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DENSITY OF STATES OF A PARTICLE IN THE GAUSSIAN RANDOM POTENTIAL

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Approximate methods are used for the calculation of the density of states of low-lying bound states of a particle in the Gaussian random potential with the Gaussian autocorrelation function. One of the methods utilizes the prognosis for the potential wells in the framework of the correlation theory. The other method derives the density of states using Bezák's statistical sum. Both methods give the same density of states in the deep energy tail where the quasiclassical results do not longer hold. The most general expression here obtained for the density od states holds for energies $E < -\eta$, where η^2 is the mean square potential fluctuation.

ПЛОТНОСТЬ ОДНОЧАСТИЧНЫХ СОСТОЯНИЙ В СЛУЧАЙНОМ ГАУССОВСКОМ ПОТЕНЦИАЛЕ

В работе для вычисления плотности низколежащих связанных одночастичных энергетических состояний в случайном гауссовском потенциале с гауссовской автокорреляционной функцией используются приближённые методы. Один из этих методов использует прогноз для потенциальных ям в рамках теории корреляций. Второй метод выводит плотность состояний, используя статистическую сумму Безака. Оба метода дают одну и ту же плотность состояний глубокоэнергетического хвоста, где уже не имеют место квазиклассические результаты. Наиболее общее выражение для плотности состояний, которое получено в работе, имеет место для энергий $E < -\eta$, где η^2 представляет собой среднеквадратичное отклонение потенциала.

I. INTRODUCTION

Recently one of the authors of [1] has presented an approximate method for calculating the density of states (d.s.) in the low energy tail of a particle in the random Gaussian potential. This method differs from the minimum counting method of Halperin and Lax (HL) [2] in that the optimal potential wells are replaced by the most probable wells. In the framework of the correlation theory, the best function prognosis (extrapolation) for the homogeneous random function $V(\mathbf{r})$, if we know its value at a point $\mathbf{r}_0$, is

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$$V(\mathbf{r}) = V(\mathbf{r}_0)\, W(\mathbf{r}-\mathbf{r}_0). \tag{1}$$

The function $W(\mathbf{r}-\mathbf{r}_0)$ is the autocorrelation function divided by the mean square fluctuation η^2, i.e.

$$\langle V(\mathbf{r})\, V(\mathbf{r}_0)\rangle = \eta^2 W(\mathbf{r}-\mathbf{r}_0) \tag{2}$$

$$\langle V(\mathbf{r})\rangle = 0.$$

In this paper we apply this method to the particle in the Gaussian random potential $V(\mathbf{r})$ with the autocorrelation function

$$W(\mathbf{r}-\mathbf{r}') = \exp\left(-\frac{(\mathbf{r}-\mathbf{r}')^2}{L^2}\right). \tag{3}$$

This problem was solved by Bezák [3] in the limit of the large correlation length L using Feynmans's path integrals. He supposed that the autocorrelation function may be approximated by

$$W(\mathbf{r}) = 1 - \frac{\mathbf{r}^2}{L^2} \tag{4}$$

and he found the averaged density matrix.

By means of the approximation (4) with the statistical prognosis (1) the problem reduces to the solution of the Schrödinger equation of the particle in the parabolic potential well. As the solution of the problem is well known, d.s. can be found by the method [1] analytically.

Since Bezák [3] also used some auxiliary approximations, he derived d.s. in the energy region

$$E > -\eta^{4/3}\left[\frac{mL^2}{2\hbar^2}\right]^{1/3} \tag{5}$$

only and showed that the condition (5) gives the region of validity of the quasiclassical approximation (see e.g. [4]). The exact form of the partition sum is derived in [5] by means of infinite products. The compact analytical form of the statistical sum has been found independently by Barta [6], and Papadopoulos [7] and Drchal and Mašek [8].

$$Z(\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2} \varphi\left(\frac{1}{2}\hbar\omega_G\beta\right) \exp\left(\frac{1}{2}\eta^2\beta^2\right) \tag{6a}$$

$$\omega_G = \frac{\eta}{L}\sqrt{\frac{2\beta}{m}}, \tag{6b}$$

where

$$\varphi(x) = \left(\frac{x}{\mathrm{sh}x}\right)^3. \tag{6c}$$

In this paper we shall find the asymptotic form of d.s. corresponding to the statistical sum (6) and we shall show the consistency of both presented theories in the low energy tail.

