A wave function for the F center obtained using the uncertainty principle

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Abstract. We propose the possibility to obtain the wave function for a bounded particle in some physical region using the uncertainty principle. The problem of the F Center in solids is developed as an example where the method works out acceptably.

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1. Introduction and Theory

The uncertainty principle is one of the fundamental principles of Quantum Mechanics. It is usually expressed as:

$$\Delta q \Delta p \geq \hbar. \tag{1}$$

Here Δq and Δp are the uncertainties in position and conjugated momentum respectively and $\hbar$ is the Planck's constant h divided by 2π. As it is well known this relation comes out when we observe a given physical region Δq with a Heisenberg microscope [1,2]. It has been used to make valuable energy estimations for some systems like the Hydrogen atom, where the energy for the ground state is known [3]. In the case of particles bounded by complicated potentials in some physical region, like electrons in solids, it is necessary to use approximate methods like variational methods to obtain the required solutions. Under these situations it is difficult to assume that the uncertainty principle could be of any help in getting reasonable estimation for some physical quantities. However, in this work we propose a method where the use of the uncertainty principle gives some useful information even in a fairly complicated physical situation.

Basically, the proposed method consists in considering for some given particle, a wave function with an estimative parameter in analogy with the variational method. However, the parameter would be estimated here using the uncertainty principle.

Thus, for a particle in a state n in a certain bounded region, we can say that the wave function will depend on a parameter α : $\psi_n(q_j, \alpha)$, where q_j are the linear position coordinates. The kinetic energy is expressed by

$$E_k = -\frac{\hbar^2}{2m} \int \psi_n(q_j, \alpha) \nabla_q^2 \psi_n(q_j, \alpha) d\tau = F_n(\alpha), \tag{2}$$

where m is the mass of the particle. Now using the uncertainty principle [1] as an approximation in the bounded region, it can be found that the following expression can be considered valid

$$p_j q_j \simeq h, \tag{3}$$

where we have just replaced the uncertainties in position and momentum by q_j and p_j respectively.

The kinetic energy now takes the form

$$E_k = \frac{p^2}{2m} = \frac{1}{2m} \sum_j p_j^2 = \frac{1}{2m} \sum_j \frac{\hbar_j^2}{q_j^2}, \qquad \hbar_j \equiv \hbar \quad \text{for all} \quad j.$$

If there are some symmetry and the estimated bounded region for state n is $a_n = q_j$; using [2] it can be concluded

$$E_k = \frac{1}{2ma_n^2} \sum_j \hbar_j^2 = F_n(\alpha). \tag{4}$$

Therefore, if $F_n(\alpha)$ is a well behaved function that depends of a good choice of $\psi(q_j, \alpha)$ the parameter that will depend on known physical quantities could be obtained. The success of the method requires a good choice of the wave function and the bounded region. To illustrate the method, we applied it to the F Center problem, which is a basic topic in defect theory of solid state physics. It mainly consists of a bounded electron in a limited crystalline region of an ionic solid.

2. The F Center problem

As is well known in solid state physics, the F Center is a crystalline defect that appears in ionic crystals after irradiation. It consists in a trapped electron in an anion vacancy. Thus, in a typical alkali halide crystal, such as NaCl, the electron occupies the place of a Cl^- ion. A simple theoretical model for an F Center considers a trapped electron in square infinite potential well [4], for which the energy is an analytical function. The expression for the transition energy between the ground

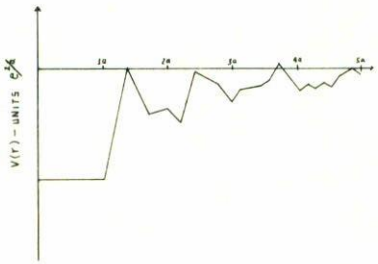

FIGURE 1. The F Center point-ion potential, in reduced units. (From Fowler [4]).

state and first excited state, named F band, is

$$E = \frac{3\pi^2 h^2}{2m} \mathrm{a}^{-2}, \tag{5}$$

where h is the Planck constant divided by 2π ,m is the electron mass and a the half length of the well, equivalent to the interionic distance of the crystalline lattice.

This model gives results close to experimental values and follows the empirical Mollows-Ivey-Law for the F band, which is [4]

$$E = 17.7a^{-1.84}, \tag{6}$$

a is the interionic distance in Angstroms and E the energy in eV.

