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1992 J. Phys. A: Math. Gen. 25 L1305

(http://iopscience.iop.org/0305-4470/25/23/007)

J. Phys. A: Math. Gen. **25** (1992) L1305–L1309. Printed in the UK

LETTER TO THE EDITOR

Levinson's theorem in semiconductor quantum dots

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Received 17 July 1992, in final form 8 September 1992

Abstract. The Levinson's theorem in a semiconductor quantum dot is analysed. If the well and barrier effective masses differ, the zero-energy wavefunction phaseshift is shown to be $\eta(0)=\pi M_b$ (M_b being the number of bound states) for even values of azimuthal quantum number l, and $\pi(M_b+1)$ for odd l. For constant effective mass, however, $\eta(0)=\pi M_b$ regardless of the parity of l. Furthermore, while $\eta\to 0$ in the large-energy limit for the constant effective mass, the essentially different behaviour of η takes place if the effective mass is non-uniform.

Recent advances in microfabrication technologies have enabled the realization of various semiconductor quantum structures, attracting considerable attention due to novel physical properties not encountered in conventional materials. Among the most interesting of them are quantum dots (or inverse superatoms) [1, 2]—spherical semiconductor quantum wells in finite-height barriers. Along with the potential, it is also the effective mass that varies in the structure. In this letter we consider the relation between the zero-energy wavefunction phaseshift and the number of bound states. This problem has been tackled in the literature since the pioneering work of Levinson [3], for both the one-dimensional and three-dimensional systems, but with the assumption of constant electron mass. Here we generalize these results allowing for the spatially dependent electron (effective) mass, as indeed is the case in real structures of that type.

A real semiconductor quantum dot (QD) is a sphere of semiconductor A embedded in semiconductor B bulk, chosen so that the conduction band edge of A is below that of B, and in that sense A makes a spherical quantum well for electrons, B being the barrier. Usually, but not necessarily, the transition (interface) between the two is abrupt, making the potential and the effective mass not only spatially dependent, but also discontinuous. In this confining potential the electron bound states may exist, their energies being characterized by radial (n) azimuthal (l), and magnetic (m) quantum numbers. Due to the spherical symmetry the Schrödinger equation for this system is separable, and (within the envelope-function effective mass approximation) its radial part $X(r)/r$ reads

$$-\frac{\hbar^2}{2}\left[\left(\frac{1}{m(r)}\frac{\mathrm{d}^2X}{\mathrm{d}r^2}\right)+\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{1}{m(r)}\right)\left(\frac{\mathrm{d}X}{\mathrm{d}r}-\frac{X}{r}\right)-\frac{1}{m(r)}\frac{l(l+1)}{r^2}X\right]+[U(r)-E]X=0 \tag{1}$$

where the potential $U(r)$ and the effective mass $m(r)$ are only radially dependent (e.g. $m(r)=m_w$ for $r<R_0$, and $m(r)=m_b$ for $r>R_0$, R_0 being the QD radius, and $U(r)$ is

0305-4470/92/231305+05$07.50

the band edge plus the self-consistent electrostatic potential). For example, in conventional QDs, with electrostatic potential neglected, $U(r)=0$ for $r>R_0$ and $U(r)=-|\Delta E_c|$ for $r<R_0$, where ΔE_c is the conduction band edge discontinuity. Solutions of (1) may be expressed via the Jost functions $f_l(\pm k, r)$, the asymptotic form $r\to+\infty$ of which is

$$f_l(\pm k, r)=\mathrm{i}^l \exp(\pm \mathrm{i}kr) \qquad k^2=\frac{2m_b}{\hbar^2}E. \tag{2}$$

The general solution of (1) is

$$X_l(k, r)=Af_l(k, r)+Bf_l(-k, r) \tag{3}$$

where A and B are constants to be determined from the boundary conditions at $r\to 0$, that have the form [4]

$$X_l(k, r\to 0)\to\frac{r^{l+1}}{(2l+1)!!} \qquad \left.\frac{\mathrm{d}X_l}{\mathrm{d}r}\right|_{r\to 0}\to\frac{(l+1)r^l}{(2l+1)!!}. \tag{4}$$

