Density of States of an Electron in a Gaussian Random Potential for \((4 - \epsilon)\)-dimensional Space

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Abstract

The density of states for the Schrödinger equation with a Gaussian random potential is calculated in a space of dimension \(d = 4 - \epsilon\) in the entire energy range including the vicinity of a mobility edge. Leading terms in \(1/\epsilon\) are taken into account for \(N \sim 1\) \((N\) is an order of perturbation theory\) while all powers of \(1/\epsilon\) are essential for \(N \gg 1\) with calculation of the expansion coefficients in the leading order in \(N\).

PACS numbers 03.65.-w, 11.10.Hi, 71.23.An

It is a common belief\(^1\),\(^2\) that the average density of states has no singularity in the point of an Anderson transition in contrast to the conductivity and localization length. Nevertheless its calculation is of principal interest because all known methods fail in the vicinity of the transition. Another reason is that the density of states and the conductivity which are determined by the average Green function \(\langle G(x, x') \rangle\) and the correlator \(\langle G_R G^A \rangle\) correspondingly are not completely independent quantities. In "parquet" approximation difficulties in both cases are of the same character and are connected with the problem of "ghost" pole\(^3\). On the other hand, to satisfy the Ward identity it is necessary to provide a strict correspondence of diagrams taken into account in the calculation of self energy and the irreducible vertex in the Bethe–Salpeter equation\(^4\). Thus no approximation for conductivity can be self-consistent before the corresponding approximation for density of
states is formulated. This problem was ignored in all existing theories except the symmetry approach suggested in Ref. 5.

For weak disorder the mobility edge is displaced near the bare band edge and the random potential can be regarded as Gaussian because the averaging is possible on scales smaller than wavelength and larger than the distance between scatterers (the so called Gaussian range of spectrum). The calculation of the average Green function for the Schrödinger equation with a Gaussian random potential is reduced to the problem of a second-order transition with \( n \)-component order parameter \( \vec{\varphi} = (\varphi_1, \varphi_2, ..., \varphi_n) \) in the limit \( n \to 0 \).

Then the coefficients in the Ginzburg–Landau Hamiltonian

\[
H\{\varphi\} = \int d^d x \left( \frac{1}{2} \kappa |\nabla \varphi|^2 + \frac{1}{2} \kappa_0^2 |\varphi|^2 + \frac{1}{4} u |\varphi|^4 \right)
\]

are related with the parameters of the disordered system by the relations

\[
c = 1/2m, \quad \kappa_0^2 = -E, \quad u = -a_0^d W^2/2,
\]

where \( d \) is the dimension of space, \( m \) and \( E \) are the particle mass and energy, \( a_0 \) is the lattice constant, and \( W \) is the amplitude of the random potential (we set \( c = 1, a_0 = 1 \) in what follows). The "wrong" sign of the coefficient of \( |\varphi|^4 \) leads to unreachability of Wilson fixed point in renormgroup equations and to the problem of "ghost" pole in "parquet" approximation. So the possibility of \((4 - \epsilon)\)-expansion was in question for many years and the number of suggestions on a value of upper critical dimension different from four was proposed. The progress was achieved in recent author’s papers, where the proper treatment of factorial divergency of perturbation series was shown to be necessary. Here we report the results for \((4 - \epsilon)\)-dimensional case with the details of calculation to be published elsewhere.

In a four-dimensional space the structure of the perturbation series for the self-energy \( \Sigma(p, \kappa) \) at \( p = 0 \) has a form

\[
\Sigma(0, \kappa) - \Sigma(0, 0) = \kappa^2 \sum_{N=1}^{\infty} u^N \sum_{K=0}^{N} A_N^K \left( \frac{\Lambda}{\kappa} \right)^K,
\]

where \( A_N^K \) are the coefficients of the perturbation series.
where \(\kappa\) is the renormalized value of \(\kappa_0\) and \(\Lambda\) is the large-momentum cutoff parameter. The analogous expansion for \(d = 4 - \epsilon\) has the form

