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I Random Matrix Theory and Localization.

**II 2D Magnetic Vortices in Thin
Superconducting Films.**

by
Alexei Bulatov

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment
of the requirements for the degree of Doctor of Philosophy, The City University
of New York.

1996


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This manuscript has been read and accepted for the Graduate Faculty in Physics in satisfaction of the dissertation requirement for the degree of Doctor of Philosophy.

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Abstract**I Random Matrix Theory and Localization.****II 2D Magnetic Vortices in Thin Superconducting Films.**

by

Alexei Bulatov

Adviser: Professor Joseph L. Birman

A Random Matrix Model with explicitly broken $U(N)$ invariance has been proposed and studied by means of effective-field theory. The effective action is constructed as a functional of the eigenvalue and eigenvector distributions. Using this effective action, the entire N -level distribution function is obtained in the mean-field approximation. This distribution was shown to be dependent on the choice of the basis. In the basis close to the diagonal, we show a smooth transition from the Gaussian Unitary Ensemble to the Poisson level distribution.

It was shown that the known analytical results on Density of States in the Impurity Band Tails in 1D problem can be reproduced by using the Random Matrix Theory approach combined with the recursion procedure.

It is shown that the Nernst coefficient in thin Superconducting films is greatly enhanced (almost two orders of magnitude) due to the long-range vortex-vortex interactions.

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Chapter 1. Introduction and review.

1.1 Introduction.

Most of the achievements of solid state physics have been related to systems with perfect (or "almost perfect") spatial periodicity, such as crystals. On the other hand, many real materials are not well described by this simple model. In the last few decades, the study of various kinds of disordered systems became one of the most important topics in condensed matter physics. These systems are quite interesting for technological applications, such as in laser technology, thermoelectric and photoelectric devices (disordered semiconductors) and computer technology. From a theoretical point of view, it is important to go beyond the one-electron band theory, which also leads to the study of disordered systems. This requires a very serious development of theory and involves many-body effects. In contrast to the "ordered" systems, in the disordered case one has to average the results over the "randomness" present in the system. Due to this averaging, the single-electron problems acquire some features of many-body problems. One of the important results in such single-electron theory, is the famous "Anderson localization" [1], related to the transition from localized to the delocalized states in the disordered tight-binding models. Another important feature is that many-body effects become important, because the single-particle excitations may not be well defined due to the disorder [2,3].

The most common theoretical approach in disordered systems is to calculate the many particle Green's functions in a perturbative manner. This approach is implemented by diagrammatic techniques and allows one to obtain the physically meaningful quantities in the form of an expansion in powers of some "small parameter". The disadvantage of this approach is that the expansion series usually diverge in the presence of a "phase transition" in the system and therefore are not very reliable to analyze the transitions. Instead of the Green's function, one may try to calculate the full distribution of the energy spectrum for the problem. In this case, the result should appear in a non-perturbative way. One of the appropriate theoretical tools for such a program seems to be the random matrix theory (RMT), which in principle enables one to obtain directly the many-level distribution function. In order to do it, one has to construct a random matrix model with reasonable physical properties, corresponding to generic kinds of random systems under study.

1.2 The Wigner-Dyson Random Matrix Theory.

Random matrix models were suggested in the work of E. Wigner [4] and developed by F. Dyson [5]. The original idea of the classical work [4] was an attempt to obtain some properties of the eigenvalues of complicated Hamiltonians, describing systems with "zero space dimensions" (i.e. nuclei), assuming that the matrix elements of the Hamiltonian are random numbers with some given statistical properties. Since then, Random Matrix Theory (RMT) has been applied in various areas of nuclear and mesoscopic physics [6].

The Wigner model [4] is based on the assumption that the matrix elements of the Hamiltonian are all random independent equally distributed Gaussian variables with the probability distribution

$$P dH = \prod_{1 \leq i, j \leq N} dH_{ij} \exp\left(-\beta \sum_{i, j} \frac{|H_{ij}|^2}{\sigma}\right). \quad (1.1)$$

As was shown in [5], there are three types of Gaussian ensembles: Orthogonal (GOE), unitary (GUE) and symplectic (GSE), depending on the symmetry of the Hamiltonian [7]. Namely GOE corresponds to the systems with time-reversal symmetry, GUE to the systems with broken time-reversal symmetry and GSE to the case when the time-reversal symmetry is not broken but the system does not have central symmetry (for example, in the presence of spin-orbit interaction). These symmetries of the Hamiltonian lead to one of the typical results of RMT, namely the "logarithmic level repulsion" when the eigenvalues of the matrix approach each other closer than the average energy distance [7,8]. According to [5], the probability distribution for the eigenvalues is

$$Pd\lambda = \prod_{1 \leq i \leq N} d\lambda_i \exp\left(-\beta \sum_{i=1}^N \frac{\lambda_i^2}{\sigma} + \alpha \sum_{i < j} \log|\lambda_i - \lambda_j|\right), \quad (1.2)$$

with α being equal to 1,2,4 for the GOE, GUE and GSE respectively.

The classical RMT was designed for the system with "zero dimensions" (like nuclei), where all states strongly overlap. For this reason, one can expect that the RMT will be applicable to the extended states in disordered systems and to the quantum-mechanical analogues of classical chaotic systems (quantum billiards) [9]. The important application of the theory of quantum billiards are the nanostructures called "quantum dots". In these systems, the electrons are scattered by the geometric boundaries of the device rather than by the impurities inside of the device [10]. As was shown in [6,11,12], the RMT can be applied to extended states in disordered systems. In [11], a powerful non-perturbative formalism based on the introduction of noncommuting Grassmanian variables, has been developed and applied to the problem of level statistics of small metallic samples. In this (microscopic) approach, the nonlinear σ -model appears and the analysis becomes quite complicated. However, the essential result of [11] coincides with that obtained from the simple RMT model with the logarithmic level repulsion. In this case, only the lowest energy mode of the corresponding nonlinear sigma-model ("zero-mode") is essential for the level evolution at small level separations. It has been also shown [13], that the zero-dimensional σ -model is equivalent to the RMT.

1.3 Localization and level repulsion.

It is known, following P.W. Anderson that some states in disordered systems should be localized [1,14]. In this case, one can expect the Poisson distribution for the

energy levels, because the degeneracy is not prohibited anymore and the level repulsion disappears. The physical reason for this effect is that the localized wave function consists of practically non-overlapping "pieces" [3], and therefore the spectrum may have degeneracy. This means, that the basic assumption of the RMT breaks down, because the different matrix elements of the Hamiltonian can not have equal weights anymore. In order to describe such states while retaining the concept of an RMT description, one may try to "break" the $U(N)$ (or $O(N)$) invariance of the probability distribution, since this invariance leads to level repulsion. However, an interesting class of Random Matrix Ensembles (RME), which seem to have both Poissonian and Gaussian limits, has been proposed in [14] by C.M. Canali, Mats Wallin and V.E. Kravtsov. In this RME, the $U(N)$ invariance is not broken, but the Gaussian probability distribution for each matrix element is replaced by some function

$$P(\{H_{i,k}\}) \sim \exp\left(-\sum_{i,k} |H_{i,k}|^\Gamma / \Delta^2\right), \quad \Gamma \ll 1.$$

The authors claim that smallness of the exponent Γ may possibly lead to the deviations from the standard GUE results. The authors relate their results to the random transfer in disordered conductors, where this type of model seem to be successful in describing the weak localization phenomena [15]. In the recent paper of Shapiro and co-workers [16], the mechanism of "spontaneous breaking" of the $U(N)$ symmetry was proposed. These results reveal a new class of matrix models, possessing both Poissonian and Gaussian

limits. However, as the authors pointed out in [16], there is no clear physical reason to choose the probability distribution in the form which they used in that work, namely:

$$Pd\Lambda = \frac{1}{Z} d\Lambda \int dU \exp(-b \text{Tr}(\Lambda U \Lambda U^+)) \quad ,$$

Here, Λ is the eigenvalue matrix and U stands for some arbitrary unitary matrix which should be integrated out (see Chapter 2 below). After the integration is performed, the system still “remembers” that the $U(N)$ symmetry was broken in the original distribution.

Another model, with $U(N)$ -symmetry explicitly broken in the action, has been introduced in [17]. In that model, the probability distribution was assumed to be

$$PdH = \frac{1}{Z} \prod_{1 \leq i < j \leq N} dH_{i,j} \exp \left[-\frac{1}{2} \sum_{1 \leq i \leq N} H_{i,i}^2 - (1 + \mu) \sum_{1 \leq j < i \leq N} H_{i,j}^2 \right].$$

Where μ is an arbitrary positive parameter. However, the analysis in [17] does not seem to be complete, since the authors had to involve the entropy arguments in their treatment, since they did not succeed in integration over the unitary group. In both works [16,17], the N -level distribution function for the eigenvalues has been obtained explicitly. In recent work [18], the one- and two-level Green's functions had been obtained by using the perturbative methods developed by E. Brézin and A. Zee. The model is formulated on a lattice, at each site of which there is prescribed to be the standard GUE matrix

model. The states on different sites are supposed to be randomly coupled. The probability distribution was taken as

$$P(H) = \frac{1}{Z} \exp\left(-N \sum_{a,b} \frac{1}{2} (M^2)_{a,b} \text{Tr}(H_{a,b} H_{b,a})\right),$$

where the matrix M^2 couples different sites of the lattice, labeled by a, b and H belongs to a standard GUE ensemble, attributed to each site. This model can be viewed as a level distribution for some Hamiltonian with partially violated symmetry [5,18]. A similar model has been studied in [19,20]. In [19], the $1/N$ expansion for the Green's functions has been developed. In [20], the results of [18] for one- and two-level Green's functions has been derived. One should note, that the model [17] can be viewed as a particular case of [18-20], when one has one state per each site. The essential results of [16,17] is that the level repulsion breaks down in some limit, when the diagonal matrix elements of the Hamiltonian are much "greater" than the off-diagonal ones. In the perturbative approach ([18-20]), one always obtains the semi-circle Wigner distribution for the density of states (DOS)

$$\rho(\lambda) = \frac{2}{\pi\lambda_0} \sqrt{1 - \frac{\lambda^2}{\lambda_0^2}}, \quad \lambda^2 \leq \lambda_0^2, \quad (1.3)$$

where $\lambda_0^2 = \alpha / \beta$ and α, β are defined in (1.2). This is not the case for [16,17]. In [18], the correlator between different levels has a "universal" form in the large N limit,

independent of the original distribution of matrix elements. The perturbative methods [18-20] enable one to calculate directly the physically-meaningful quantities, however they do not allow one to analyze the "phase transition" in the system, if there is any. From a physical point of view, one can expect the phase transition from the "localized" to the "extended" state. In this case, the non-perturbative methods of [16,17] seem to be preferable.

Another approach to the analysis of random matrices is related to the "level dynamics" [21-23], in which the distribution of eigenvalues is obtained as a result of the solution of the system of coupled "equations of motion" for the eigenvalues. The role of "time" is played by the perturbation parameter. Therefore, the Hamiltonian is expressed as $H = H_0 + t V$. Then, introducing the denotion $x_n(t)$ for the eigenvalues and new variables $p_n = V_{nn}$; $f_{mn} = |x_n - x_m| V_{mn}$ ($m \neq n$), one arrives at the system of "equations of motion" for the eigenvalues [21]:

$$\begin{aligned} dx_n / dt &= p_n \\ \frac{dp_n}{dt} &= 2 \sum_{m \neq n} \frac{f_{nm}^2}{(x_n - x_m)^3} \\ \frac{df_{nm}}{dt} &= (x_n - x_m) \sum_{l \neq n, m} \frac{f_{nl} f_{lm}}{|x_n - x_l| |x_m - x_l|} \left(\frac{1}{x_n - x_l} - \frac{1}{x_m - x_l} \right) \quad (x_n > x_m) \end{aligned} \quad (1.4)$$

It was shown in [21], that these equations of motion have an infinite number of integrals of motion. The main assumptions in [21] were that after some relaxation time the distribution function for the "dynamical system" of eigenvalues is given by a Gibbs

distribution, dependent on only two integrals of motion: the “energy” and the “angular momentum” of corresponding system of eigenvalues. The result of [21], obtained in the framework of "level dynamics" model, is quite similar to the result [17] (and also contains some undefined constant). For the random systems, the "level dynamics" approach is essentially equivalent to the RMT (see [21,22] and references there).

1.4 Work to be presented in the thesis.

In the first part of the thesis, we describe the results on the N-level distribution for a simple RMT model [24], which extends the model of Shapiro and Pichard [17], with possible application to the transition from localized to delocalized regime in tight-binding models with disorder. This model can be possibly also applied to random transfer matrices, especially to the optical transport in the quasi-1D systems with possible finite number of "channels" ([15], [25]).

One should consider the generalization of the model introduced by Shapiro and Pichard in [17]. Note, that the lack of the explicit $U(N)$ symmetry has a simple physical motivation, and in principle allows one to introduce different dimensionality. The model I will introduce and study can be considered as a particular case of model [18] with only one state per site of the lattice, but with all off-diagonal matrix elements being differently

distributed. This model seems to be reasonable from the physical point of view, for two reasons:

1) The probability distribution is clearly basis-dependent in this model, as one can expect from a physical point of view ([16]).

2) Different matrix elements have different "weights" in the distribution, which is related to the different possible "overlapping" ([17]).

