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Eigenvalue fluctuations for lattice Anderson Hamiltonians

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ABSTRACT. We consider the random Schrödinger operator $-\varepsilon^{-2}\Delta^{(d)} + \xi^{(\varepsilon)}(x)$, with $\Delta^{(d)}$ the discrete Laplacian on \mathbb{Z}^d and $\xi^{(\varepsilon)}(x)$ are bounded and independent random variables, on sets of the form $D_\varepsilon := \{x \in \mathbb{Z}^d : x\varepsilon \in D\}$ for D bounded, open and with a smooth boundary, and study the statistics of the Dirichlet eigenvalues in the limit $\varepsilon \downarrow 0$. Assuming $\mathbb{E}\xi^{(\varepsilon)}(x) = U(x\varepsilon)$ holds for some bounded and continuous function $U : D \rightarrow \mathbb{R}$, the k -th eigenvalue converges to the k -th Dirichlet eigenvalue of the homogenized operator $-\Delta + U(x)$, where Δ is the continuum Laplacian on D . Moreover, assuming that $\text{Var}(\xi^{(\varepsilon)}(x)) = V(x\varepsilon)$ for some positive and continuous $V : D \rightarrow \mathbb{R}$, we establish a multivariate central limit theorem for simple eigenvalues centered by their expectation and scaled by $\varepsilon^{-d/2}$. The limiting covariance is expressed as integral of V against the product of squares of two eigenfunctions of $-\Delta + U(x)$.

1. INTRODUCTION AND RESULTS

Random Schrödinger operators naturally arise in theories of disordered materials in solid state physics. Among the most well-studied examples is the Anderson Hamiltonian obtained by adding a random on-site potential to a homogenous kinetic term. From the perspective of conductivity theory, a question of prime interest for such operators concerns the existence of localized states, i.e., effects where the lattice structure remains relevant at all scales. On the other hand, in homogenization theory, one is more focused on the situations where lattice effects become integrated into “material constants” and a continuum limit is possible.

In the present paper we study the statistics of the eigenvalues of Anderson Hamiltonians in the “homogenization” regime, i.e., under the conditions when a non-trivial continuum limit can be taken. We will address the convergence to a continuum limit as well as the fluctuation of the eigenvalues around their mean. Our setting is as follows: Let D be a bounded open subset of \mathbb{R}^d whose boundary is $C^{1,\alpha}$ for some $\alpha > 0$. Given an $\varepsilon > 0$, we define its discretized version as

$$(1.1) \quad D_\varepsilon := \{x \in \mathbb{Z}^d : \text{dist}_\infty(x\varepsilon, D^c) > \varepsilon\}$$

where $\text{dist}_\infty(x, y)$ is the ℓ^∞ -distance in \mathbb{R}^d . For any numbers $\{\xi^{(\varepsilon)}(x) : x \in D_\varepsilon\}$, define an operator (a matrix) $H_{D_\varepsilon, \xi}$ acting on the linear space of functions $f : D_\varepsilon \rightarrow \mathbb{R}$ that vanish outside D_ε via

$$(1.2) \quad (H_{D_\varepsilon, \xi} f)(x) := -\varepsilon^{-2}(\Delta^{(d)} f)(x) + \xi^{(\varepsilon)}(x)f(x),$$

where $\Delta^{(d)}$ is the standard lattice Laplacian

$$(1.3) \quad (\Delta^{(d)} f)(x) := \sum_{y: |y-x|=1} [f(y) - f(x)].$$

We will take the potential $\xi^{(\varepsilon)}$ random subject to the following requirements:

Assumption 1.1 *There are numbers $a, b \in \mathbb{R}$ with $a < b$ and bounded continuous functions $U : D \rightarrow \mathbb{R}$ and $V : D \rightarrow [0, \infty)$ such that for each $\varepsilon > 0$, the following holds:*

(1) *the random variables $\xi^{(\varepsilon)}(x)$, $x \in D_\varepsilon$, are independent with*

$$(1.4) \quad \text{supp } \xi^{(\varepsilon)}(x) \subset [a, b], \quad x \in D_\varepsilon,$$

(2) *for any $x \in D_\varepsilon$,*

$$(1.5) \quad \mathbb{E}\xi^{(\varepsilon)}(x) = U(x\varepsilon) \quad \text{and} \quad \text{Var}(\xi^{(\varepsilon)}(x)) = V(x\varepsilon).$$

We will write \mathbb{P}_ε to denote the law of $\xi^{(\varepsilon)}$ but will not mark the ε -dependence explicitly on expectation. To ease our notations, we will also often omit marking the ε -dependence of ξ .

Our task is to relate the spectrum of $H_{D_\varepsilon, \xi}$ to that of a suitable (homogenized) continuum operator. In the leading order, this is the content of:

Theorem 1.2 *Let $\lambda_{D_\varepsilon, \xi}^{(k)}$ denote the k -th smallest eigenvalue of $H_{D_\varepsilon, \xi}$. Under Assumption 1.1, for each $k \geq 1$,*

$$(1.6) \quad \lambda_{D_\varepsilon, \xi}^{(k)} \xrightarrow[\varepsilon \downarrow 0]{\mathbb{P}} \lambda_D^{(k)},$$

where $\lambda_D^{(k)}$ is the k -th smallest eigenvalue of the operator $-\Delta + U(x)$ on $H_0^1(D)$, with Δ denoting the continuum Laplacian.

Here, as usual, $H_0^1(D)$ denotes the closure of the set of infinitely often differentiable and compactly supported functions in D with respect to the norm $\|f\|_{H^1(D)} := (\|f\|_{L^2(D)}^2 + \|\nabla f\|_{L^2(D)}^2)^{1/2}$. Thanks to our conditions on D and U , the spectrum of $-\Delta + U(x)$ is discrete with no eigenvalue more than finitely degenerate. Moreover, any orthonormal basis of eigenfunctions $\varphi_D^{(k)}$ consists of functions that are continuously differentiable on \bar{D} . See Lemma 3.1 for details.

The formula (1.6) gives the leading-order deterministic behavior of the spectrum of $H_{D_\varepsilon, \xi}$. Naturally, one is interested in the subleading terms or even a full asymptotic expansion in powers of ε . Here we take up only the modest goal of analyzing the leading order *random* term; i.e., the fluctuations of the eigenvalues around their mean. First we state a concentration estimate:

Theorem 1.3 *Under Assumption 1.1, for each $k \geq 1$, there is $c > 0$ such that for all $t > 0$ and all $\varepsilon \in (0, 1)$,*

$$(1.7) \quad \mathbb{P}_\varepsilon \left(\left| \lambda_{D_\varepsilon, \xi}^{(k)} - \mathbb{E} \lambda_{D_\varepsilon, \xi}^{(k)} \right| > t \right) \leq 4e^{-ct^2\varepsilon^{-d}}.$$

Note that, by (1.7), for every $k \geq 1$, the random variable

$$(1.8) \quad \frac{\lambda_{D_\varepsilon, \xi}^{(k)} - \mathbb{E} \lambda_{D_\varepsilon, \xi}^{(k)}}{\varepsilon^{d/2}}$$

has Gaussian tails. Our main result is then the derivation of a Gaussian asymptotic limit law. We will do this jointly for the collection of all simple eigenvalues:

Theorem 1.4 *Suppose Assumption 1.1 holds, fix $n \in \mathbb{N}$ and let $k_1, \dots, k_n \in \mathbb{N}$ be distinct indices such that the Dirichlet eigenvalues $\lambda_D^{(k_1)}, \dots, \lambda_D^{(k_n)}$ of $-\Delta + U(x)$ on D are simple. Then, in the limit as $\varepsilon \downarrow 0$, the law of the random vector*

$$(1.9) \quad \left(\frac{\lambda_{D_\varepsilon, \xi}^{(k_1)} - \mathbb{E} \lambda_{D_\varepsilon, \xi}^{(k_1)}}{\varepsilon^{d/2}}, \dots, \frac{\lambda_{D_\varepsilon, \xi}^{(k_n)} - \mathbb{E} \lambda_{D_\varepsilon, \xi}^{(k_n)}}{\varepsilon^{d/2}} \right)$$

tends weakly to a multivariate normal with mean zero and covariance matrix $\sigma_D^2 = \{\sigma_{ij}^2\}_{i,j=1}^n$ given by

$$(1.10) \quad \sigma_{ij}^2 := \int_D |\varphi_D^{(k_i)}(x)|^2 |\varphi_D^{(k_j)}(x)|^2 V(x) dx,$$

where $\varphi_D^{(i)}$ denotes the i -th normalized eigenfunction of $-\Delta + U(x)$ and $V(x)$ is the function from (1.5) characterizing the variances of $\xi^{(\varepsilon)}(x)$.

>From the perspective of the theory of random Schrödinger operators it is interesting to ponder about where the principal contribution to the fluctuations of the eigenvalues comes from. Our method of

proof indicates this quite clearly. Let $g_{D_\varepsilon, \xi}^{(k)}$ henceforth denote any eigenfunction of $H_{D_\varepsilon, \xi}$ for the eigenvalue $\lambda_{D_\varepsilon, \xi}^{(k)}$ normalized so that

$$(1.11) \quad \sum_{x \in D_\varepsilon} |g_{D_\varepsilon, \xi}^{(k)}(x)|^2 = 1.$$

Let $C_\varepsilon^{(k)}$ denote the event that $\lambda_{D_\varepsilon, \xi}^{(k)}$ is non-degenerate and note that, by (1.6), $\mathbb{P}_\varepsilon(C_\varepsilon^{(k)}) \rightarrow 1$ as $\varepsilon \downarrow 0$ for any k such that the Dirichlet eigenvalue $\lambda_D^{(k)}$ of $-\Delta + U(x)$ is non-degenerate, i.e., simple. On $C_\varepsilon^{(k)}$, write

$$(1.12) \quad T_{D_\varepsilon, \xi}^{(k)} := \sum_{x \in \mathbb{Z}^d} \varepsilon^{-2} |\nabla^{(d)} g_{D_\varepsilon, \xi}^{(k)}(x)|^2,$$

to denote the *kinetic energy* associated with the k -th eigenspace of $H_{D_\varepsilon, \xi}$, where $\nabla^{(d)} f(x)$ is the vector whose i -th component is $f(x + \hat{e}_i) - f(x)$, for \hat{e}_i denoting the i -th unit vector in \mathbb{R}^d . We regard $g_{D_\varepsilon, \xi}^{(k)}$ as extended by zero to all of \mathbb{Z}^d . We then have:

Theorem 1.5 *Suppose Assumption 1.1 holds and that $\lambda_D^{(k)}$ is simple. Then,*

$$(1.13) \quad \varepsilon^{-d} \text{Var}(T_{D_\varepsilon, \xi}^{(k)} | C_\varepsilon^{(k)}) \xrightarrow{\varepsilon \downarrow 0} 0$$

and

$$(1.14) \quad \varepsilon^{-d} \sum_{x \in D_\varepsilon} \text{Var}(g_{D_\varepsilon, \xi}^{(k)}(x)^2 | C_\varepsilon^{(k)}) \xrightarrow{\varepsilon \downarrow 0} 0.$$

The punchline of these observations is that the main fluctuation of

$$(1.15) \quad \lambda_{D_\varepsilon, \xi}^{(k)} = T_{D_\varepsilon, \xi}^{(k)} + \sum_{x \in D_\varepsilon} \xi(x) g_{D_\varepsilon, \xi}^{(k)}(x)^2$$

comes from the *potential energy* part. Based on (1.13), the exact form of the covariance is easy to explain as well: just replace $g_{D_\varepsilon, \xi}^{(k)}(x)$ by the eigenfunction $\phi_D^{(k)}$ of the limiting operator $-\Delta + U$ and note that the potential energy thus becomes a weighted sum of i.i.d. random variables, for which the central limit theorem with covariance (1.10) is well-known.

