Nonsensical models for quantum dots

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November 18, 2009

Abstract

We analyze a model proposed recently for the calculation of the energy of an exciton in a quantum dot and show that the authors made a serious mistake in the solution to the Schrödinger equation.

Not long ago Hassanabadi and Rajabi [1] proposed a simple model for a spherical quantum dot. They treated the nonrelativistic Schrödinger equation with a phenomenological potential as a quasi–exactly solvable problem so that the model parameters had to depend on the given state of the system. Although they imported particle masses, excitation energies and other model parameters from experimental data, they never contrasted their model outputs with actual experiments. More precisely, they calculated model properties and never compared them with independent physical data although they stated mischievously otherwise. Worst of all, they wrongly calculated
the excitation energy of the quantum dot by subtracting the ground state of one model from the excited state of a quite different one. Their mistake was based on the fact that their model parameters depended on the state of the problem as we already disclosed in a later comment [2].

Recently, Hassanabadi and Zarrinkamar [3] came back with a new model for the exciton in a quantum dot that we analyze in what follows.

The authors chose the nonrelativistic Hamiltonian

\[ \hat{H} = \sum_{i=e,h} \left( \frac{p_i^2}{2m_i} + \frac{1}{2}m_i\omega_0^2r_i^2 \right) - \frac{e^2}{\varepsilon|\mathbf{r}_e - \mathbf{r}_h|} \]  

(1)

where the subscripts \( e \) and \( h \) stand for the electron and the hole, respectively, and the motion is in the plane [3].

The Schrödinger equation for this problem is separable in the center of mass \( \mathbf{R} = (m_e\mathbf{r}_e + m_h\mathbf{r}_h)/(m_e + m_h) \) and relative \( \mathbf{r} = \mathbf{r}_e - \mathbf{r}_h \) coordinates and we are left with the eigenvalue equations

\[ \left( \frac{p_R^2}{2M} + \frac{1}{2}M\omega_0^2R^2 \right) Q = E_R Q \]

\[ \left( \frac{p_r^2}{2\mu} + \frac{1}{2}\mu\omega_0^2r^2 - \frac{e^2}{\varepsilon r} \right) \psi = E_r \psi \]  

(2)

where \( \mu = m_e m_h / M \) and \( M = m_e + m_h \) are the reduced and total masses, respectively. Notice the misprint in their equation (6). The first equation is just a harmonic oscillator that we do not discuss any further and the second one is separable in spherical coordinates \( \psi(\mathbf{r}) = \Phi(r)e^{im\phi} \), where \( m = 0, \pm 1, \ldots \) is the angular quantum number. On comparing their equations (8) and (9) one has the impression that the authors carried out this separation without being clearly aware of it [3].
The radial part is a solution to [3]

\[ \Phi'' + \frac{1}{r} \Phi' - \frac{m^2}{r^2} \Phi + \alpha \Phi - \beta r^2 \Phi + \frac{\gamma'}{r} \Phi = 0 \] (3)

where \( \alpha = 2\mu E_r / h^2 \), \( \beta = \mu^2 \omega_0^2 / h^2 \) and \( \gamma = 2\mu e^2 / (h^2 \varepsilon) \). This equation is not exactly solvable as everybody (except the authors) knows.

Hassanabadi and Zarrinkamar [3] proposed the ansatz

\[ \Phi(r) = r^m e^{-\sqrt{\beta} r^2 / 2} \sum_{n=0}^{\infty} a_n r^n \] (4)

and derived a recurrence relation for the coefficients that should read

\[
\begin{align*}
    a_0 &= 1 \\
    a_1 &= -\frac{\gamma}{2m + 1} \\
    a_{n+2} &= \frac{\left[2\sqrt{\beta}(m + n + 1) - \alpha\right] a_n - \gamma a_{n+1}}{(n + 2)(2m + n + 2)}
\end{align*}
\] (5)

Notice that there is a misprint in the denominator of their equation (17c).