II. MINIMUM COUNTING METHOD

Let us consider the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\Delta - V(\mathbf{r}),$$

where m is the effective mass of the particle and $V(\mathbf{r})$ is the random potential statistically defined in the previous section. We restrict ourselves to such deep states with energies E that it is sufficient to make into account merely the ground states in each negative potential fluctuation, i.e. the probability of the potential well which can give the excited state with the energy E must be negligible compared with the fluctuation giving the ground state with the same energy.

The crucial assumption used by HL was that all the eigenfunctions $f(\mathbf{r})$ with the given energy in the tail have the same shape or equivalently, that all the corresponding potential wells have the same shape. The energies of the corresponding ground states in the framework of the variational principle are given by the local minima of the averaged energy

$$E_s(\mathbf{r}_0) = \theta - V_s(\mathbf{r}_0), \tag{7}$$

where θ is the mean kinetic energy

$$\Theta = \int f(\mathbf{r}-\mathbf{r}_0)\left(-\frac{\hbar^2}{2m}\Delta\right) f(\mathbf{r}-\mathbf{r}_0)\,\mathrm{d}\mathbf{r} \tag{7a}$$

and $V_s(\mathbf{r})$ is the smoothed potential

$$V_s(\mathbf{r}_0) = \int V(\mathbf{r})\, f^2(\mathbf{r}-\mathbf{r}_0)\,\mathrm{d}\mathbf{r} \tag{7b}$$

(the wave function $f(\mathbf{r})$ can be chosen to be real).

In the low energy tail the eigenstates are placed spatially far between, so that the possibility of the simultaneous overlap between two different states is quite negligible. Then the number of the eigenstates with the energies from the interval $(E, E+\Delta E)$ is approximately equal to the number of local minima of $V_s(\mathbf{r}_0)$ with values

$$E - \Theta < V_s(\mathbf{r}_0) < E - \Theta + \Delta E.$$

HL found that except for the terms which are negligible in the low energy tail, the approximate d.s. is given by the expression

$$\varrho(E) = \frac{\sigma_1\sigma_2\sigma_3(\Theta - E)^3}{(2\pi)^2\eta^4\sigma_0^7}\exp\left(-\frac{(\Theta-E)^2}{2\eta^2\sigma_0^2}\right), \tag{8}$$

where

$$\sigma_0^2 = W_s(0) \tag{8a}$$

and σ_1^2, σ_2^2, σ_3^2 are the eigenvalues of the tensor

$$\mathscr{K} = -\nabla_y\nabla_y W_s(\mathbf{y})|_{y=0}. \tag{8b}$$

The function $W_s(\mathbf{y})$ is the smoothed autocorreletion function given by

$$W_s(\mathbf{y}) = \iint f^2(\mathbf{r}) f^2(\mathbf{r}')\, W(\mathbf{r}-\mathbf{r}'+\mathbf{y})\,\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}'.$$

Since the variational method overestimates the energy of the ground states, the formula (8) underestimates the actual d.s. HL used an approximate method to find the best shape of the wave function $f(\mathbf{r})$ for a given energy, which maximalizes the expression (8).

Instead of using this procedure the statistical prognosis was used for the potential wells in [1]. This is a good approximation for the space regions smaller than the correlation length. As the states in the deep tail are strongly localized, the function $f(\mathbf{r})$ can be found by solving the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\Delta + V(0)W(\mathbf{r})\right] f(\mathbf{r}) = Ef(\mathbf{r}). \tag{9}$$

III. GAUSSIAN AUTOCORRELATION FUNCTION

The formulae of the previous section will be now applied to the case when the autocorrelation function has the form (3). If the size of the function $f(\mathbf{r})$ is supposed to be smaller than the correlation length, the approximation (4) takes place and by solving Eq. (9) one obtains the eigenfunction of the ground state

$$f(\mathbf{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4}\exp\left(\frac{m\omega}{2\hbar}\mathbf{r}^2\right), \tag{10}$$

where ω is given by the expression

$$\omega^2 = -\frac{2V(0)}{mL^2} \tag{11}$$

and the energy of the ground state is

$$E = V(0) + \frac{3}{2}\hbar\omega. \tag{12}$$

Excluding $V(0)$ from Eqs. (11) and (12) we get

$$\frac{1}{2}m\omega^2L-\frac{3}{2}\hbar\omega+E=0. \tag{13}$$

This equation determines the dependence of the frequency ω on the energy.