It turns out that an *a priori* knowledge of (1.13–1.14) is nearly enough to justify the central limit theorem in Theorem 1.4. Indeed, let $\mathbb{E}^{(k)}$ denote the conditional expectation given $C_\varepsilon^{(k)}$ and let us, for ease of notation, drop the subindices on $\lambda_{D_\varepsilon, \xi}^{(k)}$, $T_{D_\varepsilon, \xi}^{(k)}$ and $g_{D_\varepsilon, \xi}^{(k)}$. On $C_\varepsilon^{(k)}$ we have

$$(1.16) \quad \lambda^{(k)} - \mathbb{E}^{(k)} \lambda^{(k)} = T^{(k)} - \mathbb{E}^{(k)} T^{(k)} + \sum_{x \in D_\varepsilon} \left(\xi(x) g^{(k)}(x)^2 - \mathbb{E}^{(k)} (\xi(x) g^{(k)}(x)^2) \right).$$

The sum on the right can be recast as

$$(1.17) \quad \sum_{x \in D_\varepsilon} [\xi(x) - \mathbb{E}^{(k)} \xi(x)] \mathbb{E}^{(k)} (g^{(k)}(x)^2) + \sum_{x \in D_\varepsilon} \xi(x) [g^{(k)}(x)^2 - \mathbb{E}^{(k)} (g^{(k)}(x)^2)] \\ + \sum_{x \in D_\varepsilon} \mathbb{E}^{(k)} \left((\xi(x) - \mathbb{E}^{(k)} \xi(x)) (g^{(k)}(x)^2 - \mathbb{E}^{(k)} (g^{(k)}(x)^2)) \right).$$

A routine use of the Cauchy-Schwarz inequality shows that the second moment of the latter two sums is dominated by (powers of) the sum in (1.14). Using also (1.13) we get

$$(1.18) \quad \lambda^{(k)} - \mathbb{E}^{(k)} \lambda^{(k)} = o(\varepsilon^{d/2}) + \sum_{x \in D_\varepsilon} [\xi(x) - \mathbb{E}^{(k)} \xi(x)] \mathbb{E}^{(k)} (g^{(k)}(x)^2),$$

where $o(\varepsilon^{d/2})$ represents a random variable whose variance is $o(\varepsilon^d)$. Under the assumption that the k -th eigenvalue of $-\Delta + U(x)$ is non-degenerate, the complement of $C_\varepsilon^{(k)}$ can be covered by events

from (1.7) for indices $k - 1$, k and $k + 1$. This permits us to replace the conditional expectations of $\lambda^{(k)}$ and $\xi(x)$ by unconditional ones. To get the multivariate CLT stated in Theorem 1.4, it then suffices to show

$$(1.19) \quad \varepsilon^{-d} \mathbb{E}^{(k)} \left(g^{(k)}(\lfloor \cdot / \varepsilon \rfloor)^2 \right) \xrightarrow{\varepsilon \downarrow 0} \left| \varphi_D^{(k)}(\cdot) \right|^2$$

in $L^2(D, dx)$, for any k of interest. As we will see, our proof of Theorems 1.4 and 1.5 is indeed strongly based on controlling the convergence of the discrete eigenfunctions to the continuous ones in proper L^p -norms.

2. CONNECTIONS, REMARKS AND OUTLINE

Before we delve into the proofs, let us make some connections to the existing literature. These have insofar been suppressed in order to keep the presentation focused. We then make a few remarks and give an outline of the rest of this work.

2.1 Crushed-ice problem.

Our interest in fluctuations of Dirichlet eigenvalues arose from the contemplation of the so called *crushed ice* problem. This is a problem in the continuum where one considers a bounded open set $D \subset \mathbb{R}^d$ with m balls $B(x_1, \varepsilon), \dots, B(x_m, \varepsilon)$ of radii ε removed from its interior. The positions x_1, \dots, x_m of the centers of these balls are drawn independently from a common distribution $\rho(x)dx$ on D . The principal question is how the eigenvalues of the Laplacian in

$$(2.1) \quad D_\varepsilon := D \setminus (B(x_1, \varepsilon) \cup \dots \cup B(x_m, \varepsilon))$$

behave in the limit as $\varepsilon \downarrow 0$ and $m = m(\varepsilon) \rightarrow \infty$. (The most natural boundary conditions are Neumann on ∂D and Dirichlet on $\partial B(x_i, \varepsilon)$ but all mixtures of these can be considered.)

Since its introduction by Kac in 1974, much effort went into analyzing the crushed ice problem in various regimes of dependence of m on ε . The main references include Kac [16], Huruslov and Marchenko [14], Rauch and Taylor [22]; see also the monographs by Simon [24] and Sznitman [25]. More recently, extensions to non-homogeneous kinetic terms have also been considered, e.g., by Douanla [9] and Ben-Ari [5]. The most interesting limit is obtained when

$$(2.2) \quad m(\varepsilon) \text{Cap}(B(0, \varepsilon)) \xrightarrow{\varepsilon \downarrow 0} \mu \in (0, \infty),$$

where $\text{Cap}(A)$ denotes the Newtonian capacity of A when $d \geq 3$ and the capacity corresponding to $-\Delta + 1$ when $d = 2$. The k -th Dirichlet eigenvalue of $-\Delta$ in D_ε then tends to that of the operator $-\Delta + \mu\rho(x)$ on D .

The problem of fluctuations was in this context taken up by Figari, Orlandi and Teta [10] and later by Ozawa [21]. Both of these studies infer a (single-variate) Central Limit Theorem assuming simplicity of the limiting eigenvalue but they are confined to the case of $d = 3$. Unfortunately, the proofs are very functional-analytic and (at least as claimed by Ozawa) they do not readily generalize to other dimensions. Ozawa himself calls for a probabilistic version of his result.

We believe that our approach to eigenvalue fluctuations is exactly the kind called for by Ozawa. In particular, we expect that several key steps underlying our proof of Theorem 1.4 extend to the crushed-ice problem in all dimensions. Notwithstanding, as the situation of independent and bounded potentials on a lattice is considerably simpler, we decided to start with that case first. Moreover, lattice Anderson Hamiltonians are well studied objects and so results for them are of interest in their own right. (See Subsection 2.3 for some more comments.)

2.2 Random elliptic operators.

In homogenization theory, the leading order of the eigenvalues of various random elliptic operators, whether in divergence form or not, has been studied quite thoroughly; see the book of Jikov, Kozlov and Oleinik [15]. An example of such operator (in divergence form) is the (scaled) random Laplacian,

$$(2.3) \quad \mathbf{L}^{(\varepsilon)} f(x) := \frac{1}{2} \varepsilon^{-2} \sum_{x,y: |x-y|=1} c_{xy} [f(y) - f(x)]$$

where the c_{xy} 's are non-negative random variables. Let $\lambda_{D_\varepsilon}^{(k)}$ denote the k -th eigenvalue of $\mathbf{L}^{(\varepsilon)}$ on the linear space of functions that vanish outside the set D_ε defined in (1.1). Under the assumption that (c_{xy}) is ergodic with respect to spatial shift and uniformly elliptic in the sense that

$$(2.4) \quad \exists a, b \in (0, \infty), a < b: \quad c_{xy} \in [a, b] \quad \text{almost surely,}$$

the eigenvalue $\lambda_{D_\varepsilon}^{(k)}$ converges (in probability) to the k -th smallest eigenvalue of an elliptic operator

$$(2.5) \quad \mathbf{Q}f(x) := \sum_{i,j=1}^d q_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j}(x)$$

with Dirichlet boundary conditions on ∂D , where $\mathbf{q} := (q_{ij})$ is a positive definite, symmetric matrix independent of x . While, to our knowledge, the corresponding fluctuations of the eigenvalues have not been studied, the analysis of a related effective conductance problem (Nolen [20], Rossignol [23], Biskup, Salvi and Wolff [7]) indicates that $\varepsilon^{-d/2} [\lambda_{D_\varepsilon}^{(k)} - \mathbb{E} \lambda_{D_\varepsilon}^{(k)}]$ should be asymptotically normal with mean zero and variance that is a biquadratic expression in $\nabla \varphi_D^{(k)}$ integrated over D , where $\varphi_D^{(k)}$ denotes a k -th eigenfunction of the operator \mathbf{Q} .

2.3 Anderson localization.

Our discussion of the background would not be complete without making at least some connection to the problem of Anderson localization. We focus only on spectral statistics.

When the Laplacian term in $H_{D_\varepsilon, \xi}$ is not magnified by the factor ε^{-2} , the random field $\xi^{(\varepsilon)}$ is dominant and the low-lying part of the spectrum comes from eigenfunctions that are localized at small regions independent of ε . In this case, the statistics of the spectrum in D_ε is expected to be governed by a Poisson point process. This has so far been proved in the ‘‘bulk’’ of the spectrum (Molchanov [19] in $d = 1$ and Minami [18] for general $d \geq 1$). At spectral edges there seem to be only partial results for bounded potentials at this time (Germinet and Klopp [11, 12]) although a somewhat more complete theory has been developed for some unbounded potentials (Astrauskas [1, 2], Biskup and König [6]).

In the delocalization regime, whose existence is yet to be proved, the statistics is expected to be that seen in random matrix ensembles.

2.4 Remarks.

Our first remark concerns the restriction of Theorem 1.4 to simple eigenvalues. It is clear that some restriction is needed whenever the means of two eigenvalues fall within $o(\varepsilon^{d/2})$ of each other. Although, by Theorem 1.3, the fluctuations of individual eigenvalues perhaps remain CLT-like, under degeneracy they *decide* the order and hence no Gaussian limit is possible. The precise ordering also depends on their expectations and so further control of subleading terms in (1.6) would be required in order to make a meaningful conclusion in the end. (Of course, some formulation may be possible — e.g., in terms of the Green operator or spectral density — but our present proofs would not apply anyway.)