\[
\kappa^2 + \Sigma(0, \kappa) - \Sigma(0, 0) \equiv \kappa^2 Y(\kappa) = \kappa^2 \sum_{N=0}^{\infty} (u\Lambda^{-\epsilon})^N \sum_{K=0}^{N} A_N^K(\epsilon) \left[ \frac{(\Lambda/\kappa)^\epsilon - 1}{\epsilon} \right]^K,
\]

where \(A_N^K(\epsilon)\) are the regular functions of \(\epsilon\),

\[
A_N^K(\epsilon) = \sum_{L=0}^{\infty} A_{N,L}^K \epsilon^L
\]

and \(A_0^0(\epsilon) \equiv 1\). The expansion (4) takes account of the fact that \(Y\) is a homogenious polynomial of degree \(N\) in \(\Lambda^{-\epsilon}\) and \(\kappa^{-\epsilon}\), as follows from the dimensional analysis, and that the expression (4) should be reduced to (3) in the \(\epsilon \to 0\) limit.

The quantity \(Y\) satisfies the Callan–Symanzik equation\(^8\), which follows from its relation with the vertex \(\Gamma^{(1,2)}\)\(^9\):

\[
\left( \frac{\partial}{\partial \ln \Lambda} + W(g_0, \epsilon) \frac{\partial}{\partial g_0} + V(g_0, \epsilon) \right) Y = 0,
\]

where \(g_0 = u\Lambda^{-\epsilon}, V(g_0, \epsilon) \equiv \eta_2(g_0, \epsilon)\), and the functions \(\Gamma^{(1,2)}, W(g_0, \epsilon), \) and \(\eta_2(g_0, \epsilon)\) are defined in Ref. 18. Introducing the expansions

\[
W(g_0, \epsilon) = \sum_{M=1}^{\infty} W_M(\epsilon) g_0^M = \sum_{M=1}^{\infty} \sum_{M'=0}^{\infty} W_{M,M'} g_0^M \epsilon^{M'},
\]

\[
V(g_0, \epsilon) = \sum_{M=1}^{\infty} V_M(\epsilon) g_0^M = \sum_{M=1}^{\infty} \sum_{M'=0}^{\infty} V_{M,M'} g_0^M \epsilon^{M'}
\]

and substituting expression (4) into Eq. (6), we obtain a system of equations for the functions \(A_N^K(\epsilon)\):

\[
(K+1)A_{N+1}^K(\epsilon) = (N-K)\epsilon A_N^K(\epsilon) - \sum_{M=1}^{N-K} [(N-M)W_{M+1}(\epsilon) + V_M(\epsilon)]A_{N-M}^K(\epsilon)
\]

and for the coefficients \(A_{N,L}^K\):

\[
(K+1)A_{N+1,L}^K = (N-K)A_{N,L-1}(1-\delta_{L,0}) - \sum_{M=1}^{N-K} \sum_{M'=0}^{L} [(N-M)W_{M+1,M'} + V_{M,M'}]A_{N-M}^{K,L-M'}.
\]

In the standard procedure of \(\epsilon\)-expansion\(^8\) a few first terms in series (5) are retained. In \(M\)-th order in \(\epsilon\) the coefficients \(A_{N,K,L}^{N-K,L}\) with \(K + L \leq M - 1\) are necessary for which
the closed system of the difference equations is followed from Eq. 9. Initial conditions to this system and coefficients \( W_{2,0}, V_{1,0}, \ldots \) can be derived if a few first orders of perturbation theory are calculated. By separating out the leading asymptotic term in \( N \), it is easily proved by induction that

\[
\begin{align*}
A_N^{N-K,L} &= C_{K+L}^K A_N^{N-K-L}, \\
A_N^{N-K} &= (-W_{2,0})^N \frac{\Gamma(N-\beta_0)}{\Gamma(N+1)\Gamma(-\beta_0)} \frac{(-W_{3,0})^K}{(-W_{2,0})^{2K}} \frac{(N \ln N)^K}{K!},
\end{align*}
\]

where \( \beta_0 = -V_{1,0}/W_{2,0} \), and the value of the first few coefficients in the expansion (7) equi

\[
W_1(\epsilon) = -\epsilon, \quad W_{2,0} = K_4(n + 8), \quad W_{3,0} = -3K_4^2(3n + 14), \quad V_{1,0} = -K_4(n + 2).
\]

(11)

with \( K_4 \) defined in Eq. 13. For the parquet coefficients \( A_N^{N,0} \), the result (10) is exact. The coefficients (10) do not possess the factorial growth which for \( u < 0 \) is responsible for nonperturbative contribution resulting in existence of the fluctuational tail of the density of states. This is a reason why the usual Wilson method does not work for \( u < 0 \).

