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ON DEPENDENCE OF ENERGY EIGEN VALUE ON THE ENDS OF THE INTERVAL

Abstract

Differentiability of the eigenvalue of energy with respect to the ends of the interval is investigated by the motion of the particle in the neutral field and the formula is obtained for its derivative. Using this, some important properties of the eigenvalue of the energy are revealed and a formula is obtained for it.

1. Introduction. The problem on the motion of a particle in the central field was one of the important ones in the course of the history of development of quantum mechanics since in the special Coulomb field this problem is about the hydrogen atom.

The central force field is characterized by the fact that potential energy of a particle in such a field depends only on its distance r from some center (force center). Behavior in the central force field forms foundation of atomic mechanics: the solution of the general problem on the motion of electrons in the atom is based in this or other degree on the results relating to the motion of one particle in the central force field.

There are a lot of papers devoted to the calculation of the spectrum for different fields within the bounds of non-relativistic quantum mechanics. This problem is of practical interest in the semiconductor physics in discussing quantum systems with single and multiple potential well.

In the relativistic quantum mechanics, the motion of the electron in spherically symmetric fields was investigated to the end only for the case of free particle, Coulomb fields, for the field of magnetic monopole, and combination of these fields [1-4]. Other fields allowing exact solutions in the explicit form have not been found yet [5-7].

Recently, different properties of the quantum point situated in the external potential field are under the great attention [8, 9].

From this point of view it would be very interesting to study the properties and behavior of energy values with respect to some parameter [10, 11]. In the present paper, change of the eigen values of energy with respect to the ends of the interval is studied. The expression for its derivative is found and using this, the formula for these eigen values is obtained.

2. Problem statement. It is known that the motion of a particle in the central field is described by the equation

$$-\frac{a}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{bR}{r^2} + q(r) R = ER,$$

where a and b are constants, $q(r)$ is interaction energy.

Multiplying this equation by r , we get

$$-a \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + Q(r) R = Er^2 R. \quad (2.1)$$

Here

$$Q(r) = b + q(r)r^2.$$

If we consider equation (2.1) on the bounded interval $[s_1, s_2]$, $0 < s_1 < s_2$ with the boundary condition

$$R(s_1) = 0, \quad R(s_2) = 0, \quad (2.2)$$

we get a spectral problem. In this case the eigen values of energy will depend on $s = (s_1, s_2)$ i.e. $E = E(s) = E(s_1, s_2)$. Study of this dependence and investigation of extremal properties with respect to change of the interval $[s_1, s_2]$ is of great interest from the practical point of view.

3. Calculation of the derivative of energy eigen-values. It is known that [13, p. 20] the energy eigen-values are calculated as follows:

$$E(s) = \inf_R \frac{J_1(s)}{J_2(s)}, \quad (3.1)$$

where

$$J_1(s) = \int_{s_1}^{s_2} \left[ar^2 \left(\frac{dR}{dr} \right)^2 + Q(r) R^2 \right] dr, \quad (3.2)$$

$$J_2(s) = \int_{s_1}^{s_2} r^2 R^2(r) dr. \quad (3.3)$$

Here inf is taken over all the functions $R \in C^2(s_1, s_2)$, satisfying boundary condition (2.2). Relation (3.1) determines $E(s)$ as a function dependent on $s = (s_1, s_2)$. Denote $S = \{s = (s_1, s_2) \in \mathbb{R}^2 : 0 < s_1 < s_2 < +\infty\}$.

Theorem 1. *The function $E = E(s_1, s_2)$ is differentiable with respect to s_1 and s_2 on S , and the following formula is valid*

$$\begin{aligned} \frac{\partial E}{\partial s_1} &= as_1^2 \left(\frac{\partial R(s_1)}{\partial r} \right)^2, \\ \frac{\partial E}{\partial s_2} &= -as_2^2 \left(\frac{\partial R(s_2)}{\partial r} \right)^2. \end{aligned} \quad (3.4)$$

Here $R = R(r)$ is a normalized eigen-function, i.e.

$$\int_{s_1}^{s_2} r^2 R^2(r) dr = 1.$$

Proof. Take any couples $\bar{s} = (\bar{s}_1, \bar{s}_2) \in S$, $s = (s_1, s_2) \in S$. Denote

$$\tilde{s}_1 = \max\{s_1, \bar{s}_1\}, \quad \tilde{s}_2 = \min\{s_2, \bar{s}_2\}.$$