In contrast to [18], this suggests finding the N-level distribution function in our model, which seems to be more preferable in view of possible phase transitions in the system. As we will show later, one can carry out a "mean-field" approach to the calculation of the "effective interaction" between the energy levels. It turns out, that this approach breaks down in the vicinity of a "phase transition", which indeed seems to take place in our model and looks similar to the well-known Berezinsky-Kosterlitz-Thouless (BKT) transition for magnetic vortices restricted on the 2D plane. On the "delocalized" side of the transition, one can still use the perturbation methods in a certain region of parameters. In this limit, our results should coincide with [17]. One can expect the following features: logarithmic level repulsion for small level separations and weak interaction for large level separations. By extrapolating to the localized regime, we can obtain suggestive results on a phase transition. In principle, this extrapolation should be verified by more rigorous methods.

The random transfer matrix theory [26] proved to be successful in the description of the transport in quasi-1D systems with the weak disorder. The Random Matrix approach turns out to be useful in describing the transport in quasi-1D systems beyond the limit of large conductance [27]. We believe that the model presented here may be used as a random transfer matrix model in case when there are different “overlappings” between different channels in the system.

Chapter 2. The Generalized Random Matrix Ensemble.

2.1 Polar Coordinates for Hermitian matrices.

In this section, we will review some properties of Hermitian matrices that will be used below in carrying out some “integration” over the Unitary group.

It is known [7], that any N-dimensional Hermitian matrix can be represented in a form of product

$$H = U \Lambda U^+ , \quad (2.1)$$

where U is some unitary matrix, and $\Lambda = \lambda_i \delta_{i,j}$ stands for the diagonal matrix, composed of the eigenvalues of H . This representation is analogous to usual polar coordinates with U corresponding to the “angular” and Λ to the radial coordinates. For this reason, these quantities are called “polar coordinates” for the Hermitian matrix [28]. However, the correspondence (2.1) is not one-to-one. In case of two parametrizations

$$H = U \Lambda U^+ = U_1 \Lambda_1 U_1^+ \quad (2.2)$$

we obtain from (2.2) that

$$\Lambda = \Lambda_1, \quad U_1^\dagger U = \rho = \text{diag}\{e^{i\theta_1} \dots e^{i\theta_n}\} \quad (2.3)$$

(all eigenvalues of H are supposed to be different, i. e. the matrix H is not degenerate). The set of matrices ρ forms an Abelian subgroup of $U(n)$ and is denoted as $U(1)$. The set of unitary matrices $[U]$, corresponding to the same ρ , turns out to be a subgroup of U and is called a Coset of the Unitary group $U(n)$ with respect to the Abelian subgroup $U(1)$. From (2.3), it follows that the correspondence $(\Lambda, [U]) \leftrightarrow H$ is one-to-one. For example, one can count the number of independent variables in both sides of (2.1) as: in the l.h.s., n^2 independent variables for the Hermitian matrix, on the r.h.s. n^2 variables for $U(N)$, n variables for Λ and n restrictions (2.3) on $[U]$; this makes $n^2 + n - n = n^2$ variables, the same as in the l.h.s.

Differentiating (2.1), we obtain

$$\begin{aligned} dH &= dU \Lambda U^\dagger + U \Lambda dU^\dagger + U d\Lambda U^\dagger = \\ &= dU \Lambda U^\dagger - U \Lambda U^\dagger dU U^\dagger + U d\Lambda U^\dagger \end{aligned} \quad (2.4)$$

The second line in (2.4) follows from the identity $dU U^\dagger + U dU^\dagger = 0$. From (2.4), it follows that

$$d\tilde{H} \equiv U^\dagger dH U = d\Lambda + [\delta U, \Lambda]; \quad \delta U \equiv U^\dagger dU \quad (2.5)$$

for each matrix element of H, we have

$$(d\tilde{H})_{ij} = d\lambda_i \delta_{ij} + (\delta U)_{ij} (\lambda_j - \lambda_i) \quad (2.6)$$

It can be shown that the phase volume of the Unitary group $U(N)$ is defined by means of matrix δU , which is an anti-unitary complex matrix. Since each matrix element of δU has (independent) real and imaginary parts, we obtain for the volume element in the space of Hermitian matrixes DH [28]:

$$DH = D\tilde{H} = \prod_{i < j} (\lambda_i - \lambda_j)^2 [DU] \prod_{k=1}^n d\lambda_k \quad , \quad (2.7)$$

where $[DU]$ stands for the volume element of the coset of the Unitary group.

Now, let us derive a general expression for the volume element in the space of Unitary matrices, following the general procedure [7, 28]. First of all, consider the metric defined for any square matrix M with complex elements:

$$ds^2 = \text{Tr}(dM dM^+) = \sum_{i,j=1}^n |dM_{ij}|^2 \quad (2.8)$$

In case when M is a Unitary matrix, we have

$$dU U^+ + d(U^+) U = 0 \quad ; \quad d(U^+) = -U^+ dU U^+$$

and therefore

$$\delta U = -\delta U^+ .$$

For this reason, the expression (2.8) is reduced to

$$ds^2 = \text{Tr}(dU dU^+) = -\text{Tr}(U^+ dU U^+ dU) = \text{Tr}(\delta U \delta U^+) \quad (2.9)$$

which can be rewritten as

$$ds^2 = \sum_{i,j=1}^n |\delta U_{i,j}|^2 = \sum_{k=1}^n (\delta v_j)^2 + 2 \sum_{i<j} \left\{ (\delta u_{i,j})^2 + (\delta v_{i,j})^2 \right\} , \quad (2.10)$$

where the off-diagonal and diagonal elements have been separated and

$$\delta U_{i,i} = i\delta v_i \quad , \quad \delta U_{i,j} = \delta u_{i,j} + i\delta v_{i,j} .$$

Therefore, according to [28] for the volume element we have

$$DU = 2^{\frac{n(n-1)}{2}} \prod_{k=1}^n \delta v_k \prod_{i<j} \delta u_{i,j} \delta v_{i,j} . \quad (2.11)$$

Now, let us introduce the following parametrization for the arbitrary Unitary matrix U

$$U = (I + i\Omega)(I - i\Omega)^{-1} \quad (2.12)$$

where Ω is a Hermitian matrix. The parametrization (2.12) is convenient, because it is one-to-one except for the manifold of lower dimension, defined by the conditions $\det(I + i\Omega) = 0$ or $\det(I - i\Omega) = 0$ [28]. The reason why (2.12) is one-to-one is that we can invert (2.12) in algebraic form everywhere except for the specified singular matrices Ω . Now, let us express the volume element (2.11) in terms of parameter Ω .

Differentiating (2.12), we obtain

$$\begin{aligned} dU &= i d\Omega (I - i\Omega)^{-1} + (I + i\Omega) (I - i\Omega)^{-1} i d\Omega (I - i\Omega)^{-1} = \\ &= 2 i (I - i\Omega)^{-1} d\Omega (I - i\Omega)^{-1} \end{aligned} \quad (2.13)$$

and therefore

$$\delta U = 2 i (I + i\Omega)^{-1} d\Omega (I - i\Omega)^{-1} \quad (2.14)$$

Substituting (2.14) into (2.9), we obtain

$$ds^2 = \text{Tr}(\delta U \delta U^+) = 4\text{Tr}\left((I + \Omega^2)^{-1} d\Omega (I + \Omega^2)^{-1} d\Omega\right) . \quad (2.15)$$

This gives us the following expression for the volume element [28]:

$$DU = 2^{n^2} \left[\det(I + \Omega^2)\right]^{-n} D\Omega \quad , \quad (2.16)$$

where

$$D\Omega = 2^{\frac{n(n-1)}{2}} \prod_{k=1}^n \delta \omega_k \prod_{i < j} \delta \omega_{i,j} \delta \sigma_{i,j}$$

where (2.17)

$$\Omega_{kk} = \omega_k \quad ; \quad \Omega_{i,j} = \omega_{i,j} + i\sigma_{i,j}$$

and $-\infty < \{\omega_k, \omega_{i,j}, \sigma_{i,j}\} < +\infty$. Together with expressions (2.16) and (2.17), this condition defines the measure in the space of Unitary matrices $U(N)$.

2.2 The matrix model with broken $U(N)$ invariance.

Starting with a simple matrix model which will be presented below, we will study the level distribution in both localized and delocalized regimes. Let us consider the following matrix model: suppose we have a usual GUE matrix model with quadratic action. Now, we change this model in the following way: let us "suppress" the non diagonal GUE-matrix elements $H_{i,j}$. This can also be done by changing the dispersion of

each Gaussian distributed $H_{i,j}$ by the factor $1/\varepsilon_{i,j} \equiv \left(\frac{\sigma_{i,j}}{\sigma}\right) \leq 1$, where σ is the original

GUE dispersion. In this case, the only difference compared to the GUE is that each matrix element has a different dispersion $\sigma_{ij} \leq \sigma$. The motivation for this is the following: in the systems with finite spatial dimension, one can expect that the overlap integrals between different states will be different, dependent on "how far" apart the states are, in the energy space. In the Anderson-type model, the matrix elements of H are directly related to the overlap integrals in the system. Therefore, we can expect them to have different magnitude, depending on their "position" (i,j) . For the Gaussian-distributed variables with zero average, this magnitude is controlled by dispersion of the distribution.

For the diagonal elements, suppose that $\sigma_{i,i} = \sigma$. Therefore, the distribution function for the matrix elements looks like:

$$P dH = \frac{1}{Z} \prod_{1 \leq i, j \leq N} dH_{ij} e^{-\beta \sum_{i,j} \frac{|H_{i,j}|^2}{\sigma_{i,j}}} = \frac{1}{Z} \prod_{1 \leq i, j \leq N} dH_{ij} e^{-\beta S}, \quad (2.18)$$

where

$$S = \frac{1}{\sigma} \sum_{i,j} \varepsilon_{i,j} |H_{i,j}|^2$$

and we can interpret S as an "action". It is clear that if all dispersions $\sigma_{i,j}$ are equal to σ , we have a standard GUE-ensemble with the "action" defined by (1.1):

$$S_0 = \frac{\beta}{\sigma} \text{Tr}(H^2) = \frac{\beta}{\sigma} \sum_{i,j} |H_{i,j}|^2 = \frac{\beta}{\sigma} \sum_k \lambda_k^2 \quad (2.19)$$

This action is unitary invariant, since it only depends on the eigenvalues of H .

Now, we want to find the distribution of eigenvalues of the matrix \mathbf{H} with the distribution of matrix elements (2.18). In order to do so, we have to express the distribution (2.18) in terms of the eigenvalues of H . At this point, it is essential to note

that we did not change the structure of the matrix H itself, but only changed the dispersion of the distribution of matrix elements in comparison to the standard GUE. One should note that the action in (2.18) is not basis-independent anymore, because the different weights explicitly destroy the original $U(N)$ -symmetry of the GUE. In order to determine the eigenvalue distribution, we use the parametrization as in section 2.1.

$$H = U \Lambda U^+ \quad , \quad (2.20)$$

where U is some unitary matrix and $\Lambda = \lambda_i \delta_{i,j}$ stands for the diagonal matrix, composed of the eigenvalues of H . After applying (2.20), we have to perform an integration over the unitary group U in (2.18) around some basis U_0 and this will give us the eigenvalue distribution for (2.18). Then, we can in principle analyze the "level interaction", since the effective eigenvalue distribution will contain some "potential energy" terms.

However, this integration over U is dependent on the chosen basis U_0 . In our approach, this unitary rotation plays the role of "order parameter", for which we will obtain the Ginzburg-Landau type of equations. Therefore, we are going to make the following approximation: let us first go to the basis where the matrix H is diagonal and after that consider the small $U(N)$ -rotations around this diagonal basis. One can justify that the "Gaussian" integration over the unitary rotations is possible in a certain limit. Therefore, proceeding this way, one obtains the level distribution in that basis which is

different from the one where the matrix H is diagonal. One can show, that the action in (2.18) can be written in the form

$$S = S_0 + \sum_p \varepsilon_p \text{Tr}(\Lambda W(p) \Lambda W^+(p)) \quad , \quad (2.21)$$

with

$$S_0 = \frac{\beta}{\sigma} \sum_k \lambda_k^2 \quad ; \quad \varepsilon_{ij} \equiv \sigma / \sigma_{ij} = \sum_p \varepsilon_p \exp[ip(i-j)] \quad (2.22)$$

$$W_{k,k'}(p) = \sum_m e^{-ipm} U_{k,m} U^+_{m,k'} = (UV_p U^+)_{k,k'} \quad , \quad (2.23)$$

with

$$(V_p)_{k,k'} = \delta_{k,k'} e^{ipk} \quad (2.24)$$

Since (2.23) is does not depend on the choice of the coset, it follows from (2.21)-(2.24) that in our model the coset integration is equivalent to the integration over the whole group U.

2.3 The Effective-field analysis.

In order to perform the integration over the unitary group, we have to find some convenient parametrization for the elements of the unitary group. For any unitary matrix U , we can use the parametrization (2.12) [28]:

$$U = (I + i\Omega) \times (I - i\Omega)^{-1} \quad , \quad (2.25)$$

where I stands for the unit matrix and Ω is a Hermitian matrix, which has the meaning of the "angle" of our rotation. Using the parametrization (2.25), we obtain the measure (2.16), [28]:

$$dU = \prod_{l < m} \frac{dx_{l,m} dy_{l,m}}{(\det(I + \Omega^2))^N} \prod_k dx_{k,k} = \prod_{l < m} dx_{l,m} dy_{l,m} \prod_k dx_{k,k} e^{-N \text{Tr}(\ln(I + \Omega^2))} \quad (2.26)$$

where

$$\Omega_{l,m} = x_{l,m} + i y_{l,m} = R_{l,m} e^{i \varphi_{l,m}} \quad . \quad (2.27)$$

In the delocalized regime, one can expect this "measure" to be quite important for our model.

