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A renormalization group approach to the Coulomb gap

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Abstract. The free energy of the Coulomb gap problem is expanded as a set of Feynman diagrams, using the standard diagrammatic methods of perturbation theory. The gap in the one-particle density of states due to long-ranged interactions corresponds to a renormalization of the two-point vertex function. By collecting together the leading-order logarithmic corrections we have derived the standard result for the density of states for the critical dimension, $d = 1$. This method, which is shown to be identical to the approach of Thouless, Anderson and Palmer to spin glasses, allows us to derive the strong-disorder behaviour of the density of states. The use of the renormalization group allows this derivation to be extended to all disorders, and the use of an ϵ -expansion allows the method to be extended to $d = 2$ and $d = 3$. We speculate that the renormalization group equations can also be derived diagrammatically, allowing a simple derivation of the crossover behaviour observed in the case of weak disorder.

1. Introduction

The phenomenon of the Coulomb gap has been known of for 20 years [1] and has been observed both in disordered semiconductors below the Anderson transition [2] and in the high-magnetic-field quantum Hall fluid [3]. In any system of localized electrons, when electrostatic interactions are taken into account, a soft gap appears in the density of states at the Fermi level. This classical effect is the result of the interplay of disorder, long-ranged interactions, and the discreteness of electric charge. The Hamiltonian of the system [1, 2] is

$$H[n_i] = \sum_i \phi_i n_i + e^2 \sum_{i \neq j} \frac{(n_i - \frac{1}{2})(n_j - \frac{1}{2})}{r_{ij}} \quad (1)$$

where the n_i are occupation numbers. The Hamiltonian contains two terms; the first is dependent upon disorder and the second upon Coulomb interactions. The ϕ_i are uncorrelated energies representing the effects of disorder, and macroscopic thermodynamic quantities must be obtained by averaging over them according to the distribution

$$\langle F \rangle = \langle F[\phi_i] \rangle = \int_{-\infty}^{+\infty} \prod_i \frac{d\phi_i}{\sqrt{2\pi A^2}} \exp\left(-\sum_i \frac{\phi_i^2}{2A^2}\right) F[\phi_i]. \quad (2)$$

There are two dimensionless parameters governing the problem. The one describing the relative strengths of disorder and interactions is

$$\gamma = \frac{\varepsilon_0}{A} = \frac{e^2}{aA} \quad (3)$$

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where a is the lattice spacing, so ε_0 gives a measure of the strength of the nearest-neighbour interaction. We consider the problem on a lattice, although because the system is dominated by long-range behaviour over distances of the order of the correlation length ($r \sim e^2/T$) this should be irrelevant to the physics of the problem. The standard Coulomb gap problem for strong disorder corresponds to $\gamma \ll 1$, whilst $\gamma \gg 1$ corresponds to weak disorder. The dimensionless parameter describing thermal effects is

$$\xi = \frac{\varepsilon_0}{T} = \frac{e^2}{aT}. \quad (4)$$

Because the distribution of the ϕ_i is symmetric under $\phi_i \rightarrow -\phi_i$, the Hamiltonian is symmetric under $\phi_i \rightarrow -\phi_i, n_i \rightarrow 1 - n_i$, so the chemical potential $\mu = 0$ and the total number of particles is fixed:

$$\sum_i n_i = N/2. \quad (5)$$

We would like to derive the one-particle density of states (OPDOS), $g(\varepsilon)$, defined as the distribution function of the single-site energies:

$$\varepsilon_i = \left(\frac{\partial H}{\partial n_i} \right)_{n_j} = \phi_i + e^2 \sum_{j \neq i} \frac{(n_j - \frac{1}{2})}{r_{ij}}. \quad (6)$$

At non-zero temperatures the problem was treated by Mogilyanskii and Raikh [4] and in particular it was shown that the distribution of electrons over sites obeys Fermi–Dirac statistics:

$$\langle n_i \rangle = n_{\text{FD}}(\varepsilon_i) = \frac{1}{1 + \exp(\varepsilon_i/T)}. \quad (7)$$

Once the OPDOS is known, we can derive many useful macroscopic quantities such as the screening law and the conductivity.

