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Research article

Nonlinear Pauli equation

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Appendix

Let us calculate the integral (143).

Let's move on to nondimensional coordinates, where the Bohr radius a_B is taken as the scale. In this case

$$b = b_0 a_B \tag{A1}$$

where

$$b_0 = \int\int |\mathbf{r}-\mathbf{r}'||\psi(\mathbf{r})|^2|\psi(\mathbf{r}')|^2 dV'\, dV \tag{A2}$$

Is the nondimensional parameter, which is calculated using nondimensional coordinates.

In particular, for the ground state of the hydrogen atom

$$|\psi(\mathbf{r})|^2 = \frac{1}{\pi}\exp(-2r) \tag{A3}$$

We introduce the function

$$F(\mathbf{r}) = \int |\mathbf{r}-\mathbf{r}'||\psi(\mathbf{r}')|^2 dV' \tag{A4}$$

Then we write (A2) in the form

$$b_0 = \int F(\mathbf{r})|\psi(\mathbf{r})|^2 dV \tag{A5}$$

Obviously,

$$\Delta F = 2\Phi(\mathbf{r}) \tag{A6}$$

where

$$\Phi(\mathbf{r}) = \int \frac{|\psi(\mathbf{r}')|^2}{|\mathbf{r}-\mathbf{r}'|} dV' \tag{A7}$$

The function $\Phi(\mathbf{r})$ satisfies the equation

$$\Delta\Phi = -4\pi|\psi(\mathbf{r})|^2 \tag{A8}$$

Obviously, as $r \to \infty$, the functions $F(`\mathbf{r})$ and $\Phi(\mathbf{r})$ behave as

$$F(\mathbf{r}) \to r \tag{A9}$$

and

$$\Phi(\mathbf{r}) \to \frac{1}{r} \tag{A10}$$

In addition, these functions have bounded limits as $r \to 0$, which can be easily calculated using (A3):

$$F(0) = 4\int_0^\infty r^3 \exp(-2r)\, dr = \frac{3}{2} \tag{A11}$$

$$\Phi(0) = 4\int_0^\infty r \exp(-2r)\, dr = 1 \tag{A12}$$

Because $|\psi(\mathbf{r})|^2$ depends only on r, then the function $\Phi(\mathbf{r})$ also depends only on r. Therefore, equation (A8), taking into account (A3), takes the form

$$\frac{d^2 r\Phi}{dr^2} = -4r \exp(-2r) \tag{A13}$$

The solution of equation (A13) taking into account conditions (A10) and (A12) has the form

$$\Phi = -\frac{1}{r}(r+1)\exp(-2r) + \frac{1}{r} \tag{A14}$$

Then equation (A6) takes the form

$$\frac{d^2 rF}{dr^2} = -2(r+1)\exp(-2r) + 2 \tag{A15}$$

The solution of equation (A15) taking into account conditions (A9) and (A11) has the form

$$F = -\frac{1}{2r}(r+2)\exp(-2r) + r + \frac{1}{r} \tag{A16}$$

Substituting (A3) and (A16) into (A5), one obtains

$$b_0 = \frac{35}{16} \tag{A17}$$

or, taking into account (A1),

$$b = \frac{35}{16} a_B \tag{A18}$$