The approximation giving asymptotically exact results for small \( \epsilon \) is as follows: In the lowest orders of the perturbation theory it is sufficient to retain in expansion (4) only leading order in \( 1/\epsilon \); for large \( N \) the lowest powers of \( 1/\epsilon \) should be taken into account, since the corresponding terms grow rapidly as \( N \to \infty \), but the leading order in \( N \) is sufficient for the expansion coefficients in Eq. 4. Information about the coefficients \( A_N^K(\epsilon) \) for large \( N \) can be obtained by the Lipatov method. The \( N \)th order contribution to \( \Sigma(p, \kappa) \) is calculated in a close analogy with the \( d = 4 \) case and has a form

\[
\begin{align*}
\left[ \Sigma(p, \kappa) \right]_N &= c_2 u^N \Gamma(N + b) a^N \int_0^\infty d \ln R^2 R^{-2} (\phi_c^3)^R \langle \phi_c^3 \rangle_{-R} \cdot \\
&\quad \cdot \exp \left( -N f(\kappa R) + N \epsilon \ln R + 2K_d I_4(\kappa R) \frac{1 - (\Lambda R)^{-\epsilon}}{\epsilon} \right),
\end{align*}
\]

(12)

where

\[
\begin{align*}
a &= -3K_4, \quad b = \frac{d+2}{2}, \quad c_2 = c (3K_4)^{7/2}, \\
f(x) &= -\frac{\epsilon}{2} (C + 2 + \ln \pi) - 3x^2 \left( C + \frac{1}{2} + \ln \frac{x}{2} \right), \quad \langle \phi_{c,R}^3 \rangle^R = 8 \cdot 2^{1/2} \pi^2 p K_1(p),
\end{align*}
\]

(13)
\[ I_4(x) = \tilde{I}_4 \exp(f(x)), \quad \tilde{I}_4 = \frac{16}{3} S_4, \quad S_d = 2\pi^{d/2}/\Gamma(d/2), \quad K_d = S_d(2\pi)^{-d}, \]

\(C\) is Euler’s constant, \(K_1(x)\) is a modified Bessel function, and \(c\) is a constant of order unity defined in Eq. 114 of Ref. 16. Representing the result (12) in the form of expansion (4), we have

\[
A^K_N(\epsilon) = \tilde{c}_2 \Gamma(N + b) a^N c^K_N \int_0^\infty d\ln R^2 R^{-2} \left( \epsilon + \frac{2K_d \tilde{I}_4}{N} e^f(R) - \epsilon \ln R \right)^K \cdot \exp \left( -Nf(R) + N\epsilon \ln R + 2K_d \tilde{I}_4 \frac{1}{\epsilon} \right), \tag{14}
\]

where \(\tilde{c}_2 = c_2 \langle \phi_c^3 \rangle^2 \approx 3.44 \cdot 10^{-2}\) for \(n = 0\).

As discussed in Ref. 16, for \(d = 4\) the Lipatov method reproduces the coefficients \(A^K_N(\epsilon)\) in (3) well only for \(K \ll N\), since they decrease rapidly with increasing \(K\) and accuracy \(\sim 1/N\) of the leading asymptotic expression is limited. Analogous phenomenon takes place in \((4 - \epsilon)\) dimensions: Formula (14) is valid for all \(K\) if \(N\epsilon \gg 1\) and only for \(K \ll N\) if \(N\epsilon \lesssim 1\); under these conditions the coefficients (14) satisfy Eq. 8, where only the term with \(M = 1\) is retained in the sum, which is possible for large values of \(N\) in view of factorial growth of \(A^K_N(\epsilon)\). Since the system of equations (8) determines \(A^K_N(\epsilon)\) for \(K > 0\) if \(A^0_N(\epsilon)\) are given, and the latter are well reproduced by the Lipatov method, one can determine \(A^K_N(\epsilon)\) in the region \(1 \ll N \lesssim 1/\epsilon\) for all \(K\).

