acta phys. slov. 26 (1976), No. 4

ON THE THEORY OF BOUND STATES IN A RANDOM POTENTIAL

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An approximate method is discussed for the calculation of the energy-level density of low-lying bound states in a random potential. Such states occur in regions of well-separated deep potential wells. The method utilizes the prognosis for the wells in the framework of the correlation theory. The method is suitable for the states localized in a region much smaller than the correlation length of the random potential. The presented method is compared with the theory of Halperin and Lax. The computed mean potential energies of particles in the localized states are in good agreement with the results of Halperin and Lax.

К ТЕОРИИ СВЯЗАННЫХ СОСТОЯНИЙ В СЛУЧАЙНОМ ПОТЕНЦИАЛЕ

В статье обсуждается приближённый метод для вычисления плотности энергетических уровней низколежащих связанных состояний в случайном потенциале. Такие состояния существуют в той области, где глубокие потенциальное ямы находятся на большом расстоянии друг от друга. Метод использует предсказания для потенциальных ям, полученные в рамках теории корреляции. Развиваемый метод применим для состояний, которые локализованы в области, намного меньшей, чем корреляционная длина случайного потенциала. Излагаемый метод сравнивается с теорией Гальперина и Лэкса, и рассчитанные средние потенциальные энергии частиц в локализованных состояниях находятся в хорошем согласии с этой теорией.

1. INTRODUCTION

Halperin and Lax (HL) [1] presented an approximate method for calculating the density of states $\varrho(E)$ in the low-energy tail of an electron band of a semiconductor, in the presence of a high density of impurities. In the framework of the effective scalar mass approximation the hamiltonian of the problem is $H = -\Delta/2m - V(\boldsymbol{r}) + E_0$, where m is the electron (or hole) effective mass and the constant energy E_0 is chosen such that $\langle V \rangle = 0$ (the angular brackets indicate an average over the ensemble of impurity positions). Under certain assumptions the random potential $V(\boldsymbol{r})$ obeys the Gaussian statistics with the autocorrelation function [1, 2].

$$\langle V(\boldsymbol{r})\, V(\boldsymbol{r}') \rangle = \xi W(|\boldsymbol{r} - \boldsymbol{r}'|) = \xi \exp\left(-\frac{|\boldsymbol{r} - \boldsymbol{r}'|}{L}\right), \tag{1}$$

where the mean square fluctuation ξ is proportional to the concentration of impurities and to the square of the strength of the individual impurities and to the square of the strength of the individual impurities and where the function $W(|\boldsymbol{r} - \boldsymbol{r}'|)$ depends only on the shapes of the impurity potentials. Eq. (1) presents the case of screened Coulomb impurity potentials, thus the correlation length L is identical with the screening length.

The region of energy with a small density of states is called the low energy tail. An energy E will be in the low-energy tail if $E_0 - E > 0$ is lagre compared to the energy easily obtainable from the potential fluctuations, i.e. if $(E_0 - E)/\sqrt{\xi} \gg 1$. Thus the states in the low-energy tail are bound in wells in the random potential, arising from large fluctuations in the local density of impurities.

If the energy E is deep enough in the tail, then the probability of a potential fluctuation capable to produce an excited state at E will be quite small and in the calculation of $\varrho(E)$ the presence of the excited states can be neglected.

The crucial assumption used by HL was that all the eigenstates $f(\boldsymbol{r})$, at a given energy E in the tail, have the same shape, or equivalently, that all the corresponding potential wells have the same shape. This approximation leads to an overestimate of the energy of each eigenstate and an underestimate of the density of states in the tail, where the density of states is rapidly falling. Thus the best choice of f, for any given energy E, is that which maximizes $\varrho_f(E)$. The application of the variational calculus leads to the equation for f of the form [1]

$$\left[-\frac{\Delta}{2m} - V_0(\boldsymbol{r})\right] f = (E - E_0) f \tag{2}$$

with an "average" or "optimal" potential well given by

$$V_0(\boldsymbol{r}) = -\mu \int W(\boldsymbol{r} - \boldsymbol{r}') f^2(\boldsymbol{r}')\, \mathrm{d}\boldsymbol{r}', \tag{3}$$

where μ is a Lagrange multiplier which is determined by the condition $\int f^2(\boldsymbol{r})\, \mathrm{d}\boldsymbol{r} = 1$.

States in the low-energy tail will generally be highly localized in a region of low potential and the function f must be rapidly decreasing when its argument becomes large. Assume that the characteristic size λ of f is much smaller than the correlation length L. Then for the potential V_0 with $|\boldsymbol{r} - \boldsymbol{r}_0| \gg \lambda$, where the vector $\boldsymbol{r}_0$ gives the centre of the potential well, it follows:

$$V_0(\boldsymbol{r}) = -\mu W(\boldsymbol{r} - \boldsymbol{r}_0) = -\mu \exp\left(-\frac{|\boldsymbol{r} - \boldsymbol{r}_0|}{L}\right). \tag{4}$$

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Efros [2] compared this analytical expression with the results of the HL's numerical computation. Both these functions differ at the centre of the potential well. However, at the centre of the potential well the probability of finding the electron is small and this difference can be unimportant in the quantummechanical average.