More accurate methods have been developed by several authors to obtain the energy for the F Center in alkali halide crystals, like the point-ion models and semicontinuum models [4]. In the point-ion models the discrete character of the lattice is taken in consideration to obtain the potential on the electron after adding the interaction with each ion of the lattice. It is found that the electron is in a potential well with a half-length of the order of the vacancy radius. Outside this region the electron oscillates around a Coulomb type potential. In general, this problem is solved using variational methods [4] Fig (1).

In the semicontinuum models the crystal is considered as a continuum with a cavity which contains an electron. Thus, it is possible to obtain the F Center energy values and wave functions through a spherical well with penetrable walls resolved in two regions: a cavity region where the well effect acts and a polarizable dielectric region where a coulombian effect acts. The polarization is taken into account considering that the electron charge confined in the vacancy polarizes the medium [5,6] Fig. (2).

Therefore, it is necessary to know the charge density inside the vacancy and

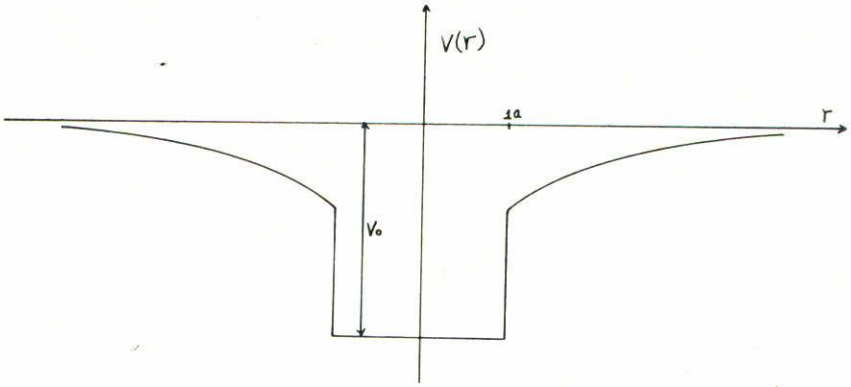

FIGURE 2. Potential used in calculating the energies of the F Center electron in the semicontinuum approach (Simpson [5]).

then the probability density which is obtained with the wave function. A solution to the problem is obtained with a variational method, which involves variational parameters in the wave function. The ground state energy and others are obtained in a self-consistent manner. Thus, in general, in the calculation, the energy term related to the potential part is too laborious to handle.

A typical method is the Simpson's classical semicontinuum method [5], which considers two contributions for obtain the well size: Madelung energy and a polarization contribution due to the cavity charge. The total contribution is V_0 and the Hamiltonian for the $r < R$ region, where R is the cavity radius, is

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V_0 \qquad r < R. \tag{7}$$

For $r > R$, a potential is constructed with the contribution for the polarizability of the medium due to electron fraction charge inside the cavity, given by

$$q = \epsilon\left(1 - \int_0^R |\psi|^2 4\pi r^2 dr\right), \tag{8}$$

where e is the electron charge, R the cavity radius and ψ the electron wave function with a variational parameter. Thus, the need for a self-consistent method is clear. The details involving this potential are in Simpson's work [5] and are not considered here. A more illustrative method is due to Fowler [6], it involves the following Hamiltonian for the region outside the cavity

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{K_0 r} \qquad r > R, \tag{9}$$

with coulombian type contribution for the potential and where m^* is the electron effective mass and K_0 the optic dielectric constant. Inside the cavity the Hamiltonian is equivalent to that of the Simpson method [5].

In the semicontinuum models, variational hydrogenic type functions are proposed. The ground state wave function is given by

$$\psi_{1s} = A(1 + \alpha r)e^{-\alpha r}, \tag{10}$$

where α is a variational parameter and the normalization constant is

$$A = \sqrt{\frac{\alpha^3}{7\pi}}. \tag{11}$$

To obtain the variational parameter, the energy W_0, is minimized in such a way that $\frac{\partial W_0}{\partial \alpha} = 0$, where $W_0 = \int \psi_0 H \psi_0 d\tau$, $d\tau = 4\pi r^2 dr$. In semicontinuum and ion point models the solution is finally searched by computer numerical methods.