Retaining in Eq. 8 only the terms with \(M = 1\) and \(M = 2\) and introducing the quantity \(X_{N,M}\) by definition

\[
A^K_N(\epsilon) = [-W_2(\epsilon)]^K \frac{\Gamma(N - \beta(\epsilon))}{\Gamma(K + 1)\Gamma(N - K - \beta(\epsilon))} A^0_{N-K}(\epsilon) X_{N,N-K} \tag{15}
\]

where \(\beta(\epsilon) = -V_1(\epsilon)/W_2(\epsilon)\), we have an equation

\[
X_{N,M} = \left( \hat{l}_M + \hat{\delta}_M \right) X_{N,M+1}, \tag{16}
\]

where

\[
\hat{l}_M \equiv h_M + e^{-i\hat{\phi}_M} \quad \gamma M = \frac{f_M}{N} e^{-2i\hat{\phi}} \quad \hat{\delta}_M \equiv e^{-2i\hat{\phi}} \tag{17}
\]

\[
h_M = -\frac{\epsilon}{W_2(\epsilon) A^0_{M+1}(\epsilon)} \frac{M + 1}{A_M(\epsilon)} - M - \beta(\epsilon) \quad f_M = \frac{W_3(\epsilon) A^0_{M-1}(\epsilon)}{W_2(\epsilon) A^0_M(\epsilon)} (M + 1 - \beta(\epsilon)) \tag{18}
\]
and $e^{-i\hat{p}}$ is the displacement operator on the distance $-1$ affecting the both arguments.

The equation (16) can be formally solved by straightforward iterations taking into account the boundary condition $X_{N,N} = 1$. The result can be expanded in powers of $\hat{\delta}_M$, terms containing a few number of operators $\hat{\delta}_M$ being essential. These terms can be explicitly calculated by induction. For $M \sim 1$ we have a result

$$A_{N}^{N-M}(\epsilon) = \frac{1}{M!} e^{N-M} \tilde{\epsilon}_2 \Gamma(N - \beta(\epsilon)) a^N (t/2\pi)^{1/2} e^{J_{\infty}(Nt \ln N - 1) + 1/t} \int_0^\infty dx e^{-\frac{1}{2}(N-1/t-x)^2} x^{M+b+\beta-f_{\infty} Nt} J(x),$$  \hspace{1cm} (19)

where

$$J(N) = \int_0^\infty d \ln R^2 R^{-2} \exp \left( -N f(R) + N \epsilon \ln R + 2Kd I_4(R) \frac{1-R^{-\epsilon}}{\epsilon} \right),$$  \hspace{1cm} (20)

and

$$t = -\frac{\epsilon a}{W_2(\epsilon)} \xrightarrow{\epsilon \to 0} \frac{3\epsilon}{n+8}, \quad f_{\infty} = \frac{W_3(\epsilon)}{aW_2(\epsilon)} \xrightarrow{\epsilon \to 0} \frac{3n+14}{n+8},$$  \hspace{1cm} (21)

which is valid in the region $Nt > 1$ or $1 - Nt \ll \epsilon^{1/2}$. For $N\epsilon \ll 1$ and $N - K \ll \ln N$ we have a result of type (5) with $A_{N}^{K,L}$ given by (10). Other regions of parameters can be also investigated but they do not make essential contributions to the sum of the perturbation series.

Two contributions are important in the sum of Eq. 4: (a) nonperturbative contribution

$$[\Sigma(0, \kappa)]_{nonpert} \equiv i \Gamma_0(\kappa^2) = i\tilde{\epsilon}_2 \kappa^2 (\kappa^\epsilon/au)^b e^{-\kappa^\epsilon/au} F(\kappa^\epsilon/au)$$  \hspace{1cm} (22)

(the limit $\Lambda \to \infty$ is taken) arising from the region of large $N$ and obtained from Eq. 4 by summation over $N$ from an arbitrary finite $N_0$ to infinity, if the coefficients $A_{N}^{N}(\epsilon)$ given by (19) are written in the form

$$A_{N}^{N}(\epsilon) = \tilde{\epsilon}_2 \Gamma(N + b) e^N a^N F(N)$$  \hspace{1cm} (23)

