A CERTAIN MODEL OF FORMATION OF A FRACTAL DIMENSIONALITY IN THE SCHROEDINGER PROBLEM

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The types of solutions which form in a one-dimensional nonlinear problem about interaction between electrons and acoustical phonons are investigated. Conditions at which the multitude of solutions is found to be fractal are indicated.

1. PROBLEM AND INTRODUCTION FORMULATION

There have been many hypotheses about the possible fractal nature of wave functions near the boundaries of a forbidden zone (see for instance [1-3]). These ideas seem quite attractive. It would be nice, however, to find a comparitively simple example in which the nature of the instability responsible for the formation of the fractal structure of the corresponding multitude would be clearly visible. For this purpose, this work examines a one-dimensional model of a system of electrons which interact with acoustical phonons. Within the method of effective mass the Schroedinger equation and the equation which describes the behavior of the phonons have the form (compare [4]; the authors assume $\hbar=2m=1$)

$$-\psi''-\alpha q'\psi=E\psi, \tag{1}$$

$$q''+a^2q-a^2\beta q|\psi|^2=0. \tag{2}$$

Here, q is the one-dimensional vector of lattice shifting, the prime indicates the value of x which is a derivative in terms of the coordinate, $a = \omega/s$, where ω and s are the frequency and phase velocity of the acoustical phonons, α and β are the constants of the bond ($\alpha > 0$ and $\beta > 0$), and the wave function $\psi(x)$ is assumed to be substantive (in this particular case this is justified). The energy of the electrons E is read off from the bottom of the conductivity zone in the ideal lattice.

It is noted that in essence an adiabatic approximation (phonons and a slow subsystem) was used in deducing these equations. For this reason the value of a is assumed to be less than the other parameters of the corresponding dimension.

Equations (1) and (2) are a nonlinear dynamic system. Assuming

$$\psi'=\varphi,\ q'=p, \tag{3}$$

this system is reduced to the standard appearance

$$
\begin{aligned}
\psi' &= \varphi, \\
q' &= p, \\
\varphi' &= -(E + ap)\psi, \\
p' &= -a^2(q - \beta\psi^2 q).
\end{aligned}
\tag{4}
$$

Generally speaking, numerical integration is required for investigating the integral trajectories of system (4). For the purpose of this work, however, it is sufficient to determine the special points and to investigate the behavior of the integral curves in their small vicinity.

2. SPECIAL POINTS AND THE SECULAR EQUATION

The special points of the system (4) are designated as ϕ_0, ψ_0, q_0, and p_0. Assuming, as usual, that

$$\psi = \psi_0 + \delta\psi,\ \varphi = \varphi_0 + \delta\varphi,\ p = p_0 + \delta p,\ q = q_0 + \delta q, \tag{5}$$

where $\delta\psi$, $\delta\phi$, δq, and δp are proportional to $e^{\lambda x}$, the following linearized system is found:

$$
\begin{aligned}
&\lambda\delta\psi - \delta\varphi = 0, \\
&\lambda\delta\varphi + a\psi_0\delta p + (E + ap_0)\delta\psi = 0, \\
&\lambda\delta q - \delta p = 0, \\
&\lambda\delta p + a^2(1 - \beta\psi_0^2)\delta q + 2a^2\beta q_0\psi_0\delta\psi = 0.
\end{aligned}
\tag{6}
$$

The determinant of this system is designated as $D(\lambda)$ and the secular equation, from which the values of λ are identified, has the form of $D(\lambda) = 0$. Assuming that the right parts of Eqs. (3) are equal to zero, it is found that

$$\varphi_0 = p_0 = 0, \tag{7}$$

$$E\psi_0 = 0, \tag{8}$$

$$(\beta\psi_0^2 - 1)q_0 = 0. \tag{9}$$

At $E \neq 0$ Eqs. (7) and (8) allow for only a trivial solution*:

$$\psi_0 = q_0 = 0,\ \lambda_{1,2} = \pm i\sqrt{E},\ \lambda_{3,4} = \pm ia. \tag{10}$$

At $E = 0$, however, the function ψ_0 remains arbitrary, while $q_0 = 0$. Here, the roots of the secular equation have the appearance

$$\lambda_{1,2} = 0,\ \lambda_{3,4} = \pm a\sqrt{\beta\psi_0^2 - 1},$$

where ψ_0 can take any value (the line of special points).

The presence of a zero root and a line of special points hinders the investigation of solutions of the examined system using the well-known methods [5]. For this reason it is expedient to somewhat alter the system (1) and (2), adding small nonlinear components to it (the latter need not have a strictly physical

*The equality of $\psi_0 = 0$ should not be confused; according to (5), the wave function is not reduced to ψ_0 alone.

sense - upon completion of the calculations the corresponding coefficients may be equated to zero).

