $\mathbf{E}$  and measure the confining potential with respect to an arbitrary reference point  $(x_0, y_0)$ , without enhancing the scope of the problem considerably. We shall therefore be concerned with a two-dimensional system described by the Hamiltonian

$$H_2 = (1/2m)[p_\perp + (e/c)\mathbf{A}_\perp]^2 + \frac{1}{2}m[\Omega_1^2(x - x_0)^2 + \Omega_2^2(y - y_0)^2] + e\mathbf{E}_\perp \cdot \mathbf{r}_\perp \quad (2)$$

where  $\mathbf{p}_\perp = (p_x, p_y)$  etc., and  $\mathbf{r}$  and  $\mathbf{p}$  obey canonical commutation relations.

As a first step we shall show that (2) may be reduced to the following standard form

$$h = p_x^2 + x^2 + b(p_y^2 + y^2) + c(xp_y - yp_x). \quad (3)$$

Then the spectrum of (3) will be determined for arbitrary real numbers  $b$  and  $c$ . The reader who is interested in the result only is referred to (21), (27) or (28).

The electric field is conveniently dealt with by completing the square given by the last two terms in (2). If we introduce

$$\bar{x}_0 \equiv x_0 - eE_x/m\Omega_1^2, \quad \bar{y}_0 \equiv y_0 - eE_y/m\Omega_2^2 \quad (4)$$

then  $H_2$  may be written:

$$H_2 = (1/2m)[p_\perp + (e/c)\mathbf{A}_\perp]^2 + \frac{1}{2}m\Omega_1^2(x - \bar{x}_0)^2 + \frac{1}{2}m\Omega_2^2(y - \bar{y}_0)^2 + G \quad (5a)$$

with the constant

$$G = \frac{1}{2}m\Omega_1^2(x_0^2 - \bar{x}_0^2) + \frac{1}{2}m\Omega_2^2(y_0^2 - \bar{y}_0^2). \quad (5b)$$

Next we make a canonical transformation

$$x_1 \equiv (\Omega_1/\omega)^{1/2}(x - \bar{x}_0), \quad x_2 \equiv (\Omega_2/\omega)^{1/2}(y - \bar{y}_0) \\ p_1 \equiv (\omega/\Omega_1)^{1/2}p_x, \quad p_2 \equiv (\omega/\Omega_2)^{1/2}p_y \quad (6)$$

and choose the gauge

$$A_x = -x_2B(\Omega_2\omega)^{1/2}/(\Omega_1 + \Omega_2), \quad A_y = x_1B(\Omega_1\omega)^{1/2}/(\Omega_1 + \Omega_2) \quad (7)$$

with  $\omega$  an as yet arbitrary parameter. Of course, the canonical commutation relations are preserved by (6), and  $\text{rot } \mathbf{A} = (0, 0, B)$  is obviously fulfilled. Equation (5a) now reads

$$H_2 - G = (\Omega_1/\omega)(p_1^2/2m + \frac{1}{2}m\omega^2\gamma^2x_1^2) + (\Omega_2/\omega)(p_2^2/2m + \frac{1}{2}m\omega^2\gamma^2x_2^2) \\ + \omega_c[(\Omega_1\Omega_2)^{1/2}/(\Omega_1 + \Omega_2)](x_1p_2 - x_2p_1). \quad (8)$$

The abbreviations

$$\omega_c \equiv eB/mc, \quad \gamma^2 \equiv 1 + \omega_c^2/(\Omega_1 + \Omega_2)^2 \quad (9)$$

have been used. Obviously (8) is of standard form (3) if one identifies:

$$b = \Omega_2/\Omega_1, \quad c = 2\omega_c(\Omega_2/\Omega_1)^{1/2}/[\omega_c^2 + (\Omega_1 + \Omega_2)^2]^{1/2} \quad (10)$$

and chooses units such that  $m\omega\gamma = 1$ .

