Canalized states in a two-dimensional quantum model of thin films

1995 J. Phys. A: Math. Gen. 28 L201

(http://iopscience.iop.org/0305-4470/28/6/004)

J. Phys. A: Math. Gen. 28 (1995) L201–L206. Printed in the UK

LETTER TO THE EDITOR

Canalized states in a two-dimensional quantum model of thin films

N Markovska, J Pop-Jordanov and E A Solov'ev†

Macedonian Academy of Sciences and Arts, PO Box 428, 91000 Skopje, Macedonia

Received 4 January 1995

Abstract. In the two-dimensional quantum model defined by Hamiltonian $\hat{H}(x,y) = -\frac{1}{2}\Delta_{x,y} + (\alpha + \lambda\cos y)[\delta(x-a) + \delta(x+a)]$ we revealed a particular solution with positive energy exponentially decreasing as $|x| \to \infty$ in spite of the tunnelling effect. The existence of these canalized states cannot be explained in terms of one-dimensional quantum theory and must be referred to as an ingenious interaction between different degrees of freedom.

We are considering the two-dimensional problem defined by Hamiltonian (atomic units are used throughout):

$$\hat{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + (\alpha + \lambda\cos y)[\delta(x-a) + \delta(x+a)]. \tag{1}$$

This Hamiltonian models the particle in a two-layer thin film of thickness 2α with 2π lattice period (see figure 1). Recently the quantum treatment of such a system has become topical owing to the achievements in understanding the physics of nanocrystalline solar cells [1].

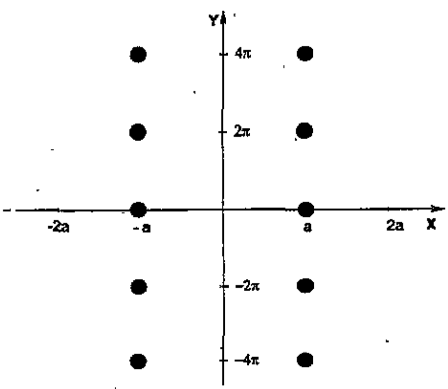

Figure 1. The pattern of the two-dimensional thin film.

† Permanent address: Department of Theoretical Physics, Institute of Physics, St Petersburg University, 198904 St Petersburg, Russia.

The wavefunction of Hamiltonian (1) satisfies the two-dimensional Schrödinger equation for a free particle:

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\psi(x,y)=E\psi(x,y) \tag{2}$$

everywhere except at the points $x=\pm a$. The presence of the δ-barrier at $x=a$ leads to the well known matching condition [2]:

$$\psi(x,y)|_{x=a+0}=\psi(x,y)|_{x=a-0} \tag{3a}$$

$$\left.\frac{\partial\psi(x,y)}{\partial x}\right|_{x=a+0}-\left.\frac{\partial\psi(x,y)}{\partial x}\right|_{x=a-0}=2(\alpha+\lambda\cos y)\psi(a,y). \tag{3b}$$

The same condition holds at $x=-a$. However, owing to the symmetry of the Hamiltonian $\hat{H}(x,y)=\hat{H}(-x,y)$ we can choose the wavefunction in symmetric or antisymmetric form: $\psi(x,y)=\pm\psi(-x,y)$, and the problem is reduced to the half-plane $x\geqslant 0$.

In this problem the boundary condition has a non-standard form of a combination of boundary conditions from scattering and solid-state theory. Namely, the scattering boundary condition for the x coordinate [3]:

$$\hat{S}\psi_{\text{in}}=e^{2i\theta}\psi_{\text{out}} \tag{4}$$

and the Bloch condition for the y coordinate [2]:

$$\psi(x,y+2\pi)=e^{2\pi ip}\psi(x,y) \tag{5}$$

where $\hat{S}$ is the S-matrix, θ is the scattering phase and p is the quasi-momentum. Therefore, the general solution can be chosen as an eigenfunction of the S-matrix with respect to the x axis with a fixed quasi-momentum along the y axis. The latter entails seeking ψ as a Fourier series with respect to the y coordinate:

$$\psi(x,y)=\sum_{n=l}^{m}c_n\begin{pmatrix}\cos k_n x\\ \sin k_n x\end{pmatrix}\exp[i(p+n)y]$$
$$+\sum_{\substack{n>m\\ n<l}}c_n\begin{pmatrix}\cosh q_n x\\ \sinh q_n x\end{pmatrix}\exp[i(p+n)y] \qquad |x|\leqslant a \tag{6a}$$

$$\psi(x,y)=\sum_{n=l}^{m}d_n\sin(k_n|x|+\theta(p))\exp[i(p+n)y]$$
$$+\sum_{\substack{n>m\\ n<l}}d_n\exp[-q_n|x|+i(p+n)y] \qquad |x|\geqslant a \tag{6b}$$

where $q_n=\sqrt{(p+n)^2-2E}$, $k_n=\sqrt{2E-(p+n)^2}$, $l=[-p-\sqrt{2E}]$ and $m=[-p+\sqrt{2E}]$. The upper circular and hyperbolic functions in equation (6a) pertain to the solutions that are symmetric in the x coordinate, the lower to the antisymmetric solutions.