Using (3) and (4), and introducing $f_l(\pm k)$ as

$$f_l(\pm k)=\lim_{r\to 0}\frac{(\pm kr)^l}{(2l+1)!!}f_l(\pm k, r) \tag{5}$$

the expression for the wavefunction $X_l(r)$ is

$$X_l(r)=\frac{m_b}{m_w}\frac{\mathrm{i}}{2k^{l+1}}[f_l(-k)f_l(k, r)-(-1)^l f_l(k)f_l(-k, r)]. \tag{6}$$

On the other hand, the asymptotic expression for $X_l(r)$ as $r\to+\infty$ may be written as

$$X_l(r)=\text{constant}\times\sin(kr-\tfrac{1}{2}l\pi+\eta_l) \tag{7}$$

where $\eta_l=\eta_l(k)$ is the phaseshift corresponding to the wavevector k. Comparing (6) and (7) we get an important relation

$$f_l(k)/f_l(-k)=\exp(2\mathrm{i}\eta_l). \tag{8}$$

Now define the function $h_l(k, r)=f_l(k, r)/f_\infty$ where f_∞ stands for $f_l(k, r)$ calculated for a large enough k (or E), such that $U(r)$ could be neglected when solving equation (1), i.e. by formally setting $U(r)=0$†. Then, f_∞ in the well and barrier reads (in further consideration subscript l will be omitted)

$$\begin{aligned} &f_\infty=\exp[-\mathrm{i}(kr-l\pi/2)] && \text{for } r>R_0\\ &f_\infty=C\exp[\mathrm{i}(k_1r-l\pi/2)]+D\exp[-\mathrm{i}(k_1r-l\pi/2)] && \text{for } r<R_0 \end{aligned} \tag{9}$$

where $k_1\equiv Rk\equiv(m_w/m_b)^{1/2}k$, and the constants C and D are determined from the boundary conditions: $X(r)$ and $(\mathrm{d}X/\mathrm{d}r-X/r)/m(r)$ are continuous for all r,

† The meaning of $E\to+\infty$ ($k\to+\infty$) in this derivation is as follows: $E\gg|U(r)|$ for all r and $kR_0\gg 1$ (so that corresponding Bessel functions may be approximated by exponential ones). Certainly, the effective mass approximation itself is valid in a limited energy interval, typically not more than 0.5 eV above the conduction band edge. Thus, all these considerations may be expected to be valid for realistic structures with not too large band offsets and also large enough QD radii, the latter being a condition for using the effective mass approximation anyway. For structure parameters not meeting the above conditions, a much more elaborate theory is required, although the derivation presented here would remain formally correct.

specifically at $r = R_0$ in this instance. For analysing the behaviour of $\eta(k)$ it is also necessary to find the ratio $f_{-\infty}/f_{\infty}$. The appropriate calculation gives

$$\lambda = \frac{f_{-\infty}}{f_{\infty}} = \frac{C(-K)+D(-K)}{C(K)+D(K)}\bigg|_{k\to+\infty} \tag{10}$$

$$C(K) = \frac{(-1)^l}{2iK_1}[(1+iK_1)-R^2(1+iK)]\exp[-i(K+K_1)] \tag{11}$$

$$D(K) = \frac{1}{2iK_1}[R^2(1+iK)-1(1+iK_1)]\exp[i(K-K_1)] \tag{12}$$

with $K = kR_0$, and $K_1 = k_1R_0$. If the effective mass spatial dependence is neglected (or there is none), i.e. $R = 1$, then $C = 0$, $D = 1$, and hence $\lambda = 1$ for all values of K.

