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ON THE PHOTO-IONIZATION OF IMPURITY CENTRES IN SEMICONDUCTORS

M. Tomak

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ON THE PHOTO-IONIZATION OF IMPURITY CENTRES IN SEMICONDUCTORS *

M. Tomak **

International Centre for Theoretical Physics, Trieste, Italy.

ABSTRACT

The dependence of the photo-ionization cross-section on photon energy is calculated. The impurity potential is assumed to be of the Hülthén potential type and bound state wave function is calculated variationally. The results show that, at least in some cases, the Hülthén potential may describe the impurity better than the hydrogen or delta function potentials.

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** Permanent address: Department of Physics, Middle East Technical University, Ankara, Turkey.

I. INTRODUCTION

The dependence of the photo-ionization cross-section on photon energy is mainly determined by the potential which binds the charge carrier to the impurity centre and the band structure of the host crystal. Several successful attempts have been made to calculate the photo-ionization cross-sections with the use of different impurity potentials. Lax [1] was the first to use hydrogenic theory. The characteristic feature of the hydrogen spectrum is that its maximum is at the photo-ionization threshold. Absorption then falls off with increasing photon energy. The experimental curves, however, show that peak ranges from above E_I to about $2E_I$, where E_I is the "observed" ionization energy [2]. This discrepancy between the hydrogen model and experimental findings has motivated a number of investigators to go beyond the hydrogenic model.

Lucovsky [3] calculated the photo-ionization cross-section by using a delta-function (or zero range model) potential for the impurity. This potential describes well only the ion-core and neglects completely the long-range Coulomb effects. It is therefore expected that the model will not account for the observed cross-sections of shallower centres. As expected, Lucovsky's model agreed very well with the measured spectrum of cross-sections, in certain cases, but the agreement was not satisfactory in some other cases. A number of calculations and experiments have been performed for improving the situation and for studying the effects of electron-lattice interaction on the photo-ionization cross-section [4]-[17].

II. PHOTO-IONIZATION CROSS-SECTIONS

In this work, we propose yet another impurity potential model with the hope that it will do better in some physically interesting cases. The impurity potential is taken to be the Hülthén potential,

$$V(r) = -\frac{e^2}{\epsilon a}\,\frac{e^{-\lambda r/a}}{1-e^{-\lambda r/a}} \qquad (1)$$

It is interesting to note that in the limit of small r the Hülthén potential behaves like a Coulomb potential, whereas for large r it decreases exponentially. This behaviour may be well suited for the description of screening effects. It is possible to solve the Schrödinger equation for $\ell = 0$ states. The wave function for the ground state is given by

$$\psi(r) = \left[\frac{4-\lambda^2}{4\pi\lambda^2 a}\right]^{1/2} e^{-r/a} \quad \frac{e^{\lambda r/2a} - e^{-\lambda r/2a}}{r} \qquad (2)$$

This model potential can be used to describe shallow impurities whose spectra are well understood in terms of the effective mass approximation (EMA). In the EMA, continuum state energies are assumed to have the same distribution as that of the perfect crystal energy bands, and the corresponding wave functions are taken to be perfect crystal Bloch functions. This obviously is not applicable for deep impurities with strong, short-range potential resulting in strongly localized ground state and drastic alteration of the continuum states in the form of resonances and antiresonances.

With these restrictions in mind, the calculation of the photo-ionization cross-section is performed in two major steps. First, the wave function (2) is used as a trial function in the EMA treatment of the impurity problem where (λ) and (a) are treated as variation parameters to minimize the energy. Fixing (λ) and (a) by this procedure determines the ground state wave function completely. Then, the final state is represented by plane waves and the matrix element between the ground and final states is calculated in the electric-dipole approximation.