We will see that the behavior of the set of local "phases" $\varphi_{l,m}$ becomes quite important.

Now, we should expand the action S from (2.18) as a functional of $\{\Omega\}$, using the parametrization (2.25). In order to do so, one can suggest the following method: let us introduce parameter t in (2.25) and express the “Hamiltonian” (2.20) in the form

$$H(t) = (1 + it\Omega)(1 - it\Omega)^{-1} \mathcal{A} (1 - it\Omega)(1 + it\Omega)^{-1} \quad (2.28)$$

We see that the parameter t really controls the value of the “angle” Ω . Therefore, the expansion in powers of Ω is equivalent to the expansion in powers of t provided that after the expansion, we put $t=1$. Differentiating (2.28) with respect to t , we obtain

$$\frac{d}{dt} H(t) = i \left[\frac{2\Omega}{1 + t^2\Omega^2}, H(t) \right], \quad (2.29)$$

where the square brackets stand for the commutator. Using this relation, we obtain the recursion relations for the coefficients in expansion $H(t) = \sum_n H_n t^n$ as

$$H_n = \frac{2i}{n} [\Omega, H_{n-1}] - \frac{i}{n} [\Omega^3, H_{n-3}]. \quad (2.30)$$

This relation enables us to obtain the expansion of the action (2.18) without lengthy calculations. Using the condition $H_0 = \mathcal{A}$, we obtain from (2.30):

$$H_1 = 2i[\Omega, A] ; H_2 = 2i^2[\Omega, [\Omega, A]] ; H_3 = \frac{2i^3}{3}[\Omega^3, A] + \frac{2i}{3}[\Omega, H_2]$$

The expansion of the "action" gives us

$$\begin{aligned} \Delta S = S_{\text{eff}} - S_0 = & 4 \frac{\beta}{\sigma} \sum_{i,k} (\varepsilon_{i,k} - 1) (\lambda_k - \lambda_i)^2 R_{i,k}^2 + N \sum_{i,k} R_{i,k}^2 + \\ & + \frac{8\beta}{\sigma} \sum_{i,j} (\lambda_i - \lambda_j)^2 \times \\ & \left\{ \sum_{k'} [\varepsilon_{i,j} - \varepsilon_{k,j}] R_{i,k} R_{k,j} R_{i,j} \sin(\phi_{i,k} + \phi_{k,j} + \phi_{j,i}) + \right. \\ & \left. \sum_{k,k'} [(\varepsilon_{i,k} + \varepsilon_{i,k'} - \varepsilon_{k,k'}) + (\varepsilon_{j,k} - \varepsilon_{j,k'} - \varepsilon_{k,k'}) - \varepsilon_{i,j} - 1] R_{i,j} R_{j,k} R_{k,k'} R_{k',i} \cos(\phi_{i,j} + \phi_{j,k} + \phi_{k,k'} + \phi_{k',i}) \right\} \\ & - \frac{1}{2} \left(-\frac{N}{2} \right) \sum_{i,j,k,k'} R_{i,j} R_{j,k} R_{k,k'} R_{k',i} \cos(\phi_{i,j} + \phi_{j,k} + \phi_{k,k'} + \phi_{k',i}) \end{aligned} \quad (2.31)$$

When the parameters $\{\varepsilon_{i,j}\}$ increase, the corresponding dispersion of non-diagonal matrix elements decreases and therefore one can expect the average hopping amplitude from one site to another to decrease. This effect is in favor of localization. From (2.31), it follows that in this case the leading correction term is of the second order in the amplitude R . Note, that in the delocalized regime, one can expect that the expansion (2.31) is not valid, since both R and ϕ fluctuate strongly. In this case, the whole "action" (2.31) is reduced to the constant term plus quadratic term $N \sum_{i,k} R_{i,k}^2$, related to

the measure on the $U(N)$ group. This term does not depend on level separation and therefore the level repulsion is restored in the limit of the delocalized regime.

The phase dependent terms are reminiscent of the Hamiltonian for the Global $O(2)$ model [29], where the Berezinsky-Kosterlitz-Thouless transition (BKT) takes place. The meaning of the BKT transition is the formation of free vortices [29]. The "free vortex" is related to the large fluctuation of phase. In our model, one can expect the large fluctuations of the phase of the wave function for the delocalized states, because the phase distribution is close to uniform. For the localized states, the phase does not have large fluctuations. The rough estimate based on the results for the global $O(2)$ model, gives us the region $\varepsilon > 1 + 4\pi / N$ for the BKT-type transition in the vicinity of the state with $\langle R \rangle = 0$. Since N is supposed to be very large, this estimate indicates that there always are some "free vortices" in our system if only $\varepsilon > 1$. We will use these qualitative considerations in order to obtain the solution for both localized and delocalized regimes, without studying the transition itself. In this case, one can use the mean-field approximation with respect to the phase angles in two different regimes.

In the localized regime, as discussed above, one can expect the level repulsion to be strongly suppressed. This is because the localized states are separated in space, the overlap is small and the system does not resist the degeneracy, i. e. there is no level repulsion. For the delocalized states, the overlap is large and the level repulsion takes place. From (2.31), we see that in the localized regime $\langle R \rangle^2 N^2 \sim 1 / (\beta (\varepsilon - 1) (\Delta \lambda)^2)$. On the other hand, the expansion of (2.12) in powers of Ω is valid if $\langle R \rangle^2 N^2 \leq 1$. This implies that $\beta (\varepsilon - 1) (\Delta \lambda)^2 \gg 1$. The condition was obtained in the exactly

solvable model [16] for the smallest level separation, where the transition took place in this limit.

Because of large phase fluctuations close to the delocalized regime, only the terms which do not depend on phase will survive. Since all $R_{i,j}$ have different indices, the probability distribution factors into a product of distributions for each $R_{i,j}$. In this case, the effective action is reduced to

$$\begin{aligned} \Delta S = S_{\text{eff}} - S_0 = & 4 \frac{\beta}{\sigma} \sum_{i,k} (\varepsilon_{i,k} - 1) (\lambda_k - \lambda_i)^2 R_{i,k}^2 + N \sum_{i,k} R_{i,k}^2 + \\ & + \frac{16\beta}{\sigma} \sum_{i,j} (\lambda_i - \lambda_j)^2 \sum_k \left[1 - \varepsilon_{i,j} + (\varepsilon_{j,k} - \varepsilon_{i,k}) \right] R_{i,j}^2 R_{j,k}^2 \\ & - \left(-\frac{N}{2} \right) \sum_{i,j,k} R_{i,j}^2 R_{j,k}^2 \end{aligned} \quad (2.32)$$

Note, that the cubic term, present in (2.31), does not contribute to (2.32). The reason is that this term is zero for the zero total phase. If we assume that the parameters $\{\varepsilon\}$ are smooth functions of their indices, we have: $\sum_{i,j} (\lambda_i - \lambda_j)^2 \sum_k (\varepsilon_{j,k} - \varepsilon_{i,k}) R_{i,j}^2 R_{j,k}^2 \approx 0$, due to the fact that the coefficient $(\varepsilon_{j,k} - \varepsilon_{i,k})$ is an oscillating function of k . At the same time, close to the delocalized regime, we can assume that all the “amplitudes” $\{R\}$ are close to each other; this will be shown to agree with the self-consistent analysis presented below. In this case, the action (2.32) can be approximated as

$$\begin{aligned}
\Delta S = S_{\text{eff}} - S_0 = & 4 \frac{\beta}{\sigma} \sum_{i,j} (\varepsilon_{i,j} - 1) (\lambda_i - \lambda_j)^2 R_{i,j}^2 + N \sum_{i,j} R_{i,j}^2 + \\
& \frac{16\beta N}{\sigma} \sum_{i,j} (\lambda_i - \lambda_j)^2 [1 - \varepsilon_{i,j}] R_{i,j}^4 + \\
& \left(\frac{N^2}{2} \right) \sum_{i,j} R_{i,j}^4
\end{aligned} \tag{2.33}$$

The expression (2.33) indicates that the minimum $\langle R \rangle = 0$ may be not a global minimum in our model. This suggests that there are some other possible “phases” corresponding to different minima of the effective action. This really reflects the fact that there is a strong basis dependence in our model and the level distribution is also basis-dependent. However, now we will concentrate on the situation close to the basis with $\langle R \rangle = 0$ and analyze the level distribution. In this case, the quartic corrections are small and the saddle-point approximation in the vicinity of $\langle R \rangle = 0$ is well justified.

We can apply the self-consistent approximation to (2.33) on the delocalized side and to analyze the level repulsion in the model. Performing the integration over the non diagonal elements of $\Omega_{i,j} \equiv x_{i,j} + i y_{i,j}$ (in polar coordinates), we finally obtain the probability distribution for the eigenvalues as

$$P d\Lambda \equiv C_N \prod_k d\lambda_k \prod_{i < j} \left[\frac{(\lambda_i - \lambda_j)^2}{\Theta_{i,j} (\lambda_i - \lambda_j)^2 + \Pi_{i,j}} \right] e^{-\rho \sum_i \lambda_i^2}, \tag{2.34}$$

where

$$\Theta_{i,j} = \frac{4\beta\varepsilon_{i,j}}{N} \quad (2.35)$$

$$\Pi_{i,j} = 1 + 16\langle R_{i,j}^2 \rangle$$

The meaning of the averaging in (2.35) is that we are averaging with respect to the distribution which parameters are dependent on the average that we are looking for. This situation is the same as in standard self-consistent approach and corresponds to the mean-field approximation. Now, let us assume that $\{\varepsilon\}$ is a smooth parameter with the typical average $\varepsilon = \langle \varepsilon \rangle$. One should note that the result of the Gaussian integration is exact, in the limit of large parameter $\beta(\varepsilon - 1)(\Delta\lambda)^2 \gg 1$ (this is also the condition for validity of our expansion (2.31)). First of all, β is supposed to be large, as described in [7,16], $\beta \sim N$. It is also important that the level repulsion should exist for the small level separations. The probability distribution for the eigenvalues can be approximated as

$$P dA \cong \frac{1}{Z} \prod_a d\lambda_a \prod_{b < c} \frac{(\lambda_b - \lambda_c)^2}{\left[\frac{1}{\gamma^2} (\lambda_b - \lambda_c)^2 + 1 \right]} \exp\left(-\frac{\beta}{\sigma} \sum_a \lambda_a^2\right) \quad (2.36)$$

where

$$\frac{1}{\gamma^2} = \frac{4\beta(\varepsilon - 1)}{N\sigma} \quad (2.37)$$

As one can see from (2.37), level repulsion exists for small level separations, where

$\frac{(\lambda_b - \lambda_c)^2}{\gamma^2} \ll 1$, but is suppressed for large separations. To our knowledge, this is the

first self-consistent calculation for the N-level distribution function, taking the basis-dependence of the eigenvectors into account. From the analysis we present here, one can expect that the level distribution strongly depends on the choice of the basis.

2.4 Density of states. Localization and level repulsion.

The distribution (2.36) looks quite similar to the one obtained in the early paper of Yukawa [21]. However, here we have explicitly derived the distribution (2.36) from a model (2.1) in the mean-field approximation. A similar model was considered in [7], where a similar result was obtained, using the maximum entropy principle [17]. In the present work, we performed the explicit integration in the mean-field approximation and the resulting distribution contains no arbitrary constants. From (2.36), we see that the effective "interaction" between the energy levels looks like:

$$V(\lambda_a - \lambda_b) = -\text{Ln} \left[\frac{(\lambda_a - \lambda_b)^2}{\frac{1}{\gamma^2} (\lambda_a - \lambda_b)^2 + 1} \right] \quad (2.38)$$

From the effective interaction between the eigenvalues, one can in principle derive all information about the level distribution (2.36), see [8, 14]. The n-level correlator is given by $\langle \rho(\lambda_1) \rho(\lambda_2) \dots \rho(\lambda_n) \rangle$, where the average is taken with the weight (2.36). Following the standard procedure, we obtain the equation for the average density of states (DOS) $\rho(\lambda)$ in the mean-field approximation as

$$\int d\lambda' \rho(\lambda') V(\lambda - \lambda') = \frac{\beta}{N\sigma} u(\lambda) + \text{const} \quad (2.39)$$

with

$$u(\lambda) = \lambda^2 \quad (2.40)$$

The equation (2.39) reduces to

$$\int d\lambda' \rho(\lambda') \left(\frac{1}{\lambda' - \lambda} - \frac{\lambda' - \lambda}{(\lambda' - \lambda)^2 + \gamma^2} \right) = \kappa \lambda, \quad (2.41)$$

where

$$\kappa \equiv \frac{4\beta}{N\sigma} \quad (2.42)$$

Equation (2.41) can be exactly solved in some cases. For example, when $\gamma \rightarrow \infty$, we have a standard "semicircle" law [8]

$$\rho(\lambda) = \frac{2}{\pi a} \sqrt{1 - \frac{\lambda^2}{a^2}}; \quad a^2 = \frac{2}{\kappa} \quad (2.43)$$

Since γ tends to infinity when $\varepsilon \rightarrow 0$, this limit corresponds to the true GUE and leads to (1.3), as it should. Using the results from the theory of singular integral equations

[15], one can obtain a solution of equation (2.41), valid in both limits $\varepsilon \rightarrow 0$ and $\varepsilon \rightarrow \infty$. This solution is

$$\rho(\lambda) = \sqrt{\frac{2\kappa}{\pi^2}} \sqrt{1 - \frac{\lambda^2}{a^2}} \left[1 + \frac{4}{3\pi} \left(\frac{1}{a^2} - \frac{\kappa}{2} \right) \left(1 + 2 \frac{\lambda^2}{a^2} \right) \right], \quad (2.44)$$

where

$$a^2 = \frac{2}{\kappa} \frac{4\gamma^2}{1 + 4\gamma^2} \quad (2.45)$$

is the width of the distribution (2.44) (fig.2.1). Strictly speaking, our results are only valid for $\varepsilon \geq 1$, since the equation (2.41) was derived in this region. The limit $\varepsilon \rightarrow \infty$ corresponds to $\gamma \rightarrow 0$. Since the width (2.45) tends to zero for small γ , the distribution (2.44) tends to a delta-function in the limit $\gamma \rightarrow 0$. This limit corresponds to the case when the level repulsion is "killed".