All standard discussions of the Coulomb gap focus on the strong-disorder problem, although we will also consider the case of weak disorder. In this case we might expect a crystalline ground state and a hard gap. However, as noted by Efros [5], the freezing temperature of a pure ionic crystal with no disorder is numerically smaller by about two orders of magnitude than ε_0 . Thus there is a very wide range of temperatures between this freezing temperature and ε_0 for which the weakly disordered Coulomb gap system behaves like a strongly correlated classical fluid.

In section 2, we demonstrate that the Coulomb gap partition function can be expanded as a series of Feynman diagrams. The general philosophy is to expand the partition function $\ln Z[\phi_i]$ as a series of diagrams and only at the last moment to perform the averaging over disorder (2). This method is identical to the method used by Thouless, Anderson, and Palmer (TAP) [8] to study the spin-glass problem; we discuss this in section 3. In the next section, section 4, we give a simple argument for the lack of any low-temperature phase transition for the critical dimensionality $d = 1$. This means that the derivation of the leading approximation to the one-particle density of states for the Coulomb gap problem given in section 5 does indeed sum the most important set of diagrams, and that any divergences in other sets of diagrams must cancel. The standard results for $d = 2$ and $d = 3$ can be obtained by means of an ϵ -expansion for $\epsilon = d - 1$, as explained in section 6. Finally, we speculate that renormalization group theory arguments can allow a derivation of the weak-disorder limit in which the standard results for the density of states break down.

2. Diagrammatic perturbation theory for the Coulomb gap

The density of states is calculated by means of a diagrammatic perturbation theory. Polyakov [6] shows how to convert classical Ising-like models into a continuous field problem, which can be expanded into the Feynman diagrams well known from quantum field theory, and we use a slightly modified version to take account of disorder.

The partition function is rewritten using the identity

$$\begin{aligned} Z[\phi_i] &= \sum_{[n_i]} \exp\left(-\frac{H[n_i, \phi_i]}{T}\right) \\ &= \sum_{[n_i]} \exp\left[\frac{1}{T} \left(\sum_i \phi_i \left(n_i - \frac{1}{2}\right) + e^2 \sum_{i \neq j} \frac{(n_i - \frac{1}{2})(n_j - \frac{1}{2})}{r_{ij}}\right)\right] \\ &= \sum_{[n_i]} \exp\left(\sum_i \frac{\phi_i}{T} \frac{d}{d\chi_i} \Big|_0 + e^2 \sum_{i \neq j} \frac{T}{r_{ij}} \frac{d}{d\chi_i} \Big|_0 \frac{d}{d\chi_j} \Big|_0\right) \exp \sum_i \frac{\chi_i (n_i - \frac{1}{2})}{T} \end{aligned} \quad (8)$$

leaving the result in a form in which the summation over $[n_i = 0, 1]$ can be easily performed, using the identities:

$$\sum_{[n_i]} \exp \sum_i \frac{\chi_i (n_i - \frac{1}{2})}{T} = \prod_i \cosh \frac{\chi_i}{2T} = \exp \sum_i \ln \cosh \frac{\chi_i}{2T} \quad (9)$$

$$\exp \sum_i \frac{\phi_i}{T} \frac{d}{d\chi_i} \exp \sum_i \ln \cosh \frac{\chi_i}{2T} = \exp \sum_i \ln \cosh \frac{\chi_i + \phi_i}{2T} \quad (10)$$

to yield the formally exact result

$$Z[\phi_i] = \exp\left(\sum_{i \neq j} \frac{-Te^2}{r_{ij}} \frac{d}{d\chi_i} \Big|_0 \frac{d}{d\chi_j} \Big|_0\right) \exp - \sum_i \ln \cosh \left(\frac{\chi_i + \phi_i}{2T}\right). \quad (11)$$

Our general approach will now be to perturbatively expand $\ln Z[\phi_i]$ as a series of connected Feynman diagrams, similar to the ‘locator’ perturbation series of Anderson [7], and only at the very last stage to perform the averaging over ϕ_i . This corresponds to the approach of Thouless, Anderson and Palmer (TAP) [8] to spin glasses.