The photo-ionization cross-section is found to be

$$\sigma_I(\hbar\omega) = \left[\left(\frac{E_{eff}}{E}\right)^2 \frac{n}{\epsilon}\right] \frac{16\pi a}{3} \frac{\hbar\omega}{E_I} \left(\frac{\hbar\omega}{E_I} - 1\right)^{3/2} a^2 S(\hbar\omega) \qquad (3)$$

where

$\frac{E_{eff}}{E}$ = the effective field ratio,

n = the index of refraction,

ϵ = the dielectric constant,

$\alpha = e^2/\hbar c$ the fine structure constant and

$$S(\hbar\omega) = C^{5/2} a^5 \frac{4-\lambda^2}{\lambda^2} \left\{1\Big/\left[\left(1 - \frac{\lambda}{2}\right)^2 + ca^2 \left(\frac{\hbar\omega}{E_I} - 1\right)\right]^2 - 1\Big/\left[\left(1 + \frac{\lambda}{2}\right)^2 + ca^2 \left(\frac{\hbar\omega}{E_I} - 1\right)\right]^2\right\}^2 \qquad (4)$$

with

$$c = (2m^* E_I/\hbar^2)$$

In the case of a Yukawa type potential

$$V(r) = -A e^2 \frac{e^{-\beta r/a}}{r} \qquad (5)$$

with the ground state wave function

$$\psi(r) = \sqrt{\beta^2/8\pi a^3}\; e^{-\beta r/a} \qquad (6)$$

the photo-ionization cross-section is found to be

$$\sigma_I(\hbar\omega) = \left[\left(\frac{E_{eff}}{E}\right)^2 \frac{n}{\epsilon}\right] \frac{16\pi a}{3} 2\left(\frac{\beta}{a}\right)^5 \left(\frac{\hbar^2}{2m^* E_I}\right)^{7/2} \frac{(\hbar\omega/E_I - 1)^{3/2}}{(\hbar\omega/E_I)^5} \cdot \qquad (7)$$

III. NUMERICAL RESULTS AND DISCUSSION

The expressions (3) and (7) can now be compared with the hydrogenic and delta function potential results: Si:P system is chosen for numerical calculations. As is well known, P is a shallow impurity in Si and the system is well studied both theoretically and experimentally. Almost all the material properties are well known. But the calculation of cross-sections requires knowledge of the quantity E_{eff}, which is the effective field at the impurity site. It is extremely difficult to calculate E_{eff}. The ratio E_{eff}/E has therefore generally been treated as an adjustable parameter to fix the absolute values of σ. It is clear that this factor does not affect the shape of $\sigma(\hbar\omega)$. In this work, the ratio is taken to be approximately equal to one.

The numerical results are tabulated in Table I and are graphically displayed in Fig.1. It is encouraging to observe that the Hülthén potential produces the correct behaviour for the photo-ionization cross-section as a function of photon energy. The cross-section shows increased adsorption at higher photon energies and displays a maximum value at about a photon energy $\hbar\omega/E_I \sim 1.07$. These features are rather satisfactory. The model is not expected to hold in the case of very deep impurities. In that case, from among the three main quantities that enter the calculation, namely initial and final state wave functions and the final state energies only the last can be calculated with sufficient accuracy. The accurate wave

functions are not available to make a direct prediction. As stressed by Pantelides [13] and Jaros [15], one is either forced to extract a wave function from the experimental data or to use numerical wave functions which lead to a large computing effort. It is clear that more accurate calculations of bound states are necessary for accurate calculations of the photo-ionization cross-sections. The effect of electron-phonon interaction on the cross-sections, which is neglected in this work, should be taken into account especially in the case of deep impurities. Work along these lines is in progress.