As our second remark we note that an important input into the proof of Theorem 1.4 is a good approximation of discrete eigenvalues by continuous ones in L^p -norm on D . The reader may then find it perplexing to find that changes in the value of $\xi(x)$ have negligible effect on the discrete eigenfunction at x . (In particular, no “corrector” needs to be invoked to compensate for rapid oscillations of the ξ -term.) This can be proved by invoking rank-one perturbation and (1.6); see Proposition 5.2 and Lemma 5.3. For a heuristic explanation, we define $\Psi^{(k)}$ by the equation

$$(2.6) \quad \varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}(x) = \varphi_D^{(k)}(x\varepsilon) + \varepsilon^2 \Psi^{(k)}(x).$$

Invoking the eigenvalue equations, we then have

$$(2.7) \quad \begin{aligned} \Delta^{(d)} \Psi^{(k)}(x) &= \varepsilon^{-2-d/2} \Delta^{(d)} g_{D_\varepsilon, \xi}^{(k)}(x) - \varepsilon^{-2} \Delta^{(d)} \varphi_D^{(k)}(\cdot \varepsilon)(x) \\ &\approx (\lambda_{D_\varepsilon, \xi}^{(k)} - \xi(x)) \varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}(x) - (\lambda_D^{(k)} - U(x\varepsilon)) \varphi_D^{(k)}(x\varepsilon), \end{aligned}$$

where we approximated the discrete Laplacian by its continuous counterpart. Assuming that $\varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}(x)$ is in fact pointwise close to $\varphi_D^{(k)}(x\varepsilon)$, we get

$$(2.8) \quad -\Delta^{(d)} \Psi^{(k)}(x) = (\xi(x) - U(x\varepsilon) + o(1)) \varphi_D^{(k)}(x\varepsilon),$$

i.e., $\Psi^{(k)}$ solves a corrector-like Poisson equation. In particular, since the Dirichlet Laplacian on D_ε is invertible, $\Psi^{(k)}$ can in principle be computed and studied.

2.5 Outline.

The remainder of this paper is organized as follows: In the next section we establish Theorem 1.2 along with some useful regularity estimates on discrete and continuous eigenfunctions. In Section 4 we prove Theorem 1.3 dealing with concentration of the law of discrete eigenvalues. Then, in Section 5, we proceed to prove our main result (Theorem 1.4). Theorem 1.5 is then derived readily as well.

3. CONVERGENCE TO CONTINUUM MODEL

We are now in a position to start the expositions of the proofs. Our first task will be to prove Theorem 1.2 dealing with the leading-order convergence of the random eigenvalues to those of the continuum problem. Let us begin by fixing some notation.

3.1 Notations.

We will henceforth assume that D is a bounded open set in \mathbb{R}^d with $C^{1,\alpha}$ -boundary for some $\alpha > 0$ and that Assumption 1.1 holds. We write

$$(3.1) \quad \Omega_{a,b} := [a, b]^{\mathbb{Z}^d},$$

for a set that supports \mathbb{P}_ε for every $\varepsilon > 0$. Recalling the notation $g_{D_\varepsilon, \xi}^{(k)}$ for the k -th eigenvector of $H_{D_\varepsilon, \xi}$ normalized as in (1.11), we similarly write $\varphi_D^{(k)}$ for an eigenfunction of $-\Delta + U(x)$ corresponding to $\lambda_D^{(k)}$ normalized so that $\int_D |\varphi_D^{(k)}(x)|^2 dx = 1$. These eigenfunctions are unique up to a sign as soon as the corresponding eigenvalue is non-degenerate.

We will write $\|f\|_p$ for the canonical ℓ^p -norm of \mathbb{R} - or \mathbb{R}^d -valued functions f on \mathbb{Z}^d . When $p = 2$, we use $\langle f, h \rangle$ to denote the associated inner product in $\ell^2(\mathbb{Z}^d)$. All functions defined *a priori* only on D_ε will be regarded as extended by zero to $\mathbb{Z}^d \setminus D_\varepsilon$. In order to control convergence to the continuum

problem, it will sometimes be convenient to work with the scaled ℓ^p -norm,

$$(3.2) \quad \|f\|_{\varepsilon,p} := \left(\varepsilon^d \sum_{x \in \mathbb{Z}^d} |f(x)|^p \right)^{1/p}.$$

This implies, e.g., that

$$(3.3) \quad \|\varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}\|_{\varepsilon,2} = 1.$$

We will sometimes use $\langle f, g \rangle_{\varepsilon,2}$ to denote the inner product associated with $\|\cdot\|_{\varepsilon,2}$. For functions f, g of a continuum variable, we write the norms as $\|f\|_{L^p(\mathbb{R}^d)}$ and the inner product in $L^2(\mathbb{R}^d)$ as $\langle f, g \rangle_{L^2(\mathbb{R}^d)}$.

3.2 Regularity bounds.

Our starting point are some regularity estimates on both the continuum and discrete eigenvalues and eigenfunctions. Note that, in our earlier convention, $\lambda_{D_\varepsilon,0}^{(k)}$ corresponds to the k -th eigenvalue of $-\varepsilon^{-2}\Delta^{(d)}$ with Dirichlet boundary conditions on D_ε^c . Recall that $C^{1,\alpha}(A)$ denotes the set of functions that are continuously differentiable on the interior of A with a uniform estimate on α -Hölder norm of the gradient.

Lemma 3.1 *For all $k \geq 1$*

$$(3.4) \quad \sup_{0 < \varepsilon < 1} \sup_{\xi \in \Omega_{a,b}} |\lambda_{D_\varepsilon, \xi}^{(k)} - \lambda_{D_\varepsilon, 0}^{(k)}| \leq \max\{|b|, |a|\}.$$

Similarly, both $-\Delta$ and $-\Delta + U(x)$ have compact resolvent on $H_0^1(D)$ and their spectrum thus consists of isolated, finitely degenerate eigenvalues. Moreover, if $\lambda_{D,0}^{(k)}$ denotes the k -th eigenvalue of $-\Delta$ on $H_0^1(D)$, then

$$(3.5) \quad |\lambda_D^{(k)} - \lambda_{D,0}^{(k)}| \leq \|U\|_\infty.$$

In addition, any eigenfunction $\varphi_D^{(k)}$ of $-\Delta + U(x)$ obeys

$$(3.6) \quad \varphi_D^{(k)} \in C^{1,\alpha}(\bar{D}).$$

Proof. The estimates (3.4–3.5) are consequences of the Minimax Theorem. The regularity of the eigenfunction follows from the regularity of the boundary of D via, e.g., Corollary 8.36 of Gilbarg and Trudinger [13]. \square

The following estimate will be quite convenient for the derivations in the rest of the paper:

Lemma 3.2 *For $k \geq 1$, there is a constant $c = c(k, a, b, D)$, such that*

$$(3.7) \quad \sup_{\xi \in \Omega_{a,b}} \|g_{D_\varepsilon, \xi}^{(k)}\|_\infty \leq c \varepsilon^{d/2}.$$

Proof. Let g be an eigenfunction of $H_{D_\varepsilon, \xi}$ for an eigenvalue λ normalized so that $\|g\|_2 = 1$. The key observation is that the inner product $\langle \delta_x, e^{t\Delta^{(d)}} \delta_y \rangle$, with $\Delta^{(d)}$ taken with respect to the Dirichlet boundary condition, coincides with the transition probability $p_t(x, y)$ of a continuous-time (constant-speed) simple random walk on \mathbb{Z}^d killed upon exit from D_ε . The eigenvalue equation and the Feynman-Kac

formula imply

$$(3.8) \quad \begin{aligned} g(x) &= e^{\lambda t} \left(e^{t\varepsilon^{-2}(\Delta^{(d)} - \varepsilon^2 \xi)} g \right)(x) \\ &= e^{\lambda t} E^x \left(\exp \left\{ \int_0^{\varepsilon^{-2}t} \varepsilon^2 \xi(X_s) ds \right\} g(X_{t\varepsilon^{-2}}) \right), \end{aligned}$$

where the expectation is over random walks (X_s) started at x . Taking absolute values, bounding $|\xi(x_i)|$ by $\|\xi\|_\infty$ and writing the result using the semigroup, we get

$$(3.9) \quad |g(x)| \leq e^{(\lambda + \|\xi\|_\infty)t} \sum_{y \in D_\varepsilon} p_{\varepsilon^{-2}t}(x, y) |g(y)|.$$

Applying the Cauchy-Schwarz inequality and using that g is normalized yields

$$(3.10) \quad g(x)^2 \leq e^{2(\lambda + \|\xi\|_\infty)t} \sum_{y \in D_\varepsilon} p_{\varepsilon^{-2}t}(x, y)^2 \leq e^{2(\lambda + \|\xi\|_\infty)t} p_{2\varepsilon^{-2}t}(x, x),$$

where the second inequality follows by the fact that p_t is reversible with respect to the counting measure. But $p_t(x, x)$ is non-decreasing in D_ε and so it is bounded by the corresponding quantity on \mathbb{Z}^d . The local central limit theorem (or other methods to control heat kernels) then yield $p_t(x, x) \leq Ct^{-d/2}$ for all $t \geq 1$. Setting $t := 1$ in (3.10), the claim follows. \square

Note that Lemma 3.2 and the fact that $|D_\varepsilon| = O(\varepsilon^{-d})$ imply

$$(3.11) \quad \sup_{p \in [1, \infty]} \sup_{0 < \varepsilon < 1} \sup_{\xi \in \Omega_{a,b}} \|\varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}\|_{\varepsilon, p} < \infty$$

for all $k \geq 1$.

3.3 Continuum interpolation.

Having dispensed with regularity issues, we now proceed to develop tools that will help us approximate discrete eigenfunctions by continuous ones. The piece-wise constant approximation is a natural first candidate: For any function $f: \mathbb{Z}^d \rightarrow \mathbb{R}$, set

$$(3.12) \quad \bar{f}(x) := \varepsilon^{-d/2} f(\lfloor x/\varepsilon \rfloor), \quad x \in \mathbb{R}^d.$$

The scaling ensures that, automatically, $\langle f, h \rangle = \langle \bar{f}, \bar{h} \rangle_{L^2(\mathbb{R}^d)}$. Unfortunately, our need to control the kinetic energy makes this approximation less attractive in detailed estimates. Instead, we will use an approximation by piece-wise linear interpolations over lattice cells. The following lemma can be extracted from the proof of Lemma 2.1 in Becker and König [4]:

Lemma 3.3 *There is a constant $C = C(d)$ for which the following holds: For any function $f: \mathbb{Z}^d \rightarrow \mathbb{R}$ and any $\varepsilon \in (0, 1)$, there is a function $\tilde{f}: \mathbb{R}^d \rightarrow \mathbb{R}$ such that*

- 1 *the map $f \mapsto \tilde{f}$ is linear,*
- 2 *\tilde{f} is continuous on \mathbb{R}^d and $\tilde{f}(x\varepsilon) = f(x)$ for all $x \in \mathbb{Z}^d$,*
- 3 *for any $x \in \mathbb{Z}^d$ and any $y \in \varepsilon x + [0, \varepsilon]^d$ we have*

$$(3.13) \quad |\tilde{f}(y)| \leq \max_{z \in x + \{0,1\}^d} |f(z)|,$$

and

$$(3.14) \quad |\tilde{f}(y) - f(x)| \leq d \max_{z \in x + \{0,1\}^d} |\nabla^{(d)} f(z)|,$$

4 for all $p \in [1, \infty]$ we have

$$(3.15) \quad \|\tilde{f}\|_{L^p(\mathbb{R}^d)} \leq C(d)\|f\|_{\varepsilon,p},$$

and

$$(3.16) \quad \left| \|\tilde{f}\|_{L^2(\mathbb{R}^d)} - \|f\|_{\varepsilon,2} \right| \leq C(d)\|\nabla^{(d)}f\|_{\varepsilon,2},$$

5 \tilde{f} is piece-wise linear and thus a.e. differentiable with

$$(3.17) \quad \|\nabla\tilde{f}\|_{L^2(\mathbb{R}^d)} = \varepsilon^{-1}\|\nabla^{(d)}f\|_{\varepsilon,2}.$$

Proof. Although most of these are already contained in the proof of [4, Lemma 2.1], we provide an independent proof as the desired statements are hard to glean from the notations used there. A key point is that for any $y = (y_1, \dots, y_d) \in [0, 1]^d$ there is a permutation σ of $\{1, \dots, d\}$ such that $y_{\sigma(1)} \geq \dots \geq y_{\sigma(d)}$. Moreover, when all components of y are distinct, such a σ is unique.