In summary, we propose an effective-field theory to study the random matrix model (2.18). We construct the effective action and show that for $\beta \sim \mathbf{N}$ in the vicinity of the basis with $\langle R \rangle = 0$ the model does not have the phase transition to the localized phase. Therefore, the mean-field approximation is reliable and the corrections are small. Note, that in the case $\beta \sim \mathbf{N}^2$ the level repulsion is "killed". In this case, we derive

from (21) $V(\lambda_a - \lambda_b) = -\text{Ln} \left[\frac{(\lambda_a - \lambda_b)^2}{(\lambda_a - \lambda_b)^2 + \frac{c}{N}} \right]$, with $c = \frac{1}{\beta(\varepsilon - 1)} \geq 0$. From the

effective action (2.33), the density of states and the higher-order correlators can be obtained. One should note, that the alternative methods of Grassmanian integration [16] allow one to obtain only certain correlators of the N-level distribution function. In our approach, we directly obtain this distribution function.

2.5 Open problems.

1. While the analysis given is valid in the vicinity of “almost-diagonal” basis $\langle R \rangle = 0$ we have an indication in equation (2.33) that, outside of this region, a higher-order quartic term dominates, which is the hint of the first-order kind of phase transition to the localized phase. This will be investigated separately in the future research.
2. From the analysis presented above, we can conclude that the matrix model (2.18) incorporates both standard GUE and the Poisson level distributions as limiting cases. In the intermediate regime, we have to obtain the effective “interaction” between levels. The transition between the two limiting cases is dependent on the set of parameters $\varepsilon_{i,j}$. This set of parameters contains the information of the effective number of “overlapping” between the different sites of the system. In principle, one can expect that the effective dimensionality of the system is “encoded” in the set of parameters $\varepsilon_{i,j}$. However, it is still not clear how to obtain that effective dimensionality from the given set of parameters. This would be extremely important for the localization problems, since it is known that dimensionality plays a crucial role in these phenomena.
3. An interesting application of our RMT model seems to be the random transfer-matrix theory with possible different distribution for different off-diagonal elements. This may be relevant to the quasi-1D systems with possible different “overlapping” between different channels, in particular to some problems of optical transport [24].

Chapter 3. The Random Matrix Theory of Impurity band Tails.

3.1 Introduction.

In this chapter, the problem of the impurity band tails is considered from the point of view of a suitably chosen Random Matrix Model. Namely, it will be shown that an appropriate model is the “banded” random matrix model with diagonal disorder which will be studied by means of a recursive method [29] in the large- N limit. When the diagonal matrix elements are independent and Gaussian-distributed [30], we obtain the density of states (DOS) in the “tail” outside of the band in the large- N limit. We obtain agreement with the Lifshitz-Halperin-Lax results [31,32] on the impurity band tails in 1D. As far as we know, this is the first use of Random Matrix Models in this context.

Impurity levels occur due to violation of the translation invariance of the effective potential, acting on the electron in the crystal [33]. Physically, impurity band tails occur in case of high concentration of impurity atoms in the crystal. Because of the impurities, one obtains some finite density of single-electron states in the “gap” region, forbidden for the spectrum of periodic problem [31]. These contributions to the single-electron density of states are called impurity-band tails. In this region, the density of states is extremely small and is entirely due to the impurities. It turns out [31,32], that these “tails” exist due to the large fluctuations of the local field, acting on the single electron. Particularly [32], the most important are the fluctuations that are able to create bound states of the electron

beyond the boundary of the unperturbed spectrum. Therefore, there is some “optimal” large fluctuation of the local field, which gives the most important contribution to the density of states at each point of the “tail” [31,32]. This fact has been explicitly used in [32], where the density of states has been obtained in the region smaller than the bandwidth of the unperturbed problem (which was assumed to be infinite). For this reason, the method of [31,32] is called the method of “optimal fluctuation”.

In this part of the work, we are going to apply a suitably chosen Random Matrix Model to the analysis of the impurity-band tails in a 1D disordered chain without making an assumption about the large width of the conductance band. We consider a simple 1D chain with diagonal disorder and show that RMT together with recursion methods [29,30] enables us to reproduce the well-known results [31,32] on the density of states in the impurity band tails in all regions of the spectrum.

3.2 The model.

Let us consider the simplest model with a hopping Hamiltonian in 1D [29]:

$$H = \sum_n (h_n |n\rangle \langle n| + V|n\rangle \langle n+1| + V|n\rangle \langle n-1|) \quad (3.1)$$

The diagonal elements $\{h_n\}$ are disordered, and this represents fluctuations of the potential energy on a given site. The constant V equals $1/4$ of the band width in the

case of no disorder and can be expressed in terms of the effective mass m^* and the size of the unit cell a as

$$V = \frac{1}{2 m^* a^2} \quad (3.2)$$

The diagonal elements are assumed to be independent, and equally distributed, Gaussian random variables, [30], so that

$$\begin{aligned} h_n &= \langle h \rangle + \delta h_n, \\ \langle \delta h_n, \delta h_{n'} \rangle &= \sigma \delta_{n,n'} \end{aligned} \quad (3.3)$$

Our objective is to calculate the density of states for this model, especially in the energy region near the edge of the spectrum.

3.3 The results on the Impurity band tails in 1D.

Let us consider an approach to RMT, introduced in [30]. This method requires calculation of the inverse matrix

$$(R_n)_{i,j} = \left(\frac{1}{H_n - z} \right)_{i,j}, \quad (3.4)$$

where the index n stands for the “size” of the $n \times n$ matrix. In RMT, it is assumed that $n \gg 1$. Now, we employ the following expression for the inverse of a matrix A [30]:

$$(A^{-1})_{i,j} = \frac{\partial}{\partial A_{i,j}} \text{Ln} [\det A]. \quad (3.5)$$

This is a general expression easily seen to follow from the definition of the determinant of a matrix. In our case (3.4), we have:

$$(R_n)_{i,j} = \frac{\partial}{\partial H_{i,j}} \text{Ln} [\det (H_n - z)] \quad (3.6)$$

and

$$\text{Tr} (R_n) = -\frac{\partial}{\partial z} \text{Ln} [\det (H_n - z)] \quad (3.7)$$

Now, we will obtain a recursive relation [29], when the size of matrix is increased from $n-1$ to n . From (3.7), we obtain

$$\text{Tr} (R_n) - \text{Tr} (R_{n-1}) = -\frac{\partial}{\partial z} \text{Ln} \left[\frac{\det (H_n - z)}{\det (H_{n-1} - z)} \right] \quad (3.8)$$

The structure of the matrices we consider is shown in fig. 3.1. For this case, we have

$$\frac{\det(H_n - z)}{\det(H_{n-1} - z)} = h_n - z - \sum_{i,j=1}^{n-1} V_i V_j (R_{n-1})_{i,j} \quad (3.9)$$

and therefore

$$\text{Tr}(R_n) - \text{Tr}(R_{n-1}) = -\frac{\partial}{\partial z} \text{Ln} \left[h_n - z - \sum_{i,j=1}^{n-1} V_i V_j (R_{n-1})_{i,j} \right] \quad (3.10)$$

where $V_j = (H_h)_{j,n}$. For the case of a one-band matrix (fig. 1), (3.10) is reduced to

$$\text{Tr}(R_n) - \text{Tr}(R_{n-1}) = -\frac{\partial}{\partial z} \text{Ln} \left[h_n - z - V^2 (R_{n-1})_{n-1,n-1} \right]. \quad (3.11)$$

Introducing the “average” quantities

$$U_n = \frac{1}{n} \text{Tr}(R_n) \quad (3.12)$$

we obtain

$$U_n - U_{n-1} + \frac{1}{n} U_{n-1} = -\frac{\partial}{\partial z} \frac{1}{n} \text{Ln} \left[h_n - z - V^2 (R_{n-1})_{n-1,n-1} \right]. \quad (3.13)$$

We also observe that

$$(R_{n-1})_{n-1,n-1} = \frac{1}{h_{n-1} - z - V^2(R_{n-2})_{n-2,n-2}} \quad (3.14)$$

This implies that the elements $(R_n)_{n,n}$ of the inverse matrix may have a stable point $(R_n)_{n,n} \rightarrow R$. In case when there is diagonal disorder ($\delta h_n \neq 0$), the quantity (3.14) turns out to be self-averaging [30], which means that we can average both sides of (3.14) over the disorder (3.3). In case of no diagonal disorder, we immediately obtain the result for the fixed point, familiar from RMT:

$$R = \frac{1}{V^2} \left[-\frac{z}{2} + \sqrt{\left(\frac{z}{2}\right)^2 - V^2} \right] \quad (3.15)$$

and

$$U = \left(-\frac{\partial}{\partial z} \right) \text{Ln} \left[-z - V^2 R(z) \right] \quad (3.16)$$

with the density of states, proportional to $\text{Im}(U)$

$$\rho(z) \sim \frac{1}{\sqrt{1 - \left(\frac{z}{2V}\right)^2}}, \quad (3.17)$$

which is the answer previously obtained for the 1D chain with no disorder [29], and where $4V$ is the bandwidth. In the presence of disorder $\{h_n\} \neq 0$, and assuming (3.3) we obtain a system of equations

$$R(z) = \int dx P(x) \frac{1}{x - z - V^2 R(z)} \quad (3.18)$$

$$U(z) = \left(1 + V^2 \frac{\partial R(z)}{\partial z}\right) R(z)$$

Note, that the first of the equations (3.18) exactly coincides with the equation for the trace of the inverse matrix (resolvent) in case of full matrix with equally distributed non-diagonal elements and large diagonal disorder [30]. The second equation of the system (3.18) indicates that there is a relation between the two different resolvents: $R(z)$ for the full matrix and $U(z)$ for the band matrix.

The first equation of (3.18) can be rewritten as

$$R(z) = \frac{1}{i\sqrt{\sigma}} \int_0^{+\infty} d\eta \exp(-\eta^2/2) \exp\left[i\eta \left(\frac{z + V^2 R(z) + i\varepsilon}{\sqrt{\sigma}}\right)\right] \quad (3.19)$$

$(\varepsilon \rightarrow 0)$

In the saddle-point approximation,

$$R(z) \approx \frac{1}{i} \sqrt{\frac{2\pi}{\sigma}} \exp\left[-\frac{(z + V^2 R(z))^2}{2\sigma}\right]. \quad (3.20)$$

Assuming that $z \geq 2V$, but $|z/2 - V| \cong V$, we can still use (3.15) as the first approximation. Then, we obtain from (3.20):

$$R(z) = \frac{1}{i} \sqrt{\frac{2\pi}{\sigma}} \exp\left[-\frac{1}{2\sigma} \left((2V)^{\frac{3}{2}} \sqrt{\frac{z}{2} - V} + \frac{5}{4} \sqrt{V} \left(\frac{z}{2} - V\right)^{\frac{3}{2}} + \dots \right)\right]. \quad (3.21)$$

Taking (3.21) into account, we arrive at the following expression for the DOS:

$$\rho(z) \sim \frac{1}{\sqrt{\frac{z}{2} - V}} \exp\left[-\frac{1}{2\sigma} \left((2V)^{\frac{3}{2}} \sqrt{\frac{z}{2} - V} + \frac{5}{4} \sqrt{V} \left(\frac{z}{2} - V\right)^{\frac{3}{2}} + \dots \right)\right]. \quad (3.22)$$

3.4 Discussion and comparison with other results.

From (3.22), it follows that the exponent contains the term $\left(\frac{z}{2} - V\right)^{3/2}$, which is typical for the continuous 1D problem with “white noise” [32], plus some additional terms. One has to note, that in our case the fluctuations of our potential are not exactly delta-correlated; the correlation radius is the size of the “cell” $a \sim 1/\sqrt{2V}$. We believe that the complicated behavior (3.22) near the band edge is a consequence of a finite correlation radius in the discrete model. One should note, that the 3/2-power dependence takes place for $|z - 2V|/D^{2/3} \sim 2 - 3$ where $D^{2/3} \sim \sqrt{\sigma}$, see in [32,33]. In our case, this means that $|z - 2V|/V \sim 2 - 3$. In this region, the second term in the exponent is the leading one and we obtain qualitative agreement with [31,32]. One should note, that the asymptotic solution (3.22) is just the first-order iteration for equation (3.19) and is not exact. For this reason, the 3/2-power term has a different numerical coefficient in front of it, namely we find $5/4 \sqrt{2}$, while the value $4/3 \sqrt{2}$ is in the literature [32,33]. On the other hand, in the vicinity of the band edge we obtain the square root term in the exponent, agreeing with [34]. For large z , it follows from (3.20) that the DOS behaves like $\rho(z) \sim \exp\left[-\frac{z^2}{2\sigma}\right]$, according to [32,35].