(the formula (46) of Ref. 16 is used); (b) the quasiparquet contribution arising from the terms with coefficients $A_{N}^{N-K,L}$ with $K \sim L \sim 1$ given by (10)

$$[Y(\kappa)]_{quasipart} = \left[ \Delta + \frac{W_{3,0}}{W_{2,0}} u \kappa^{-\epsilon} \ln \Delta \right]^{\beta_0}, \quad \Delta \equiv 1 + W_{2,0} a u \kappa^{-\epsilon} - \Lambda^{-\epsilon}/\epsilon.$$  \hspace{1cm} (24)
To logarithmic accuracy, the quantity $\Delta$ in the logarithm can be replaced by its minimum value $\bar{\Delta} \sim \epsilon \ln \epsilon$ (determined by Eqs. (26)–(30) presented below), and in the limit $\Lambda \to \infty$ the result (24) can be written in the form

$$[Y(\kappa)]_{\text{quasiparq}} = [1 + W_{2,0} \tilde{u} \kappa^{-\epsilon}]^{\delta_0}, \quad \tilde{u} \equiv u \left[1 + \frac{W_{3,0}}{W_{2,0}} \epsilon \ln \bar{\Delta}\right],$$

which differs from the parquet result only in that $u$ is replaced by $\tilde{u}$. It can be proved that such replacement occurs in all parquet formulas employed in calculating the density of states.

The rest of the calculations are similar to those described in Ref. 15. The damping $\Gamma$, the renormalized energy $E$, and the density of states $\nu$ are determined in parametric form as functions of the bare energy $E_B$ by the equations

$$\Gamma = \Gamma_c \left(1 + \frac{\epsilon x}{2}\right)^{2/\epsilon} \sin \varphi, \quad E = -\Gamma_c \left(1 + \frac{\epsilon x}{2}\right)^{2/\epsilon} \cos \varphi,$$

$$-E_B + E_c = \Gamma_c \left(\frac{\epsilon x}{2}\right)^{1/4} \left(1 + \frac{\epsilon x}{2}\right)^{2/\epsilon-1/4} \left(\cos \left(\varphi + \frac{\varphi}{4x}\right) - \text{tg} \left(\frac{1 + 2\epsilon x}{3}\right) \sin \left(\varphi + \frac{\varphi}{4x}\right)\right),$$

$$\nu = \frac{\Gamma_c}{4\pi |\tilde{u}|} \left(1 + \frac{\epsilon x}{2}\right)^{2/\epsilon} \left((1 + \frac{2}{\epsilon x})^{-1/4} \sin \left(\varphi + \frac{\varphi}{4x}\right) \left[1 - \frac{R_0^2}{2(1 + \epsilon x/2)}\right] - \left(1 + \frac{2}{\epsilon x}\right)^{-3/4} \sin \left(\varphi + \frac{3\varphi}{4x}\right)\right),$$

$$\Gamma_c = \left(\frac{8K_4 |\tilde{u}|}{\epsilon}\right)^{2/\epsilon}, \quad E_c \simeq 2u \int \frac{d^d k}{(2\pi)^d k^2} \frac{1}{\epsilon}, \quad R_0 \approx \left(\frac{\epsilon}{3 \ln(1/\epsilon)}\right)^{1/2},$$

where $x(\varphi)$ is a single-valued function in the interval $0 < \varphi < \pi$, similar to the function shown in Fig. 2 of Ref. 15 and determined by equation

$$\sin \left(\varphi + \frac{\varphi}{4x}\right) = \frac{e^{-4x/3}}{x^{1/4}} I(x) \cos \frac{\varphi(1 + 2\epsilon x)}{3}$$