Given $y \in x\varepsilon + [0, \varepsilon]^d$ let thus σ be a permutation that puts the components of $y - x\varepsilon$ in non-increasing ordering. Writing the reordered components of $y/\varepsilon - x$ as $1 \geq \alpha_1 \geq \dots \geq \alpha_d \geq 0$, we have

$$(3.18) \quad y = x\varepsilon + \varepsilon \sum_{i=1}^d \alpha_i \hat{e}_{\sigma(i)}.$$

We then define

$$(3.19) \quad \tilde{f}(y) := f(x) + \sum_{i=1}^d \alpha_i (\nabla_{\sigma(i)}^{(d)} f)(x + \hat{e}_{\sigma(1)} + \dots + \hat{e}_{\sigma(i-1)}),$$

where, we recall, $(\nabla_i^{(d)} f)(x) := f(x + \hat{e}_i) - f(x)$.

Our first task is to check that \tilde{f} is well defined. Obviously, the α_j 's are determined by y so we only have to check that the definition does not depend on σ , if there is more than one for the same y . That happens only when $\alpha_i = \alpha_{i+1}$ for some $i = 0, \dots, d-1$ (where $\alpha_0 := 1$ by convention). Then (3.18) holds also for σ replaced by permutation σ' which agrees with σ except at indices $i, i+1$ where $\sigma'(i) := \sigma(i+1)$ and $\sigma'(i+1) := \sigma(i)$. Abbreviating $z := x + \hat{e}_{\sigma(1)} + \dots + \hat{e}_{\sigma(i-1)}$, the two possible expressions for $\tilde{f}(y)$ will agree if and only if

$$(3.20) \quad (\nabla_{\sigma(i)} f)(z) + (\nabla_{\sigma(i+1)} f)(z + \hat{e}_{\sigma(i)}) = (\nabla_{\sigma(i+1)} f)(z) + (\nabla_{\sigma(i)} f)(z + \hat{e}_{\sigma(i+1)}) \dots$$

As is readily verified, both of these are equal to $f(z + \hat{e}_{\sigma(i)} + \hat{e}_{\sigma(i+1)}) - f(z)$. Hence, \tilde{f} is consistent. The map $f \mapsto \tilde{f}$ is obviously linear, thus proving (1).

We now move to checking continuity of \tilde{f} . First note that (3.19) extends to all points in the closed "cube" $\mathcal{C}(x) := x\varepsilon + [0, \varepsilon]^d$. In light of uniform continuity of \tilde{f} on the open "cube," the extension is continuous, and thus independent of σ (if more than one σ corresponds to the same boundary point). Now pick $y \in \mathcal{C}(x) \cap \mathcal{C}(x + \hat{e}_i)$. As $f(x) + \nabla_i^{(d)} f(x) = f(x + \hat{e}_i)$, taking (3.19) on $\mathcal{C}(x)$ with $\sigma(1) := i$ and $\alpha_1 := 1$ has the same value as (3.19) on $\mathcal{C}(x + \hat{e}_i)$ with $\sigma(d) := i$ and $\alpha_d := 0$. Hence, the expressions for \tilde{f} on $\mathcal{C}(x)$ and $\mathcal{C}(x + \hat{e}_i)$ agree on the common "side" $\mathcal{C}(x) \cap \mathcal{C}(x + \hat{e}_i)$ and \tilde{f} is thus continuous on \mathbb{R}^d . Conclusion (2) is readily checked.

It remains to prove the stated bounds. For that we first note that (3.19) can be recast as

$$(3.21) \quad \tilde{f}(y) = \sum_{i=0}^d (\alpha_i - \alpha_{i+1}) f(x + \hat{e}_{\sigma(1)} + \dots + \hat{e}_{\sigma(i)})$$

where $\alpha_0 := 1$. Using that $\alpha_i - \alpha_{i+1}$ are non-negative and sum up to one, we get (3.13). This immediately yields (3.15). Similarly, (3.19) and the fact that $|\alpha_i| \leq 1$ directly show (3.14). To get (3.16) from this, abbreviate $h(y) := \tilde{f}(y) - f(\lfloor y/\varepsilon \rfloor)$. Squaring (3.14), bounding the maximum (of squares) by a sum and integrating over $y \in \mathbb{R}^d$ yields

$$(3.22) \quad \|h\|_{L^2(\mathbb{R}^d)} \leq C(d) \|\nabla^{(d)} f\|_{\varepsilon,2}.$$

But the L^2 -norm of $y \mapsto f(\lfloor y/\varepsilon \rfloor)$ is $\|f\|_{\varepsilon,2}$ and so we get (3.16) by the triangle inequality.

Concerning (3.17), define $W_\sigma := \bigcup_{x \in \mathbb{Z}^d} \{\varepsilon x + z : z \in [0, \varepsilon)^d, z_{\sigma(1)} > \dots > z_{\sigma(d)}\}$ and note that \tilde{f} is piece-wise linear on W_σ with

$$(3.23) \quad \nabla_{\sigma(i)} \tilde{f}(y) = \varepsilon^{-1} (\nabla_{\sigma(i)}^{(d)} f)(\lfloor y/\varepsilon \rfloor + \hat{e}_{\sigma(1)} + \dots + \hat{e}_{\sigma(i-1)}), \quad y \in W_\sigma.$$

This implies

$$(3.24) \quad \int_{W_\sigma} |\nabla f(y)|^2 dy = \varepsilon^{-2} \sum_{i=1}^d \sum_{x \in \mathbb{Z}^d} |(\nabla_{\sigma(i)}^{(d)} f)(x)|^2 \int \mathbf{1}_{\{1 \geq \alpha_1 > \dots > \alpha_d \geq 0\}} d\alpha_1 \dots d\alpha_d.$$

The integral on the right equals $(d!)^{-1}$ so we get (3.17) by summing over all admissible σ and using that W_σ 's cover \mathbb{R}^d up to a set of zero Lebesgue measure. \square

Our next item of concern is an approximation of functions on the lattice by piecewise constant modifications. For each $L \geq 1$ and any $f: \mathbb{Z}^d \rightarrow \mathbb{R}$, denote

$$(3.25) \quad f_L(x) := f(L \lfloor x/L \rfloor).$$

Then we have:

Lemma 3.4 *There exists a constant $C(d) < \infty$ such that, for any $L \geq 1$ and any $f: \mathbb{Z}^d \rightarrow \mathbb{R}$,*

$$(3.26) \quad \|f - f_L\|_1 < C(d)L \|\nabla^{(d)} f\|_1.$$

Proof. Consider the box $B_k := x_0 + \{0, \dots, k-1\}^d$. The triangle inequality shows

$$(3.27) \quad \sum_{x \in B_k \setminus B_{k-1}} |f(x) - f(x_0)| \leq \sum_{x \in B_{k-1} \setminus B_{k-2}} \left(|f(x) - f(x_0)| + \sum_{z \in \{0,1\}^d} \sum_{i=1}^d |(\nabla_i^{(d)} f)(x+z)| \right).$$

This implies

$$(3.28) \quad \sum_{x \in B_L} |f(x) - f(x_0)| \leq 2^d \sqrt{d} L \sum_{x \in B_L} |(\nabla^{(d)} f)(x)|.$$

The claim follows by summing over $x_0 \in (L\mathbb{Z})^d$. \square

3.4 Convergence of eigenfunctions/eigenvalues.

Having dispensed with regularity issues, we now proceed to tackle convergence statements. We will employ a standard trick: Instead of individual eigenvalues, we will work with their sums

$$(3.29) \quad \Lambda_k^\varepsilon(\xi) := \sum_{i=1}^k \lambda_{\mathcal{D}_\varepsilon, \xi}^{(i)} \quad \text{and} \quad \Lambda_k := \sum_{i=1}^k \lambda_{\mathcal{D}}^{(i)}.$$

These quantities are better suited for dealing with degeneracy because they are concave in ξ and, in fact, admit a variational characterization (sometimes dubbed the Ky Fan Maximum Principle [17]) of

the form

$$(3.30) \quad \Lambda_k^\varepsilon(\xi) = \inf_{\substack{h_1, \dots, h_k \\ \text{ONS}}} \sum_{i=1}^k (\varepsilon^{-2} \|\nabla^{(d)} h_i\|_2^2 + \langle \xi, h_i^2 \rangle)$$

and

$$(3.31) \quad \Lambda_k = \inf_{\substack{\psi_1, \dots, \psi_k \\ \text{ONS}}} \sum_{i=1}^k (\|\nabla \psi_i\|_{L^2(\mathbb{R}^d)}^2 + \langle U, \psi_i^2 \rangle_{L^2(\mathbb{R}^d)}).$$

Here the acronym ‘‘ONS’’ indicates that the k -tuple of functions form an orthonormal system in the subspace corresponding to Dirichlet boundary conditions (and, in the latter case, also tacitly assumes that the functions are in the domain of the gradient). Substituting actual eigenfunctions shows that the sums of eigenvalues are no smaller than the infima but the complementary bound requires a bit of work. The argument actually yields a quantitative form of the Ky Fan Maximum Principle which will be quite suitable for our later needs:

Lemma 3.5 *Consider a separable Hilbert space \mathcal{H} and a self-adjoint linear operator \hat{H} on \mathcal{H} which is bounded from below and has compact resolvent. Let $\{\varphi_i : i \geq 1\}$ be an orthonormal basis of eigenfunctions of \hat{H} corresponding to eigenvalues λ_i that we assume obey $\lambda_{i+1} \geq \lambda_i$ for all $i \geq 1$. Let $\hat{\Pi}_k$ denote the orthogonal projection onto $\{\varphi_1, \dots, \varphi_k\}^\perp$. Then for any ONS ψ_1, \dots, ψ_k that lies in the domain of \hat{H} ,*

$$(3.32) \quad \sum_{i=1}^k \langle \psi_i, \hat{H} \psi_i \rangle - (\lambda_1 + \dots + \lambda_k) \geq (\lambda_{k+1} - \lambda_k) \sum_{i=1}^k \|\hat{\Pi}_k \psi_i\|^2.$$

Proof. We provide a proof as it is very short. The argument parallels the derivation of Lemma 3.2 in Barekat [3]. Since ψ_1, \dots, ψ_k is an ONS and \mathcal{H} is separable, we may extend it into an orthonormal (countable) basis $\{\psi_i : i \geq 1\}$. Denoting $a_{ij} := \langle \psi_i, \varphi_j \rangle$, the Parseval identity yields

$$(3.33) \quad b_j := \sum_{i=1}^k |a_{ij}|^2 \leq \sum_{i \geq 1} |a_{ij}|^2 = \langle \varphi_j, \varphi_j \rangle = 1.$$

Since $\sum_{j \geq 1} b_j = k$, we have $\sum_{j > k} b_j = \sum_{j=1}^k (1 - b_j)$ and it thus follows that

$$(3.34) \quad \begin{aligned} \sum_{i=1}^k \langle \psi_i, \hat{H} \psi_i \rangle &= \sum_{i=1}^k \sum_{j \geq 1} \lambda_j |a_{ij}|^2 = \sum_{j \geq 1} b_j \lambda_j \\ &\geq \sum_{j=1}^k \lambda_j b_j + \lambda_{k+1} \sum_{j > k} b_j \\ &= \lambda_1 + \dots + \lambda_k + \sum_{j=1}^k (\lambda_{k+1} - \lambda_j) (1 - b_j) \\ &\geq \lambda_1 + \dots + \lambda_k + (\lambda_{k+1} - \lambda_k) \sum_{j=1}^k (1 - b_j). \end{aligned}$$

Writing the last sum as $\sum_{j > k} b_j$ we easily see that it equals $\sum_{i=1}^k \|\hat{\Pi}_k \psi_i\|^2$. \square

Our next goal, formulated in Propositions 3.6 and 3.7 below, is to establish convergence $\Lambda_k^\varepsilon(\xi) \rightarrow \Lambda_k$ in probability. Throughout we assume the setting in Assumption 1.1.