One should note that although we investigated the density of states in the band “tails” inside of the “gap” region, our basic equation (3.18) is also applicable to the density of states inside of the conduction band. In this region, one can also expect some deviation from the result for the density of states (3.17), valid in the absence of noise in the system. This will be examined in future work.

We conclude that using the modified recursion method for random banded matrices, presented in this paper, one can study the density of states of the discrete 1D chain both inside and outside of the conduction band analytically in the entire region. Outside of the band, we obtain the exponential “Lifshitz tails” for the density of states.

In the work of J. D’Anna and A. Zee [36], a similar formalism has been independently developed. Their RG method is essentially equivalent to our “recursion” procedure. However, we have applied this method to the case of 1D chain as opposed to the “full” matrix in [36] and we studied specifically the problem of impurity band tails, which was not addressed in [36].

3.5 Open problems.

1. We showed that the new recursive procedure together with the banded random matrix model allows us to reproduce the results on the DOS in the impurity band tails for the simple 1D chain with diagonal disorder. The next step is to generalize our model for the higher dimensions (2D and 3D). In principle, this is possible due to the fact that the problems for tight-binding Hamiltonian in higher dimensions can be “mapped” onto the tight-binding model for the 1D chain [29], analogous to the one considered above (3.1). However, the structure of coefficients for (3.1) is dependent on the dimensionality and may become quite complicated. This problem requires additional analysis.

2. Another interesting problem is to calculate the higher-order correlators for our model. In principle, this will enable us to analyze the conductivity of our system. This can be done in the framework of our approach. For example, in [36] the higher correlators for the case of “full” matrix have been obtained using quite similar approach.

3. It is interesting to apply (3.18) to examine the change of the DOS inside of the band due to impurities. The general formulation should also apply in this case.

Chapter 4 The Effect of Temporal Noise on the Single-Electron

Transport in Long Biological Molecules

4.1 Introduction.

We apply a simple model for the single-electron transport with the temporal noise. This model assumes that the correlation time for the noise is much smaller than any other characteristic time scale in the system. We show that for long molecules, the effects of the temporal noise cause destruction of the phase coherence and therefore the ballistic transfer does not exist. In particular, the time-dependence of the reaction rate in the typical experiments on the single-electron transport, exhibits a power-law decay as a function of time, as opposed to the exponential or stretched exponential decay, the latter is typical for the systems with no temporal noise. Experimental measurements are proposed.

The problem of the single-electron transfer in long biological molecules is quite important from both experimental and theoretical points of view [37-41]. By now, there exist a number of theoretical models, explaining some particular features of the process [38-41]. It is essential that the adiabatic approach [40], is not appropriate for the transfer in long biological molecules due to large donor-acceptor separations and therefore very weak coupling between the sites. The transfer mechanism becomes non-adiabatic and

dependent in a complicated way upon the geometry and size of the system. For this reason, the tight-binding model for the single-electron transfer in long biological molecules has been established [38] and developed in number of works [39,41]. This model has many advantages, including the possibility of taking into account the relative energies of different attached molecular groups. Using the Green's function techniques, developed in [39], it is possible to obtain the quantities measured in experiment (such as reaction rates) directly from the tight-binding model with a reasonable amount of computation efforts [39,41].

On the other hand, all the above mentioned models do not consistently take into account the effects of dissipation in a large system with many degrees of freedom, such as a long molecule. The electron transfer has been essentially treated in a pure quantum-mechanical sense, which leads to the ballistic model of the electron transfer [41]. However, the long molecule itself has many internal degrees of freedom (for example, the backbone exhibits some thermal fluctuations). This additional "noise" is always present and as we show below, it destroys the electron phase coherence and therefore leads to the suppression of the ballistic electron transfer. This effect is especially important for the long-range electron transfer, where the ballistic contribution becomes negligible.

4.2 Formulation of the model.

In this part of the thesis, we are going to address the influence of noise on the single-electron transfer. In order to do this, we apply the model [42-46], which was first proposed in [42] to study the electron transport in disordered 1D metallic chains, where it could be solved exactly. Afterwards, this model was applied [44-46] to different problems in systems with “dynamical disorder” (for example, the influence of phonons on the electron transport). In our case, the model can not be solved analytically, but it leads to simple equations in the long-time region, which are convenient for numerical simulations.

The model is formulated in terms of the Anderson tight-binding Hamiltonian in second-quantised form with a_k , a_k^+ being destruction/annihilation operators on the site

$$H = \sum_{k,l} (a_k^+ a_l V_{k,l} + a_l^+ a_k V_{k,l}^*) \quad (4.1)$$

where the matrix elements $V_{k,l}$ represent the transition amplitude for the electron between the sites k and l and are assumed to have some random (“noisy”) component:

$$\begin{aligned} V_{k,l} &= \langle V_{k,l} \rangle + \delta V_{k,l} \\ \langle \delta V_{i,j} \delta V_{k,l} \rangle &= (a^2)_{i,j} \delta(t-t') [\delta_{i,k} \delta_{j,l} + \delta_{i,l} \delta_{j,k}] \end{aligned} \quad (4.2)$$

i.e. we assume Gaussian white noise for the fluctuations of the hopping amplitudes [42,44]. Now, one can show that the model (4.1, 4.2) can be exactly reduced to the Focker-Planck equation. For the metallic chains, it was possible to solve the model exactly, due to the translational invariance; in biological molecules, we do not have this option.

4.3 The results on the Rate Constant.

In noisy systems, one has to work with the density matrix operator (not with the wave function) of the electrons, defined by

$$\rho_{m,n} = a_m^\dagger a_n \quad , \quad (4.3)$$

where m and n label different sites, and

$$i\hbar \frac{\partial}{\partial t} (\rho_{m,n}) = \sum_k (\rho_{k,m} V_{k,n} - \rho_{n,k} V_{m,k}) \quad , \quad (4.4)$$

where the amplitudes $V_{k,l}$ are defined by (4.2). Further analysis is based on Furutsu-Novikov theorem [43], which holds for the Gaussian noise (4.2) and a smooth functional

ρ :

$$\langle \rho_{m,k} [\delta V_{n,k}(t)] \delta V_{n,k}(t) \rangle = \int dt' \sum_{p,q} \langle \delta V_{n,k}(t) \delta V_{p,q}(t') \rangle \left\langle \frac{\delta \rho_{m,k}(t)}{\delta (\delta V_{p,q}(t'))} \right\rangle, \quad (4.5)$$

where $\langle \dots \rangle$ stands for the averaging over the Gaussian random process (4.2) and

$\frac{\delta}{\delta (\delta V_{p,q})}$ is a variation with respect to this process. The formula can be viewed as a

generalization of the partial integration formula to the case when ρ is a smooth functional

of a Gaussian-distributed functions $\delta V_{i,j}$. In order to average both sides of (4.4), we

have to calculate the functional derivative

$$\begin{aligned} \text{ih} \left\langle \frac{\delta \rho_{n,m}(t)}{\delta [\delta V_{p,q}(t)]} \right\rangle &= \sum_k \left\{ \rho_{k,m} \Delta_{k,n} (\delta_{k,p} \delta_{n,q} + \delta_{k,q} \delta_{n,p}) - \right. \\ &\quad \left. - \rho_{k,n} \Delta_{k,m} (\delta_{m,p} \delta_{k,q} + \delta_{m,q} \delta_{k,p}) \right\} \end{aligned}$$

where the symbol $\Delta_{i,j}$ is defined as

$$\Delta_{i,j} = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are connected} \\ 0, & \text{if not} \end{cases}$$

Using this expression and the formula (4.5), we average both sides of (4.4) and obtain the equation of motion for $\langle \rho_{n,m} \rangle$, which is the density matrix, averaged with respect to the noise (4.2):

$$\begin{aligned}
ih \frac{\partial}{\partial t} \langle \rho_{n,m} \rangle &= \sum_k \left(\langle \rho_{k,m} \rangle \langle V_{k,n} \rangle - \langle \rho_{n,k} \rangle \langle V_{m,k} \rangle \right) + \\
&+ \frac{4}{ih} \left\{ \langle \rho_{n,m} \rangle \sum_k \left(\frac{(a^2)_{n,k} \Delta_{n,k} + (a^2)_{m,k} \Delta_{m,k}}{2} \right) - \delta_{m,n} \sum_k \langle \rho_{k,k} \rangle (a^2)_{n,k} \Delta_{n,k} - \right. \\
&\left. -(a^2)_{m,n} \Delta_{m,n} \langle \rho_{n,m} \rangle \right\} \quad (4.6)
\end{aligned}$$

Note, that the r.h.s. of (4.6) consists of two parts: the “ballistic” part, related to the average quantities $\langle V_{i,j} \rangle$, and the diffusion part, related to the fluctuations of V .

According to (4.6), the off-diagonal density matrix elements $\langle \rho_{n,m} \rangle$ decay in time with the typical relaxation time

$$\tau_r \cong \left(\frac{\hbar^2}{4a^2} \right) \cong \frac{\hbar^2}{\langle \delta V^2 \rangle \tau_{\text{corr}}} \quad (4.7)$$

where τ_{corr} is the correlation time, defined by $a^2_{i,j} = \langle \delta V^2 \rangle_{i,j} \tau_{\text{corr}}$. In our model, the correlation time is assumed to be much smaller than any other characteristic time in the system, which enables one to take the limit when the correlation time tends to zero.

On the other hand, the diagonal matrix elements do not decay in time and the total probability is conserved. From the equation (4.6), it follows that the diagonal matrix elements of the density matrix obey the discrete analog of the Focker-Planck type equation with the “convective” term, dependent on the non-diagonal matrix elements of the density matrix. This term describes the ballistic (coherent) mode of the electron transfer [41]. In the long-time limit, the off-diagonal matrix elements decay and the ballistic terms disappear. Therefore, in the long-time limit, we have a pure diffusion for the diagonal matrix elements of the density matrix.

Let us estimate the relaxation time for the non-diagonal elements of the density matrix. We take $\tau_{\text{corr}} \sim 10^{-13} \div 10^{-14}$ s (for example, due to phonons). As it was obtained in [42], the approximation [4.2] is reasonable when the phonon band width is much smaller than the temperature. If we assume it to be ~ 10 K, then for the fluctuations of the hopping amplitudes we can roughly take ~ 1 K as an estimate. This gives us $\langle \delta V^2 \rangle \sim (10^{-4} \text{ eV})^2$. Then, we obtain from (4.7) $\tau_r \sim 10^{-7} - 10^{-8}$ s. For the effective diffusion coefficient, we have $D \sim d^2 / \tau_r \sim 10^7 - 10^8 \left(\frac{\text{\AA}}{\text{s}} \right)^2$. From the experimental data [41], it looks like D can be roughly estimated as $10^5 \div 10^6 \left(\frac{\text{\AA}}{\text{s}} \right)^2$. Therefore, we have a considerable (1-2 orders of magnitude) discrepancy. However, one should note that these values strongly depend on the specific geometry, and the results of [41] exhibit the same order of magnitude variations, for different molecules and different locations of the acceptor and donor. From the above stated arguments, it is clear that the diffusive regime of the single-electron transfer is valid if the molecule is sufficiently

long, so that the off-diagonal matrix elements of the density matrix become negligibly small. One can estimate the “cross-over” length from the “ballistic” to the diffusion regime as $L \sim \text{const} \sqrt{D\tau_r}$, where τ_r is the relaxation time, given by (4.7) and $\text{const} \cong 8$, as was shown in [42] for the case of the chain with translational invariance. This estimate gives us: $L \sim 5 \div 10 \text{ \AA}$, which is less than the typical range of the experiments [1,5]. Therefore, one should expect that the single-electron transfer has a diffusion, and not ballistic nature for these samples.

4.4 The transition from ballistic to diffusive transport regime.

Now, let us analyze the situation when the phase coherence is not broken and the correlations of hopping amplitudes do not depend on time. Then, we have a complicated system of overlapping between different sites. In the limiting case of many overlapping sites, one can expect the system to behave similarly to the electron in a random potential (random with respect to coordinate, as opposed to the temporal randomness in our basic model). The model of electron in a 1D spatially random white-noise potential can be solved [47,48] with the following result for the transmission probability:

$$\langle |T|^2 \rangle = \frac{4}{\sqrt{\pi}} e^{-z} \int_0^{\infty} \frac{dx x^2 \exp(-x^2)}{\text{ch}(\sqrt{z}\sqrt{x})} , \quad (4.8)$$

where

$$z = \frac{m_e L}{h^2} \frac{\sigma_v}{E} ; \quad \langle \delta V(x) \delta V(x') \rangle = 2\sigma_v \delta(x-x') , \quad (4.9)$$

E stands for the energy of the electron and L is the size of the system. For the low energies, which correspond to the long-time limit, we obtain from (4.8, 4.9):

$$\langle |T|^2 \rangle \cong \frac{1920}{\sqrt{\pi}} \frac{1}{z^3} e^{-z} = \frac{1920}{\sqrt{\pi}} \left(\frac{E}{E_0} \right)^3 \exp\left(-\frac{E_0}{E} \right) ; \quad E_0 = \frac{m_e L}{h^2} \sigma_v . \quad (4.10)$$

The asymptotic (4.10) is correct, if $t \gg h/E_0$. Comparing to (4.7) and taking the same values for the rest of the quantities as before, we obtain

$$t_0 / \tau_r \sim 10^2 / L \left(\overset{0}{\text{Å}} \right) \quad (4.11)$$

Therefore, for sufficiently short molecules, there is a region where the temporal disorder model is valid, but the spatial is not.