Obviously, wavefunction (6) satisfies Schrödinger equation (2) and boundary conditions (4), (5). The coefficients of expansion in equation (6) and scattering phase $\theta(p)$ are determined from matching condition (3) which takes the form of three-term recurrence relations for coefficients d_n (see the appendix). These recurrence relations have two linearly independent solutions. The physical solution has to decrease as $n \to \pm\infty$. This type of solution has asymptotics:

$$d_n = \left(\frac{\lambda e^a}{2}\right)^{|n|} \frac{1}{\Gamma(|n+p|-\alpha+1)} \left(1 + O\left(\frac{1}{n}\right)\right). \tag{7}$$

The requirement for the decrease in the coefficients d_n on both sides ($n \to -\infty$ and $n \to +\infty$) determines $\theta = \theta(p)$. The alternative solutions increase at least on one side with asymptotics

$$d_n = \left(\frac{\lambda e^a}{2}\right)^{-|n|} \Gamma(|n+p|-\alpha+1) \left(1 + O\left(\frac{1}{n}\right)\right) \tag{8}$$

so that for them the series in (6) diverge.

On examining the complete set of wavefunctions (6) we have revealed a particular solution of unusual type:

$$\psi(x,y) = c_0 \begin{pmatrix} \cos k_0 x \\ \sin k_0 x \end{pmatrix} \exp(ipy) + \sum_{n=1}^{\infty} c_n \begin{pmatrix} \cosh q_n x \\ \sinh q_n x \end{pmatrix} \exp[i(p+n)y] \qquad |x| \leqslant a$$

$$\psi(x,y) = \sum_{n=1}^{\infty} d_n \exp[-q_n|x| + i(p+n)y] \qquad |x| \geqslant a. \tag{9}$$

The surprising property of these states is their location in the vicinity of the y axis. We have to emphasize that these canalized states occur above the boundary of the continuous spectrum ($E > 0$) and wavefunction (6*a*) contains a component with positive energy with respect to the x coordinate. This is the way in which one could expect the particle to propagate in all directions due to the tunnelling effect. Thus the existence of canalized states cannot be explained in the framework of one-dimensional quantum theory and must be referred to an ingenious interaction between different degrees of freedom.

It follows from equation (A2) that canalized states exist only with the additional restriction:

$$c_0 \begin{pmatrix} \cos k_0 a \\ \sin k_0 a \end{pmatrix} = 0 \tag{10}$$

which provides the connection between k_0 and a: $k_0 a = (j + \frac{1}{2})\pi$ for the symmetric and $k_0 a = j\pi$ for the antisymmetric case, where j is integer. Consequently, the condition $q_1^2 = (p+1)^2 - 2E \geqslant 0$ restricts the quasi-momentum region where this type of state exists:

$$p \geqslant p_{\min} = \frac{(j + \frac{1}{2})^2 \pi^2}{2a^2} - \frac{1}{2} \tag{11a}$$

for symmetric states and

$$p \geqslant p_{\min} = \frac{j^2 \pi^2}{2a^2} - \frac{1}{2} \tag{11b}$$

for antisymmetric states.

To prove the existence of canalized states (9) let us introduce the following transformation:

$$D_n = c_n \begin{pmatrix} \cosh q_n a \\ \sinh q_n a \end{pmatrix} = d_n \exp(-q_n a). \tag{12}$$

Using this transformation, the recurrence relations for the coefficients of the special kind of solution will be

$$(\beta_1 - \alpha) D_1 = \tfrac{1}{2}\lambda D_2 \qquad n = 1$$
$$(\beta_n - \alpha) D_n = \tfrac{1}{2}\lambda (D_{n+1} + D_{n-1}) \qquad n \geqslant 2. \tag{13}$$

The coefficient c_0 is determined from equation (A.7) which takes the form

$$c_0 k_0 \begin{pmatrix} -\sin k_0 a \\ \cos k_0 a \end{pmatrix} = \lambda d_1 \exp(-q_1 a). \tag{14}$$