Calculate the increment of the functional (3.1). For that at first we calculate the increment of the functional J_1 ([12, p. 182]).

$$\Delta J_1 \equiv J_1(\bar{s}) - J_1(s) = \int_{\tilde{s}_1}^{\tilde{s}_2} \left[ar^2 \left(\frac{d\bar{R}}{dr} \right)^2 + Q(r) \bar{R}^2 \right] dr -$$

$$- \int_{s_1}^{s_2} \left[ar^2 \left(\frac{dR}{dr} \right)^2 + Q(r) R^2 \right] dr.$$

For simplicity of the statement we denote

$$A(R) = ar^2 \left(\frac{dR}{dr} \right)^2 + Q(r) R^2. \quad (3.5)$$

Then

$$\begin{aligned} \Delta J_1 \equiv & \left[\int_{\tilde{s}_1}^{\tilde{s}_2} A(\bar{R}) dr - \int_{\tilde{s}_1}^{\tilde{s}_2} A(\bar{R}) dr \right] + \left[\int_{\tilde{s}_1}^{\tilde{s}_2} A(\bar{R}) dr - \int_{\tilde{s}_1}^{\tilde{s}_2} A(\bar{R}) dr \right] + \\ & + \left[\int_{\tilde{s}_1}^{\tilde{s}_2} A(R) dr - \int_{s_1}^{s_2} A(R) dr \right]. \end{aligned}$$

It is clear that

$$\int_{\tilde{s}_1}^{\tilde{s}_2} A(\bar{R}) dr - \int_{\tilde{s}_1}^{\tilde{s}_2} A(\bar{R}) dr = A(\bar{R}(\tilde{s}_2)) (\tilde{s}_2 - \tilde{s}_2) - A(\bar{R}(\tilde{s}_1)) (\tilde{s}_1 - \tilde{s}_1) + o(\|\Delta s\|),$$

where

$$\|\Delta s\| = \sqrt{|\Delta s_1|^2 + |\Delta s_2|^2}.$$

Taking this into account, we have

$$\begin{aligned} \Delta J_1 = & \int_{\tilde{s}_1}^{\tilde{s}_2} A(R) dr + A(\bar{R}(\tilde{s}_2)) (\tilde{s}_2 - \tilde{s}_2) - A(\bar{R}(\tilde{s}_1)) (\tilde{s}_1 - \tilde{s}_1) + \\ & + A(R(\tilde{s}_2)) (\tilde{s}_2 - s_2) - A(R(\tilde{s}_1)) (\tilde{s}_1 - s_1) + o(\|\Delta s\|). \end{aligned}$$

Here

$$\Delta A(R) = A(\bar{R}) - A(R).$$

Taking into attention expression (3.5), we get

$$\Delta A(R) = 2ar^2 \frac{dR}{dr} \frac{d\Delta R}{dr} + 2Q(r) R\Delta R + 2ar^2 \left(\frac{d\Delta R}{dr} \right)^2 + 2Q(r) (\Delta R)^2.$$

Here $\Delta R = \bar{R} - R$.

Then

$$\begin{aligned} \Delta J_1 = & 2 \int_{\tilde{s}_1}^{\tilde{s}_2} \left[ar^2 \frac{dR}{dr} \frac{d\Delta R}{dr} + 2Q(r) R\Delta R \right] dr + \\ & + A(R(\tilde{s}_2)) (\tilde{s}_2 - s_2) - A(R(\tilde{s}_1)) (\tilde{s}_1 - s_1) + \\ & + A(R(\tilde{s}_2)) (\tilde{s}_2 - s_2) - A(R(\tilde{s}_1)) (\tilde{s}_1 - s_1) + \delta_1(\Delta s, \Delta R). \end{aligned} \quad (3.6)$$

Here

$$\begin{aligned} & \delta(\Delta s, \Delta u) [A(\bar{R}(\tilde{s}_2)) - A(R(\tilde{s}_2))] (\bar{s}_1 - \tilde{s}_1) - \\ & - [A(\bar{R}(\tilde{s}_1)) - A(R(\tilde{s}_1))] (\bar{s}_1 - \tilde{s}_1) + 2ar^2 \left(\frac{d\Delta R}{dr}\right)^2 + 2Q(r) (\Delta R)^2. \end{aligned}$$