Proposition 3.6 For any $\delta > 0$,

$$(3.35) \quad \lim_{\varepsilon \downarrow 0} \mathbb{P}_\varepsilon(\Lambda_k^\varepsilon(\xi) \geq \Lambda_k + \delta) = 0.$$

Proof. Consider (a choice of) an ONS of the first k eigenfunctions $\varphi_D^{(1)}, \dots, \varphi_D^{(k)}$ of $-\Delta + U$. By Lemma 3.1 all of these are $C^{1,\alpha}$. Now define

$$(3.36) \quad f_i(x) := \begin{cases} \varphi_D^{(i)}(x\varepsilon), & \text{if } x \in D_\varepsilon, \\ 0, & \text{otherwise.} \end{cases}$$

Thanks to uniform continuity of the eigenfunctions, we then have

$$(3.37) \quad \langle f_i, f_j \rangle_{\varepsilon,2} \xrightarrow{\varepsilon \downarrow 0} \langle \varphi_D^{(i)}, \varphi_D^{(j)} \rangle_{L^2(D)} = \delta_{ij}$$

and so for ε small the functions f_1, \dots, f_k are nearly mutually orthogonal. Applying the Gram-Schmidt orthogonalization procedure, we see that there are functions $\{h_i^\varepsilon\}_{i=1}^k$ and coefficients $\{a_{ij}(\varepsilon)\}_{1 \leq i, j \leq k}$ such that

$$(3.38) \quad h_i^\varepsilon = \sum_{j=1}^k (\delta_{ij} + a_{ij}(\varepsilon)) f_j, \quad i = 1, \dots, k,$$

with

$$(3.39) \quad \langle h_i^\varepsilon, h_j^\varepsilon \rangle_{\varepsilon,2} = \delta_{ij} \quad \text{and} \quad \max_{i,j} |a_{ij}(\varepsilon)| \xrightarrow{\varepsilon \downarrow 0} 0.$$

Moreover, the definition of f_i and the $C^{1,\alpha}$ -regularity of the eigenfunctions imply

$$(3.40) \quad \sup_{\substack{y \in D \\ \text{dist}_\infty(y, D^c) > 2\varepsilon}} \left| \nabla \varphi_D^{(i)}(y) - \varepsilon^{-1} (\nabla^{(d)} f_i)(\lfloor y/\varepsilon \rfloor) \right| \xrightarrow{\varepsilon \downarrow 0} 0$$

and same continues to hold for h_i^ε instead of f_i as well. Hereby we get

$$(3.41) \quad \varepsilon^{-1} \|\nabla^{(d)} h_i^\varepsilon\|_{\varepsilon,2} \xrightarrow{\varepsilon \downarrow 0} \|\nabla \varphi_D^{(i)}\|_{L^2(\mathbb{R}^d)}$$

and, by continuity of U , also

$$(3.42) \quad \langle U(\varepsilon \cdot), (h_i^\varepsilon)^2 \rangle_{\varepsilon,2} \xrightarrow{\varepsilon \downarrow 0} \langle U, \varphi_D^{(i)} \rangle_{L^2(\mathbb{R}^d)}.$$

Once the two sides in each of these limit statements (for all $i = 1, \dots, k$) are within some $\delta \in (0, 1)$ of each other, the variational characterization (3.30) yields

$$(3.43) \quad \Lambda_k^\varepsilon(\xi) \leq \Lambda_k + 2k\delta + \sum_{i=1}^k \langle \xi - U(\varepsilon \cdot), (h_i^\varepsilon)^2 \rangle_{\varepsilon,2}.$$

Invoking a union bound we obtain

$$(3.44) \quad \mathbb{P}_\varepsilon(\Lambda_k^\varepsilon(\xi) \geq \Lambda_k + 3k\delta) \leq \sum_{i=1}^k \mathbb{P}_\varepsilon\left(\langle \xi - U(\varepsilon \cdot), (h_i^\varepsilon)^2 \rangle_{\varepsilon,2} \geq \delta\right).$$

The Chebyshev inequality now shows

$$(3.45) \quad \mathbb{P}_\varepsilon\left(\langle \xi - U(\varepsilon \cdot), (h_i^\varepsilon)^2 \rangle_{\varepsilon,2} \geq \delta\right) \leq \frac{C}{\delta^2} \sum_{x \in D_\varepsilon} \varepsilon^{2d} h_i^\varepsilon(x)^4,$$

where C is a uniform bound on $\text{Var}(\xi(x))$. But the h_i^ε 's are bounded and since $\|h_i^\varepsilon\|_{\varepsilon,2} = 1$, the right-hand side is proportional to ε^d . As δ was arbitrary, the claim follows. \square

Proposition 3.7 For any $\delta > 0$,

$$(3.46) \quad \lim_{\varepsilon \downarrow 0} \mathbb{P}_\varepsilon(\Lambda_k^\varepsilon(\xi) \leq \Lambda_k - \delta) = 0.$$

Proof. Let $g_{D_\varepsilon, \xi}^{(1)}, \dots, g_{D_\varepsilon, \xi}^{(k)}$ be (a choice of) an ONS of the first k eigenfunctions of $H_{D_\varepsilon, \xi}$ and let $\tilde{g}_{1, \xi}^\varepsilon, \dots, \tilde{g}_{k, \xi}^\varepsilon$ denote the continuum interpolations of $\varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(1)}, \dots, \varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}$, respectively, as described in Lemma 3.3. The uniform bound (3.4) on the eigenvalues ensures

$$(3.47) \quad \sup_{\xi \in \Omega_{a,b}} \sup_{0 < \varepsilon < 1} \varepsilon^{-1} \|\nabla^{(d)} g_{D_\varepsilon, \xi}^{(i)}\|_2 < \infty$$

and so, in light of Lemma 3.3(4),

$$(3.48) \quad \sup_{\xi \in \Omega_{a,b}} \left| \langle \tilde{g}_{i, \xi}^\varepsilon, \tilde{g}_{j, \xi}^\varepsilon \rangle_{L^2(\mathbb{R}^d)} - \delta_{ij} \right| \xrightarrow{\varepsilon \downarrow 0} 0.$$

Invoking again the Gram-Schmidt orthogonalization, we can thus find functions $\tilde{h}_{1, \xi}^\varepsilon, \dots, \tilde{h}_{k, \xi}^\varepsilon$ and coefficients $a_{ij}(\xi, \varepsilon)$ such that

$$(3.49) \quad \tilde{h}_{i, \xi}^\varepsilon = \sum_{j=1}^k (\delta_{ij} + a_{ij}(\xi, \varepsilon)) \tilde{g}_{j, \xi}^\varepsilon, \quad i = 1, \dots, k,$$

for which

$$(3.50) \quad \langle \tilde{h}_{i, \xi}^\varepsilon, \tilde{h}_{j, \xi}^\varepsilon \rangle_{L^2(\mathbb{R}^d)} = \delta_{ij} \quad \text{and} \quad \max_{ij} \sup_{\xi \in \Omega_{a,b}} |a_{ij}(\xi, \varepsilon)| \xrightarrow{\varepsilon \downarrow 0} 0.$$

Thanks to the definition of D_ε , both the $\tilde{g}_{i, \xi}^\varepsilon$'s and $\tilde{h}_{i, \xi}^\varepsilon$'s are supported in D .

Lemma 3.3(5), (3.47) and (3.49–3.50) guarantee

$$(3.51) \quad \sup_{\xi \in \Omega_{a,b}} \left| \|\nabla \tilde{h}_{i, \xi}^\varepsilon\|_{L^2(\mathbb{R}^d)}^2 - \varepsilon^{-2} \|\nabla^{(d)} g_{D_\varepsilon, \xi}^{(i)}\|_2^2 \right| \xrightarrow{\varepsilon \downarrow 0} 0$$

while (3.14) ensures

$$(3.52) \quad \sup_{\xi \in \Omega_{a,b}} \left| \langle U, (\tilde{h}_{i, \xi}^\varepsilon)^2 \rangle_{L^2(\mathbb{R}^d)} - \langle U(\varepsilon \cdot), (g_{D_\varepsilon, \xi}^{(i)})^2 \rangle \right| \xrightarrow{\varepsilon \downarrow 0} 0.$$

Once both suprema on the left are less than some $\delta > 0$, using the $\tilde{h}_{i, \xi}^\varepsilon$ as the ψ_i 's in (3.31) and noting that the $g_{D_\varepsilon, \xi}^{(i)}$'s achieve the infimum in (3.30), yields

$$(3.53) \quad \Lambda_k \leq \Lambda_k^\varepsilon(\xi) + 2k\delta + \sum_{i=1}^k \langle U(\varepsilon \cdot) - \xi, (g_{D_\varepsilon, \xi}^{(i)})^2 \rangle.$$

Now consider the piece-wise constant approximation $f_L(x) = f(L[x/L])$ to the function $f(x) := (g_{D_\varepsilon, \xi}^{(i)}(x))^2$. Since $\|\nabla^{(d)}(g^2)\|_1 \leq C(d) \|g\|_2 \|\nabla^{(d)} g\|_2$, Lemma 3.4, (3.47) and the boundedness of $U - \xi$ give

$$(3.54) \quad \langle U(\varepsilon \cdot) - \xi, (g_{D_\varepsilon, \xi}^{(i)})^2 \rangle \leq \langle U(\varepsilon \cdot) - \xi, ((g_{D_\varepsilon, \xi}^{(i)})^2)_L \rangle + CL\varepsilon$$

for some C independent of ξ . Setting $B_L(x) := Lx + \{0, \dots, L-1\}^d$, on the event

$$(3.55) \quad F_{L, \varepsilon} := \bigcap_{\substack{x \in (L\mathbb{Z})^d \\ B_L(x) \cap D_\varepsilon \neq \emptyset}} \left\{ \xi : \left| \sum_{z \in B_L(x)} U(z\varepsilon) - \xi(z) \right| < \delta L^d \right\}$$

we in turn have

$$(3.56) \quad \langle U(\varepsilon \cdot) - \xi, ((g_{D\varepsilon, \xi}^{(i)})^2)_L \rangle \leq \delta(1 + CL\varepsilon),$$

again by Lemma 3.4. Assuming that $CL\varepsilon \leq \delta$, we thus get

$$(3.57) \quad \mathbb{P}(\Lambda_k \geq \Lambda_k^\varepsilon(\xi) + 5k\delta) \leq \mathbb{P}_\varepsilon(F_{L, \varepsilon}^c).$$