The diagram rules for the series expansion of $\ln Z$ are as follows, where $n_{FD}(\phi)$ is the Fermi–Dirac function.

(i) Each vertex i with n_i lines coming out of it gives a factor of

$$-\left(T \frac{d}{d\phi_i}\right)^{n_i} \ln \cosh \frac{\phi_i}{2T} = \left(T \frac{d}{d\phi_i}\right)^{n_i-1} \left(n_{FD}(\phi_i) - \frac{1}{2}\right). \quad (12)$$

(ii) Each line from i to j gives a factor of

$$\frac{-e^2}{r_{ij} T}. \quad (13)$$

(iii) There is a symmetry factor $1/|G|$, where $|G|$ is a combinatorial factor equal to the order of the symmetry group of the diagram. This standard factor [9] is well known from statistical and quantum field theories.

When it comes to averaging over disorder, we note that the disorder-averaged bare n -point vertex function is

$$\int_{-\infty}^{\infty} g_0(\phi) d\phi \left(T \frac{d}{d\phi}\right)^n \ln \cosh \frac{\phi}{2T}. \quad (14)$$

Integrating this by parts, we can see that it equals

$$\int_{-\infty}^{\infty} T dx \left(\frac{d}{dx} \right)^{n-2} g(Tx) \left(\frac{d}{dx} \right)^2 \ln \cosh x \approx \pi T^{n-1} \left(\frac{d}{dx} \right)_{x=0}^{n-2} g(x) \quad (15)$$

so for all non-pathological distributions of disorder (such as, for example, the Gaussian (2)) the bare two-point vertex function is

$$\lambda_2 = \frac{\pi T a^d}{A} \quad (16)$$

(where d is the dimensionality of space) and higher vertex functions disappear like powers of T/A :

$$\lambda_n \propto \left(\frac{T}{A} \right)^{n-1} \quad (17)$$

and so are negligible in our calculations to leading logarithmic order. In the case of a ‘top-hat’ distribution of local site energies, as used in numerical simulations, the λ_n disappear like $\exp(-A/T)$ for $n > 2$. Thus to leading order, only two-point vertices survive after averaging. Note that the bare two-point vertex function is proportional to the non-interacting density of states g_0 , and that the renormalized two-point vertex function is given, after averaging, by

$$\left\langle \text{sech}^2 \frac{\varepsilon_i}{2T} \right\rangle = T a^d g \quad (18)$$

where g is the density of states at the Fermi level as a function of temperature.

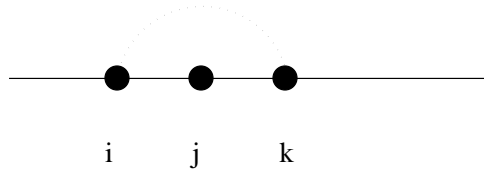


Figure 1. An example of a Feynman diagram containing a connection; this represents the possibility $i = k$.

3. The relationship between the Coulomb gap and the TAP treatment of spin glasses

The idea of performing a diagrammatic expansion of $\ln Z$ and of only performing the averages over disorder at the last moment is identical to the TAP theory of spin glasses [8]. The Coulomb gap problem is in some senses simpler than the spin-glass problem, because for $A \gg T$ only two-point vertices survive after averaging. The only reason that the field theory is not a trivial ϕ^2 -theory is the possibility that more than one vertex could represent the same site, so if for example $i = k$, then ϕ_i and ϕ_k will no longer be independent. We represent this case by Feynman diagrams including ‘connections’ (see figure 1). As in the diagrams for the conductivity of a dirty metal [13], it is these connections which make the theory non-trivial, in that there are one-particle irreducible diagrams [9] more complex than a single bare two-point vertex.

