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Published in:
EQEC '05. European Quantum Electronics Conference, 2005.

Link to article, DOI:
[10.1109/EQEC.2005.1567176](https://doi.org/10.1109/EQEC.2005.1567176)

Publication date:
2005

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Kristensen, P. T., Markussen, T., Tromborg, B., & Mørk, J. (2005). Influence of wetting layer wave functions on carrier capture in quantum dots. In *EQEC '05. European Quantum Electronics Conference, 2005*. (Vol. 29B, pp. 3-3). [1567176] IEEE. <https://doi.org/10.1109/EQEC.2005.1567176>

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Influence of wetting layer wave functions on carrier capture in quantum dots

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The properties of lasers and optical amplifiers based on active quantum dot (QD) materials are strongly influenced by the attainable rate of carrier injection into the dots. It is well-known that carrier capture from the extended continuum states can be mediated by carrier-carrier (Auger) as well as carrier-phonon scattering [1,2]. In both cases the capture time depends strongly on adequate descriptions of the corresponding wave functions. While the discrete bound state wave functions are usually found by solving the Schrödinger equation in the full potential (including the dot), the continuum wave functions are usually approximated by simple plane waves [1]. The plane wave approximation, however, does not take into account the influence of the QD potential on the extended states. To remedy this problem, the use of so-called orthogonalized plane waves has been suggested. This more elaborate approach uses plane waves modified so as to be orthogonal to the bound dot states [2]. In this work we numerically solve the effective mass Schrödinger equation and show that the capture times are strongly influenced by details of the continuum states not accounted for by the approximate wave functions.

We consider phonon mediated relaxation of carriers in conical quantum dots on a thin wetting layer (WL), as shown in Fig. 1 (top left). Using the rotational symmetry, the problem of solving the Schrödinger equation is reduced to two dimensions, making a finite element method (FEM) efficient. The calculated eigenstates are subsequently used for calculating the capture times as a function of dot radius, r_0 , for fixed cone angle. Furthermore, we compare these times to the results obtained using Bessel function (BF) solutions for the WL without QD and orthogonalized Bessel functions (OBF), defined as: $|OBF\rangle = |BF\rangle - \langle QD|BF\rangle|QD\rangle$.

The calculated capture times are shown in Fig. 1 (middle) for a WL thickness of 2 nm. For small radii, the curves for all three WL descriptions converge and rise significantly, the reason being that the bound QD state becomes less confined in the dot area for small radii and eventually becomes unbound. For radii $4.5 \text{ nm} < r_0 < 6.5 \text{ nm}$, the capture times for the OBF and the FEM solutions both increase, showing qualitatively the same behaviour, whereas the capture times of the BF solutions decrease. This indicates that in this range OBF do provide better approximations to the true states than BF, although the absolute deviation may be quite large. For larger radii the capture times for the FEM solutions are seen to rapidly increase. This is because the WL states with energies close to the band edge are squeezed out of the QD area, a feature accounted for by neither the BF nor the OBF approximations.

Fig. 1 (bottom) shows radial probability densities (at $r_0 = 6.25 \text{ nm}$ and $z = 0 \text{ nm}$) for the QD state and the three WL states corresponding to magnetic quantum number $m_z = 0$. The picture illustrates how the larger overlap of the BF with the QD state can explain the smaller capture times as compared to the OBF. Also it illustrates that neither of the two approximations resembles the FEM solution, each yielding approximately the same absolute error.

We conclude that calculations of capture times for phonon mediated carrier capture from a wetting layer into a quantum dot depend critically on the approximations used for the wetting layer wave functions.

Figure 1

top: Schematics of the model and contour plot of the radial probability density of the bound state in the (r,z) -plane.

middle: Capture times as function of dot radius calculated using 3 different types of wetting layer states.

bottom: Radial ($z=0$) probability densities for the three different wetting layer states and the bound state. All three wetting layer states have energies $E_w = E_{dot} + \hbar\omega_{LO}$.

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