Let us now turn to the determination of the spectrum of (3). Instead of giving the solution in an elegant and deductive form we shall indicate the way to it in a more inductive manner.

The form of  $h$  suggests that we play with the commutation relations of the operators  $p_x^2 + x^2$ ,  $p_y^2 + y^2$ , and the angular momentum  $z$ -component  $xp_y - yp_x$ . One is readily led to consider the three operators

$$L_1 \equiv \frac{1}{4}(p_x^2 + x^2 - p_y^2 - y^2), \quad L_2 \equiv \frac{1}{2}(p_x p_y + x y), \quad L_3 \equiv \frac{1}{2}(x p_y - y p_x), \quad (11)$$

and one can easily verify that these satisfy the angular momentum commutation relations:

$$[L_i, L_j] = i\hbar \epsilon_{ijk} L_k \quad (12)$$

In other words: the  $L_i$  form the Lie algebra (under commutation) of the special unitary group in two dimensions,  $SU(2)$ , or likewise the special orthogonal group in three dimensions,  $SO(3)$ . The  $L_i$  may therefore be interpreted as infinitesimal generators of 'rotations'. Thus one is prompted to ask: what are the 'rotational' symmetries of the Hamiltonian (3)? The answer may be found by writing  $h$  in the form

$$h = (b+1)(2J+1) + 2(1-b)L_1 + 2cL_3 \quad (13)$$

where

$$J \equiv \frac{1}{4}(p_x^2 + x^2 + p_y^2 + y^2 - 2) \quad (14)$$

is easily verified to be a Casimir operator, i.e.

$$[J, L_i] = 0, \quad i = 1, 2, 3. \quad (15)$$

Moreover, a straightforward calculation yields

$$L_1^2 + L_2^2 + L_3^2 = J(J+1) \quad (16)$$

for the standard quadratic Casimir invariant of the Lie algebra (12). Therefore, the spectrum of  $J$  is well known; it consists of all half integers (greater or equal to zero).

Now, by virtue of (13), the problem would be solved if the spectrum of  $(1-b)L_1 + cL_3$  was known. Since any transformation  $L_1 \rightarrow \alpha L_1 + \beta L_3$ ,  $L_3 \rightarrow -\beta L_1 + \alpha L_3$ ,  $L_2 \rightarrow L_2$  with  $\alpha^2 + \beta^2 = 1$  leaves the commutation relations (12) and the Casimir operator  $L_1^2 + L_2^2 + L_3^2$  invariant, the three generators

$$\mathcal{L}_1 \equiv [cL_1 + (b-1)L_3]/d, \quad \mathcal{L}_2 \equiv L_2, \quad \mathcal{L}_3 \equiv [cL_3 + (1-b)L_1]/d \quad (17)$$

constitute the same Lie algebra as the three  $L_i$ , and preserve the relation (16), i.e.

$$[\mathcal{L}_i, \mathcal{L}_j] = i\hbar \epsilon_{ijk} \mathcal{L}_k; \quad \mathcal{L}_1^2 + \mathcal{L}_2^2 + \mathcal{L}_3^2 = J(J+1) \quad (18)$$

as long as  $d$  is one of the roots of the equation

$$d^2 = c^2 + (1-b)^2. \quad (19)$$

Thus,

$$h = (b+1)(2J+1) + 2d\mathcal{L}_3 \quad (20)$$

is invariant with respect to 'rotations' generated by  $\mathcal{L}_3$ :  $[h, \mathcal{L}_3] = 0$ . Choosing the 3-axis as the quantisation axis one has  $\{j, j-1, \dots, -j+1, -j\}$  as the set of possible eigenvalues of  $\mathcal{L}_3$  for any fixed eigenvalue  $j$  of  $J$ . From (20) the spectrum of  $h$  is then given by:

$$\text{spec}[h] = \{(b+1)j + [c^2 + (b-1)^2]^{1/2}l\}, \quad (21)$$

$$j \in \{1, 2, 3, \dots\}, \quad l \in \{j-1, j-3, \dots, -j+3, -j+1\}.$$

The spectrum consists of multiplets numbered by a natural number  $j$ , with multiplicity  $j$ . The level spacing within a multiplet is  $2[c^2 + (b-1)^2]^{1/2}$ ; also the spacing between centre-of-mass position of the multiplet is a constant,  $b+1$ . The levels of neighbouring multiplets do not overlap only if  $j-1 < (b+1)/\{2[c^2 + (b-1)^2]^{1/2}\}$ .