A standard large-deviation estimate bounds $\mathbb{P}_\varepsilon(F_{L, \varepsilon}^c) \leq c(\varepsilon L)^{-d} e^{-cL^d}$. Choosing, e.g., $L = c\delta/\varepsilon$ for some c sufficiently small, the claim follows. \square

We are now ready to conclude:

Proof of Theorem 1.2. By Propositions 3.6 and 3.7 we have

$$(3.58) \quad \Lambda_k^\varepsilon(\xi) \xrightarrow[\varepsilon \downarrow 0]{\mathbb{P}} \Lambda_k, \quad k \geq 1.$$

Then

$$(3.59) \quad \lambda_{D\varepsilon, \xi}^{(k)} = \Lambda_k^\varepsilon(\xi) - \Lambda_{k-1}^\varepsilon(\xi) \xrightarrow[\varepsilon \downarrow 0]{\mathbb{P}} \Lambda_k - \Lambda_{k-1} = \lambda_D^{(k)}$$

for all $k \geq 1$ as well. \square

The proof of Proposition 3.7 gives us the following additional fact:

Corollary 3.8 *Given any choice of $\xi \mapsto g_{D\varepsilon, \xi}^{(1)}, \dots, g_{D\varepsilon, \xi}^{(k)}$, let $\tilde{g}_{1, \xi}^\varepsilon, \dots, \tilde{g}_{k, \xi}^\varepsilon$ denote the continuum interpolations of $\varepsilon^{-d/2} g_{D\varepsilon, \xi}^{(1)}, \dots, \varepsilon^{-d/2} g_{D\varepsilon, \xi}^{(k)}$ as constructed in Lemma 3.3. Assume $\lambda_D^{(k+1)} > \lambda_D^{(k)}$ and let $\hat{\Pi}_k$ denote the orthogonal projection on $\{\varphi_D^{(1)}, \dots, \varphi_D^{(k)}\}^\perp$. Then, for any $\delta' > 0$, there is an event $E_{k, \varepsilon, \delta'}$ such that*

$$(3.60) \quad \left\{ \xi : \sum_{i=1}^k \|\hat{\Pi}_k \tilde{g}_{i, \xi}^\varepsilon\|_{L^2(\mathbb{R}^d)} > \delta' \right\} \subseteq E_{k, \varepsilon, \delta'} \quad \text{and} \quad \lim_{\varepsilon \downarrow 0} \mathbb{P}_\varepsilon(E_{k, \varepsilon, \delta'}) = 0.$$

Proof. An inspection of the proof of Proposition 3.7 reveals that

$$(3.61) \quad \left\{ \xi : \sum_{i=1}^k \left(\|\nabla \tilde{h}_{i, \xi}^\varepsilon\|_{L^2(\mathbb{R}^d)}^2 + \langle U, (\tilde{h}_{i, \xi}^\varepsilon)^2 \rangle_{L^2(\mathbb{R}^d)} \right) \geq \Lambda_k - \delta' \right\}$$

is a subset of the event $E_{k, \varepsilon, \delta'} := F_{L, \varepsilon}^c$, where $F_{L, \varepsilon}$ is the event in (3.55) with proper choices of δ and L . Thanks to Lemma 3.5, the inclusion in (3.60) thus holds for $\tilde{h}_{i, \xi}^\varepsilon$ instead of $\tilde{g}_{i, \xi}^\varepsilon$. Adjusting δ slightly, the identities (3.49–3.50) then yield the same for the $\tilde{g}_{i, \xi}^\varepsilon$'s. \square

Remark 3.9 Note that under the assumption $\lambda_D^{(k+1)} > \lambda_D^{(k)}$ the space $\{\varphi_D^{(1)}, \dots, \varphi_D^{(k)}\}^\perp$, and thus also the projection $\hat{\Pi}_k$, is independent of the choice of the eigenfunction basis. The formulation (3.60) avoids having to deal with questions about the measurability of eigenfunctions and/or the Hilbert-space projections.

4. CONCENTRATION ESTIMATE

We now move to the proof of a concentration estimate for eigenfunctions around their mean. The proof actually boils down to a well-known concentration inequality due to Talagrand that we recast into a form adapted to our needs:

Theorem 4.1 (Theorem 6.6 of [26]) *Let $N \in \mathbb{N}$ and let $|\cdot|_2$ denote the Euclidean norm on \mathbb{R}^N . Let $f: [-1, 1]^N \rightarrow \mathbb{R}$ be concave and Lipschitz continuous with*

$$(4.1) \quad L := \sup_{\xi, \eta \in [-1, 1]^N} \frac{|f(\xi) - f(\eta)|}{|\xi - \eta|_2} < \infty.$$

Then for any product probability measure P on $[-1, 1]^N$ and any $t > 0$,

$$(4.2) \quad P(|f - \text{med}(f)| > t) \leq 4 \exp \left\{ -\frac{t^2}{16L^2} \right\},$$

where $\text{med}(f)$ denotes the median of f .

Proof of Theorem 1.3. We will first prove concentration for the quantity $\Lambda_k^\varepsilon(\xi)$ and then extract the desired statement from it. In light of Theorem 4.1, it suffices to derive a good bound on the Lipschitz constant for $f(\xi) := \Lambda_k^\varepsilon(\xi)$. Fix ξ and let $\{g_{D_\varepsilon, \xi}^{(i)} : i = 1, \dots, k\}$ be a set of eigenfunctions satisfying (1.11) that achieve the corresponding eigenvalues $\{\lambda_{D_\varepsilon, \xi}^{(i)} : i = 1, \dots, k\}$, respectively. For any η , the variational characterization (3.30) of $\Lambda_k^\varepsilon(\xi)$ yields

$$(4.3) \quad \Lambda_k^\varepsilon(\xi) - \Lambda_k^\varepsilon(\eta) \leq \sum_{x \in D_\varepsilon} (\xi(x) - \eta(x)) \sum_{j=1}^k |g_{D_\varepsilon, \eta}^{(j)}(x)|^2.$$

Peeling off the sum over j and applying the Cauchy-Schwarz inequality, we obtain

$$(4.4) \quad \Lambda_k^\varepsilon(\xi) - \Lambda_k^\varepsilon(\eta) \leq |\xi - \eta|_2 \sum_{j=1}^k \left(\sum_{x \in D_\varepsilon} |g_{D_\varepsilon, \eta}^{(j)}(x)|^4 \right)^{1/2}.$$

But Lemma 3.2 ensures that $|g_{D_\varepsilon, \eta}^{(j)}(x)| \leq c\varepsilon^{d/2}$, and the normalization convention (1.11) then gives

$$(4.5) \quad \Lambda_k^\varepsilon(\xi) - \Lambda_k^\varepsilon(\eta) \leq kc\varepsilon^{d/2} |\xi - \eta|_2.$$

Since this is valid for all η, ξ , the same estimate applies to $|\Lambda_k^\varepsilon(\xi) - \Lambda_k^\varepsilon(\eta)|$ as well.

Now fix $t > 0$. Talagrand's inequality readily yields

$$(4.6) \quad \mathbb{P}_\varepsilon(|\Lambda_k^\varepsilon - \text{med}(\Lambda_k^\varepsilon)| > t) \leq 4 \exp\{-ct^2\varepsilon^{-d}\}.$$

But that implies the same bound also for $\text{med}(\Lambda_k^\varepsilon)$ replaced by $\mathbb{E}\Lambda_k^\varepsilon$. Since $\Lambda_k^\varepsilon(\xi)$ is the sum of the first k eigenvalues, the desired inequality for a single eigenvalue follows by considering the differences $\Lambda_k^\varepsilon(\xi) - \Lambda_{k-1}^\varepsilon(\xi)$. \square

Remark 4.2 We note that, thanks to pointwise boundedness of the support of ξ and the Lipschitz property of the eigenfunction, the proof could equally well be based on Azuma's inequality.

For later purposes we restate the concentration bound in a slightly different form:

Lemma 4.3 *Let $k \geq 1$. There is a constant $c > 0$ such that for any $t > 0$,*

$$(4.7) \quad \max_{x \in D_\varepsilon} \mathbb{P}_\varepsilon \left(\sup_{\xi(x) \in [a, b]} |\lambda_{D_\varepsilon, \xi}^{(k)} - \lambda_D^{(k)}| > t \right) \leq 4 \exp\{-ct^2\varepsilon^{-d}\}$$

holds for all sufficiently small ε .

Proof. Let $t > 0$ be fixed. From Theorem 1.3 we know that $\lambda_{D_\varepsilon, \xi}^{(k)} \rightarrow \lambda_D^{(k)}$ in probability. Since the eigenvalues are uniformly bounded, this implies

$$(4.8) \quad \left| \mathbb{E} \lambda_{D_\varepsilon, \xi}^{(k)} - \lambda_D^{(k)} \right| < \frac{2}{3} t$$

for $\varepsilon > 0$ sufficiently small. Moreover, (4.5) gives

$$(4.9) \quad \sup_{\substack{\xi^{(y)} = \eta^{(y)} \\ \forall y \neq x}} \left| \lambda_{D_\varepsilon, \xi}^{(k)} - \lambda_{D_\varepsilon, \eta}^{(k)} \right| \leq c \varepsilon^{d/2} < \frac{1}{3} t,$$

once ε is sufficiently small. Hence, the probability in (4.7) is bounded by the probability that $\lambda_{D_\varepsilon, \xi}^{(k)}$ deviates from its mean by more than $t/3$. This is estimated using Theorem 1.3. \square

5. GAUSSIAN LIMIT LAW

We are now finally ready to address the main aspect of this work, which is the limit theorem for fluctuations of asymptotically non-degenerate eigenvalues. The main idea is quite simple and is inspired by the recent work on fluctuations of effective conductivity in the random conductance model (Biskup, Salvi and Wolff [7]). Consider an ordering of the vertices in D_ε into a sequence $x_1, \dots, x_{|D_\varepsilon|}$ and let $\mathcal{F}_m := \sigma(\xi(x_1), \dots, \xi(x_m))$. Then

$$(5.1) \quad \lambda_{D_\varepsilon, \xi}^{(k)} - \mathbb{E} \lambda_{D_\varepsilon, \xi}^{(k)} = \sum_{m=1}^{|D_\varepsilon|} \left(\mathbb{E}(\lambda_{D_\varepsilon, \xi}^{(k)} | \mathcal{F}_m) - \mathbb{E}(\lambda_{D_\varepsilon, \xi}^{(k)} | \mathcal{F}_{m-1}) \right)$$

represents the fluctuation of the k -th eigenvalue as a martingale. We may then apply the Martingale Central Limit Theorem due to Brown [8] which asserts that a family

$$(5.2) \quad \{(M_m^\varepsilon, \mathcal{F}_m) : m = 0, \dots, n(\varepsilon)\}$$

of square-integrable \mathbb{R}^V -valued martingales such that

- (0) $M_0^\varepsilon = 0$ and $n(\varepsilon) \rightarrow \infty$ as $\varepsilon \downarrow 0$,
- (1) there is a finite v -dimensional square matrix $\sigma^2 = \{\sigma_{ij}^2\}$ for which

$$(5.3) \quad \varepsilon^{-d} \sum_{m=1}^{n(\varepsilon)} E \left((M_m^\varepsilon - M_{m-1}^\varepsilon)(M_m^\varepsilon - M_{m-1}^\varepsilon)^\top | \mathcal{F}_{m-1} \right) \xrightarrow[\varepsilon \downarrow 0]{\mathbb{P}} \sigma^2,$$