3. THE MODIFIED SYSTEM OF EQUATIONS

One of the components of interest suggests itself - it describes (the small!) anharmonism of lattice oscillations. With its consideration Eq. (2) assumes the appearance

$$q''=a^2(\beta\psi^2-1)q+\sigma q^2, \qquad (2')$$

where σ is the constant of the anharmonism ($\sigma > 0$). Analogously, a component nonlinear in terms of ψ must be introduced into the right part of Eq. (1). Its simplest form, which conforms with the condition of gradient invariance, is $|\psi|^2\psi$. Thus, considering the function of ψ significant, as before, it is found that

$$\psi''+(E+\alpha p)\psi+\eta\psi^3=0, \qquad (1')$$

where η is the parameter, whose sign is subject to identification (below it will be evident that it must agree with the sign of E). It is stressed that unlike the anharmonic component, the additional member in (1') has only a formally mathematical sense and upon completion of the calculations the maximal transition of $\eta \to 0$ should be met.

Instead of the linearized system (6), the following is now found:

$$\begin{gathered}\lambda\delta\psi-\delta\varphi=0,\\ \lambda\delta\varphi+(E+\alpha p_0+3\eta\psi_0^2)\,\delta\psi+\alpha\psi_0\,\delta p=0,\\ \lambda\delta q-\delta p=0,\\ \lambda\delta p-[a^2(\beta\psi_0^2-1)+2\sigma q_0]\,\delta q+2a^2\beta\psi_0 q_0\,\delta\psi=0.\end{gathered} \qquad (6')$$

The trivial special point here is not altered, just as the behavior of the solutions in its vicinity is not altered. The nontrivial special point, however, is now determined by the relations

$$\varphi_0=p_0=0,\ \psi_0^2=-E/\eta,\ \ q_0=a^2(\beta\psi_0^2-1)\,\sigma^{-1}. \qquad (11)$$

It is evident that the examined special point exists only when sign η = -sign E and E approaches zero along with η, which the author will hypothesize. Now the case of $E \to 0$ is of interest, where the relation $|E/\eta|$ remains finite (factually ψ_0^2 is determined from the normalization condition). The determinant of system (6') here assumes the appearance

$$D(\lambda)=\lambda^4+(\sigma q_0-2E)\,\lambda^2+2\alpha\beta q_0 a^2\psi_0^2\lambda-2E\sigma q_0. \qquad (12)$$

At low values (but still not equal to zero) of E, σ and η of the root $D(\lambda)$ are given by the expressions

$$\begin{gathered}\lambda_1=\frac{\sigma|\eta|}{\alpha\beta a^2}\operatorname{sign}E,\\ \lambda_{2,3}=\frac{1\pm i\sqrt{3}}{2}R^{1/3},\ \lambda_4=-R^{1/3},\end{gathered} \qquad (13)$$

where

$$R=\left[2\alpha\beta\alpha'\sigma^{-1}\left|\frac{E}{\eta}\right|\left(\beta\left|\frac{E}{\eta}\right|+1\right)\right] \tag{14}$$

(for the sake of determinateness, it is assumed that $|E/\eta| > 1$).

According to [5], it follows that at $E \to +0$ (when $\eta < 0$) near the special point there is one and only one periodic trajectory, where it is of the saddle type.* This means that permitted solutions of the Schroedinger equation appear which are described by homoclinic integral curves. As is known (see, for instance, [6]), their multitude has a fractal dimension. Generally speaking, selection of the specific integral curve which corresponds to an energy of $E = 0$, is determined by the boundary conditions on the ends of the large (formally - infinitely large) sample. It is known, however, that for homoclinic curves such a procedure is physically senseless, since even the smallest variations in the boundary conditions lead to quite large changes in the solution. In fact, the case of "spatial noise" must occur here, i.e., powerful and disordered changes in the wave function with a shift from point to point.

It is clear that the examined solutions correspond to less than complete energy since they are associated with the trivial special point. Because of this, it is precisely they which must be physically realized.

Apparently analogous results are also acquired with interaction between electrons and optical lattice oscillations. However, consideration of interaction with acoustical oscillations, despite its relative weakness, seems attractive due to its universal nature.

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REFERENCES

1. H. Aoki, J. Phys. C, vol. 16, p. 205, 1983.
2. C. M. Soukoulis and E. N. Economou, Phys. Rev. Lett., vol. 52, p. 565, 1984.
3. M. Cohen, E. N. Economou, and C. M. Soukoulis, J. Noncryst. Sol., vols. 59-60, p. 25, 1983.
4. F. V. Kusmartsev and E. I. Rashba, FTP, vol. 18, p. 691, 1984.
5. L. P. Shil'nikov, Matem. Sb., vol. 77(119), p. 461, 1968.
6. V. S. Afraimovich and Ya. B. Pesin, UMN, vol. 39, no. 3(236), p. 135, 1984.

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*It should be noted that demonstration of Shil'nikov's theorem [5] is based on a hypothesis about the existence of a loop in the separatrix with a specific value of a certain parameter. For this hypothesis to be confirmed, it is sufficient to have (in the problem here) four free parameters, whose adjustment ensures "linking" of the two separatrices, one of which belongs to a stable separatrix surface, while the other belongs to an unstable separatrix surface. As is evident from Eqs. (1') and (2'), such parameters are present in the problem. Naturally, the situation with the loop of the separatrix is not approximate. With a change in the parameters, this loop is broken down, engendering approximate objects - stable or saddle maximal cycles. In the problem here, the latter possibility is realized.