Let us compare these models in the region where both of them are valid. For the temporal profile of the reaction rate, limited by the electron transfer, we obtain from (4.10)

$$k(t) \cong \text{const} \frac{\sqrt{E_0}}{t^{7/2}} \exp(-\sqrt{2E_0} t) \quad (4.12)$$

In the temporal disorder model (4.6), the transfer rate exhibits the diffusion-type behavior in the long-time limit. In the time domain, we have:

$$k(t) \cong \text{const} \frac{1}{t^{d/2+1}} \exp\left(-\frac{L^2}{4 D t}\right) \cong \text{const} \frac{1}{t^{d/2+1}} \quad (4.13)$$

where d stands for the effective number of neighbors for the effective electron path and from the quasi-1D structures of molecules, $d \sim 1 - 2$.

So, for the “temporal” noise we obtain an asymptotics (4.13), while for the “static” noise we have (4.12).

4.5 Conclusions and future work.

In conclusion, one can expect to distinguish the type of disorder in the long molecules by analyzing the long-time “tails” of the reaction rate. As we mentioned before, it requires the size of the system and the observation times to be large enough, namely $L \geq 8\sqrt{D\tau} \sim 5-10 \text{ \AA}$, as it was mentioned before. One can expect that these conditions are satisfied for typical experiments on the single-electron transfer in biological molecules.

The next step is to apply the “temporal noise” model described above, to some realistic biological molecule in order to compare with existing results and experiments. The analysis presented here shows that one can expect significant deviations from “ballistic” picture for the long-range electron transfer.

II. 2D Vortices in thin superconducting films.

In the second part of the research, the collective effects of 2D magnetic vortex-vortex interactions in thin superconducting films, which cause a significant enhancement of the Nernst coefficient in such systems, have been studied.

Chapter 5. 2D magnetic vortices in thin superconductor films.

5.1 Introduction.

The vortex-vortex interaction for the magnetic vortices in the usual case of “thick” superconducting films, when the thickness of the film d is much larger than the London penetration length, $d \gg \lambda_L$ [49], is given by

$$U_{12}(|\mathbf{r}_1 - \mathbf{r}_2|) = \frac{1}{2\lambda_L^2} \left(\frac{\Phi_0}{2\pi} \right)^2 K_0 \left(\frac{|\mathbf{r}_1 - \mathbf{r}_2|}{\lambda_L} \right) ,$$

where \mathbf{r}_1 , \mathbf{r}_2 denote positions of vortices, Φ_0 stands for the elementary flux and $K_0(z)$ is the zero-order Bessel function of imaginary argument [49]. This vortex-vortex interaction is short-ranged and decays exponentially at a distance of the order of London penetration length [49]. The physical reason for this is that the electromagnetic field between the vortices is totally screened by the superconducting currents at the distance of the order of London penetration length.

On the other hand, in case when the vortices are restricted to the 2D plane, the vortex-vortex interaction becomes long-ranged, as opposed to the usual case of 3D magnetic vortices in the “thick” superconducting films [49,50]. This happens due to the fact that in thin superconducting films, the electromagnetic field can not be totally

screened by superconducting currents and therefore does not decay exponentially as a function of vortex-vortex separation. Due to this effect, the interaction between vortices may cause significant enhancement of galvano-magnetic effects in thin superconducting films, as opposed to thick films. In particular, the Nernst coefficient acquires a contribution, proportional to the second power of the external magnetic field. This contribution exceeds the linear single-vortex term for relatively small magnetic fields, and suggests a study of the effect of non-equilibrium vortex-antivortex pair production by some external currents, which may lead to the same order of magnitude for the transverse voltage, as one can expect for the Nernst effect in thin films. One can expect that this effect gives an explanation for unusually high values of the dc-voltage in recent experiments of A. Gerber and G. Deutcher [51] on ac-to-dc conversion in thin superconducting granular films subjected to both static magnetic field and ac external currents.

In normal metals, thermo-magnetic effects appear to be hardly observable [52]. Particularly, we are interested in the Nernst effect that accounts for appearance of a transverse electric field E_y in presence of both external magnetic field H_z and the temperature gradient $\nabla_x T$ as

$$E_y = N \nabla_x T, \quad (5.1)$$

where N is the Nernst coefficient [52]. In normal metal, the Nernst coefficient can be estimated as $N \approx (\Omega \tau) Q = (\Omega \tau) \frac{\pi^2}{3e} \frac{T}{E_F} \cong (\Omega \tau) 10^{-8} T$, where Q stands for the thermoelectric coefficient, τ stands for the mean free time, e is an elementary charge, Ω is a cyclotron frequency, E_F stands for the Fermi energy and T for the temperature in energy units [52]. This estimate gives us for $H \sim 10^3 - 10^4$ Gauss the electric field $E \sim 10^{-9} - 10^{-10}$ V/cm.

However, these effects are enhanced by about three orders of magnitude in superconducting (SC) phases of metals due to the motion of magnetic vortices [53,54]. In the SC phase, this effect occurs because the *excess* of magnetic vortices of one sign of vorticity (e.g. "+") move in the external temperature gradient with some drift velocity V_x and produce the electric current ([54])

$$E_y = \frac{1}{c} V_x \Phi_0 N_+ \quad (5.2)$$

Here, $N_+ = H_z / \Phi_0$ is the vortex concentration, Φ_0 - unit flux. The drift velocity is obtained from the equilibrium condition between the "thermodynamic" and "viscous" [53] forces, acting on the vortex line

$$S_1 \nabla T = \eta V_x ,$$

and we see that the vortex velocity is related to the entropy S_1 carried by one vortex [53] and the effective viscosity η [55] $\eta \approx \Phi_0 H_{c2}(0) \sigma_n / c^2$ where σ_n is a conductivity of normal metal. This leads to the expression for the Nernst coefficient as

$$N = \frac{S_1}{c\eta} H_z \quad , \quad (5.3)$$

which turns out to be a linear function of weak external magnetic field (in absence of vortex pinning). Theoretical estimates of S_1 [53]

$$S_1 = \frac{(\Phi_0)^2 T}{24 \lambda_L^2 \Delta_0^2} \quad ,$$

where $\Delta_0 = \frac{3.5}{2} T_C$ stands for the energy gap at $T=0$, give correct order of magnitude for electric field (5.1) as high as $10^{-6} \div 10^{-7}$ V/cm for $\nabla_x T \sim 1$ K/cm [56]. One should note that the estimate [53] was made for thick films, when the thickness d is much greater than the London penetration length λ_L .

The exact solution for S_1 for magnetic field close to the upper critical field H_{c2} was given by Caroli and Maki [57]. In this limit, $S_1 \sim (H_{c2} - H)$ which yields

$$N \sim H_{c2} - H \quad , \quad H \rightarrow H_{c2} \quad . \quad (5.4)$$

The solution [57] is applicable both to thick and thin films, when

$$d \leq \lambda_L. \quad (5.5)$$

Indeed, near H_{c2} the second-order phase transition takes place and the order parameter tends to zero as $\sqrt{H_{c2} - H}$ which makes the result [57] exact, since the effects of vortex interaction are negligible.

As we mentioned above, the pair vortex-vortex interaction is essentially short-ranged in thick SC films. However, as it was shown by Pearl, this interaction becomes long-ranged in case of thin films [49]. The force acting between the two vortices in the near-2D films (see condition (5.5)) is given as

$$F_{12} = \begin{cases} \frac{Q_{3D}^2}{r^2}, & r \gg \lambda_L \\ \frac{Q_{2D}^2}{r}, & r \leq \lambda_L \end{cases}; \quad \lambda_L \equiv \frac{\lambda_L^2}{d} \quad (5.6)$$

$$Q_{3D} \equiv \frac{\Phi_0}{2\pi}, \quad Q_{2D} \equiv \frac{\Phi_0}{2\pi\sqrt{2}\lambda_L}$$

The long-distance behavior of the interaction turns out to be precisely the 3D-Coulomb law with the effective charge Q_{3D} . This happens because in thin SC films the magnetic field is not totally screened by the SC currents (see in [49], p.60).

Usually, the properties of the 2D SC films are considered close to the SC transition temperature T_c , where the crossover parameter λ_{\perp} in (5.6) can be very large and even greater than the film largest dimension, R . In such case, the 2D Coulomb Gas Model (CGM, see in [50]), ignoring the 3D Coulomb "tails" and, therefore, considering the limit $\lambda_{\perp} \gg R$, is a very useful description of 2D vortex ensemble. As a consequence, the lower critical field H_{c1} for thin films happens to be several orders of magnitude smaller than for thick films [58]. In thin films, the vortex-antivortex pairs can be easily created either thermally, leading to Berezinskii-Kosterlitz-Thouless transition (see in [50]), or by applying electric current, causing peculiarities of the energy dissipation rate in the resistive state [59-61].

5.2 Formulation of the model.

The objective of the present research was to show that the galvano-magnetic effects in thin films are significantly enhanced in comparison with similar effects in thick films in a certain range of parameters, where the 2D CGM [50,58] is still valid and the crossover distance λ_{\perp} in (5.6) is not much larger than R , according to the 2D CGM. Considering the Nernst effect, we show that this enhancement comes from the long-range interaction between the vortices, given by (5.6). We also show that the dc-voltage across the film may occur even in the absence of any temperature gradients in case some steady gradient of non-equilibrium vortex-antivortex pair concentration is produced by some external current. The estimated values of dc-voltage across the sample appear to be comparable to the unusually high values of dc-voltage, observed by Gerber and Deutcher [31] in thin granular superconducting films subjected to both ac-current and external transverse magnetic field.

The idea is that, since the effective charges of "vortex Coulomb gas" and the crossover distance λ_{\perp} in Pearl's formula (5.6) depend on the average SC density n_s , [50], even a small gradient of n_s may strongly disturb the equilibrium of vortices, producing additional driving forces acting on the system. If this gradient is steady but non-equilibrium, these driving forces can result in a steady current of vortices, giving rise to the voltage (5.2).

5.3 The results on the Nernst coefficient.

To describe this effect, one should derive an expression for the total force acting on the ensemble of vortices in case when external sources produce a steady non-equilibrium distribution of normal component, resulting in the change $\Delta n_s = \tilde{n}_s - n_s$ of superconducting component density from the equilibrium value n_s to some nonequilibrium concentration \tilde{n}_s . We show, that even small gradients $\nabla(\Delta n_s)$ may cause significant forces, acting on the vortex ensemble. As a consequence, we have a large flow of vortices and some finite voltage across the sample. We show, that in a certain region of parameters, this voltage may exceed the usual (single-vortex) contribution. This effect is specific for the thin films, when (5.5) is satisfied.

The infinitesimal work of external sources, creating some deviation δn_s , can be represented as

$$\delta W = \int \xi \delta n_s dV, \quad (5.7)$$

where ξ has to be chosen so that the solution of the energy balance equation

$$\xi + \frac{\delta F(\tilde{n}_s)}{\delta \tilde{n}_s} = 0 \quad (5.8)$$

is satisfied for the steady-state solution \tilde{n}_s . In (5.8), F stands for the free energy of the superconductor which can be taken in Ginzburg-Landau form [49] as

$$F = \int d^2x \int_{-d/2}^{d/2} dz \left[\frac{\nabla^2 (\nabla \sqrt{n_s})^2}{4m} + \frac{\hbar^2}{4m} n_s \left(\nabla \Theta - \frac{2e}{\hbar c} \mathbf{A} \right)^2 + a n_s + \frac{b n_s^2}{2} \right] + \int d^2x \int_{-\infty}^{\infty} dz \frac{(\mathbf{B} - \mathbf{H})^2}{8\pi} , \quad (5.9)$$

where \mathbf{B} , \mathbf{H} are total and external magnetic fields, respectively, \mathbf{A} -vector potential and Θ is the phase of order parameter $\Psi = \sqrt{n_s} e^{i\Theta}$. Parameters a , b , m have the same meaning as in BCS theory [49]. In (5.9), the film is located in the (x, y) plane in the region $-d/2 \leq z \leq d/2$.