- (2) for each $\delta > 0$,

$$(5.4) \quad \varepsilon^{-d} \sum_{m=1}^{n(\varepsilon)} E \left(|M_m^\varepsilon - M_{m-1}^\varepsilon|^2 \mathbf{1}_{\{|M_m^\varepsilon - M_{m-1}^\varepsilon| > \delta \varepsilon^{d/2}\}} | \mathcal{F}_{m-1} \right) \xrightarrow[\varepsilon \downarrow 0]{\mathbb{P}} 0,$$

satisfies

$$(5.5) \quad \varepsilon^{-d/2} M_{n(\varepsilon)}^\varepsilon \xrightarrow[\varepsilon \downarrow 0]{\text{law}} \mathcal{N}(0, \sigma^2).$$

The proof of Theorem 1.4 thus reduces to verification of the premises (0-2) of this result for

$$(5.6) \quad M_n^\varepsilon := \sum_{m=1}^n \left(\mathbb{E}(\lambda_{D_\varepsilon, \xi}^{(k)} | \mathcal{F}_m) - \mathbb{E}(\lambda_{D_\varepsilon, \xi}^{(k)} | \mathcal{F}_{m-1}) \right)$$

and $n_\varepsilon := |D_\varepsilon|$.

The condition (0) is checked immediately, but the control of the limits in (1) and (2) will require a more explicit expression for the martingale differences. Here we note that, for any function $f = f(\xi_1, \dots, \xi_n)$

on \mathbb{R}^n that is absolutely continuous in each variable and for any collection ξ_1, \dots, ξ_n of bounded independent random variables we have, for $\mathcal{F}_m := \sigma(\xi_1, \dots, \xi_m)$,

$$(5.7) \quad \mathbb{E}(f|\mathcal{F}_m) - \mathbb{E}(f|\mathcal{F}_{m-1}) = \widehat{\mathbb{E}} \int_{\widehat{\xi}_m}^{\xi_m} \frac{\partial f}{\partial \xi_m}(\xi_1, \dots, \xi_{m-1}, \xi, \widehat{\xi}_{m+1}, \dots, \widehat{\xi}_n) d\tilde{\xi},$$

where the expectation is over the collection of random variables $\widehat{\xi}$, which are copies of ξ independent of ξ . The integral is in the sense of Riemann, and we use the corresponding notation to explicate the sign change upon exchanging the limits of integration. To validate the condition of absolute continuity (and justify the use of the Fundamental Theorem of Calculus), we prove:

Lemma 5.1 *The function $\xi \mapsto \lambda_{D_\varepsilon, \xi}^{(k)}$ is everywhere right and left differentiable with respect to each $\xi(x)$. The set of points where the two derivatives disagree is at most countably infinite; else the derivative exists and is continuous in $\xi(x)$. The partial derivatives $\frac{\partial}{\partial \xi(x)^\pm} \lambda_{D_\varepsilon, \xi}^{(k)}$ are bounded and, except at countably many values of $\xi(x)$,*

$$(5.8) \quad \frac{\partial}{\partial \xi(x)} \lambda_{D_\varepsilon, \xi}^{(k)} = |g_{D_\varepsilon, \xi}^{(k)}(x)|^2$$

for any possible choice of $g_{D_\varepsilon, \xi}^{(k)}$. (I.e., all choices give the same result.)

Proof. Note that $\lambda_{D_\varepsilon, \xi}^{(k)} = \Lambda_k^\varepsilon(\xi) - \Lambda_{k-1}^\varepsilon(\xi)$. Since $\xi \mapsto \Lambda_k^\varepsilon(\xi)$ is concave — being the infimum of a family of linear functions — it is right and left differentiable in $\xi(x)$ at all values. The derivatives are non-increasing and ordered so there are at most countably many points where they disagree. Moreover, at differentiability points of Λ_k^ε , (4.3) yields

$$(5.9) \quad \frac{\partial}{\partial \xi(x)} \Lambda_k^\varepsilon(\xi) = \sum_{j=1}^k |g_{D_\varepsilon, \xi}^{(j)}(x)|^2$$

for any choice of eigenfunctions $g_{D_\varepsilon, \xi}^{(1)}, \dots, g_{D_\varepsilon, \xi}^{(k)}$. At common differentiability points of both $\Lambda_k^\varepsilon(\xi)$ and $\Lambda_{k-1}^\varepsilon(\xi)$, we then get (5.8). \square

The upshot of Lemma 5.1 is that we are permitted to use (5.8) in (5.7) with no provisos on eigenvalue degeneracy. Our goal is to replace the modulus-squared of $g_{D_\varepsilon, \xi}^{(k)}$ by that pertaining to the corresponding eigenfunction in the continuum problem. However, there is a subtle issue arising from the integration with respect to the dummy variable $\tilde{\xi}$ in (5.7). Indeed, with this variable in place of $\xi(x)$, the configuration $\tilde{\xi}$ may not even be in the support of \mathbb{P}_ε . We handle this with the help of:

Lemma 5.2 *Given $k \geq 1$ and a configuration ξ , suppose that $\lambda_{D_\varepsilon, \xi}^{(k)}$ remains simple as $\xi(x)$ varies through an interval $[a, b]$. Then for any ξ' satisfying $\xi(y) = \xi'(y)$ for $y \neq x$ and for any $\xi(x), \xi'(x) \in [a, b]$,*

$$(5.10) \quad |g_{D_\varepsilon, \xi'}^{(k)}(x)| = |g_{D_\varepsilon, \xi}^{(k)}(x)| \exp \left\{ \int_{\xi(x)}^{\xi'(x)} G_{D_\varepsilon}^{(k)}(x, x; \tilde{\xi}) d\tilde{\xi}(x) \right\},$$

where $\tilde{\xi}$ is the configuration that agrees with ξ (and ξ') outside x where it equals $\tilde{\xi}(x)$ and

$$(5.11) \quad G_{D_\varepsilon}^{(k)}(x, y; \xi) := \langle \delta_x, (H_{D_\varepsilon, \xi} - \lambda_{D_\varepsilon, \xi}^{(k)})^{-1} (1 - \widehat{P}_k) \delta_y \rangle_{\ell^2(\mathbb{Z}^d)}$$

with \widehat{P}_k denoting the orthogonal projection on $\text{Ker}(\lambda_{D_\varepsilon, \xi}^{(k)} - H_{D_\varepsilon, \xi})$.

Proof. To make notations brief, let us write λ , resp., g for the relevant eigenvalue, resp., eigenfunction. Since the eigenvalue is simple, Rayleigh's perturbation theory ensures that the eigenfunction is unique

up to normalization and overall sign. In particular, (5.8) holds. Moreover, also the eigenfunction g — with the sign fixed at x , for instance — is differentiable in $\xi(x)$. Taking the derivative of the eigenvalue equation, we get

$$(5.12) \quad (\lambda - H_{D_\varepsilon, \xi}) \frac{\partial g}{\partial \xi(x)} = g(x) \mathbf{1}_{\{x\}} - |g(x)|^2 g.$$

Interpreting the right-hand side as $(1 - \widehat{P}_k)(g(x) \mathbf{1}_{\{x\}})$, we can now invert $\lambda - H_{D_\varepsilon, \xi}$ to obtain

$$(5.13) \quad \frac{\partial}{\partial \xi(x)} g(y) = G_{D_\varepsilon}^{(k)}(y, x; \xi) g(x).$$

Evaluating at x , we get an autonomous ODE for $g(x)$. Solving yields (5.10). \square

Our next aim will be to show that, whenever $\lambda_D^{(k)}$ is simple, the term in the exponent of (5.10) actually tends to zero as $\varepsilon \downarrow 0$.

Lemma 5.3 *For $k \geq 1$ let δ be such that $0 < \delta < \frac{1}{3} \min\{\lambda_D^{(k)} - \lambda_D^{(k-1)}, \lambda_D^{(k+1)} - \lambda_D^{(k)}\}$ and set*

$$(5.14) \quad A_{k, \varepsilon} := \bigcap_{x \in D_\varepsilon} \left\{ \xi : \sup_{\xi_x \in [a, b]} |\lambda_{D_\varepsilon, \xi}^{(i)} - \lambda_D^{(i)}| < \delta, i = k-1, k, k+1 \right\}.$$

Then

$$(5.15) \quad \max_{x \in D_\varepsilon} \sup_{\xi'_x \in [a, b]} \sup_{\xi \in A_{k, \varepsilon}} \left| \int_{\xi_x}^{\xi'_x} G_{D_\varepsilon}^{(k)}(x, x; \xi) d\xi_x \right| \xrightarrow{\varepsilon \downarrow 0} 0.$$

Proof. Take k such that $\lambda_D^{(k)}$ is simple and note that, for $\xi \in A_{k, \varepsilon}$, the eigenvalue $\lambda_{D_\varepsilon, \xi}^{(k)}$ remains simple for all values of $\xi(x)$. Then

$$(5.16) \quad G_{D_\varepsilon}^{(k)}(x, x; \xi) = \sum_{\substack{i \geq 1 \\ i \neq k}} \frac{1}{\lambda_{D_\varepsilon, \xi}^{(i)} - \lambda_{D_\varepsilon, \xi}^{(k)}} |g_{D_\varepsilon, \xi}^{(i)}(x)|^2.$$

Thanks to (3.4) and the fact that the eigenvalues of $-\varepsilon^{-2} \Delta^{(d)}$ are close to those of the continuum problem, for each $R > 0$ there is $K > k$ such that, for any sufficiently small $\varepsilon > 0$,

$$(5.17) \quad i \geq K \quad \Rightarrow \quad \lambda_{D_\varepsilon, \xi}^{(i)} \geq \lambda_{D_\varepsilon, \xi}^{(k)} + R$$

uniformly in $\xi \in \Omega_{a, b}$. The corresponding part of the above sum is then bounded by

$$(5.18) \quad 0 \leq \sum_{i \geq K} \frac{1}{\lambda_{D_\varepsilon, \xi}^{(i)} - \lambda_{D_\varepsilon, \xi}^{(k)}} |g_{D_\varepsilon, \xi}^{(i)}(x)|^2 \leq \frac{1}{R} \sum_{i \geq K} |g_{D_\varepsilon, \xi}^{(i)}(x)|^2 \leq \frac{1}{R},$$

where we used the Plancherel formula to bound the second sum by $\langle \delta_x, \delta_x \rangle_2 = 1$. This reduces an estimate of $G_{D_\varepsilon}^{(k)}(x, x; \xi)$ to a finite number of terms.

