Energy levels of an elecrton bound on a donor-acceptor pair

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The problem of the dependence of the binding energy of an electron in a donor-acceptor pair on the distance R between the donor and acceptor is examined. It is shown that the critical distance R_c is an essential singularity at which an infinite number of levels converge.

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An electron has bound states on a donor-acceptor pair if the distance R between the donor and acceptor exceeds a critical magnitude R_c. A variational calculation using a single-parameter wave function gives $R_c = 1.75\ a_B$, where a_B is the Bohr radius of the electron. However, as shown in Ref. 2, where the problem of the energy levels of an electron bound on a proton and a negatively charged meson was solved, the variational function gives a rather poor approximation, since the exact value of R_c is 0.639 a_B. Thus the variational method underestimates by more than an order of magnitude (a factor of 20) the value of the impurity concentration up to which bound electronic states in a donor-acceptor pairs exist. It is interesting to analyze the behavior of the electron energy E near the point R_c. Below we shall show that the point R_c is an essential singularity of the function $E(R)$. The function $E(R)$ is multivalued, and an infinite number of branches converge at the point $R = R_c$.

The solution of the Shrödinger equation in elliptical coordinates for an electron bound on a donor-acceptor pair reduces to solving two ordinary differential equations[2,3]:

$$\frac{d}{d\xi}\left[(\xi^2-1)\frac{dM}{d\xi}\right]+\left[\lambda^2+\frac{1}{4}+\epsilon\xi^2-m^2(\xi^2-1)^{-1}\right]M=0,\qquad \infty>\xi\geqslant 1,\qquad (1)$$

$$\frac{d}{d\eta}\left[(1-\eta^2)\frac{dN}{d\eta}\right]-\left[\lambda^2+\frac{1}{4}+\epsilon\eta^2+m^2(1-\eta^2)^{-1}\right]N=0,\qquad -1\leqslant\eta\leqslant 1.\qquad (2)$$

Here $\epsilon = ER^2/4E_B a_B^2$, E_B is the Bohr energy of an electron, m is the magnetic quantum number, λ is the separation constant, and $\psi = M(\xi)N(\eta)\exp(im\varphi)$.

We shall examine the problem of the energy states with $m=0$, to which the ground state belongs. For $\epsilon = 0$ the solution, finite at $\xi = 1$, has the form

$$M(\xi) = F\left(\frac{1}{2}+i\lambda,\ \frac{1}{2}-i\lambda;\ \frac{1-\xi}{2}\right),\qquad (3)$$

where $F(\alpha,\beta;\gamma;z)$ is the hypergeometric function. The region of bound states coresponds to real values of λ. The value $\lambda = 0$ corresponds to $R_c = 0.639a_B$.[2] For $R/R_c - 1 \ll 1$, $|\epsilon| \ll 1$. In this case it is possible to determine the behavior in two intersecting regions. For $1/|\sqrt{|\epsilon|} \gg \xi \gg 1$, we obtain from (3)

$$M(\xi) = \frac{1}{\pi}\sqrt{\frac{2}{\xi}}\left\{\frac{1}{\lambda}\sin\left(\lambda \ln\frac{\xi}{2}\right) + 4(\ln 2)\cos\left(\lambda \ln\frac{\xi}{2}\right)\right\}. \tag{4}$$

In the region $\xi \gg 1$ Eq. (1) has the solution (finite for $\xi \to \infty$)

$$M(\xi) = \frac{C}{\sqrt{\xi}} K_{i\lambda}(\xi\sqrt{-\epsilon}), \tag{5}$$

where C is a constant, and $K_{i\lambda}(z)$ is a modified Bessel function of the third kind. Joining (4) and (5) in the region $1\sqrt{|\epsilon|} \gg \xi \gg 1$ leads to an equation relating λ and ϵ. In the lowest approximation with respect to λ we have

$$\frac{\sin\left(\frac{\lambda}{2}\ln|\epsilon|\right) + \lambda\gamma\cos\left(\frac{\lambda}{2}\ln|\epsilon|\right)}{\cos\left(\frac{\lambda}{2}\ln|\epsilon|\right) - \lambda\gamma\sin\left(\frac{\lambda}{2}\ln|\epsilon|\right)} = 4\lambda \ln 2\,; \tag{6}$$

where γ is Euler's constant. From (6) we obtain an explicit relation between ϵ and λ

$$\lambda_n = 2\pi n(8\ln 2 - 2\gamma - \ln|\epsilon|)^{-1}, \tag{7}$$

where $n = 1,2, \ldots$ is an arbitrary positive integer.

On the other hand, for $\lambda \ll 1$, it follows from (2) that

$$\lambda^2 = A(R - R_c), \tag{8}$$

where

$$A = -2\int_{-1}^{1} d\eta\, \eta N_0^2(\eta)\left[\int_{-1}^{1} d\eta_1 N_0^2(\eta_1)\right]^{-1} > 0, \tag{9}$$

$N_0(\eta)$ is the solution of Eq. (3) for $\epsilon = 0$, $\lambda = 0$, $m = 0$. From (7) and (8) we obtain ϵ as a function of $R - R_c$

$$\epsilon_n = -256\exp\left[-2\gamma - \frac{2\pi n}{\sqrt{A(R - R_c)}}\right]. \tag{10}$$

Thus the point R_c is an essential singularity of the function $\epsilon(R)$. An infinite number of levels converges at this point.

The procedure for determining R_c is as follows. From Eq. (1) we find the value of λ, for which the indices of differential equation (1) converge in the vicinity of the point $\xi = \infty$ and then we solve (2) with the value obtained for λ. The solutions are independent of m for $\xi \to \infty$. For this reason, the quantity R_c is the same for all levels.

Thus the change in the levels of the system with the transition from $R \rightarrow \infty$ to $R = R_c$ can be viewed as follows. For $R \rightarrow \infty$ the elecrton is located near the donor and has a hydrogenlike spectrum of levels. As the donor and acceptor approach each other, the energy of the ground state decreases (in absolute magnitude) and the distance between the levels decreases simultaneously. In addition, the energy of all levels approaches zero for $R \rightarrow R_c$, i.e., all levels clump together at the point R_c and for each branch of $\epsilon_n(R)$ the point R_c is an essential singularity.

[1]J. J. Hopfield, "Physics of semiconductors," Proc. of the 7th Intern. Conf., Paris, 1964, p. 725.
[2]A. S. Wightman, Phys. Rev. 77, 521 (1950).
[3]L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, Moscow, 1963, p. 331.

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