

Comments

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Comment on “Coulomb-diamagnetic problem in two dimensions”

R. K. Pandey and V. S. Varma

Department of Physics and Astrophysics, University of Delhi, Delhi 110 007 India

(Received 10 October 1989)

It is shown that the conjecture proposed in a recent communication [Chhajlany, Mal'nev, and Kumar, Phys. Rev. A **39**, 5082 (1989)] regarding energy eigenvalues of the Coulomb-diamagnetic problem in two dimensions is not correct because it leads to non-normalizable solutions. Their results (i) disagree with an exact solution of the problem that exists for a specific relation between the associated coupling constants, (ii) disagree with the eigenvalues calculated by the method of Hill determinants for arbitrary values of these couplings, and (iii) violate strict variational upper bounds. We are able to verify numerically that the energy levels of the system calculated by the method of Hill determinants do indeed show a $3\hbar\omega_c/2$ spacing near the zero-field ionization threshold.

Recently Chhajlany, Mal'nev, and Kumar¹ (CMK) have reported what they conjecture to be the exact energy eigenvalues of the Coulomb-diamagnetic problem in two dimensions. We wish to point out that their conjecture, although elegant, is not correct. For convenience we shall adopt the same notation as CMK and the reader is referred to that paper for an explanation of the symbols.

Working with two-dimensional cylindrical coordinates, CMK consider the radial equation

$$R'' + (1/\xi)R' + [\gamma - m^2/\xi^2 + \alpha/\xi - \xi^2]R = 0 \quad (1)$$

in terms of the dimensionless radial variable ξ , the other dimensionless variables being related to the energy E , the Rydberg constant \mathcal{R} , and the cyclotron frequency ω_c by

$$\gamma = 4E/(\hbar\omega_c) - 2m, \quad \alpha^2 = 16\mathcal{R}/(\hbar\omega_c). \quad (2)$$

Writing the radial wave function as

$$R(\xi) = \xi^{|m|} \exp(-\xi^2/2) \exp(-\beta\xi) \sum_{n=0}^{\infty} a_n \xi^n, \quad a_0 \neq 0 \quad (3)$$

CMK reduce Eq. (1) to the following four-term recursion relation:

$$n(n+p-1)a_n + [\alpha - \beta(p+2n-2)]a_{n-1} + (\delta + \beta^2 - 2n + 4)a_{n-2} + 2\beta a_{n-3} = 0, \quad (4)$$

where $p = 2|m| + 1$ and $\delta = \gamma - p - 1$. At this stage, they propose a conjecture whose physical basis is never clarified and claim that on requiring the multipliers of a_k and a_{2k} to vanish in (4) above, the energy spectrum of the problem is given by the simple expression

$$E_{km} = (\hbar\omega_c/2)(2k + m + |m| + 1) - \mathcal{R}/(k + |m| + 1/2)^2. \quad (5)$$

The validity of the conjecture seems to hinge on the fact that the energy spectrum (5) coincides with the Coulomb spectrum in the limit $\omega_c \rightarrow 0$ and with the Landau spectrum in the limit $\mathcal{R} \rightarrow 0$, in addition to displaying equal spacing in the limit of large n near the zero-field ionization threshold (for which fact there seems to be some experimental evidence²). That the expression for the energy given by Eq. (5) agrees with the expected result in the limits stated above unfortunately cannot ensure that it is correct for all values of ω_c and \mathcal{R} . While the solutions reported by CMK are indeed mathematical solutions of the differential equation (1), in order to assert that they are eigensolutions, we must be able to demonstrate the normalizability of the associated wave functions.

