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THE EXACT INSTANTON SOLUTION FOR THE CONDUCTIVITY OF A DISORDERED SOLID

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1. Introduction

One can study the physical properties of disordered systems for Fermi-energies deep in the localized tail in a systematic way. This was done first for the density of states by Lifshitz [1]. Mott and Davis [2] have calculated the frequency-dependent conductivity $\sigma(\omega)$ in the same limit. The conductivity is then determined by the probability of finding two deep potential wells with eigenvalues at $E\pm\omega$. Because of the repulsion of energy levels by tunneling these wells must be separated by a minimal distance proportional to $\ln\,\omega$. In the one-dimensional case, to which we will restrict our considerations for simplicity, this implies that the conductivity will be proportional to $\omega^2 \ln^2\omega$ [2].
These qualitative arguments can be made more explicit by calculating the semiclassical limit of a certain functional integral.The interesting results come from nontrivial saddle-points and cannot be reached by ordinary perturbation theory. For the density of states this has been done already in a number of papers [3-6]. However, to the authors knowledge, there exists only one analogous calculation of the conductivity [7]. In the present work we start from a supersymmetric formulation of the problem. As a first step we only present the exact solution of the saddle-point equation. The calculation of the fluctuations around it shall be published in a forthcoming publication.
The saddle-point equation corresponds to the classical motion of a particle in a two-dimensional nonlinear and

anisotropic potential. It is of the type considered in a different context by Garnier [8], who proved its integrability already in 1919. There are, in fact many possibilities to solve it: one can separate the coordinates in the corresponding Hamilton- Jacobi equation [9,10], one can use the integrability of the nonlinear Schrödinger equation with two components [11] which in the stationary case is equivalent to our problem and one can work with a certain ansatz like in [12-14]. We choose the last possibility as it gives the instanton solution in the most direct way. But before we give the exact result in Sect.4 we present an approximate instanton solution in Sect.3.

2.The saddle-point equation

We consider the model of a free electron in a white-noise-potential V(x) given by the Hamiltonian

$$H = -\frac{d^2}{dx^2} + V(x) \quad , \quad \langle V(x)V(x')\rangle = 2\gamma\delta(x-x') \qquad (1)$$

setting $h/2\pi=2m=1$. In general the dimension does not play a crucial role in the instanton approach [3-7]. We concentrate therefore on one dimension and express the conductivity σ with the help of a correlation function $S_2(x)$ ([7]):

$$\mathrm{Re}\,\sigma(\omega) = -\frac{e^2\omega^2\pi}{2} \int dx\, x^2\, S_2(x) \qquad (2)$$

The correlation function can be expressed in terms of averaged Greens functions:

$$S_2(x) = \frac{1}{2\pi^2}\,\mathrm{Re}\,\left(\mathcal{G}^{-+}(x) - \mathcal{G}^{--}(x)\right) \quad , \qquad (3)$$

where

$$\mathcal{G}^{\alpha\beta}(x) = \langle\, G(E-\tfrac{\omega}{2}+\alpha i0^+;0,x)\; G(E+\tfrac{\omega}{2}+\beta i0^+;x,0)\,\rangle . \qquad (4)$$

Next we write the Greens functions as functional integrals over commuting fields ϕ_i and anticommuting fields χ_i and carry out the average. This results in a supersymmetric field theory [15]. The product of advanced and retarded Greens functions for instance, is given by

$$\mathcal{G}^{-+}(x) = \frac{|E|^2}{16\gamma^2} \int \mathcal{D}(\Psi_i,\Psi_i^*)\; \chi_1(0)\chi_1^*(\tilde{x})\chi_2(\tilde{x})\chi_2^*(0)\; e^{-S} \qquad (5)$$