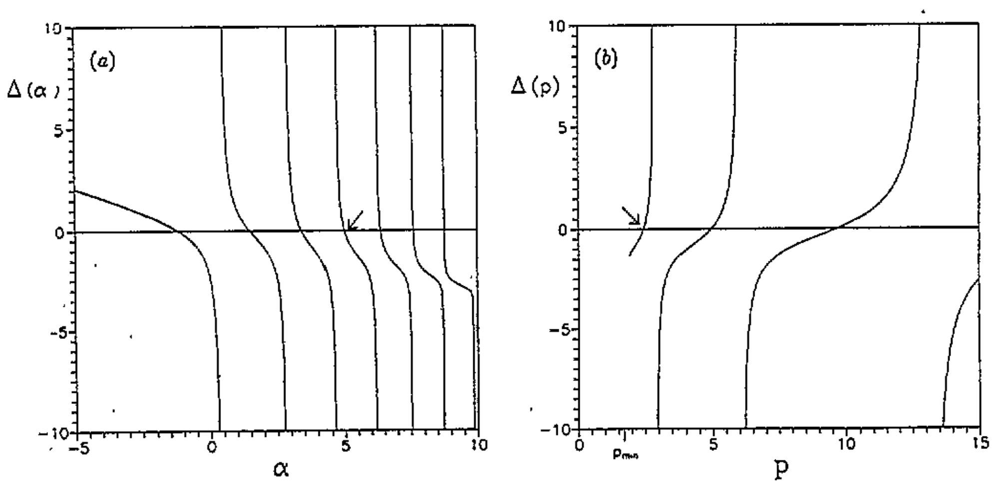

Figure 2. Continued fraction (16) as a function: (*a*) α ($\lambda = 5$, $a = 5$, $p = 2.5$ and $j = 3$); and (*b*) $p = 2.5$ ($\alpha = 5$, $\lambda = 5$, $a = 5$, and $j = 3$). The arrow indicates the root corresponding to the quantum state in figure 3.

Relations (13) can be rewritten in the form of an eigenvalue problem with respect to parameter α:

$$\hat{\mathbf{A}} \mathbf{D}_j = \alpha_j \mathbf{D}_j \tag{15}$$

where

$$\hat{\mathbf{A}} = \begin{pmatrix} \beta_1 & -\frac{1}{2}\lambda & 0 & 0 & \dots \\ -\frac{1}{2}\lambda & \beta_2 & -\frac{1}{2}\lambda & 0 & \dots \\ 0 & -\frac{1}{2}\lambda & \beta_3 & -\frac{1}{2}\lambda & \dots \\ \vdots & \vdots & \vdots & \vdots & \end{pmatrix}.$$

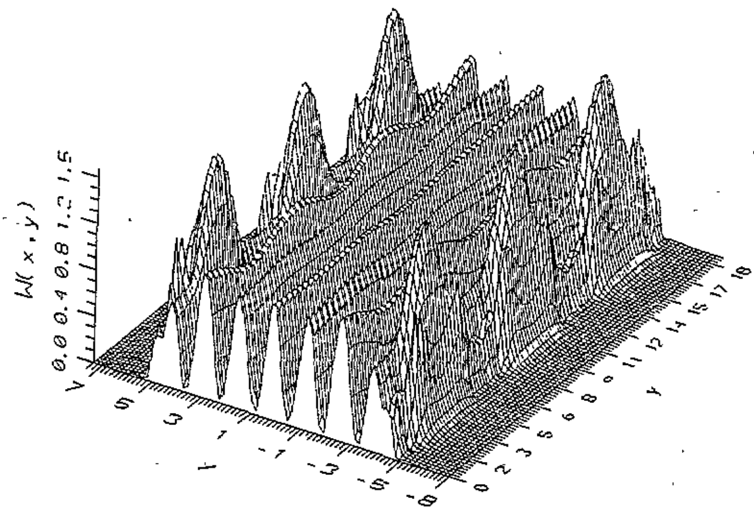

Figure 3. The space distribution of probability density $W(x, y)$ for a canalized state at $\alpha = 5$, $\lambda = 5$, $a = 5$, $p = 2.5$ and $j = 3$.

This approach is an analogue of the Sturmian representation for hydrogen where instead of the energy the charge of the nucleus is quantized [4]. The operator $\hat{\mathbf{A}}$ is Hermitian and well-defined in Hilbert space. Therefore the eigenvalue problem has an infinite set of solutions with real eigenvalues α. The numerical procedure for finding the eigenvalues of three-diagonal matrix $\hat{\mathbf{A}}$ can be reduced to the calculation of the zeros of the related continued fraction

$$\Delta = 2\beta_1 - 2\alpha - \frac{\lambda^2}{(2\beta_2 - 2\alpha -} \frac{\lambda^2}{(2\beta_3 - 2\alpha -} \cdots \frac{\lambda^2}{(2\beta_n - 2\alpha -} \cdots. \tag{16}$$

Figure 2(a) shows Δ as a function of α at $a = 5$, $\lambda = 5$, $p = 2.5$ and $j = 3$. From figure 2(a) one can see that the plot has a tangent-like form with an infinite number of roots α_j on the right-hand side. Figure 2(b) illustrates the dependence of Δ on the quasi-momentum at fixed values of the parameters determining Hamiltonian (1). The density of probability $W(x, y) = |\psi(x, y)|^2$ corresponding to the solution indicated in figure 2 by the arrow is shown in figure 3.