where

$$I(x) = \tilde{c}_2 \left(\frac{3}{4}\right)^{1/4} \left(\frac{\pi t}{2}\right)^{1/2} e^{-f_\infty + f_\infty (1+\epsilon x/2) \ln [\Delta(1+\epsilon x/2)/t]} \int_0^\infty dz e^{-\frac{1}{2}(\epsilon x/2t - z)^2} z^{b + \beta - f_\infty (1+\epsilon x/2)} J(z)$$
The expressions (26–30) are simplified drastically in two overlapping regions. For large $|E|$, when $x \gg \ln(1/\epsilon)$, the right-hand side of (29) is small and the quantity $\varphi$ is close to 0 or $\pi$, so for $\Gamma(E)$ and $\nu(E)$ we have asymptotic expressions

$$
\Gamma(E) = \begin{cases} 
\frac{\pi}{8} \epsilon E \left[ (E/\Gamma_c)^{\epsilon/2} - 1 \right]^{-1}, & E \gg \Gamma \\
\Gamma_0(E) \left[ 1 - (|E|/\Gamma_c)^{-\epsilon/2} \right]^{-1/4}, & -E \gg \Gamma 
\end{cases}
$$

(32)

$$
\nu(E) = \begin{cases} 
\frac{1}{2} K_4 E^{(d-2)/2} \left[ 1 - \left( \frac{E}{\Gamma_c} \right)^{-\epsilon/2} \right]^{-1/4}, & E \gg \Gamma \\
\frac{\Gamma_0(E)}{4\pi |\bar{u}|} \left( 1 - \frac{R_0}{2} \left( \frac{|E|}{\Gamma_c} \right)^{-\epsilon/2} - \left[ 1 - \left( \frac{|E|}{\Gamma_c} \right)^{-\epsilon/2} \right]^{1/2} \right) , & -E \gg \Gamma 
\end{cases}
$$

(33)

$(\Gamma_0(E) \equiv \Gamma_0(|\kappa|^2))$ which give an illusion of ghost pole. For small $|E|$, when $x \lesssim \epsilon^{-1/2}$, Eq. 29 takes the form

$$
\sin(\varphi + \varphi/4x) = I(0) \cos(\varphi/3) \frac{e^{-4x/3}}{x^{1/4}}, \quad I(0) \sim \epsilon^{-7/12} \left( \ln \frac{1}{\epsilon} \right)^{17/12},
$$

(34)

and the ghost pole is shifted from the real axis into the complex plane on the distance $\sim \epsilon \ln(1/\epsilon)$.

For large positive $E$ Eq. 32 gives the inverse relaxation time appearing in the kinetic equation while for large negative $E$ the damping $\Gamma$ becomes purely nonperturbative. The function $\nu(E)$ for large positive $E$ goes over to the density of states of an ideal system, and for large negative $E$ the following result is obtained for the fluctuational tail

$$
\nu(E) = \frac{K_4}{\pi} \Gamma_0(E) |E|^{-\epsilon/2} \ln \frac{1}{R_0} = \tilde{c}_2 K_4 \left( \frac{2\pi}{3} \ln \frac{1}{R_0} \right)^{1/2} R_0^{-3} |E|^{(d-2)/2} \left[ \frac{I_4 |E|^{\epsilon/2}}{4|u|} \right]^{(d+1)/2} \cdot \exp \left( \frac{2K_d I_4(R_0)}{\epsilon} - \frac{I_4(R_0)|E|^{\epsilon/2}}{4|u|R_0^\kappa} \right),
$$

(35)

the energy dependence of which is identical to that obtained in Ref. 22 and 23 and corresponds to Lifshitz’s law; the divergence in the limit $\epsilon \to 0$ is removed for a finite cutoff parameter $\Lambda$.

It is interesting, that for $\epsilon x \ll 1$ formulas (26–30) have the same functional form as in the $d = 4$ case, i.e. the behavior of all physical quantities in the vicinity of a mobility edge.
is effectively four-dimensional. As in Refs. 15 and 16, the phase transition point shifts into the complex plain, and the density of states has no singularities for real $E$ in accordance with widely accepted but not proved ideas.

I am grateful to the participants of the seminars at the Institute for Physical Problems and the Physics Institute of the Academy of Sciences for their interest in this work.

This work was performed with the financial support of the International Science Foundation and the Russian government (grants MOH000 and MOH300) and the Russian Fund for Fundamental Research (grant 96-02-19527).
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