STATIONARY STATES OF AN ELECTRON IN THE FIELD OF A HOLE IN AN IONIC CRYSTAL

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An approximate solution is given of the Schrödinger equation for S-states of an electron in the field of a hole, when the potential energy of the electron has the form \(-\frac{e^2}{r}[1 + \exp(-qr)].\)

INTRODUCTION

According to Haken [1] the potential energy of the interaction of an electron and hole in an ionic crystal, taking into consideration their interaction with the optical lattice vibrations, has the form

\[
U(R) = -\frac{e^2}{\varepsilon R} \left( 1 + \gamma \frac{e^{-\beta R} + e^{-\beta R}}{2} \right).
\]

In paper [2] this formula was derived in a more general way and it was shown that it holds exactly when the relative impulse \(P\) of an electron with respect to a hole is zero and remains approximately valid when this impulse is small. An electron and a hole interact most strongly with phonons, whose absolute value of the wave vector \(k\) is \(0\). It will be shown here that if we confine ourselves to interaction with such phonons, then formula (1) holds for arbitrary \(P\), its importance thus being extended. We shall confine ourselves below to the special case when \(m_1 = m_2\) and \(\gamma = 1\) and give an approximate solution of the Schrödinger equation for the s-states of an electron in the field of a hole.

POTENTIAL ENERGY OF ELECTRON-HOLE INTERACTION IN IONIC CRYSTAL

Let us consider the case when the effective mass of an electron equals the effective mass of a hole. The Hamiltonian (4) from paper [2] here has the form

\[
H = \frac{p^2}{m} - \frac{e^2}{\varepsilon R} + \sum_k \left( \hbar \omega_k + \frac{\hbar^2 \beta^2}{4m} a_k a_k + \right.
\]

\[
\left. + \sum_k 2 \cos \left( \frac{k \cdot r}{2} \right) (V_k a_k + V_k^* a_k^*) \right).
\]

We apply the following unitary transformation to this Hamiltonian

\[
p = \exp \left( -\frac{i}{\hbar} S \right) P \exp \left( \frac{i}{\hbar} S \right),
\]

\[
r = \exp \left( -\frac{i}{\hbar} S \right) R \exp \left( \frac{i}{\hbar} S \right),
\]

\[
a_k = \exp \left( -\frac{i}{\hbar} S \right) a_k \exp \left( \frac{i}{\hbar} S \right),
\]

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and require that

\[ -\frac{i}{\hbar} [S, A_i] + A_i = 0, \quad (4) \]

where

\[ A_i = \sum_k \left( \hbar \omega_k + \frac{\hbar^2 k^2}{4m} \right) a_k^\dagger a_k, \quad A_i = \sum_k 2 \cos \left( \frac{k \cdot R}{2} \right) (V_k a_k + V_k^* a_k^\dagger). \quad (5) \]

Requirement (7) from paper [2] becomes the above condition when \( P = 0 \). We now require condition (4) to be satisfied for \( P \neq 0 \). For \( S \) we get

\[ S = -\frac{\hbar}{2} \sum_k \frac{2 \cos \left( \frac{k \cdot R}{2} \right)}{\hbar \omega_k + \frac{\hbar^2 k^2}{4m}} (V_k a_k - V_k^* a_k^\dagger). \quad (6) \]

Using the results of paper [2] we get

\[ H = e^{\frac{i}{\hbar} S} \frac{P^2}{m} e^{\frac{i}{\hbar} S} - \frac{e^2}{eR} (1 + \gamma e^{-\omega_0}) + \sum_k \hbar \omega_k a_k^\dagger a_k, \quad (7) \]

where \( \gamma = e/\varepsilon_0 - 1, \quad q = \sqrt{\frac{2m \omega_0}{\hbar}}, \quad \varepsilon \) is the static and \( \varepsilon_0 \) the optical dielectric constant, \( \omega \) the frequency of the optical vibrations of the lattice and \( m \) the effective mass of the particles in question.

Let us rewrite the term \( e^{\frac{i}{\hbar} S} \frac{P^2}{m} e^{\frac{i}{\hbar} S} \) in the Hamiltonian (7). Using the commutation law

\[ F(r) P^2 - P^2 F(r) = 2i\hbar (\nabla F) \cdot P + \hbar^2 (\Delta F) \quad (8) \]

and the fact that the operator \( P \) commutes with the operators \( a_k^\dagger \) and \( a_k \), we get

\[ e^{\frac{i}{\hbar} S} \frac{P^2}{m} e^{\frac{i}{\hbar} S} = \frac{1}{m} \left[ P^2 + 2(\nabla S) \cdot P + (\nabla S)^2 \right] \cdot i\hbar (\nabla \cdot \nabla S). \quad (9) \]

According to (6)

\[ \nabla S = i\hbar \sum_k \frac{k \sin \left( \frac{k \cdot R}{2} \right)}{\hbar \omega_k + \frac{\hbar^2 k^2}{4m}} (V_k a_k - V_k^* a_k^\dagger). \quad (10) \]

In the case of optical vibrations \( V_k \) is proportional to \( 1/k \), so that for \( k \to 0, \nabla S \to 0 \) and thus for \( k \sim 0 \) we can write

\[ e^{\frac{i}{\hbar} S} \frac{P^2}{m} e^{\frac{i}{\hbar} S} \simeq \frac{P^2}{m}. \]

We have thus arrived at the result that when the interaction of an electron and hole with phonons for which \( k \sim 0 \) is taken into consideration, then their Hamiltonian can be written as follows:

\[ H = \frac{P^2}{m} - \frac{e^2}{eR} (1 + \gamma e^{-\omega_0}). \quad (11) \]