In the next section we will show that a certain set of Feynman diagrams (see figure 2) which we will call the ‘maximally crossed’ diagrams, are larger by $O(A/\varepsilon_0)$ than any others, and thus dominate the expression for the density of states.

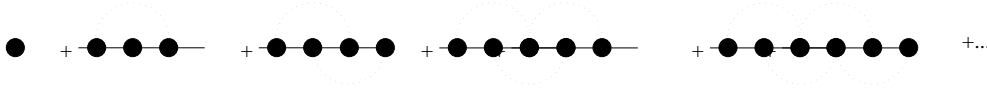


Figure 2. Diagrams contributing to the standard Coulomb gap density of states; these ‘maximally crossed’ diagrams are larger by $O(A/\varepsilon_0)$ than all others.

This behaviour is identical to that of spin glasses, for which a certain set of diagrams is larger than any others by $O(z)$ where z , the coordination number, is assumed large. However, in spin glasses, the sum of a set of loop diagrams incorporating four-point vertices diverges at the spin-glass temperature, signalling the onset of replica symmetry breaking (RSB). However the TAP approach allows expansions around frozen-in spins, and the method is ‘fail-safe’ in the sense that if we are expanding about a state which is not a global minimum of energy, we will get negative or zero eigenvectors of the response matrix, and a negative or infinite susceptibility. The low-temperature state is marginally stable [11] (meaning that the eigenvalues of the stability matrix are distributed all the way down to zero) but the TAP method holds up under these circumstances. The marginal stability of the system is precisely due to the exponentially large number of metastable states.

In section 4 we note that there exists a simple physical argument for why no such phase transition can occur at low temperature in the Coulomb gap problem for $d = 1$. Thus any sets of diagrams whose sums do diverge at low temperatures must cancel with other such diagrams. For $d = 2$ and $d = 3$ the question of whether or not a glass transition exists is inconclusive, although this does not affect our arguments.

Anderson [10] demonstrates a derivation of the low-temperature distribution of effective local fields in the spin-glass problem which is exactly analogous to the standard derivation of the density of states in the Coulomb gap [2]. However, because of the onset of RSB at low temperatures, following a rather intricate method due to Bray and Moore [11] is necessary in order to perform a perturbation theory expansion around the non-trivial ground state of the spin glass, although their method is based on a locator perturbation theory—essentially the same as our calculation in this paper. Bray and Moore define a Green’s function, which when averaged over disorder, gives exactly (18).

The Coulomb gap is effectively a variant of the random-field ferromagnet with long-ranged interactions. Bray [12] confirms that whilst the random-field ferromagnet displays low-temperature anomalies in the specific heat (again due to marginal stability), it does not have RSB.

4. The absence of a low-temperature phase transition for $d = 1$

As mentioned in the previous section, we are performing a perturbation expansion around a trivial ground state. Thus it is essential that we sum the diagrams at a temperature higher than that of any phase transition, and we will show that for $d = 1$ there is no such transition. Consider a 1-d Coulomb gap system with small but finite disorder, $\gamma \gg 1$, at $T = 0$. The system will form into domains of perfect ionic crystals separated by domain walls. Suppose that the density of domain walls is N , and hence that the mean number of sites in a single domain is N^{-1} : the limit $\gamma \gg 1$ corresponds to $N \ll 1$. Then it is possible to make a simple argument similar to that of Imry and Ma [14], showing that the free energy has a

minimum for a finite domain wall density, of order

$$N_c \sim \frac{A^2}{\varepsilon_0^2} \quad (19)$$

and so any disorder, no matter how small, destroys long-range order for $d = 1$. Thus for this critical dimensionality there is no low-temperature phase transition, and we are safe in the knowledge that our perturbation theory is around a stable minimum.

Vojta [15] shows that within the uncontrolled approximation of the spherical model, the Coulomb gap system has a low-temperature transition to a phase with long-range order for $d > 4$, whereas for $d \leq 4$ there is no such transition. Monte Carlo simulations are inconclusive on the question of whether there is a phase transition for $d = 2, d = 3$ or not [16, 17]. Studies of a related system, the Coulomb glass, show a phase transition for $d = 3$ [18] but not for $d = 2$ [19]. All of the numerical simulations show clearly that the Coulomb gap is well developed at temperatures well above that of the suspected glass transition. This gives us a justification for disregarding the glass transition and performing an expansion around the trivial ground state.