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Table 1. Photo Ionization Cross Sections (10^{-15} cm^2)

$\hbar\omega/E_I$	HYDROGEN	DELTA	YUKAWA	HÜLTHEN
1.02	2.30	0.007	0.22	5.66
1.04	2.18	0.02	0.55	8.86
1.06	2.07	0.03	0.92	9.77
1.08	1.97	0.05	1.29	9.60
1.10	1.87	0.06	1.65	8.98
1.12	1.78	0.07	1.98	8.22
1.14	1.70	0.09	2.29	7.45
1.20	1.48	0.14	3.02	5.48
1.26	1.29	0.17	3.51	4.09
1.32	1.14	0.21	3.80	3.14
1.38	1.01	0.23	3.94	2.47
1.42	0.93	0.25	3.97	2.13
1.48	0.83	0.28	3.94	1.74
1.54	0.74	0.29	3.86	1.44
1.60	0.67	0.30	3.73	1.21
1.70	0.56	0.31	3.47	0.93
1.80	0.48	0.32	3.18	0.74
1.90	0.41	0.32	2.90	0.59
2.00	0.36	0.33	2.63	0.49
2.20	0.27	0.32	2.14	0.35

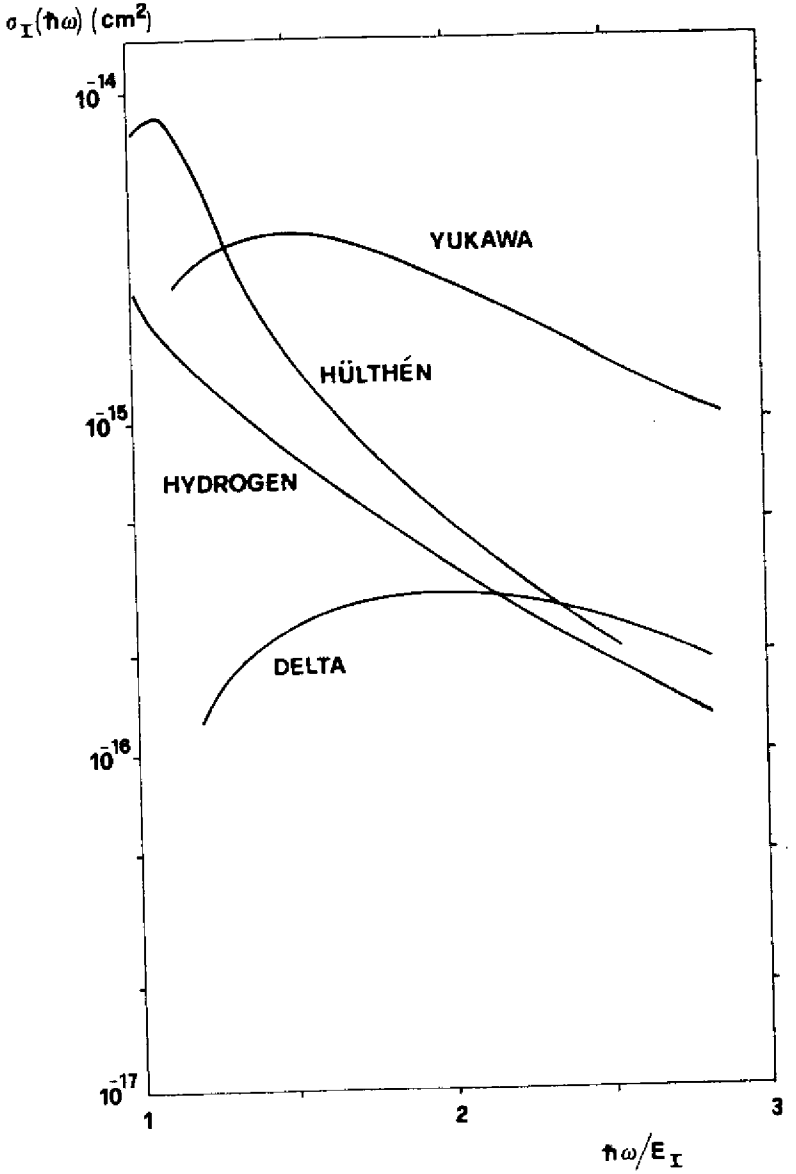

Fig. 1

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