It is clear from (3.6) that

$$\begin{aligned} \Delta J_1 = & 2 \int_{\tilde{s}_1}^{\tilde{s}_2} \left[a \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - Q(r) R \right] \Delta R dr + 2ar^2 \frac{dR}{dr} \Delta R \Big|_{\tilde{s}_1}^{\tilde{s}_1} + \\ & + A(R(\tilde{s}_2)) (\bar{s}_2 - s_2) - A(R(\tilde{s}_1)) (\bar{s}_1 - s_1) + \delta_1(\Delta s, \Delta R). \end{aligned} \tag{3.7}$$

Considering that $R = R(r)$ satisfies equation (2.1), we have

$$\begin{aligned} \Delta J_1 = & 2 \int_{\tilde{s}_1}^{\tilde{s}_2} Er^2 R \Delta R dr + J_{11} + J_{12} + A(R(\tilde{s}_2)) (\bar{s}_2 - s_2) - \\ & - A(R(\tilde{s}_1)) (\bar{s}_1 - s_1) + \delta_1(\Delta s, \Delta R), \end{aligned} \tag{3.8}$$

where

$$\begin{aligned} J_{11} &= -2a\tilde{s}_1^2 \frac{dR(\tilde{s}_1)}{dr} \Delta R(\tilde{s}_1), \\ J_{12} &= 2a\tilde{s}_2^2 \frac{dR(\tilde{s}_2)}{dr} \Delta R(\tilde{s}_2). \end{aligned}$$

Taking into account boundary conditions (2.2), we calculate $\Delta R(\tilde{s}_1)$ and $\Delta R(\tilde{s}_2)$.

$$\begin{aligned} \Delta R(\tilde{s}_1) &= \bar{R}(\tilde{s}_1) - R(\tilde{s}_1) = [\bar{R}(\tilde{s}_1) - \bar{R}(\bar{s}_1)] + [R(s_1) - R(\tilde{s}_1)] = \\ &= \frac{d\bar{R}(\tilde{s}_1)}{dr} (\bar{s}_1 - \tilde{s}_1) = \frac{dR(\tilde{s}_1)}{dr} (\bar{s}_1 - \tilde{s}_1) + \frac{dR(\tilde{s}_1)}{dr} (s_1 - \tilde{s}_1) - \\ &- \frac{d\Delta R(\tilde{s}_1)}{dr} (\bar{s}_1 - \tilde{s}_1) = \frac{dR(\tilde{s}_1)}{dr} (\bar{s}_1 - s_1) - \frac{d\Delta R(\tilde{s}_1)}{dr} (\bar{s}_1 - \tilde{s}_1). \end{aligned}$$

Similarly,

$$\Delta R(\tilde{s}_2) = -\frac{dR(\tilde{s}_2)}{dr} (\bar{s}_1 - s_1) - \frac{d\Delta R(\tilde{s}_2)}{dr} (\bar{s}_1 - \tilde{s}_1).$$

Taking this into account in the expression of the functions J_{11} and J_{12} we get

$$\begin{aligned} J_{11} &= 2a\tilde{s}_1^2 \left(\frac{dR(\tilde{s}_1)}{dr}\right)^2 (\bar{s}_1 - s_1) + 2a\tilde{s}_1^2 \frac{dR(\tilde{s}_1)}{dr} (\bar{s}_1 - \tilde{s}_1). \\ J_{12} &= -2a\tilde{s}_2^2 \left(\frac{dR(\tilde{s}_2)}{dr}\right) (\bar{s}_2 - s_2) - 2a\tilde{s}_2^2 \frac{d\Delta R(\tilde{s}_2)}{dr} (\bar{s}_2 - \tilde{s}_2). \end{aligned}$$

Substituting the obtained expressions J_{11} , J_{12} in (38), we have

$$\Delta J_1 = 2 \int_{\tilde{s}_1}^{\tilde{s}_2} Er^2 R \Delta R dr + 2a\tilde{s}_1^2 \left(\frac{dR(\tilde{s}_1)}{dr}\right)^2 (\bar{s}_1 - s_1) -$$

$$\begin{aligned}
 & -2a\tilde{s}_2^2 \left(\frac{dR(\tilde{s}_2)}{dr} \right)^2 (\bar{s}_2 - s_2) + \\
 & + A(R(\tilde{s}_2))(\bar{s}_2 - s_2) - A(R(\tilde{s}_1))(\bar{s}_1 - s_1) + \delta_2(\Delta s, \Delta R), \quad (3.9)
 \end{aligned}$$

where

$$\delta_2(\Delta s, \Delta R) = \delta_1(\Delta s, \Delta R) - 2as_1^2 \frac{d\Delta R(\tilde{s}_1)}{dr} (\bar{s}_1 - \tilde{s}_1) - 2a\tilde{s}_2^2 \frac{d\Delta R(\tilde{s}_2)}{dr} (\bar{s}_2 - \tilde{s}_2).$$