5. Deriving the density of states within perturbation theory

We discuss first the critical dimensionality $d = 1$, because the divergences encountered here are logarithmic and hence tractable to the renormalization group. We mention later how the results are modified for the more severe divergences for $d = 2, d = 3$. We aim to derive the results of Raikh and Efros [20] for the Coulomb gap with strong disorder:

$$g = g_\infty = \frac{g_0}{1 + e^2 g_0 \ln(\varepsilon_0/T)} \quad (20)$$

and to show how these are modified for weak disorder to the crossover behaviour observed by Pikus and Efros [21]:

$$g \approx \frac{A}{\varepsilon_0} g_\infty + \frac{1}{e^2} \exp(-\alpha \varepsilon_0/T). \quad (21)$$

We note that heuristically, we expect the low-disorder density of states to behave like the Boltzmann function $\exp(-\alpha \varepsilon_0/T)$ where the typical energy of excitations is $\alpha \varepsilon_0$.

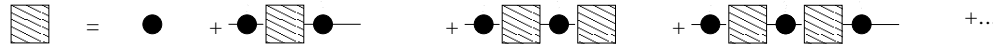


Figure 3. The Dyson equation giving all the leading logarithmic terms in the density of states.

We have already discussed how the diagrammatic perturbation expansion can be obtained. The ‘maximally crossed’ diagrams (see figure 2 for maximally crossed diagrams to order g_0^2) are larger by $\mathcal{O}(\varepsilon_0/A)$ than any diagrams containing unpaired vertices. Before averaging over disorder these diagrams give

$$\begin{aligned} \text{sech}^2\left(\frac{\phi_i}{2T}\right) &= \text{sech}^2\left(\frac{\varepsilon_i}{2T}\right) - \text{sech}^4\left(\frac{\varepsilon_i}{2T}\right) \text{sech}^2\left(\frac{\varepsilon_j}{2T}\right) \left(-\frac{e^2}{r_{ij}T}\right)^2 \\ &\quad - \text{sech}^4\left(\frac{\varepsilon_i}{2T}\right) \text{sech}^4\left(\frac{\varepsilon_j}{2T}\right) \left(-\frac{e^2}{r_{ij}T}\right)^3 \\ &\quad - \text{sech}^6\left(\frac{\varepsilon_i}{2T}\right) \text{sech}^4\left(\frac{\varepsilon_j}{2T}\right) \left(-\frac{e^2}{r_{ij}T}\right)^4 + \dots \end{aligned} \quad (22)$$

We first perform the spatial integration, then by inspection sum the series. As the final step of the calculation, we can now perform the averaging over disorder (2) to give, using (18), and to logarithmic accuracy,

$$g \approx g_0 - \frac{e^2 g_0^2}{2} \ln\left(1 + \frac{\varepsilon_0^2}{T^2}\right) + \dots \approx g_0 - e^2 g_0^2 \ln \frac{\varepsilon_0}{T}. \quad (23)$$

As we would expect, there is the same logarithmic behaviour for a $(1/r^d)$ -potential for d spatial dimensions. For the Coulomb gap for $d = 1$ the divergences are sufficiently mild that we can collect together the leading-order logarithmic terms depicted in figure 3 to give an expansion for g in terms of g_0 :

$$g \approx g_0 - e^2 g_0^2 \ln \frac{\varepsilon_0}{T} + e^4 g_0^2 \ln^2 \frac{\varepsilon_0}{T} - \dots \quad (24)$$

so the strong-disorder case can be derived as a resummation of all the leading-order logarithmic terms. A more satisfactory mechanism for collecting together all terms of the same magnitude is to use the renormalization group equations, and instead of considering a perturbation expansion for g , to derive an expansion for the β -function. This is discussed in the next section.