with $\tilde{x}=x\sqrt{|E|}$ and the action

$$S = -\frac{1}{4}\,\varepsilon^{3/2} i \int dx\, \Big\{ \Big|\frac{d\Psi_1}{dx}\Big|^2 - \Big|\frac{d\Psi_2}{dx}\Big|^2 + (1+\bar{\omega})|\Psi_1|^2 - (1-\bar{\omega})|\Psi_2|^2 + \frac{i}{4}\left(|\Psi_1|^2 - |\Psi_2|^2\right)^2 \Big\} \quad , \qquad (6)$$

where Ψ_i is a short-hand notation for $(\phi_i,\phi_i^*,\chi_i,\chi_i^*)$. In (6) we already introduced by a simple rescaling the dimensionless parameters of the theory, namely $\varepsilon=|E|/\gamma^{2/3}$ and $\bar{\omega}=\omega/2|E|$. The relevant saddle-point of (6) lies in the complex plane. We go from $\Psi_i=0$ in the direction of steepest descent by rotating the real and imaginary part of Ψ_i such, that $|\Psi_1|^2 \to i|\Psi_1|^2$ and $|\Psi_2|^2 \to -i|\Psi_2|^2$. Thus we obtain a real action:

$$S = \frac{1}{4}\varepsilon^{3/2} \int dx \; \{ |\frac{d\Psi_1}{dx}|^2 + |\frac{d\Psi_2}{dx}|^2 + (1+\bar{\omega})|\Psi_1|^2 + (1-\bar{\omega})|\Psi_2|^2 - \frac{1}{4}(|\Psi_1|^2 + |\Psi_2|^2)^2 \} \quad . \qquad (7)$$

In deriving the saddle-point equation we may neglect the anticommuting fields. Furthermore we consider only the real part of ϕ_1 as the action (7) is invariant with respect to rotations in the complex ϕ_1- and ϕ_2-plane separately. The saddle-point condition $\delta S=0$ gives than the classical problem of motion in a wine bottle like potential

$$\left(\frac{d^2}{dx^2} + \frac{1}{2}\vec{\phi}^2 - 1 \mp \bar{\omega}\right)\phi_{1/2} = 0 \quad , \qquad (8)$$

known as the Garnier-problem [8,9,12]. The instanton solutions of (8) are the only one with finite action. They approach $\vec{\phi}=0$ at the boundaries $x\to\pm\infty$ and therefore must have *zero energy*. There exists a second *constant of motion*

$$K = \frac{1}{4}(\phi_1 p_2 - \phi_2 p_1)^2 + \bar{\omega}\left(p_1^2 + \frac{\phi_1^4}{4} - p_2^2 - \frac{\phi_2^4}{4} - (1+\bar{\omega})\phi_1^2 - (1-\bar{\omega})\phi_2^2\right)$$

with $p_i = d\phi_i/dx$, which has been found in [9]. It also must be zero for the instanton solutions, because of their boundary conditions. A complete set of instanton solutions depends therefore on two parameters.

A mathematical investigation of equations like (8) can be found in [9,11]. Here we look for the solution with finite action relevant to the conductivity problem. The usual arguments about two nearly degenerate potential wells lead

us to expect that it looks like a two instanton solution. A first indication about it gives the approximate consideration in the next section.

3. Approximate solution

In close analogy to [2,7] we start with two isolated one instanton solutions:

$$g_{1/2} = \frac{2\sqrt{1\pm\eta}}{\cosh(\sqrt{1\pm\eta}\,(x\pm D/2))} \qquad (9)$$

of the equations

$$\left(-\frac{d^2}{dx^2} + V_{1/2}\right) g_{1/2} = (-1\mp\eta)\, g_{1/2} \,, \quad V_i = -\frac{g_i^2}{2} \quad . \qquad (10)$$