The characteristic size λ of the function (10) can be defined as the distance for which the exponential factor will decrease on the value e^{-3}. Following further considerations regarding the size of the eigenfunction, the condition

$$\lambda^2=6\hbar/m\omega\ll L^2$$

must hold. Using (13) the corresponding condition for the energies is

$$|E|\gg 15\hbar^2/mL^2,\qquad E<0. \tag{14}$$

If this condition is satisfied, the size of the ground state function is smaller than the correlation length L. From the intuitive point of view the inequality (14) means that the kinetic energy of the particle in the potential well of the characteristic size L being of the order $\hbar^2/2mL^2$, it must be much smaller than the depth of the potential well. To write the expression for d.s. one has to compute the quantities

$$\Theta=\frac{3}{4}\hbar\omega,\quad \sigma_0^2=\left(1+\frac{2\hbar}{m\omega L^2}\right)^{-3/2},\quad \sigma_1^2=\sigma_2^2=\sigma_3^2=\frac{2}{L^2}\sigma_0^{10/3}. \tag{15}$$

We have used the formulae (8a, b), (10).

For the energies in the deep tail we get after substitution into (8) the asymptotic form of d.s. as

$$\varrho(E)=\frac{|E|^3}{\pi^2\sqrt{2}\,L^3\eta^4}\exp\left(-\frac{1}{2}\left(\frac{E}{\eta}\right)^2-3\left|\frac{E}{\eta}\right|^{3/2}\sqrt{\frac{\hbar^2}{2mL^2\eta}}\right). \tag{16}$$

The terms of the orders $|E|$, $|E|^{1/2}$, $|E|^0$ are neglected in the argument of the exponential function. In the preexponential factor only the leading term is kept.

Our calculations neglect the presence of the excited states in each minimum. The ground state with the energy E is generated by the potential well with the depth $V_0=E-\frac{3}{2}\hbar\omega$, the first excited state with the same energy is generated by the well with the depth $V_1=E-\frac{5}{2}\hbar\omega$. As follows from the Gaussian statistics the ratio of the probabilities of both potential wells is of the order

$$\exp\left(-\frac{1}{2\eta^2}(V_1^2-V_0^2)\right).$$

The requirement of neglecting the excited states then leads to the condition

$$|E|\gg\eta\left(\frac{\eta mL^2}{2\hbar^2}\right)^{1/3}. \tag{17}$$

This condition is just opposite to that of Bezák (5).

The use of the minimum counting method assumes a one-to-one correspondence between energy states and minima, which is only valid if the spread of the wave function associated with each minimum is small compared to the mean separation between minima, i.e. if

$$\lambda^3<\left(\int_{-\infty}^{E_1}\varrho(E)\,dE\right)^{-1}. \tag{18}$$

When only minima below some cut-off energy E_1 are to be counted and $\lambda^2=6\hbar L(2m|E|)^{-1/2}$ is the characteristic size of the wave function, a "safe" condition can be written with $E_1=0$, which gives

$$|E|>\frac{18\sqrt[3]{4}\,\hbar^2}{\pi^{8/3}mL^2}. \tag{19}$$

This is not any new condition and is less stringent than the condition (14).

IV. CONSISTENCY WITH BEZÁK'S THEORY

Bezák's results for d.s. are confined to be quasiclassical approximation. We show how to get the asymptotical form of d.s. for the wide range of negative energies from the statistical sum (6). We do not follow the direct way, which uses the formula

$$\varrho(E)=\frac{1}{2\pi i}\int_{-i\infty+\delta}^{+i\infty+\delta}Z(\beta)\exp(\beta E)\,d\beta,$$

because the function to be integrated strongly oscillates for imaginary β. Therefore we use another method (see Appendix) which gives for $|E|\gg\eta, E<0$ the approximate form

$$\varrho(E)=\frac{1}{\sqrt{2\pi\eta^2}}\left(\frac{m\eta^2}{2\pi\hbar^2|E|}\right)^{3/2}\varphi\left(\sqrt{\frac{\hbar^2|E|^3}{2L^2\eta m\eta^3}}\right)\exp\left(-\frac{E^2}{2\eta^2}\right). \tag{20}$$

(The function $\varphi(x)$ is defined by (6c)).