From the recursion relation (4) it is clear that the dominant asymptotic behavior of the ratio of the coefficients is

$$\lim_{n \rightarrow \infty} (a_n/a_{n-1}) \sim (2/n)^{1/2}. \quad (6)$$

This implies that the series $\sum_n a_n \xi^n$ behaves asymptotically as $\exp(\xi^2)$ which renders the radial wave function non-normalizable for arbitrary values of the energy—as indeed should be the case. The two conditions imposed by CMK [that the multipliers of a_k and a_{2k} in (4) vanish for some finite k] do not alter the asymptotic behavior of the coefficients a_n . Hence the solutions of the differential equation (1) associated with the energies (5) for general ω_c and \mathcal{R} will also be non-normalizable.

For a more explicit demonstration that the energy ei-

genvalues of the system are not given by (4), one can construct, for specific relations between the couplings, solutions in which the series $\sum_n a_n \xi^n$ in the wave function terminates for n equal to some N^3 , so that there can be no doubt about the normalizability of such solutions. For this we require $a_{N+1}(\alpha, \delta, \beta) = 0$ and the terms multiplying the coefficients a_{N-1} and a_{N-2} in (4) for $n = N + 2$ to vanish. This implies that $\delta = 2N, \beta = 0$ and ensures that a_{N+1} and all higher coefficients are zero. One can construct an infinite number of such solutions, but for our purposes the simplest will suffice. Thus for $N = 1$ we have $a_2 = 0$ and $\delta = 2$ with $\beta = 0$. This yields $\mathcal{R}/(\hbar\omega_c) = (2|m| + 1)/8$ for which

$$R_{1m}(\xi) = \{1 - 4[\mathcal{R}/(\hbar\omega_c)]^{1/2} \xi / (2|m| + 1)\} \xi^{|m|} \times \exp(-\xi^2/2) \quad (7)$$

and

$$\epsilon_{1m} = (m + |m| + 2)\hbar\omega_c/2. \quad (8)$$

Notice that the solutions carry the subscripts 1 as they possess one node since the wave functions $R_{1m}(\xi)$ vanish at $\xi = (2|m| + 1)(\hbar\omega_c/\mathcal{R})^{1/2}/4$. One can verify by direct substitution that (7) and (8) are indeed solutions of (1). The corresponding CMK energies for $\mathcal{R}/(\hbar\omega_c) = (2|m| + 1)/8$ are given by

$$E_{1m} = [(|m| + m + 3) - (2|m| + 1)/(2|m| + 3)^2] \hbar\omega_c/2. \quad (9)$$

Clearly the CMK conjecture does not agree with Eq. (8) and must therefore be wrong.

For general values of \mathcal{R} and ω_c there are, of course, a number of numerical techniques for calculating eigenvalue spectra. In the present case we choose the method of Hill determinants⁴ (HD). The normalizability of the solutions generated by this method have recently been established.⁵ The energies of the two of the lowest states calculated by the HD method for $m = 0$ and in units of $\hbar = \mu = c = 1$ are shown in Fig. 1 as solid lines. The CMK results are shown as dashed lines for comparison. The energies have been plotted as functions of ω_c and \mathcal{R} , which for convenience have been constrained by the relation $\omega_c + \mathcal{R} = 10$. On comparison we notice that the HD and CMK results agree with each other only in the limits when either $\omega_c \rightarrow 0$ or $\mathcal{R} \rightarrow 0$. Notice that whereas Eq. (4) suggests a linear dependence of the energy on ω_c and \mathcal{R} , the HD results are curves which always lie below the straight lines given by Eq. (5). However, numerical calculations show that the CMK results come closer to the HD values as we go to higher and higher values of the excitation quantum number.

We have also checked that the exact solution for the first excited state energy as given by (8) is $\epsilon_{10} = \frac{80}{9}$ for $\omega_c = \frac{80}{9}$ and $\mathcal{R} = \frac{10}{9}$. The HD result agrees to 16 significant places. The corresponding CMK result, as given by Eq. (9), is $E_{10} = \frac{1040}{81}$.

To put the issue completely beyond doubt, we carry out a variational calculation for the two lowest energy levels for a given m . The purpose is to show that the

CMK results violate the strict variational upper bounds and must therefore be unequivocally ruled out.