As follows from (5.7), the external force acting on the vortex ensemble is defined as $\mathbf{f} = \delta W / \delta \boldsymbol{\rho}$, or

$$\mathbf{f} = \int \xi \frac{\delta}{\delta \boldsymbol{\rho}} (\tilde{n}_s) dV , \quad (5.10)$$

where $\boldsymbol{\rho}$ is a center of mass coordinate for the vortex ensemble. If $\Delta n_s = \tilde{n}_s - n_s$ is small, then we can make an expansion in (5.8), which gives

$$\xi + \frac{\delta^2 F}{\delta n_s^2} \Delta n_s = 0 . \quad (5.11)$$

Substitution of eq. (5.11) into (5.10) yields

$$f = - \int \frac{\delta^2 F}{\delta n_s^2} \Delta n_s \frac{\delta}{\delta \rho} (\tilde{n}_s) dV \quad (5.12)$$

Since we are looking for linear response, we should substitute the non-perturbed solution $\tilde{n}_s \approx n_s$ into (5.12). A variation of (5.9) gives

$$b n_s + a + \frac{\nabla^2}{4m} \left(\nabla \Theta - \frac{2e}{hc} \mathbf{A} \right)^2 - \frac{\hbar^2}{4m} \frac{\nabla^2 \sqrt{n_s}}{\sqrt{n_s}} = 0 \quad (5.13)$$

for such a solution. The vortices are well defined if the correlation length ξ , determining the size of vortex core, obeys the condition

$$\xi^2 N_s \ll 1 \quad (5.14)$$

of low density of vortices. Therefore, the last term on the l.h.s. of (5.13) can be omitted, as being non-zero in the vicinity of cores only. It allows us to consider n_s as a smooth variable and to find $\delta^2 F / \delta n_s^2 = b$, which does not depend on center of mass coordinate ρ of the vortex ensemble. Taking into account that a also does not depend on ρ , we obtain

$$\frac{\delta}{\delta \rho} (n_s) = \left(-\frac{1}{b} \right) \frac{\delta}{\delta \rho} \left[\frac{\hbar^2}{4m} \left(\nabla \Theta - \frac{2e}{\hbar c} \mathbf{A} \right)^2 \right] \quad (5.15)$$

Substituting (5.15) into (5.12) and integrating by parts, we finally get

$$f = \int dV \nabla(\Delta n_s) \frac{\hbar^2}{4m} \left(\nabla \Theta - \frac{2e}{\hbar c} \mathbf{A} \right)^2 \quad (5.16)$$

where the fact that the phase and the vector potential depend on $(\mathbf{x} - \rho)$ as: $\Theta(\mathbf{x} - \rho)$, $\mathbf{A}(\mathbf{x} - \rho)$ was taken into account. Using the definition of electric current

$\mathbf{J} = -c \frac{\delta F}{\delta \mathbf{A}}$ and introducing the 2D current $\mathbf{I} \equiv \int_{-d/2}^{d/2} dz \mathbf{J}$ we can rewrite (5.16) as

$$f = \int d^2x \frac{2\pi}{c^2} \lambda_{\perp} \mathbf{I}^2 \frac{\nabla(\Delta n_s)}{n_s} \quad (5.17)$$

The distribution of currents $\mathbf{I}(\mathbf{x})$ can be taken as a sum of currents, produced by each vortex. Making use of the Pearl's solution, we obtain [49]:

$$\mathbf{I}(\mathbf{q}) = \sum_j \frac{c\Phi_0}{2\pi} \frac{\mathbf{i} \mathbf{q} \times \mathbf{n}}{q(1 + \lambda_{\perp} q)} e^{i \mathbf{q} \cdot \mathbf{x}_j} \quad (5.18)$$

where $\{x_j\}$ are coordinates of vortex cores, $n_j = (0,0,\pm 1)$ is a unit vector along z-axis, \pm stands according to the vorticity of j-th vortex. The vortex ensemble may be treated as the charged 2D Coulomb gas [50,58], where the screening is possible. However, as shown by S. Doniach and B. Huberman in [58], the net effective charge (read the net paramagnetic moment) in the presence of the external magnetic field remains unscreened at large distances. In our case, it means that the harmonic with $q \sim 1/R$ in (5.18), is not affected by screening (compare to [51]). Note that this harmonic gives the main contribution to (5.18). It allows us to omit the rest of harmonics in (5.18) and after substitution of (5.18) into (5.17), to obtain

$$\mathbf{f} = \frac{\nabla \Delta n_s}{n_s} \frac{\Phi_0^2 \lambda_{\perp} N_s^2}{2\pi} \frac{R^2}{\left(1 + \frac{\lambda_{\perp}}{R}\right)^2} \quad (5.19)$$

Now, we can estimate the drift velocity of the equilibrium ensemble of vortices by assuming that the motion is described in terms of viscous flow [55] with the total viscous force $\mathbf{f}_{\eta} = -\mathbf{V}_d \eta N_s R^2 d$, balancing the external force \mathbf{f} . Consequently, after substituting \mathbf{V}_d into (5.2), we obtain expression for the transverse electric field

$$E_y = N_1 \frac{\nabla_x (\tilde{n}_s - n_s)}{n_s}, \quad N_1 \equiv \frac{\Phi_0}{2\pi c \eta} \frac{\lambda_{\perp} H_z |H_z|}{\left(1 + \frac{\lambda_{\perp}}{R}\right)^2} d \quad (5.20)$$

Note that in the 3D case the corresponding term disappears as $\lambda_1^2 / R^2 \rightarrow 0$ due to the absence of long-range forces.

Strictly speaking, this relation is only valid far from the upper critical line $H_{c2}(T)$ in the phase diagram of superconductor. The line $H = H^*(T) < H_{c2}(T)$ may exist, such that for $H \geq H^*(T)$ our approximation, based on the 2D Qoulomb Gas Model (QGM), is no longer valid and the solution should smoothly transform into (5.4), according to [57]. We can estimate $H^*(T)$ by implementing the requirement that in the presence of external field H_z the solution for the average density n_s does not significantly change. This gives us

$$H^*(T) = \frac{H_c}{2} \left(1 + \frac{\lambda_1}{R} \right) \sqrt{\frac{d}{\lambda_1}} \sqrt{1 - \frac{T}{T_c}} , \quad (5.21)$$

where the relation [49] $a = -\frac{H_c^2}{4\pi n_s(0)} \left(1 - \frac{T}{T_c} \right)$ for the Ginzburg-Landau coefficient in terms of the critical field H_c and superconducting component density $n_s(0)$ at $T=0$ was employed.

The 2D CGM assumes the limit $\lambda_1 \gg R$, in which there is no limitation on H_z , since H^* in (5.21) is formally infinite. In realistic case, when T is not too close to T_c , this field can be considerably smaller than H_c . It implies that the superposition principle for currents is no longer valid for $H > H^*(T)$, as the superconducting density

n_s changes significantly. This means that the 2D CGM is not applicable to this case. However, we will only attempt to estimate the maximum value of the coefficient N_1 , supposedly achieved at $H \approx H^*(T)$. A substitution of (5.21) into (5.20) gives us

$$N_{\max} = \frac{\Phi_0}{c \eta} \frac{H_c^2}{4\pi} \left(1 - \frac{T}{T_c}\right) \quad (5.22)$$

In (5.20), we can express $\nabla(\tilde{n}_s - n_s)$ in terms of some temperature gradient, if there is any in the system. For $T \rightarrow 0$, one finds $\frac{\nabla(\tilde{n}_s - n_s)}{n_s} \sim -e^{-\Delta/T} \nabla T$ where Δ stands for the superconducting gap. After comparing with (5.1), it results in $N \sim e^{-\Delta/T} \rightarrow 0$. For T near (but not too close to) T_c we have $\frac{\nabla(\tilde{n}_s - n_s)}{n_s} \sim -\frac{\nabla T}{T_c}$ and consequently

$$N = \frac{N_1}{T_c} \quad (5.23)$$

for equation (5.1). Taking into account typical values

$H_c \sim 10^3 \div 10^4$ G, $\eta \sim 10^{-6} \div 10^{-7}$ e.g.u. one arrives at the estimate

$$E_y \leq (10^{-1} \div 10^{-4}) \frac{\nabla T}{T_c} \text{ (V/cm)} \quad (5.24)$$

Therefore, for temperature gradients as small as $0.1 T_c / \text{cm}$ the produced voltage may be of the order of mV/cm , exceeding the characteristic values of Nernst voltage in thick films [53,56] by several orders of magnitude.

5.4 Comparison to the 3D case.

It is interesting to compare the result (5.22) for the Nernst coefficient to that obtained for thick films [53]. Using the results [53] and (5.22), one obtains the estimate

$$\frac{E^{(2D)}}{E^{(3D)}} \cong \frac{H}{H_c} \frac{\lambda_L^2(T) \lambda_L(0)}{\xi(0) \left(d + \frac{\lambda_L^2(T)}{R} \right)^2} \quad (5.25)$$

where $E^{(2D)}$ and $E^{(3D)}$ stand for the value of the transverse electric field in thin and thick films, respectively. Let us take a case, when $\lambda_L^2 / d \ll R$ and $\lambda_L \cong 1000 \text{ \AA}$,

$\xi \approx d \cong 100 \text{ \AA}$. From (5.25), we get $\frac{E^{(2D)}}{E^{(3D)}} \sim \frac{H}{H_c} \times 10^3$. In this case, (5.21) implies

that $H^* \cong 0.1 H_c$. Thus, we have $E^{(2D)} / E^{(3D)} \sim 10^2$.

Analyzing (5.25), one arrives at the conclusion that for the fields as high as $H \geq H_{cr}$ where

$$H_{cr} = \frac{H_c^2}{H_{c2}} \left(1 + \frac{\lambda_{\perp}}{R}\right)^2 \frac{d}{\lambda_{\perp}} \quad (5.26)$$

the collective contribution to the Nernst voltage (5.21) exceeds the one-vortex term (5.25). Note that the crossover field H_{cr} turns out to be smaller than H^* (5.21). This means that in this region our calculations and the 2D Coulomb gas model are still valid. However, when λ_{\perp} become considerably large in comparison to the characteristic size of the system R , H_{cr} is of the same order as H_c implying that the interaction effects are insignificant in the very vicinity of T_c .

In case the nonequilibrium gradient in (5.20) exists due to a gradient ∇n_r in vortex-antivortex pair density, created by an external current, the estimate for E_y turns out to be as

$$E_y \leq -(10^{-1} \div 10^{-4}) \xi^2 \nabla n_r \quad (\text{V/cm}) \quad (5.27)$$

where it was assumed that for the high density of pairs the lower estimate for \tilde{n}_s should be $\tilde{n}_s \approx n_s(1 - \xi^2 n_r)$ (compare with [50,62]).

It is worth noting that the external inhomogeneous pair-breaking microwave radiation may produce the steady non-equilibrium gradient of the normal component in thin SC film. It should also produce the gradient of the SC density and, consequently, the driving forces acting on vortices. Then, (5.20) is still valid and the dc voltage is proportional to the square of the external magnetic field. In this case, the dc voltage does not contain the linear terms $\sim H_z$, as opposed to the Nernst effect.

5.5 Comparison to the experiment.

Now, let us consider the recent experiment [51] on the ac-to-dc conversion in thin superconducting granular films subjected to both static magnetic field and ac. external currents. The dc-voltage measured across the sample was dependent upon the external magnetic field H and amplitude of the applied ac-current. As mentioned by the authors in [51], the voltage of the order of tens of microvolts was observed at ac-frequencies as low as ~ 10 Hz ruling out an explanation in terms of the inverse Josephson effect. The results of [51] have several peculiar features:

- I) For small external magnetic fields, the dc-voltage has an odd component as a function of H_z .

- ii) When the direction of the sample is reversed, the induced voltage changes sign. The direction of sample was defined as a direction from the grounded side to the side subjected to external ac-current [51].
- iii) The effect has a threshold with respect to the ac-current amplitude and the typical values of the voltage vary from ~ 10 mV/cm to ~ 1 mV/cm .
- iy) The dc voltage has its maximum values for $H \approx H_c \approx 10^4$ G and $T \approx T_c$.

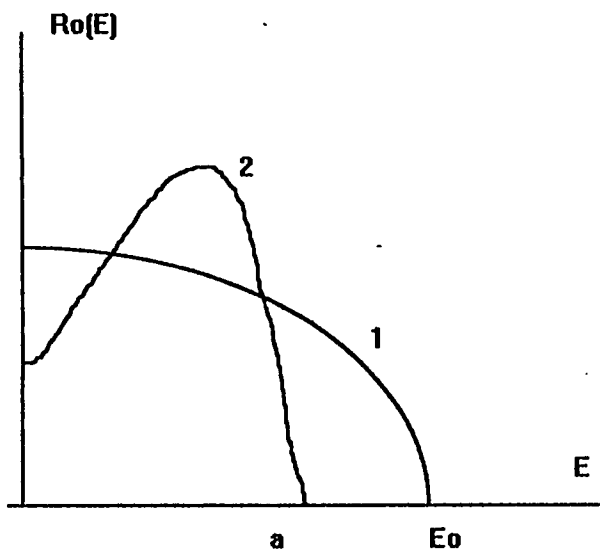
These features can be understood within the framework of the model presented above. Indeed, general symmetry and time-reverse considerations imply a presence of some steady current changing its sign after time reversal. This can be due either to the Nernst effect (enhanced, as it was shown above) in some uncontrollably small temperature gradient, or inhomogeneity of vortex pair creation by the external ac-current. Feature (ii) gives a hint of this possibility. The pair creation mechanism seems to be more realistic, because the simple analysis of data [51] shows that the dc-voltage increases almost linearly with the current amplitude above the threshold. This behavior resembles the regime considered before in [59,60], when the density of vortex pairs increases linearly with current. As was emphasized in [59,60], the conditions for pair creation in thin films are very sensitive to different parameters of the film, including the temperature. Therefore, a small temperature gradient can produce a pair concentration gradient which in its turn causes the unipolar vortex motion and creates dc-voltage.