We have written the instantons in this form in order to show the analogy with the quantum mechanical eigenvalues of a potential well. They are solutions of our problem (8) in the limit of an infinite separation D when $\eta=\bar{\omega}$. To obtain a solution for a finite distance D we apply ordinary perturbation theory of two nearly degenerate eigenstates [16]. Due to the overlap matrix element $t=4\,exp(-D)$ the energy splitting increases. If we set it equal to $\bar{\omega}$:

$$\bar{\omega} = \sqrt{\eta^2 + t^2} \qquad (11)$$

we get an approximate solution of (8):

$$\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} = \begin{pmatrix}\cos\theta\\ \sin\theta\end{pmatrix} g_1 + \begin{pmatrix}\sin\theta\\ -\cos\theta\end{pmatrix} g_2 \quad . \qquad (12)$$

The angle θ is determined by

$$t=\bar{\omega}\, \sin 2\theta \quad , \quad \eta=\bar{\omega}\, \cos 2\theta \quad . \qquad (13)$$

One can see from (11), that there exists a minimal distance equal $\ln 4/\bar{\omega}$ where both potential wells have the same depth and the angle θ equals $\pi/4$. It will be seen later, that the exact instanton-solution has the same qualitative behaviour as (12). But to calculate the fluctuations around the saddle point of (7) we need the exact instanton solution.

4. The exact instanton solution

As already mentioned in the introduction, we have different possibilities to find an exact solution of (8). There exist a lot of similarities to the nonlinear Schrödinger equation for which the N-soliton solutions are given in [13,14]. We follow this very direct way to find the two instanton solution of (8).

We interpret $-\vec{\phi}^2/2$ as potential $V(x)$ and investigate the solutions of

$$L_k\, \phi(x,k) = \left(-\frac{d^2}{dx^2} + V(x) - k^2\right) \phi(x,k) = 0 \qquad (14)$$

in dependence on k. It is known from [13] that the two instanton can be found with the ansatz

$$\phi(x,k) = (k^2 + a_1(x)k + a_2(x))\, e^{ikx} \quad . \qquad (15)$$

Comparing (14) with (8) we see, that we look for a potential V with two eigenvalues at the following values of k:

$$\kappa_{1/2} = i\sqrt{1\pm\bar{\omega}} = 2iu_{1/2} \quad . \qquad (16)$$

Because of $L_{\kappa_i}=L_{\kappa_i^*}$ the relations

$$\phi(x,\kappa_i^*) + \alpha_i\, \phi(x,\kappa_i) = 0 \; ; i=1,2 \qquad (17)$$

must be fulfilled with some free parameters α_i. On the contrary, already these α_i determine uniquely the functions $a_i(x)$ in (15). By inserting (15) in (14) the potential is given by $V=2i\, da_1/dx$.

To fulfill the selfconsistency condition $V=-\phi^2/2$, it is very convenient [13] to define

$$\psi(x,k) = \frac{\phi(x,k)}{R(k)} = \left(1 + \sum_{n=1}^{2} \frac{\psi_n\, e^{-i\kappa_n x}}{k-\kappa_n}\right) e^{ikx} \qquad (18)$$

with $R(k)=(k-\kappa_1)(k-\kappa_2)$. The residua ψ_n of $\psi(x,k)$ at κ_n are eigenfunctions of (14) at $1\pm\bar{\omega}$. They are determined by (17) which is now written as

$$\sum_{i=1}^{2} \left(\frac{e^{i(\kappa_n^*-\kappa_i)x}}{\kappa_n^*-\kappa_i} + c_i\delta_{in} \right) \psi_i = - e^{i\kappa_n^*} \qquad (19)$$

with the new free parameters $c_i=\alpha_i R'(\kappa_i)/R(\kappa_i^*)$.

