Physica Scripta

COMMENT

Comment on Inverse problem from discrete spectrum in the $D = 2$ dimensional space (2014 *Phys. Scr.* **89** 085201)

Francisco M Fernández

INIFTA, División Química Teórica, Blvd. 113 S/N, Sucursal 4, Casilla de Correo 16, 1900 La Plata, Argentina

E-mail: fernande@quimica.unlp.edu.ar

RECEIVED
4 May 2021

REVISED
15 September 2021

ACCEPTED FOR PUBLICATION
13 January 2022

PUBLISHED
3 February 2022

Abstract

We analyse a method for the construction of the potential-energy function from the moments of the ground-state density. The sum rule on which some expressions are based appear to be wrong, as well as the moments and potential-energy functions derived for some illustrative examples.

Some time ago Lombard and Yekken [1] (LY from now on) studied the possibility of constructing the potential-energy function of a quantum-mechanical system from its discrete spectrum. The proposed method is based on the moments of the ground-state density and the main equation stems from a suitable sum rule. The purpose of this Comment is the analysis of the sum rule and some of the results that LY derived from it.

LY restricted their study to a nonrelativistic quantum-mechanical problem in two dimensions with a central-field potential $V(r)$ and chose the dimensionless Hamiltonian operator

$$H = T + V(r), \quad T = -\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}, \tag{1}$$

in polar coordinates (r, ϕ), where $\hbar = 2$ and $M = 1$, the latter being the particle mass. It is worth mentioning that there is a simple and rigorous way to derive dimensionless physical equations that make this process clearer [2].

In what follows the eigenvectors of this operator are denoted $|n,\ m\rangle$, where $n = 1, 2, \ldots$ and $m = 0, \pm 1, \pm 2, \ldots$ are the radial and angular-momentum quantum numbers, respectively. We find this choice more convenient than the notation $m = |m| = 1, 2, \ldots$ followed by LY. In the coordinate representation these bound states can be written

$$\langle \mathbf{r}|n,\ m\rangle = \psi_{n,m}(\mathbf{r}) = R_{n,m}(r)\frac{e^{im\phi}}{\sqrt{2\pi}}, \tag{2}$$

because the Schrödinger equation is separable.

If A is a linear operator it is not difficult to prove that

$$\langle 1,\ 0|[[H,\ A],\ A]|1,\ 0\rangle = 2\sum_{n=1}^{\infty}\sum_{m=-\infty}^{\infty}(E_{1,0} - E_{n,m})\ |\langle n,\ m|\ A|1{,}0\rangle|^2, \tag{3}$$

where $[A, B] = AB - BA$ is the well known quantum-mechanical commutator. For the particular case

$$A = r^j e^{ik\phi},\ j = 0,\ 1,\ldots,\ k = 0,\ \pm 1,\ldots, \tag{4}$$

we have $\langle n,\ m|\ A|1,\ 0\rangle = 0$ for all $m \neq k$. On the other hand, it follows from the double commutator

$$[[H,\ A],\ A] = 2e^{2ik\phi}r^{2j-2}(k^2 - j^2), \tag{5}$$

that

$$\langle 1,\ 0|[[H,\ A],\ A]|1,\ 0\rangle = 2(k^2 - j^2)\delta_{k,0}\langle 1,\ 0|\ r^{2j-2}\ |1{,}0\rangle_r, \tag{6}$$

where the $\langle\rangle_r$ means that the integral in the matrix element is carried out only over the radial variable. The resulting sum rule

$$\sum_{n=1}^{\infty}(E_{1,0}-E_{n,k})\,|\langle n,\,k|\,A|1,0\rangle|^2=(k^2-j^2)\delta_{k,0}\langle 1,\,0|\,r^{2j-2}\,|1,0\rangle_r, \tag{7}$$

yields a nontrivial result only for $k=0$

$$\sum_{n=1}^{\infty}(E_{n,0}-E_{1,0})\,|\langle n,\,0|\,r^j\,|1,0\rangle_r|^2=j^2\langle 1,\,0|\,r^{2j-2}\,|1,0\rangle_r. \tag{8}$$

Several results in LY's paper appear to be wrong. First, the term $-\phi^2$ is not expected in the double commutator in LY's equation (6). On assuming that this is a typo, the expectation value of LY's equation (6) reads $2m^2\langle 1,\,0|\,r^{2m-2}e^{\pm 2im\phi}|1,\,0\rangle=2m^2\langle 1,\,0|\,r^{2m-2}|1,\,\pm 2m\rangle=0$ for all m; therefore, it is not clear where the right-hand side of LY's equation (7) comes from. For this reason, one may doubt about all the equations stemming from the LY's sum rule (7). The correct sum rule is given by present equations (7) or (8).

In the first illustrative example, LY derived the potential-energy function consistent with the ground state

$$\psi_{1,0}=(1+br)e^{-ar^2/2}. \tag{9}$$

Present result

$$\psi_{1,0}^{-1}T\psi_{1,0}=\frac{b^2-2a}{br+1}-a^2r^2-\frac{b}{r}+4a, \tag{10}$$

is in disagreement with LY's potential (17) and their energy $E_{1,0}=2a$. The expectation value

$$\langle r^{2m}\rangle=\frac{2\sqrt{a}\;b\Gamma(m+3/2)+[a+b^2(m+1)]\Gamma(m+1)}{a^m(a+\sqrt{\pi}\,\sqrt{a}\;b+b^2)}, \tag{11}$$

calculated with the function (9) does not agree with the one in LY's equation (18). In our opinion, LY's potential-energy function (21) is not consistent with their proposed bound state (20).

LY showed some results from an iterative method for the construction of the potential-energy function for some illustrative examples. It is not clear to us if they were obtained from the apparently wrong expressions just discussed.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

Francisco M Fernández https://orcid.org/0000-0003-0393-790X

References

[1] Lombard R J and Yekken R 2014 *Phys. Scr.* **89** 085201
[2] Fernández F M 2020 Dimensionless equations in non-relativistic quantum mechanicsarXiv:2005.05377