Note that the typical size of a granule in [51] was of the order of $10^{-3} \div 10^{-4}$ cm with thickness of film being about 10^{-6} cm. In dirty superconductor, one should expect λ_L to increase up to $\sim 10^4 \text{ \AA}$ (see [49]). Going back to (5.21), we see that the range of applicability of the CGM expands to $H^* \cong H_c$. In this case, the crossover field H_{cr} , given by (5.26), is of the order $H_{cr} \cong H_c(\xi/\lambda_L) \ll H_c$. There is another interesting feature of the results [51], which can probably be prescribed to some vortex pinning inside a grain. The odd component of dc-voltage as a function of the external magnetic field has well-pronounced peaks. As it was mentioned by the authors [51], those peaks approximately corresponded to the penetration of one additional elementary flux into the grain. The reason for that might be a finite vortex pinning, which we did not take into account. One can expect that the penetration of one additional flux into the grain may change the balance between the collective forces considered above and pinning and cause a finite flow of vortices.

5.6 Open problems.

However, the more detailed interpretation of the results [31] requires some additional analysis, which should probably take into account some percolation properties of the samples. For example, here we only concentrated on the voltage component which was antisymmetric with respect to the external field. In [51], both symmetric and

antisymmetric components were observed. For that symmetric component, our simple considerations of a "steady flux" flow may be reconsidered. In fact, for the odd component we had for the local electric field $E \sim \mathbf{j}(\mathbf{H}) \times \mathbf{H}$ where $\mathbf{j}(\mathbf{H})$ stands for the gradient of some thermodynamical variable. This seems to be the only possibility to satisfy both the features (i) and (ii) due to the general considerations of T-invariance and feature (ii). However, for even component we may have $\mathbf{j} \sim \mathbf{H} \times \mathbf{D}$, where \mathbf{D} is some vector, characterizing asymmetry of the sample. This gives $E \sim \mathbf{D} (\mathbf{H})^2$. Another interesting feature is that this model predicts that the transverse dc-voltage is strongly affected by the external pair-breaking radiation, applied to the sample. This prediction can be checked in experiment. The more detailed analysis of these problems is suggested as the subject of further research.



1- The “semicircle” law (1.3).

2- The qualitative sketch for (2.44).

Figure 2.1

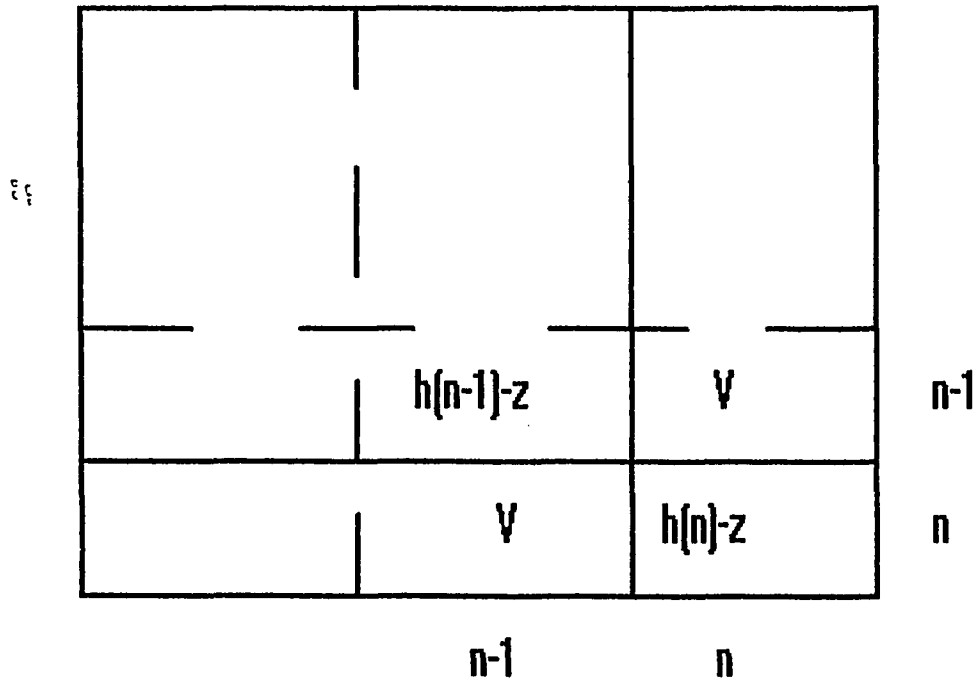


Figure 3.1

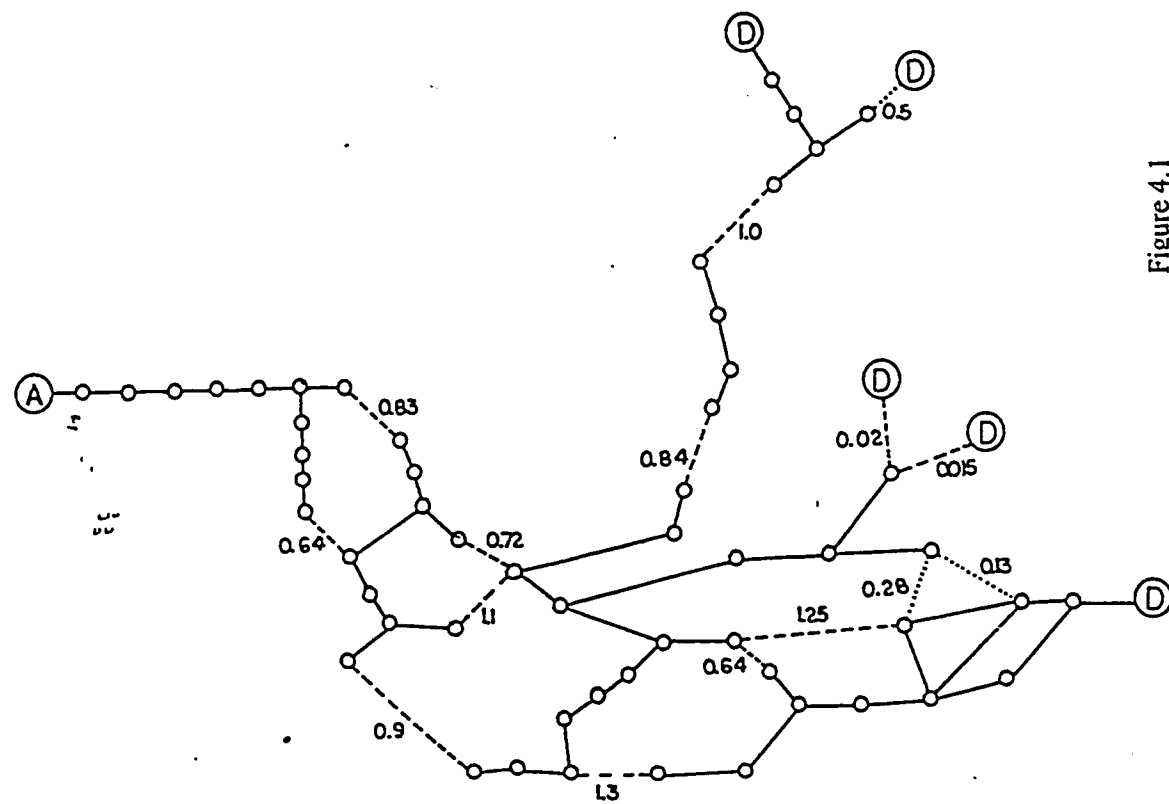


FIG. 5. His81: relevant structure.

Figure 4.1

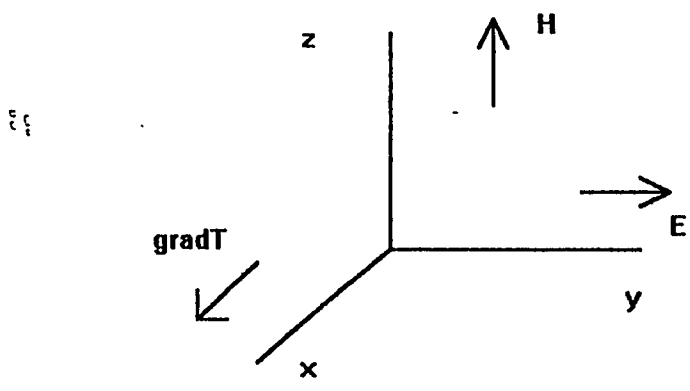


Figure 5.1

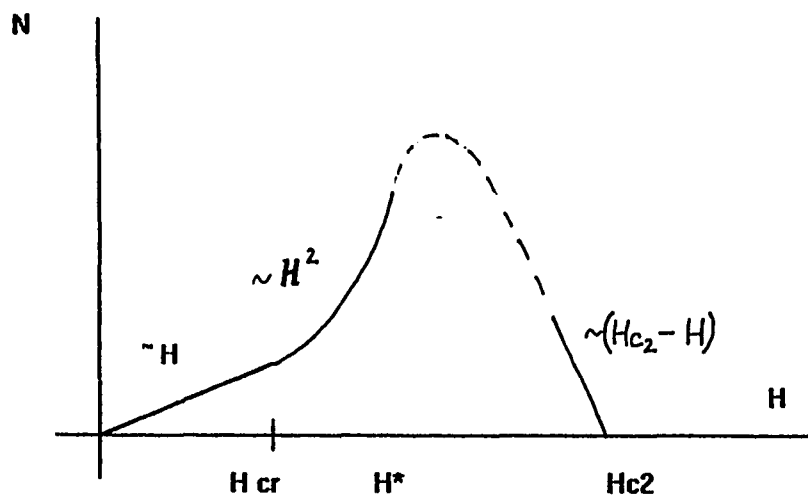


Figure 5.2

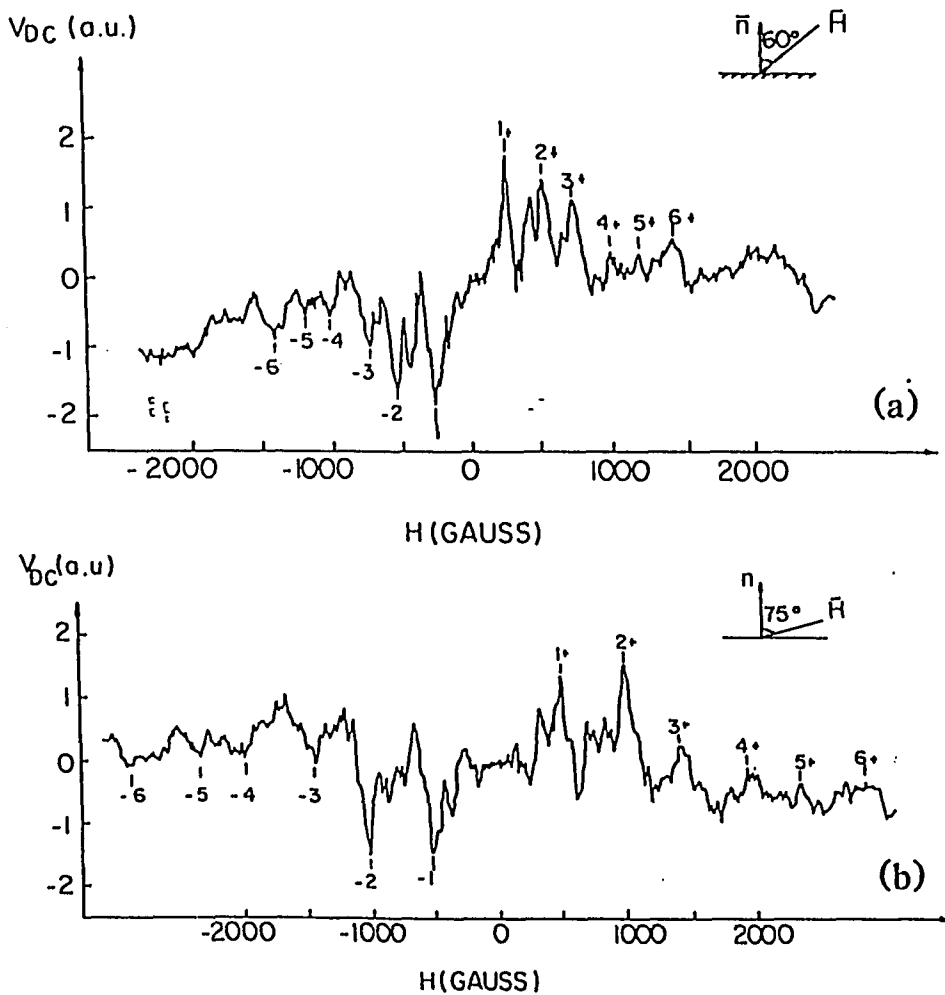


FIG. 3. Typical voltage pattern as a function of an external dc magnetic field measured in a Pb sample close to the percolation threshold, with a residual resistivity in the superconducting state of some percent of its normal value ($1.6 \text{ k}\Omega/\text{sq}$). The magnetic field is applied at an angle of (a) 60° from the normal to the sample's surface and (b) 75° . The marked peaks were arbitrarily determined as the most pronounced characteristic features of the pattern, having their "twins" in the reversed field. The pattern width is inversely proportional to the cosine of the angle between the applied field and the normal to the sample's surface. $T=4.2 \text{ K}$. ac current frequency is 100 kHz ; amplitude is 5 mA . Figure 5.3

III References

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Supplement: publications

The generalized Random Matrix Model

A. Bulatov, D. Schmeltzer and Joseph L. Birman, Phys. Rev. B52, 13792 (1995).

The Nernst effect in Thin SC films

**Anatoly Kuklov, Alexei Bulatov and Joseph L. Birman, Phys. Rev. Lett. v72 p.2274
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