Now we consider the function

$$\Omega(x,k) = \psi(x,k)\psi^*(x,k^*) \quad .$$

The residuum at $k\,\infty$ is equal to $a_1+a_1^*$ and must vanish for real V. Comparing it with all the other residua gives the condition $c_i=-c_i^*$. By inserting an expansion of $\psi(x,k)$ in powers of $1/k$ into (14), we find that the residuum of $k\Omega(x,k)$ at $k\,\infty$ is equal to $V(x)/2$. Once again we use the fact that the sum over all residua of $k\Omega$ vanishes and find

$$V(x)/2 = -\sum_{i=1}^{2} \psi_i^* \psi_i \; c_i(\kappa_i^* - \kappa_i) \quad . \tag{20}$$

Now, we can fulfil the condition $V = -\vec{\phi}^2/2$ if we set

$$2\psi_i b_i = \phi_i \tag{21}$$

and

$$c_i = |b_i|^2/(\kappa_i^* - \kappa_i) \quad . \tag{22}$$

The general solution of (19,21,22) containes two parameters b_i as it must be. It represents the exact solution of (8):

$$\phi_{1/2}(x) = 8u_{1/2} \; \frac{e^{f_{1/2}} \pm e^{2f_{2/1} + f_{1/2} - D_0}}{1 + e^{2f_1} + e^{2f_2} + 4e^{2(f_1+f_2-D_0)}} \; , \tag{23}$$

where we have introduced

$$f_i = 2u_i x - \ln|b_i| \tag{24}$$

and the minimal distance D_0 between the solitons, defined by

$$2e^{-D_0} = (u_1 - u_2)/(u_1 + u_2) \quad . \tag{25}$$

The two degrees of freedom b_i correspond to a general shift of the x-coordinate which we will keep fixed in the following and to the distance between the instantons.

To make the result more transparent and to show the similarity with the approximate solution, we introduce instead of f_i the new parameters x_i:

$$x_1 = f_1 + \ln\sqrt{1 + \exp(-2\Delta f(x))} = s(x) + D(x)/2 \tag{26}$$

$$x_2 = f_2 - D_0 + \ln 2 - \ln\sqrt{1 + \exp(-2\Delta f(x))} = s(x) - D(x)/2$$

with $\Delta f(x) = f_1 - f_2$. We choose the b_i in (24) such that

$$\Delta f(x) = 2(u_1 - u_2)x + x_0 \tag{27}$$

and

$$s(x) = (u_1 + u_2)x \; , \tag{28}$$

where the new parameter x_0 determines the spacing between the instantons. By introducing the angle $\theta(x)$

$$\sin\theta(x) = \frac{\exp(-\Delta f(x))}{\sqrt{1 + \exp(-2\Delta f(x))}} \tag{29}$$

and with the help of (26) we rewrite (23) as follows

$$\phi_1(x) = 8u_1 \frac{\cos\theta(x) e^{-x_1} + \sin\theta(x) e^{x_2}}{1 + e^{-2x_1} + e^{2x_2}} \tag{30}$$

$$\phi_2(x) = 8u_2 \frac{\sin\theta(x) e^{-x_1} - \cos\theta(x) e^{x_2}}{1 + e^{-2x_1} + e^{2x_2}} \quad .$$

It is interesting that the distance $D(x)$, introduced in (25), depends on the angle $\theta(x)$ in the same way as in the approximate solution:

$$\exp(-D(x)) = \exp(-D_0) \; \sin 2\theta(x) \quad . \tag{31}$$

The formulas (32) represent the final result of this paper, where the parameters x_1, x_2 and θ are determined by subsequently inserting the expressions (16),(25-29) and (31). These form a family of zero-energy solutions parametrized by x_0 corresponding to varying distances between the instantons. These solutions are similar in structure to the approximate solutions found in Sect.3. The only difference is that the angle θ and the distance D now depend slightly on x, and the g_i have changed a little bit. One finds (12) to be a good approximation for small $\bar{\omega}$ and one has the advantage of a systematic way of improving it. One can see that the minimal distance between the instantons which is so important for the conductivity comes in very naturally without any additional constraint as in [7]. The exact solution (30) seems to be a good starting point to calculate the fluctuations around the extremum and to give an expression for the conductivity. This will be done in a subsequent publication.

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