We now consider the two cases separately:

(i) The azimuthal quantum number l is even ($l = 0, 2, 4, \ldots$). Then

$$C(K)+D(K) = \frac{\sin K_1}{K_1}(R^2-1)+\cos K_1 + i\frac{K}{K_1}R^2\sin K_1 = f_{\infty} \tag{13}$$

and therefore

$$h(K)/h(-K) = \exp[2i[\eta(K)+K+\omega(K)]] \tag{14}$$

where $\omega(K)$ is the argument of the complex number $C(-K)+D(-K)$. Equation (14) is valid for all $K \geq 0$, i.e. $E \geq 0$. Now $\omega(K)$ should be explored very carefully. Bearing in mind that $\omega(K)$ is (taken to be) a continuous function of K, it is given by

$$\omega(K) = -\tan^{-1}\left[\frac{R^2K}{K_1\cot K_1-(1-R^2)}\right]+\omega(0)-\pi N(K) \tag{15}$$

where $\omega(0)$ is an integer multiple of π, and $N(K)$, or $N(K_1)$ is given in figure 1. In the special case of constant effective mass ($R = 1$), $\omega(K) = -K+\omega(0)$.

We also note that, from (6), bound states are obtained from $f(k) = 0$, the solutions being on the negative part of the imaginary k axis (the very special case $f(0) = 0$, i.e. the possibility of zero-energy bound state, will be discussed elsewhere). Bearing (13) in mind, we conclude that the number of solutions of $h(K)$ is equal to the number of solutions of $f(k)$, i.e. *equal to the number of bound states* M_b.

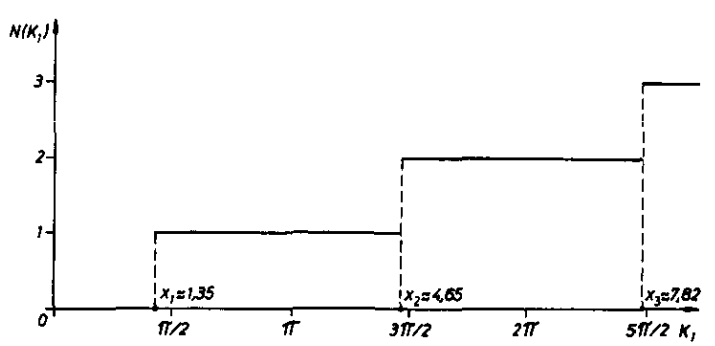

Figure 1. An example dependence of $N(K_1)$, equation (19) in the case of $R < 1$ (specifically $R^2 = 0.7$), typically encountered in semiconductor QDs. Values x_i are the solutions of $K_1\cot K_1-(1-R^2) = 0$, with $R^2 = m_w/m_b$. If $R > 1$, the x_i are then in the intervals $(\pi/2, \pi)$, $(3\pi/2, 2\pi)$, ...

Next, we integrate the function $h'(K)/h(K)$ along a semicircular contour C, with radius K_{max}, belonging to the bottom half of the complex K plane, that encompasses all M_b bound states. The result of the integration should be

$$I=\frac{1}{2\pi i}\oint_C \frac{h'(K)}{h(K)}\,dK=-M_b \tag{16}$$

and the explicit integration along C, with $K_{max}\to+\infty$, gives

$$\pi I=[\eta(K_{max})-\eta(0)]+K[\omega(K)-\omega(0)]. \tag{17}$$

The phaseshift for very large K, $\eta(K_{max})$, is determined from

$$\tan(\eta+K)=\frac{R^2K}{K_1\cot K_1-(1-R^2)}. \tag{18}$$

Since $\eta(K)$ is a continuous function, assuming that for $R=1$ $\eta(K)$ tends to zero in the large-K limit, we have

$$\eta(K\to+\infty)=\tan^{-1}\left[\frac{R^2K}{K_1\cot K_1-(1-R^2)}\right]-K+\pi N(K) \tag{19}$$

with $N(K)$ given in figure 1. From (17) and (19) we find†

$$\eta(0)=\pi M_b. \tag{20}$$

Therefore, Levinson's theorem remains valid for the non-uniform effective mass case, $R\neq 1$ as well, provided the azimuthal quantum number l is even.