At this point the authors treated this problem as if it were the textbook harmonic oscillator or hydrogen atom and based on the argument that “the series must be bounded for \( n = n_r \)” they chose

\[ \alpha = 2\sqrt{\beta}(m + n_r + 1) - \gamma \frac{a_{n_r+1}}{a_{n_r}} \] (6)

and supposedly obtained the exact energies and wavefunctions

\[ E_{0,m} = 2\hbar \omega_0 (m + 1) + \frac{4\mu e^4}{\varepsilon h^2 (2m + 1)} \] (7)

\[ \Phi_{0,m}(r) = N_{0m} r^m e^{-\sqrt{\beta} r^2 / 2} \left(1 - \frac{\gamma r}{2m + 1}\right) \] (8)
respectively, for $n_r = 0$. However, the reader may verify that $\Phi_{0,m}(r)$ is not a solution to Eq. (3) unless the additional condition

$$2\sqrt{\beta}(2m + 1) - \gamma^2 = 0$$

is satisfied.

As we said above, this model is not exactly solvable. However, one can obtain solutions for particular values of the model parameters with the well known consequence that they have to depend on the quantum numbers of the chosen state. We already discussed this feature of quasi–exactly solvable problems in our earlier criticism of the Hassanabadi and Rajabi’s paper [2] but the former author did not appear to take notice. Under such conditions the energy should be

$$E_{0,m} = \hbar\omega_0(m + 2)$$

We can easily trace the mistake in Hassanabadi and Zarrinkamar’s reasoning to the fact that Eq. (5) is a three–term recurrence relation. Therefore, the condition $a_{n_r+2} = 0$ alone is insufficient to force $a_j = 0$ for $j > n_r + 2$ as in the well known cases of the pure harmonic or Coulomb interactions. In order to have an exact solution we should set the model parameters so that $a_{n_r+2} = 0$ and $a_{n_r+3} = 0$ which accounts for the additional condition (9) in the particular case $n_r = 0$.

In addition to what has been said, notice that the wavefunction $\Phi_{0,0}(r)$ with $m = 0$

$$\Phi_{0,0}(r) = N_0 e^{-\sqrt{\beta}r^2/2}(1 - \gamma r)$$

exhibits a node, as shown in their Fig. 2 [3], and therefore it cannot be part of a ground state. In other words, the authors failed to obtain the ground–state
wavefunction of their model.

We conclude that all the results obtained by Hassanabadi and Zarrinkamar [3] from “the elegant idea of series method” are based on wrong equations and therefore completely useless. Even if they had not made the mistakes just indicated their results would have been utterly useless because they never tested the output of their model. They were satisfied with the calculation of an “exciton energy for various states” that are mere numbers without any meaning.

It is also curious that the authors stated that “the results are comparable to those of variational exact diagonalization, full configuration interaction, Hartree–Fock and 1/N methods”. However, they did not provide any reference or comparison to support their claims. If the authors had tried any such comparison they would have probably realized their mistake. Besides, it is not clear to us what they meant for full configuration interaction and Hartree–Fock with respect to their fully separable model.

The authors also claimed that their approach “could be fitted for any desired material” meaning that they input some experimental data and output results that they never compared with independent data. Nowadays, this strategy seems to be sufficient for publishing a paper in certain journals [1,3].

The reader may wonder why a supposedly respectable journal published such a paper. Well, that journal has a long history of publishing wrong, nonsensical and ridiculous papers as we have already denounced in earlier articles [4–11]. You may find, for example, solutions to the linear and nonlinear Schrödinger equation that are not square integrable, power series expansion of well known functions that are unphysical solutions to physical or
unphysical equations, useless power series approaches to models for non-linear dynamics, and many other such horrific examples [4–11]. The editors and referees of that journal are satisfied, for example, with a model for a prey–predator system that predicts a negative number of rabbits [7].

References

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