In this paper we wish to point out that the potential shape given by Eq. (4) is just the shape which can be predicted in the framework of the correlation theory and to show how this prediction can be utilized for the calculation of $\varrho(E)$. We have also presented some calculations with the autocorrelation function given by (1) and the results are compared with those computed by HL. Namely, we have computed the mean potential energy of a localized particle.

II. PROGNOSIS FOR THE POTENTIAL WELL

In the framework of the correlation theory the best prognosis (or extrapolation) for a homogeneous random function $V(\boldsymbol{r})$, if we know its value at a point $\boldsymbol{r}_0$, is [3, 4]

$$V(\boldsymbol{r}) = V(\boldsymbol{r}_0)\, W(\boldsymbol{r}-\boldsymbol{r}_0)\,. \tag{5}$$

Indeed, if the function W in Eq. (5) is identical with the correlation function W defined by Eq. (1), then the mean square fluctuation of $V(\boldsymbol{r})$ from its prediction (5) is minimum and there holds

$$\langle (V(\boldsymbol{r}) - V(\boldsymbol{r}_0)\, W(\boldsymbol{r}-\boldsymbol{r}_0))^2 \rangle = \langle V^2(\boldsymbol{r}) \rangle (1 - W^2(\boldsymbol{r}-\boldsymbol{r}_0))\,. \tag{6}$$

This expression and therefore also the probability (Chebyshev's inequality) that $V(\boldsymbol{r})$ differs from the value given by the prediction (5), will be small as long as W is near to unity, i.e. as long as $|\boldsymbol{r}-\boldsymbol{r}_0| \ll L$. Now, it is clear that the prognosis (5) is suitable for the localized states with $\lambda \ll L$. The prognosis (5) for a given energy E gives all the potential wells of the same shape and therefore it supports the central assumption made by HL.

If we now solve the Schrödinger equation for the ground state with the potential of the shape (5), we shall obtain a condition saying what the value of the potential $V(\boldsymbol{r}_0)$ has to be, in order that the ground-state energy may equal E. This condition generally does not give an isolated point $\boldsymbol{r}_0$ but surfaces on which $V(\boldsymbol{r}_0)$ has the required value. It is natural to choose this point so that the approximation may be improved. Therefore we require for the first approximation of the perturbation calculus to have the minimum value, that is for the expression

$$\{\int [V(\boldsymbol{r}_0)\, W(\boldsymbol{r}-\boldsymbol{r}_0) - V(\boldsymbol{r})]\, f_E^2(\boldsymbol{r}-\boldsymbol{r}_0)\, \mathrm{d}\boldsymbol{r}\}^2 \tag{7}$$

to be minimum if $V(\boldsymbol{r}_0)$ corresponds to the ground state $f_E(\boldsymbol{r})$ with the energy E. This requires for the "smoothed" potential

$$\int V(\boldsymbol{r}) f_E^2(\boldsymbol{r}-\boldsymbol{r}_0)\, \mathrm{d}\boldsymbol{r} \tag{8}$$

to be a minimum as a function of $\boldsymbol{r}_0$. This is, however, an equivalent requirement with that made by HL in order to find the position of large negative fluctuations of wells in $V(\boldsymbol{r})$.

The present treatment differs from that given by HL only in the choice of the function f, therefore the formal expression for the density of states (Eqs. (3, 5) and (3, 23) of HL) remains unchanged and it can be used in this case as well. We have mentioned above that the best choice of f is that which maximizes $\varrho_f(E)$, hence our approach is less correct than that of HL. However, as long as E is deep in the tail, the prognosis (5) has the high probability and the difference is expected to be small. The advantage of the present method is its simplicity and possibility to perform some calculations analytically. Further, since the prognosis (5) does not depend on the distribution function of the potential, it can also be used for non-Gaussian distributions.

III. RESULTS

For the potential well of the shape (5) with the autocorrelation function (1) the Schrödinger equation has the exact solution for the ground state [5]. This solution is (with $\boldsymbol{r}_0 \equiv 0$)

$$S(r) = \sqrt{4\pi}\, r\, f(r) = C J_p(\mathrm{e}^{-r/2L})\,, \tag{9}$$

where J_p is the Bessel function of the order p and

$$\frac{p^2}{4} = \nu = (E_0 - E)\frac{2mL^2}{\hbar^2} > 0 \tag{10}$$

$$\frac{\beta^2}{4} = v = -V(\boldsymbol{r}_0 \equiv 0)\frac{2mL^2}{\hbar^2} > 0\,.$$