(ii) The azimuthal number l is odd ($l=1,3,5,\ldots$). Performing the same procedure as for even l we arrive at the expression for $h(K)$.

$$h(K)=\frac{f(K)K_1\exp(iK)}{R^2K\cos K_1+i[K_1\sin K_1-(R^2-1)\cos K_1]}. \tag{21}$$

If $R\neq 1$, then one of the solutions of $h(K)$ is in $K=0$, but if $R=1$ then $h(0)\neq 0$. In the case $R\neq 1$ the $\omega(K)$ dependence can be written as

$$\omega(K)=\tan^{-1}\left[\frac{R^2K}{K_1\cot K_1+(1-R^2)}\right]-\pi N_1(K)+\omega(0) \tag{22}$$

where $N_1(K)$ is equal to $N(K)$, given in figure 1, except that the x_i are solutions of $K_1\tan K_1+(1-R^2)=0$. The constant $\omega(0)+\pi/2$ is equal to an arbitrary integer (L) multiple of π. On the other hand, if $R=1$ the difference $\Delta\omega=\omega(K)-\omega(0)$ cannot be obtained directly from (22), because $\omega(0)$ also depends on R: now it has to be written as $L\pi$, therefore $\Delta\omega=-K$ for $R=1$.

With the same conditions as for even l, the phaseshift $\gamma(K\to+\infty)$ can be written as

$$\eta(K\to+\infty)=-\tan^{-1}\left[\frac{R^2K}{K_1\tan K_1+(1-R^2)}\right]+\pi N_1(K)-K+\frac{\pi}{2}. \tag{23}$$

Obviously, from (23), $\eta(K\to+\infty)$ equals zero for $R=1$.

† As often quoted in literature [5] the quantity of physical interest is $\eta(0)-\eta(K\to+\infty)$. All the results in this paper may be considered in terms of this quantity, but we have adopted the usual convention $\eta(K\to+\infty)\to 0$ for $R=1$ (constant effective mass case), and evaluate $\eta(0)$ explicitly.

Finally, since $K = 0$ is one of the zeros of $h(K)$ if $R \neq 1$, the semicircular integration contour used above has to be changed, and a semi-annular contour that circumvents zero, with the inner radius K_ε ($K_\varepsilon \to 0$), used instead. Proceeding along the same lines as for even l we get

$$\eta(0) = \pi(M_b + 1) \tag{24}$$

while for $R = 1$ the contour remains semicircular, leading to

$$\eta(0) = \pi M_b . \tag{25}$$

It may seem unusual that the phase undergoes an abrupt change when R varies smoothly when crossing unity ($m_w = m_b$), while the physics apparently should not change. The same kind of discontinuity also appears in the constant effective mass case, when the system parameters are varied so that a bound state just appears, or disappears ($l = 0$ and $f_l(0) = 0$, equation (5.15) in [4]). Certainly, physically measurable quantities, like electron density, depending on the wavefunction modulus, will not undergo any abrupt change.

In conclusion, the zero-energy phase shift $\eta(0)$ in the quantum dot is found to be equal to π times the number of bound levels M_b only if the effective mass is constant. If the effective mass is non-uniform, as indeed it is in real systems, the above expression remains valid for even values of the azimuthal quantum number l only. For odd l values, however, $\eta(0) = \pi(M_b + 1)$. These results may be of importance for the fully self-consistent solution procedure that includes both bound and continuum states in semiconductor QDs.

Another interesting result is that the asymptotic behaviour of the phaseshift $\eta(K)$ in the large-energy limit is also essentially different in the constant effective mass, and spatially dependent effective mass cases, $\eta(K)$ tending to zero in the former, and being K dependent, (19) and (23), in the latter.

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