For the energies

$$-\eta\left(\frac{\eta mL^2}{2\hbar^2}\right)^{1/3}<E<-\eta \tag{21}$$

we get in agreement with Bezák [3] the asymptotical behaviour of the quasiclassical approximation

$$\varrho_c(E)=\frac{m^{3/2}\eta^{1/2}}{4\pi^2\hbar^3}\left|\frac{\eta}{E}\right|^{3/2}\exp\left(-\frac{E^2}{2\eta^2}\right). \tag{22}$$

On the other hand, for the states in the deep energy tail (17) the asymptotic form according to Eq. (20) is

$$\varrho_{HL}(E)=\frac{1}{2\pi^2}\left|\frac{E}{\eta}\right|^3\frac{1}{L^3\eta}\exp\left(-\frac{E^2}{2\eta^2}-3\left|\frac{E}{\eta}\right|^{3/2}\sqrt{\frac{\hbar^2}{2mL^2\eta}}\right). \tag{23}$$

This function is in agreement with the result (16) derived by the modified minimum counting method. Both the approximations (22) and (23) are only special cases of formula (20), which is valid for the wide range of negative energies.

It is interesting to compare the quasiclassical approximation and the approximation (16) for the deep states (17). We obtain

$$\frac{\varrho_c(E)}{\varrho_{HL}(E)}=\left(\frac{mL^2\eta^4}{2\hbar^2E^3}\right)^{3/2}\exp\left(3\left|\frac{E}{\eta}\right|^{3/2}\sqrt{\frac{\hbar^2}{2L^2M\eta}}\right)\gg 1.$$

This inequality shows that the quantum effects shift the energy levels to higher energies.

We note that the quasiclassical approximation (22) does not depend on the size of the autocorrelation function; on the other hand the approximations (16) or (20) depend both on the correlation length L and on Plancks constant $\hbar$. It would be interesting to probe how d.s. depends on the form of the autocorrelation function.

In the previous consideration we have not discussed the physical foundation of the presented model. To apply the last results to real cases the following questions should be reconsidered: *i*) is the single band approximation well founded? (At least the investigated energies must not exceed the half of the forbidden band); *ii*) is the Gaussian distribution law valid for deep potential fluctuations? [4]; *iii*) how to choose the autocorrelation function, is the approximation (4) reasonable enough?

APPENDIX

The assymptotic form of d.s.

For the Gaussian random potential the dominant term in d.s. for negative energies is

$$\exp\left(-\frac{1}{2}\left|\frac{E}{\eta}\right|^2\right),$$

therefore we can write

$$\varrho(E)=g(E)\exp\left(-\frac{1}{2}\left|\frac{E}{\eta}\right|^2\right). \tag{A1}$$

The statistical sum corresponding to d.s. (A1) is given by

$$Z(\beta)=\int_{-\infty}^{-\infty}\varrho(E)\exp(-\beta E)\,\mathrm{d}E$$

$$=\exp\left(\frac{1}{2}\eta^2\beta^2\right)\int_{-\infty}^{+\infty}g(E)\exp\left(-\frac{1}{2}\left(\frac{E}{\eta}+\eta\beta\right)^2\right)\mathrm{d}E. \tag{A2}$$

From (A2) it is clear that for $\eta\beta\gg 1$ the most considerable contribution in integral (A2) is given by the large negative energies. The function

$$\exp\left(-\frac{1}{2}\left(\frac{E}{\eta}+\eta\beta\right)^2\right)$$

has a maximum for $E=E_{max}=-\eta^2\beta$ and the width of this maximum is of the order η. For $\eta\beta\gg 1$ the relative width of this maximum is small, so we can write approximately

$$Z(\beta)\doteq\exp\left(\frac{1}{2}\eta^2\beta^2\right)g(-\eta^2\beta)\int_{-\infty}^{+\infty}\exp\left(-\frac{1}{2}\left(\frac{E}{\eta}+\eta\beta\right)^2\right)\mathrm{d}E= \tag{A3}$$

$$=\sqrt{2\pi\eta^2}\,\varrho(-\eta^2\beta)\exp(\eta^2\beta^2)\quad\text{for}\quad\eta\beta\gg 1.$$

For $\beta=-E\eta^{-2}$ we get the result

$$\varrho(E)=\frac{1}{\sqrt{2\pi\eta^2}}Z\left(-\frac{E}{\eta^2}\right)\exp\left(-\left(\frac{E}{\eta}\right)^2\right),\quad |E|\gg\eta,\quad E<0. \tag{A4}$$

This is the asymptotic form of d.s. for deep tails.

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