We choose as our trial functions

$$\psi_1(\xi) = \xi^{|m|} \exp(-\xi^2/2),$$

$$\psi_2(\xi) = \xi^{|m|+1} \exp(-\xi^2/2),$$

and carry out a standard two-parameter linear variation calculation for the energy levels. We obtain a quadratic equation for the dimensionless variable γ which for $m = 0$ is given by

$$(1 - \pi/4)\gamma^2 - (5 - \pi - \sqrt{\pi}\alpha/2)\gamma + 6 - \pi - 2\sqrt{\pi}\alpha + (\pi/2 - 1)\alpha^2 = 0.$$

We choose $m = 0$ in order to make contact with the Hill determinant calculations reported above. The lower root of this equation provides an upper bound to the ground-state energy and the larger root an upper bound to the first excited state energy of the system.⁶ These are also plotted in Fig. 1 as dotted curves and it is evident that both these bounds are violated by the CMK results, demonstrating explicitly that the CMK results cannot be correct. The HD results are always less than or equal to the variational bounds. At $\omega_c = \frac{80}{9}$ and $\mathcal{R} = \frac{10}{9}$, both the variational and HD results for the first excited state agree with the exact result $\frac{80}{9}$ given by (8) to 16 significant places.

Thus the energy eigenvalues of the Coulomb-

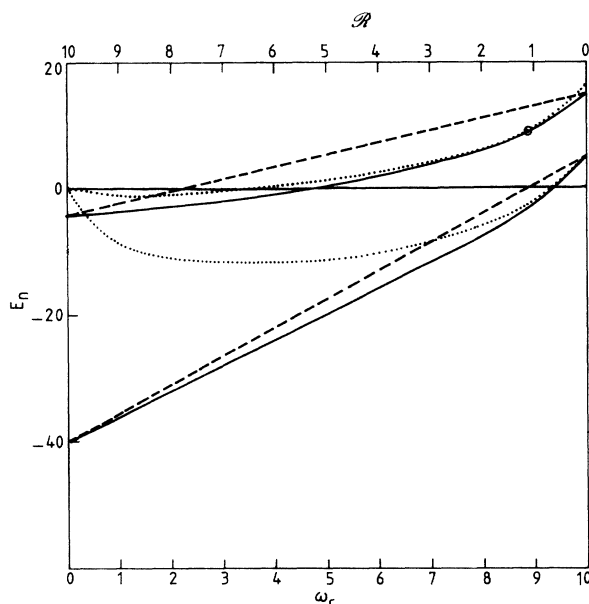


FIG. 1. Energies of the two lowest states of the Coulomb-diamagnetic problem as given (i) by CMK (shown as dashed lines), (ii) by HD calculations (shown as solid curves), and (iii) by variational calculations which provide strict upper bounds (shown as dotted lines) are plotted (for $m = 0$ and in units of $\hbar = \mu = c = 1$) as function of ω_c (\mathcal{R} being constrained by the relation $\omega_c + \mathcal{R} = 10$). An exact solution has also been indicated.

diamagnetic problem in two dimensions are clearly not linear functions of the cyclotron frequency ω_c and the Rydberg constant \mathcal{R} as conjectured by CMK, although the departure from linearity becomes progressively smaller for increasing values of the principal quantum number.

Finally we address ourselves to the question of the equal spacing of energy levels near the zero-field ionization threshold. Here two findings are significant. Our numerical calculations show that the levels calculated by the HD method do indeed show equal separation of $3\hbar\omega_c/2$ near zero energy in this limit. We have also

found that the CMK results approach more and more closely the energy levels calculated by the HD method in the limit of large n —the principal quantum number. Thus the equal spacing of energy levels near the zero-field ionization threshold that CMK demonstrate to be true for their conjecture cannot be taken as evidence that their results are correct, rather they are a consequence of the fact that the CMK results approach the actual levels more and more closely in the limit $n \rightarrow \infty$. Details of these calculations and a discussion of other features of this system will be reported in a separate communication.

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