Passing from the point \tilde{s}_1, \tilde{s}_2 to s_1, s_2 , we have

$$\begin{aligned}
 \Delta J_1 = & 2 \int_{s_1}^{s_2} Er^2 R \Delta R dr + 2as_1^2 \left(\frac{dR(s_1)}{dr} \right) (\bar{s}_1 - s_1) - \\
 & - 2a\tilde{s}_2^2 \left(\frac{dR(\tilde{s}_2)}{dr} \right)^2 (\bar{s}_2 - s_2) + \\
 & + A(R(s_2))(\bar{s}_2 - s_2) - A(R(s_1))(\bar{s}_1 - s_1) + \delta_3(\Delta s, \Delta R), \quad (3.10)
 \end{aligned}$$

Here

$$\begin{aligned}
 \delta_3(\Delta s, \Delta R) = & \delta_2(\Delta s, \Delta R) + \int_{\tilde{s}_1}^{\tilde{s}_2} Er^2 R \Delta R dr - \int_{s_1}^{s_2} Er^2 R \Delta R dr + \\
 & + 2 \left[a\tilde{s}_1^2 \left(\frac{dR(\tilde{s}_1)}{dr} \right)^2 - as_1^2 \left(\frac{dR(s_1)}{dr} \right)^2 \right] (\bar{s}_1 - s_1) - \\
 & - 2 \left[a\tilde{s}_2^2 \left(\frac{dR(\tilde{s}_2)}{dr} \right)^2 - as_2^2 \left(\frac{dR(s_2)}{dr} \right)^2 \right] (\bar{s}_2 - s_2) + \\
 & + [A(R(\tilde{s}_2)) - A(R(s_2))](\bar{s}_2 - s_2) - [A(R(\tilde{s}_1)) - A(R(s_1))](\bar{s}_1 - s_1).
 \end{aligned}$$

Now calculate the increment of the function $J_2(s)$:

$$\begin{aligned}
 \Delta J_2 \equiv J_2(\bar{s}) - J_2(s) = & \int_{\bar{s}_1}^{\bar{s}_2} r^2 \bar{R}^2 dr - \int_{s_1}^{s_2} r^2 R^2 dr = \int_{s_1}^{s_2} r^2 R \Delta R dr - \\
 & - s_2^2 R^2(s_2)(\bar{s}_2 - s_2) + s_1^2 R^2(s_1)(\bar{s}_1 - s_1) + o(\|\Delta s\|). \quad (3.11)
 \end{aligned}$$

Denote

$$I(s) = \frac{J_1(s)}{J_2(s)}.$$

Then

$$\delta I(s) = \frac{\delta J_1 J_2 - J_1 \delta J_2}{J_2^2} = \frac{\delta J_1}{J_2} - \frac{J_1}{J_2} \delta J_2.$$

Taking into account (3.1), hence we get

$$\delta I(s) = \frac{1}{J_2} \delta J_1 - E(s) \cdot \delta J_2 \quad (3.12)$$

If we show

$$\delta_3(\Delta s, \Delta R) = o(\|\Delta s\|),$$

from (3.10) we find $\delta J_1(s)$.

To prove this, by the substitution of $\xi = \frac{r-s_1}{s_2-s_1}$ we reduce equation (2.1) to the equation given on the interval $[0, 1]$. The coefficients of this equation depend on s_1, s_2 . Using the results of the work [14] and the form of the function $\delta_3(\Delta s, \Delta R)$, we see

$$\delta_3(\Delta s, \Delta R) = o(\|\Delta s\|).$$

Let $R = R(r)$ be a normalized eigen-function in the domain $[s_1, s_2]$, i.e.