The energy of the ground state is given by the first root of the equation

$$J_p(\beta) = 0\,. \tag{11}$$

The normalization constant C can be expressed as follows [7]:

$$C^{-2} = J_{p+1}^2(\beta)\frac{\mathrm{d}\,\beta^2}{\mathrm{d}p^2}\,. \tag{12}$$

For large values of p for the first root of Eq. (9) the asymptotical expression is known [6] from which it follows for the potential depth v (below we use the units $L = 1$ and $\hbar^2/2mL^2 = 1$):

$$v=\left(1+\frac{1.169055}{\sqrt[3]{\nu}}+\frac{0.410006}{\sqrt[3]{\nu^2}}-\frac{0.0010075}{\nu}-\right.$$

$$\left.-\frac{0.014347}{\nu\sqrt[3]{\nu}}+\frac{0.004444}{\nu\sqrt[3]{\nu^2}}-\ldots\right)^2. \tag{13}$$

To compare our results with those obtained by HL we computed the mean value of the potential energy of the particle in the ground state. This quantity was chosen as it has an analytical (asymptotical) expression and as it dominantly determines the

Table 1

log ν	ν	v	μ	$\bar{V}$	$\bar{V}_{\mathrm{HL}}$
3.00	1000	1256.65	1354	1080.38	1065.60
2.75	562.3	740.61	810	617.41	606.79
2.5	316.2	440.59	491.3	354.04	346.49
2.25	177.8	265.00	302.1	203.82	198.40
2.00	100	161.51	188.6	117.93	114.00
1.75	56.2	99.87	120.2	68.57	65.73
1.50	31.6	62.88	78.4	40.17	38.11
1.25	17.78	40.42	52.5	23.73	22.24
1.00	10	26.58	36.2	14.15	13.03

exponent of the exponential factor of $\varrho(E)$ in the tail [1]. The mean potential energy is given by

$$\bar{V}\equiv -v\int_0^\infty \mathrm{e}^{-r}S^2(r)\,\mathrm{d}r=-v\left(\frac{\mathrm{d}v}{\mathrm{d}\nu}\right)^{-1}. \tag{14}$$

In Table 1 are given the values v and $\bar{V}$ for large values of the energy ν and they are compared with the mean values of the potential energies $\bar{V}_{\mathrm{HL}}$ computed by HL and with the values of the Lagrange multiplier μ. This multiplier cannot be considered to be identical with the depth of the potential well, it will be, however, very close to v for the states deep in the tail, i.e. for $\nu\to\infty$. As it can be seen the agreement is very good.

The function $S(r)$ has the maximum for $r=r_{max}$ given by [6]

$$r_{max}\approx 2\ln\frac{\beta}{p+0.808618\sqrt[3]{p}}\approx 1.319\frac{1}{\sqrt[3]{\nu}}. \tag{15}$$

The prognosis (5), as we have mentioned above, can be considered a good one, as long as the particle is localized in the region of a size much smaller than the correlation length. This requires $r_{max}\ll 1$ or equivalently

$$\sqrt[3]{\nu}\gg 1. \tag{16}$$

This will be satisfied only in the tail. If we define the size of the function $S(r)$ from its exponent on the large distance, $S(r)\sim\mathrm{e}^{-r/2}$, then instead of (10) we shall obtain that $\sqrt{\nu}\gg 1$. This is however, fulfilled in the tail if Eq. (16) holds. Reasonably well the size of the wave function can be identified with the classically allowed region, i.e. one can define λ as r for which $\nu=v\mathrm{e}^{-r/2}$. From this it follows for a large ν

$$\lambda\approx\frac{2.34}{\sqrt[3]{\nu}}. \tag{17}$$

Thus, the criterion (16) has to be roughly twice stronger. If we consider this criterion, then the results given in Tab. 1 can be considered as reliable only for very large values of ν (roughly for $\nu>100$) and in this region the agreement with the results of HL is really very good.

Efros [2] used for the size of the wave function an expression differing from (17) only by the numerical factor and showed that this expression can be successfully used for the computation of the relative positions of the maxima of the wave functions. This is evident comparing the formulae (17) and (15).

REFERENCES

[1] Halperin B. I., Lax M., Phys. Rev. *148* (1966), 722.
[2] Efros A. L., UFN *111* (1973), 451.
[3] Svešnikov A. A., *Prikladnyje metody teorii slučajnych funkcij.* Nauka, Moskva 1968.
[4] Rozanov Ju. A., *Slučajnyje processy.* Nauka, Moskva 1971.
[5] Flügge S., *Practical Quantum Mechanics I.* Springer Verlag, N.Y. 1971. (Russian translation, Fljugge Z., *Zadači po kvantovoj mechanike,* Mir, Moskva 1974, Zadača 75).
[6] Janke E., Emde F., *Tablici funkcij s formulami i krivymi.* GIFML, izd. 3, Moskva 1959.
[7] Watson G. N., *Theory of Bessel Functions.* Univ. Press, Cambridge 1944.

Received July 23rd, 1975