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ELEMENTARY PROOF OF THE EXTREMUM PROPERTY OF THE REAL NODELESS SOLUTION OF THE SCHRÖDINGER EQUATION

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Элементарное доказательство экстремального свойства безузлового решения уравнения Шредингера

Дано элементарное доказательство экстремального свойства безузлового решения уравнения Шредингера.

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Elementary Proof of the Extremum Property of the Real Nodeless Solution of the Schrödinger Equation

A simple proof of the extremal property (3) of the real nodeless solution $\Omega_0(x)$ of Schrödinger equation (1) is given.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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The real nodeless solution $\Omega_0(x)$ of the Schrödinger equation in the nonrelativistic quantum mechanics

$$H\Omega_0 = E_0\Omega_0 , \qquad (1)$$

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + V(x) , \qquad (2)$$

is well known (see, e.g., ref.[1], volume I, chapter VI) to give to the functional of the energy

$$\epsilon(\Omega) = \int \Omega^* H\Omega \, dx / \int \Omega^* \Omega \, dx \qquad (3)$$

its minimal value E_0:

$$\epsilon(\Omega) > E_0 = \epsilon(\Omega_0) \qquad (4)$$

if the function $U(x)$,

$$U(x) = \Omega(x)/\Omega_0(x) , \qquad (5)$$

is not constant.The proof[1]of this property ,though being not very complicated, is not simple enough to be included in the text-book of quantum mechanics.

We give here the elementary proof of inequality (4).

1. From (5), (2) and (1) it follows

$$(H-E_0)\Omega = -\frac{1}{2}\Omega_0\frac{\partial^2 U}{\partial x^2} - \frac{\partial U}{\partial x}\frac{\partial \Omega_0}{\partial x} \quad (6)$$

and

$$\{\epsilon(U\Omega_0) - E_0\}\int \Omega_0^2 U^* U dx = \\ = -\int dx[\frac{1}{2}\Omega_0^2 U^* \frac{\partial^2 U}{\partial x^2} + \Omega_0 U^* \frac{\partial U}{\partial x}\frac{\partial \Omega_0}{\partial x}]. \quad (7)$$

Integration by parts here gives

$$\epsilon(\Omega) = E_0 + \frac{1}{2}\int dx \Omega_0^2 \frac{\partial U^*}{\partial x}\frac{\partial U}{\partial x} / \int dx \Omega_0^2 U^* U , \quad (8)$$

this equality results in (4).

2. Let us now take as Ω_0 the real solution of eq. (1), which has zeroes. Then (8) gives that $\epsilon(\Omega) > \epsilon(\Omega_0)$ if functions Ω and Ω_0 have the same zeroes. If, on the contrary, $\Omega_0(x_0)=0$ and $\Omega(x_0)\neq 0$ for some x_0, then the function $U(x)$ has a singularity at the point $x=x_0$; now the transition from (7) to (8) is incorrect and so may be eq. (4).

REFERENCES

1. Courant R., Gilbert D. Metody Matematicheskoi Fiziki, vol. I, Gostekhteoretizdat, Moscow, 1951.

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