3. Method with the uncertainty principle

In order to make an estimation of the variational type parameters we set up the following arguments:

i) It is considered that for the electron inside the cavity (F Center), the approximation given by (3) is valid.

ii) Similarly to the simple model of the box [3,4], is considered that the electron is confined in a cubic cavity of equal sides of a magnitude equivalent to vacancy diameter d; thus the following relationship will be valid

$$P_x d = \gamma\hbar, \qquad P_y d = \gamma\hbar, \qquad P_z d = \gamma\hbar \tag{12}$$

with $\gamma > 1$, factor *ad hoc* to make both sides equivalent due to the uncertainty expressions (3). The cavity radius is in general smaller than the vacancy radius [5,6,7]. When an anion is out of the crystal, the ions around this place move to the cavity center. The evaluation of ion displacements is made by the balance force methods and the cavity radius, it could be shortened up to 70% of lattice constant [7]. There are several contributions to the forces that displace the ions, such as electrostatic forces and repulsive Born-Mayer Type forces, principally. Therefore, it can be assumed

$$d = ka \qquad 1 < k < 2, \tag{13}$$

with a as the interionic distance. In a reasonable manner we can make $\gamma = K$

Crystal	$\alpha(a.u.)^{-1}$	$\alpha_s^{(a)}(a.u.)^{-1}$	$\alpha_F^{(b)}(a.u.)^{-1}$
NaBr	0.469	0.491	
KBr	0.425		
RbBr	0.407	0.441	
NaI	0.397		
RbI	0.546		
NaCl	0.497	0.511	0.560
KCl	0.445	0.471	
RbCl	0.426		
LiF	0.696		
NaF	0.605		
KF	0.525		
RbF	0.498		

TABLE I. Values of α calculated with Eq. (16) and compared to variational parameters obtained using Simpson and Fowler methods (a) From Ref. [8], (b) From Ref. [5].

and the expression for the kinetic energy is

$$E_k = \frac{3\hbar^2}{2ma^2} = F_0(\alpha), \tag{14}$$

which follows from (4).

On the other hand

$$F_0(\alpha) = \frac{\hbar^2}{2m}\int_0^\infty \psi_0 \nabla^2 \psi_0 4\pi r^2 dr$$

$$= \frac{3\hbar^2\alpha^2}{14m}, \tag{15}$$

with the wave function (10) for ψ_0.

Finally, using (14) and (15), the value can be estimated for the parameter α

$$\alpha \equiv \frac{\sqrt{7}}{a}. \tag{16}$$

It can be noted that it depends on the interionic distance a and permits a quickly estimation of the wave function.

4. Conclusions

In Table I are shown the values obtained using (16) for the parameter α compared to the values obtained using the laborious semicontinuum methods [5,8].

From the same Table, we observe that values obtained using the uncertainty principle are of the order of the normal variational parameters.

Even though, the proposition stated here can be utilized in this case, for a quick solution of the parameter α making use of the equation (16), but cannot replace variational methods already used in an extensive study of the F band.

Energy transition of the ground state to the first excited state in determined by the shape of the potential, as can be observe in the works of Simpson and Fowler [5,6]. The energy values of the levels calculated with theses methods are sensible to coulombian tails of the potential (Fig. 2.).

With the use of the uncertainty principle this kind of information is not taken into account and it is only suggested that the particle is in a potential well, so its use will be very limited.

In such cases, in relation with the semicontinuum methods, the parameter α obtained using the uncertainty principle gives a useful approximation, which can be observe in Table I.

Using expression (16) we were able to obtain some information for F Center with the estimated parameters on the wave function for all alkali halides according to the lattice constant 2a, and we are able to obtain an empirical ground state wave function for the F Center. Therefore, we can estimate any dynamical quantity of interest. Particularly, an estimation of the electron position can be done, that is

$$\langle r \rangle = \int_0^\infty \psi_0 r \psi_0 4\pi r^2 dr. \tag{17}$$

Solving the integral we finally obtained

$$\langle r \rangle = \frac{15}{7\alpha}. \tag{18}$$

After substitution of α it gives $\langle r \rangle = 0.80$a. It means that $K = 1.6$ for a box with length sides equivalent to the electron average position. This is in agreement with the proposed arguments. Thus, the method gave rough information of the F Center problem and could also be good for estimative calculations for other defects in solids, such as excitons, and very possible could be useful for some problem in other fields of physics apart of solid state.

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Resumen. Se propone la posibilidad de obtener la función de onda de una partícula confinada en una región física usando el principio de incertidumbre. El problema del Centro F en sólidos se desarrolla como un ejemplo donde el método trabaja aceptablemente.