$$J_2(s) = \int_{s_1}^{s_2} r^2 R^2(r) dr = 1. \tag{3.13}$$

Then from (3.12) we have

$$\begin{aligned} \delta I(s) &= 2 \int_{s_1}^{s_2} E r^2 R \Delta R dr - 2 a s_1^2 \left(\frac{dR(s_1)}{dr} \right)^2 (\bar{s}_1 - s_1) - \\ &+ 2 a s_2^2 \left(\frac{dR(s_2)}{dr} \right)^2 (\bar{s}_2 - s_2) + A(R(s_2)) (\bar{s}_1 - s_1) - A(R(s_1)) (\bar{s}_1 - s_1) - \\ &- \int_{s_1}^{s_2} E r^2 R \Delta R dr + E \cdot s_2^2 R^2(s_2) (\bar{s}_2 - s_2) + E \cdot s_1^2 R^2(s_1) (\bar{s}_1 - s_1). \end{aligned}$$

Here, taking into account expression (3.5) for $A(R)$, under boundary conditions (2.2) and get the equality

$$\delta I(s) = a s_1^2 \left(\frac{dR(s_1)}{dr} \right)^2 (\bar{s}_1 - s_1) - a s_2^2 \left(\frac{dR(s_2)}{dr} \right)^2 (\bar{s}_2 - s_2).$$

Taking into attention (3.1), hence we get

$$\delta E = a s_1^2 \left(\frac{dR(s_1)}{dr} \right)^2 (\bar{s}_1 - s_1) - a s_2^2 \left(\frac{dR(s_2)}{dr} \right)^2 (\bar{s}_2 - s_2),$$

i.e.

$$\begin{aligned} \frac{\partial E}{\partial s_1} &= a s_1^2 \left(\frac{dR(s_1)}{dr} \right)^2, \\ \frac{\partial E}{\partial s_2} &= -a s_2^2 \left(\frac{dR(s_2)}{dr} \right)^2. \end{aligned}$$

The theorem is proved.

4. Formula for energy eigen-values

From the obtained expressions (3.4) it follows that the energy eigen-values don't decrease with respect to S_1 and don't increase with respect to S_2 . This is directly obtained from the condition

$$\frac{\partial E}{\partial s_1} = as_1^2 \left(\frac{dR(s_1)}{dr} \right)^2 \geq 0, \quad \frac{\partial E}{\partial s_2} = -as_2^2 \left(\frac{dR(s_2)}{dr} \right)^2 \leq 0$$

Note this known fact was reflected in [13, p. 28].

Theorem 2. *If $Q(r) = b + r^2q(r) = const$, i.e. $q(r) = \frac{c}{r^2}$, then for the first energy eigen-value of problem (2.1), (2.1) on the interval, $[s_1, s_2]$ the following formula is true*

$$E(s_1, s_2) = \frac{a}{2} \left[s_2^2 \left(\frac{dR(s_2)}{dr} \right)^2 - s_1^2 \left(\frac{dR(s_1)}{dr} \right)^2 \right]. \tag{4.1}$$

Proof. Let $Q(r) = Q = const$. We write equation (2.1) in the equivalent form

$$-\frac{a}{t^2} \frac{d}{dr} \left(r^2 \frac{dR\left(\frac{r}{t}\right)}{dr} \right) + Q = E \frac{r^2}{t^2} R\left(\frac{r}{t}\right), \quad \frac{r}{t} \in (s_1, s_2).$$

Denote

$$\bar{R}(r) = R\left(\frac{r}{t}\right).$$

Then

$$\frac{d\bar{R}}{dr} = \frac{1}{t} \frac{dR(y)}{dy},$$

where $y = \frac{r}{t}$. Taking this into account, we see that $\bar{R}(r)$ is an eigen-function, $\frac{E}{t^2}$ is an eigen-value of problem (2.1) (2.2) on the interval $[ts_1, ts_2]$. Then by the results of theorem 1, we have

$$-\frac{2}{t^3 E} = as_1^2 \left(\frac{dR\left(\frac{r}{t}\right)}{dr} \right)^2 - as_2^2 \left(\frac{dR\left(\frac{r}{t}\right)}{dr} \right)^2.$$

Having accepted $t = 1$, we get (4.1).

The theorem is proved.

This shows that the quantities $\frac{dR(s_1)}{dr}$ and $\frac{dR(s_2)}{dr}$ uniquely determine the energy eigen-values.

5. Conclusions. The properties of energy eigen-values with respect to the ends of the interval is studied by the motion of the particle in the neutral field, and the formula is obtained for its derivative. These formulae enable to investigate different extremal properties of the energy eigen-values.

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