Obviously, the phenomenon considered here is not only a particular feature of the given model but should also exist in three-dimensional many-layer problems with a more realistic description of the layers. Similar (from the mathematical point of view) discrete states with non-standard boundary properties have been revealed in the one-dimensional non-stationary Schrödinger equation [6], which models the multi-photon ionization of an atom in a strong laser field.

This work was supported by the Macedonian Academy of Sciences and Arts under Grant 09-548/1. One of us (JP-J) appreciated stimulating discussions with Professor M Gretzel.

Appendix

Substituting wavefunction (6) into condition of smoothness (3a) we obtain the relation between the coefficients in the interior ($|x| < a$) and exterior ($|x| > a$) regions:

$$d_n \exp(-q_n a) = c_n \begin{pmatrix} \cosh q_n a \\ \sinh q_n a \end{pmatrix} \qquad n < l, n > m \tag{A1}$$

$$d_n \sin(k_n a + \theta) = c_n \begin{pmatrix} \cos k_n a \\ \sin k_n a \end{pmatrix} \qquad l \leqslant n \leqslant m. \tag{A2}$$

The condition for the jump in the first derivative (3*b*) in representation (6) transforms into a three-term recurrent relation for coefficients d_n:

(i) for $n < l$ and $n > m + 1$

$$d_n \exp(-q_n a)(\beta_n - \alpha) = \tfrac{1}{2}\lambda d_{n+1} \exp(-q_{n+1} a) + \tfrac{1}{2}\lambda d_{n-1} \exp(-q_{n-1} a) \tag{A3}$$

(ii) for $l + 1 < n < m$

$$d_n(\beta_n - \alpha) \sin \mu_n = \tfrac{1}{2}\lambda d_{n+1} \sin \mu_{n+1} + \tfrac{1}{2}\lambda d_{n-1} \sin \mu_{n-1} \tag{A4}$$

where $\mu_n = k_n a + \theta$ and

$$\beta_n = \begin{cases} q_n \begin{pmatrix} 1 + \exp(-2q_n a) \\ 1 - \exp(-2q_n a) \end{pmatrix}^{-1} & n < l, n > m \\ -\tfrac{1}{2}k_n \cot \mu_n + \tfrac{1}{2} \begin{pmatrix} -\tan k_n a \\ \cot k_n a \end{pmatrix} & l \leqslant n \leqslant m \end{cases}$$

(as before the upper and lower functions in β_n correspond to symmetric and antisymmetric states, respectively). The relations in the vicinity of the transitional indexes $n = l$ and $n = m$ are:

$$d_l \exp(-q_l a)(\beta_l - \alpha) = \tfrac{1}{2}\lambda d_{l+1} \sin \mu_{l+1} + \tfrac{1}{2}\lambda d_{l-1} \exp(-q_{l-1} a) \tag{A5}$$

$$d_{l+1}(\beta_{l+1} - \alpha) \sin \mu_{l+1} = \tfrac{1}{2}\lambda d_{l+2} \sin \mu_{l+2} + \tfrac{1}{2}\lambda d_l \exp(-q_l a) \tag{A6}$$

$$d_m(\beta_m - \alpha) \sin \mu_m = \tfrac{1}{2}\lambda d_{m+1} \exp(-q_{m+1} a) + \tfrac{1}{2}\lambda d_{m-1} \sin \mu_{m-1} \tag{A7}$$

$$d_{m+1} \exp(-q_{m+1} a)(\beta_{m+1} - \alpha) = \tfrac{1}{2}\lambda d_{m+2} \exp(-q_{m+2} a) + \tfrac{1}{2}\lambda d_m \sin \mu_m. \tag{A8}$$

References

[1] O'Reagan B and Graetzel M 1991 *Nature* 353 737; Special Graetzel Cell issue 1994 *Solar Energy Materials and Solar Cells* vol 32 (Amsterdam: Elsevier)

[2] Messiah A 1970 *Quantum Mechanics* vols I, II (Amsterdam: North-Holland)

[3] Newton R G 1966 *Scattering Theory of Waves and Particles* (New York: McGraw-Hill)

[4] Fock V A 1976 *Fundamentals of Quantum Mechanics* (Moscow: Nauka) (in Russian)

[5] Jones W B and Thron W J 1980 *Continued Fractions. Analytic Theory and Applications* (Reading, MA: Addison-Wesley)

[6] Kazanskii A K, Ostrovskii V N and Solov'ev E A 1976 *Sov. Phys.–JETP* 43 254