6. Renormalization group theory

We begin the renormalization group treatment by noting that we wish to express the renormalization group equations in terms of dimensionless quantities, such as the partition function Z (8), and

$$\Gamma = e^2 a^{d-1} g \quad (25)$$

which is the probability that any site is within the gap. We will express Γ in terms of ξ , where

$$\xi = \frac{r_T}{a} = \frac{\varepsilon_0}{T} \quad (26)$$

where the correlation length associated with a temperature T is [22]

$$r_T = \frac{e^2}{T}. \quad (27)$$

The β -function is

$$\beta(\Gamma) = \frac{d \ln \Gamma}{d \ln \xi} = \beta_0 + \beta_1 \Gamma + \beta_2 \Gamma^2 + \dots \quad (28)$$

For the case of strong disorder, solving the following equation for the β -function:

$$\beta(\Gamma) = -\Gamma \quad (29)$$

together with the boundary condition $\Gamma \rightarrow \Gamma_0$ as $\xi \rightarrow 0$, gives

$$\Gamma = \frac{\Gamma_0}{1 + \Gamma_0 \ln \xi} \quad g_T(0) = \frac{g_0}{1 + e^2 g_0 \ln(\varepsilon_0/T)} \approx \frac{1}{e^2 \ln(\varepsilon_0/T)} \quad (30)$$

which is exactly the result of Raikh and Efros for the density of states for $d = 1$ with strong disorder (20). In other dimensionalities, an ε -expansion gives the β -function as

$$\beta(\Gamma) = -(d - 1) - \Gamma \quad (31)$$

which can again be solved with the boundary condition $\Gamma \rightarrow \Gamma_0$ as $\xi \rightarrow 0$ to give

$$\Gamma \propto \xi^{-(d-1)} \quad g_T(0) \propto \frac{T^{d-1}}{e^2 d} \quad (32)$$

which is the standard result of Efros and Shklovskii [2]. Thus we reach our main conclusion, that the TAP method for solving the spin-glass problem is an identical approximation to the Efros–Shklovskii method for obtaining the density of states of the Coulomb gap.

We note that the $(d - 1)$ -term can be derived using hyperscaling. The system has a critical point which has been moved to $T = 0$, and the correlation length (27) implies a critical index $\nu = 1$, so from hyperscaling, the heat capacity must be proportional to T^{d-2} and the density of states to T^{d-1} .

In the limit of weak disorder $\gamma \gg 1$, the standard results for the density of states break down [21], and in this section we explain how to use the renormalization group equation to derive the behaviour in this regime. The renormalization which we are performing corresponds to a change in the disorder, γ , of the system. As noted in section 5, we expect a Boltzmann-like behaviour for the density of states at low disorder:

$$\Gamma = \Gamma_* \exp\left(-\frac{\varepsilon_0}{T}\right) \quad \ln \Gamma / \Gamma_* = -\xi \quad \beta(\Gamma) = \ln \Gamma / \Gamma_* \quad (33)$$

where Γ_* is an order unity constant. This β -function is a result which we expect to be universal at low disorder. By solving equation (28) for the modified β -function which crosses over between the weak-disorder and strong-disorder limits,

$$\beta(\Gamma) \approx -(d - 1) - \Gamma \quad (\Gamma \ll 1) \quad (34)$$

$$\beta(\Gamma) \approx \ln \Gamma / \Gamma_* \quad (\Gamma \sim \Gamma_*) \quad (35)$$

with again the same boundary conditions $\Gamma \rightarrow \Gamma_0$ as $\xi \rightarrow 0$, we obtain a density of states with a crossover behaviour which for $d = 2$ coincides with that (21) observed in the numerical simulations by Pikus and Efros [21].