There is an alternative way to arrive at the result (21). It is straightforward and slightly more tedious, but better suited for the determination of wavefunctions. The simple idea is to find the canonical transformation  $\mathbf{U}$  of four-dimensional phase space,  $\mathbf{P}' \equiv (p_x, p_y, x, y)$  ('t' denotes the transposed vector), which diagonalises the quadratic form (3). To be more specific we write (3) in the form

$$h = \mathbf{P}'\mathbf{M}\mathbf{P}, \quad \mathbf{M} = \begin{pmatrix} 1 & 0 & 0 & -c/2 \\ 0 & b & c/2 & 0 \\ 0 & c/2 & 1 & 0 \\ -c/2 & 0 & 0 & b \end{pmatrix} \quad (22)$$

and diagonalise  $\mathbf{M}$ . One finds that the orthogonal matrix

$$\mathbf{U} = (s_+ - s_-)^{-2} \begin{pmatrix} 1 & 1 & -s_+ & -s_- \\ -1 & 1 & -s_- & s_+ \\ s_+ & s_- & 1 & 1 \\ s_- & -s_+ & -1 & 1 \end{pmatrix} \quad (23)$$

with the abbreviations

$$cs_{\pm} \equiv b-1 \pm d \quad (24)$$

diagonalises  $\mathbf{M}$ :

$$\text{diag}[\mathbf{U}\mathbf{M}\mathbf{U}'] = \frac{1}{2}(1+b-d, 1+b+d, 1+b-d, 1+b+d). \quad (25)$$

Here  $d$  denotes the positive root of (19). In terms of the rotated operators  $\mathbf{P}' = \mathbf{U}\mathbf{P}$  the Hamiltonian  $h$  may therefore be written

$$h = \frac{1}{2}(cs_- + 2)(p_x'^2 + x'^2) + \frac{1}{2}(cs_+ + 2)(p_y'^2 + y'^2). \quad (26)$$

Since the transformation is canonical (i.e.  $[x', p_x'] = i\hbar$ ,  $[x', p_y'] = 0$  etc.)  $h$  is simply identified as the linear superposition of two independent harmonic oscillators. Its spectrum may therefore be written

$$\text{Spec}[h] = \{(b+1)(n_x + n_y + 1) + d(n_y - n_x)\}, \quad n_{x,y} \in \{0, 1, 2, \dots\}. \quad (27)$$

Of course, (27) is identical to (21), one only needs to identify  $j = n_x + n_y + 1$  and  $l = n_y - n_x$ .

Wavefunctions may now be constructed as usual by applying the appropriate number of creation operators  $a_{x,y}^{\dagger}$  to the ground state  $\psi'_{00}$  which is identical to the unprimed ground state determined by  $a_{x,y}\psi_{00} = 0$ .

Finally, let us translate the solution back to the original physical problem (8). By (21) and (10) the energy levels of  $H_2$  can be written as

$$\varepsilon_{jl} = G + \frac{1}{2}[\omega_c^2 + (\Omega_1 + \Omega_2)^2]^{1/2}j + \frac{1}{2}[\omega_c^2 + (\Omega_1 - \Omega_2)^2]^{1/2}l, \quad (28)$$

where again  $j \in \{1, 2, \dots\}$  and  $l \in \{j-1, j-3, \dots, -j+1\}$ .

## References

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