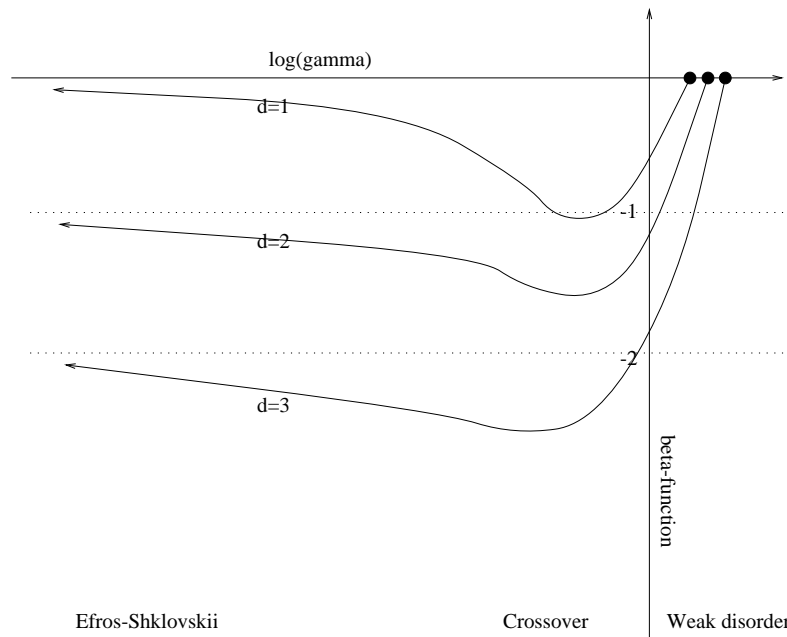


Figure 4. The scaling β -function $d \ln \Gamma / d \ln \xi$ plotted as a function of $\ln \Gamma$.

All the information in equations (29), (34), (35) can be summarized as in figure 4. Any glassy phase transition or crystallization such as those discussed in section 4 would

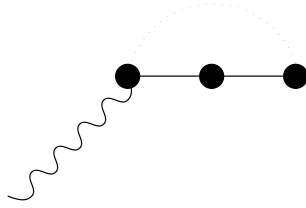


Figure 5. The first non-zero term in the perturbative expansion of the β -function. The wavy line represents a $(\phi \, d/d\phi)$ -term.

constitute a breaking of universality in the region $\ln \Gamma \sim 0$. However, even for infinitesimal disorder, the site energies will have a spread of order ε_0 and Γ will be of order unity, so this region is of little physical significance.

As noted earlier, there is a crossover between the strong-disorder (Efros–Shklovskii) and weak-disorder (Boltzmann) behaviour. For $d = 1$ this occurs at a value of

$$\Gamma = \Gamma_c = a + b \ln \Gamma_* \quad (36)$$

with a and b order unity constants, whilst for $d = 2$ the modified renormalization group equations give exactly the DOS observed in [21].

The corrections to hyperscaling in the RHS of (28) can be obtained as a systematic perturbation series by using the identity

$$\frac{d(\ln Z)}{d \ln T} = \left\langle - \sum_i \phi_i \frac{d \ln Z[\phi_i]}{d \phi_i} \right\rangle - \left\langle e^2 \frac{d \ln Z[\phi_i]}{de^2} \right\rangle \quad (37)$$

which follows from (11). Thus we can develop a perturbation theory for β , the first non-zero term of which (see figure 5) corresponds to the standard Coulomb gap result (29), (34). We believe that by evaluating further terms in the series we will obtain a series which interpolates smoothly between (34) and (35).

7. Conclusions

The essence of our paper is in linking two separate pieces of physics, the spin-glass problem, and that of the Coulomb gap. We have demonstrated that the standard results for the density of states in the Coulomb gap can be derived by a method identical to the TAP method in spin-glass theory. The Coulomb gap density of states plays the part of the renormalized two-point vertex function in an effective-field theory. For $d = 1$ we can perform the renormalization directly by summing a dominant set of diagrams to obtain the strong-disorder limit of the Coulomb gap. The results for $d = 1$ suggest the use of the renormalization group to derive this result for any dimensionality, and to extend the result to the case of weak disorder. It is shown how a diagrammatic expansion for the β -function can be used to derive the renormalization group equations. We hope to use this formalism to derive the properties of systems with weak disorder in a future paper.

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