On $A_{k, \varepsilon}$ (5.8) and Lemma 3.2 show, for all ε sufficiently small,

$$(5.19) \quad \forall \xi \in A_{k, \varepsilon} : \quad \sup_{\xi(x) \in [a, b]} |\lambda_{D_\varepsilon, \xi}^{(i)} - \lambda_{D_\varepsilon, \xi}^{(k)}| > \frac{\delta}{3} - c\varepsilon^d |b - a| > \frac{\delta}{4}, \quad i = k-1, k+1.$$

The sum of first K terms in (5.16) can thus be bounded by $cK\delta^{-1}\varepsilon^d$, uniformly on $A_{k, \varepsilon}$. This permits us to take $R \rightarrow \infty$ simultaneously with $\varepsilon \downarrow 0$ and conclude the claim. \square

Given $\varepsilon > 0$, consider now an ordering $x_1, \dots, x_{|D_\varepsilon|}$ of vertices of D_ε and given $\xi, \widehat{\xi} \in \Omega_{a,b}$, denote by $\widehat{\xi}^{(m)}$ the configuration

$$(5.20) \quad \widehat{\xi}^{(m)}(x_i) := \begin{cases} \xi(x_i), & \text{if } i \leq m, \\ \widehat{\xi}(x_i), & \text{if } i > m. \end{cases}$$

Hereafter, we regard $\widehat{\xi}$ as an independent copy of ξ and denote the corresponding expectation by $\widehat{\mathbb{E}}$. Let $\mathcal{F}_m := \sigma(\xi(x_1), \dots, \xi(x_m))$. The martingale difference can then be written with the help of Lemma 5.1 as

$$(5.21) \quad \begin{aligned} Z_m^{(i)} &:= \mathbb{E}(\lambda_{D_\varepsilon, \xi}^{(i)} | \mathcal{F}_m) - \mathbb{E}(\lambda_{D_\varepsilon, \xi}^{(i)} | \mathcal{F}_{m-1}) \\ &= \widehat{\mathbb{E}}\left(\lambda_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(i)} - \lambda_{D_\varepsilon, \widehat{\xi}^{(m-1)}}^{(i)}\right) \\ &= \widehat{\mathbb{E}}\left(\int_{\widehat{\xi}^{(m)}(x_m)}^{\xi(x_m)} |g_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(i)}(x_m)|^2 d\widehat{\xi}\right), \end{aligned}$$

where $\widehat{\xi}^{(m)}$ is the configuration that equals ξ on $\{x_1, \dots, x_{m-1}\}$, takes value $\widehat{\xi}$ at x_m , and coincides with $\widehat{\xi}$ on $\{x_{m+1}, \dots, x_{|D_\varepsilon|}\}$. Notice that Lemma 3.2 immediately gives

$$(5.22) \quad |Z_m^{(i)}| \leq c\varepsilon^d$$

for some constant $c < \infty$. In particular, condition (2) in the abovementioned Martingale Central Limit Theorem holds trivially. For condition (1), we will proceed, as mentioned before, by replacing the square of the discrete eigenfunction by its corresponding continuum counterpart. The key estimate is stated in:

Proposition 5.4 *Suppose $\lambda_D^{(i)}$ and $\lambda_D^{(j)}$ are simple. Abbreviate $B_\varepsilon(x) := \varepsilon x + [0, \varepsilon)^d$.*

$$(5.23) \quad \mathbb{E} \left| \sum_{m=1}^{|D_\varepsilon|} \left(\mathbb{E}((\varepsilon^{-d} Z_m^{(i)})(\varepsilon^{-d} Z_m^{(j)}) | \mathcal{F}_{m-1}) - \int_{B_\varepsilon(x_m)} dy V(y) |\varphi_D^{(i)}(y)|^2 |\varphi_D^{(j)}(y)|^2 \right) \right| \xrightarrow{\varepsilon \downarrow 0} 0.$$

The proof of this proposition will be done in several steps. Recall the definition of event $A_{k,\varepsilon}$ and note that, on $A_{k,\varepsilon}$ the eigenfunction $g_{D_\varepsilon, \xi}^{(k)}$ is unique up to a sign and, in particular, there is a unique measurable version of $\xi \mapsto |g_{D_\varepsilon, \xi}^{(k)}(x)|^2$ for each x . In light of the concentration bound in Lemma 4.3 we have

$$(5.24) \quad \lambda_D^{(k)} \text{ simple} \quad \Rightarrow \quad \mathbb{P}_\varepsilon(A_{k,\varepsilon}) \xrightarrow{\varepsilon \downarrow 0} 1.$$

Our first replacement step is the content of:

Lemma 5.5 *Suppose $\lambda_D^{(k)}$ is simple. Then*

$$(5.25) \quad \varepsilon^{-d} \sum_{m=1}^{|D_\varepsilon|} \mathbb{E} \left(\left| Z_m^{(k)} - (\xi(x_m) - U(\varepsilon x_m)) \mathbb{E} \left(|g_{D_\varepsilon, \xi}^{(k)}(x_m)|^2 \mathbf{1}_{A_{k,\varepsilon}} | \mathcal{F}_m \right) \right|^2 \right) \xrightarrow{\varepsilon \downarrow 0} 0.$$

Proof. Inserting the indicator of $\widehat{\xi}^{(m)} \in A_{k,\varepsilon}$ and/or its complement into the third line of (5.21) and applying the boundedness of the discrete eigenfunctions from Lemma 3.2 shows

$$(5.26) \quad \left| Z_m^{(k)} - \widehat{\mathbb{E}} \left(\mathbf{1}_{\{\widehat{\xi}^{(m)} \in A_{k,\varepsilon}\}} \int_{\widehat{\xi}^{(m)}(x_m)}^{\xi(x_m)} |g_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(k)}(x_m)|^2 d\widehat{\xi} \right) \right| \leq c\varepsilon^d \mathbb{E}(\mathbf{1}_{A_{k,\varepsilon}^c} | \mathcal{F}_m),$$

where, we recall, the expectation $\widehat{\mathbb{E}}$ affects only $\widehat{\xi}$ and so $\widehat{\mathbb{E}}(\mathbf{1}_{\{\widehat{\xi}^{(m)} \notin A_{k,\varepsilon}\}}) = \mathbb{E}(\mathbf{1}_{A_{k,\varepsilon}^c} | \mathcal{F}_m)$. Abbreviate temporarily

$$(5.27) \quad F_m(\tilde{\xi}) := \exp \left\{ 2 \int_{\tilde{\xi}(x_m)}^{\tilde{\xi}} G_{D_\varepsilon}^{(k)}(x_m, x_m; \tilde{\xi}') d\tilde{\xi}' \right\}.$$

On the event $\{\widehat{\xi}^{(m)} \in A_{k,\varepsilon}\}$, Lemmas 5.1 and 5.2 along with $\widehat{\xi}^{(m)}(x_m) = \xi(x_m)$ yield

$$(5.28) \quad \begin{aligned} & \int_{\widehat{\xi}(x_m)}^{\xi(x_m)} |g_{D_\varepsilon, \tilde{\xi}^{(m)}}^{(k)}(x_m)|^2 d\tilde{\xi} - (\xi(x_m) - \widehat{\xi}(x_m)) |g_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(k)}(x_m)|^2 \\ &= \int_{\widehat{\xi}(x_m)}^{\xi(x_m)} \left(|g_{D_\varepsilon, \tilde{\xi}^{(m)}}^{(k)}(x_m)|^2 - |g_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(k)}(x_m)|^2 \right) d\tilde{\xi} \\ &= |g_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(k)}(x_m)|^2 \int_{\widehat{\xi}(x_m)}^{\xi(x_m)} (F_m(\tilde{\xi}) - 1) d\tilde{\xi}. \end{aligned}$$

Lemma 5.3 then bounds the difference $F_m(\tilde{\xi}) - 1$ uniformly by $e^{\delta(\varepsilon)} - 1$ for some $\delta(\varepsilon) > 0$ that tends to zero as $\varepsilon \downarrow 0$. Thanks to the uniform boundedness of the eigenfunctions, this and (5.26) yield

$$(5.29) \quad \left| Z_m^{(k)} - \widehat{\mathbb{E}} \left(\mathbf{1}_{\{\widehat{\xi}^{(m)} \in A_{k,\varepsilon}\}} (\xi(x_m) - \widehat{\xi}(x_m)) |g_{D_\varepsilon, \widehat{\xi}^{(m)}}^{(k)}(x_m)|^2 \right) \right| \leq c\varepsilon^d \mathbb{E}(\mathbf{1}_{A_{k,\varepsilon}^c} | \mathcal{F}_m) + c\varepsilon^d (e^{\delta(\varepsilon)} - 1).$$

The configuration $\widehat{\xi}^{(m)}$ does not depend on $\widehat{\xi}(x_m)$, and so we may take expectation with respect to $\widehat{\xi}(x_m)$ and effectively replace it by $U(\varepsilon x_m)$. Recasting $\widehat{\mathbb{E}}$ as conditional expectation given \mathcal{F}_m and using that $\xi(x_m)$ is \mathcal{F}_m -measurable, we thus conclude

$$(5.30) \quad \left| Z_m^{(k)} - (\xi(x_m) - U(\varepsilon x_m)) \mathbb{E} \left(|g_{D_\varepsilon, \xi}^{(k)}(x_m)|^2 \mathbf{1}_{A_{k,\varepsilon}} \mid \mathcal{F}_m \right) \right| \leq c\varepsilon^d \mathbb{E}(\mathbf{1}_{A_{k,\varepsilon}^c} | \mathcal{F}_m) + c\varepsilon^d (e^{\delta(\varepsilon)} - 1).$$

Squaring this and taking another expectation shows that the left-hand-side of (5.25) is bounded by $c\varepsilon^d |D_\varepsilon|$ times $\mathbb{P}_\varepsilon(A_{k,\varepsilon}^c) + (e^{\delta(\varepsilon)} - 1)$. By (5.24), this tends to zero as claimed. \square

Next we note:

Lemma 5.6 *Suppose $\lambda_D^{(k)}$ is simple. Then*

$$(5.31) \quad \sum_{m=1}^{|D_\varepsilon|} \int_{B_\varepsilon(x_m)} dy \mathbb{E} \left(\left| |\varphi_D^{(k)}(y)|^2 - \varepsilon^{-d} |g_{D_\varepsilon, \xi}^{(k)}(x_m)|^2 \mathbf{1}_{A_{k,\varepsilon}} \right| \right) \xrightarrow{\varepsilon \downarrow 0} 0$$

Proof. Recall the setting of Corollary 3.8 and, in particular, given the scaled discrete eigenfunctions $\varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(1)}, \dots, \varepsilon^{-d/2} g_{D_\varepsilon, \xi}^{(k)}$, let $\tilde{g}_{1, \xi}^\varepsilon, \dots, \tilde{g}_{k, \xi}^\varepsilon$ denote their continuum interpolations. As $\lambda_D^{(k)}$ is simple, Corollary 3.8 guarantees that these functions project almost entirely onto the closed linear span of $\{\varphi_D^{(1)}, \dots, \varphi_D^{(\ell)}\}$ for both $\ell = k - 1$ and $\ell = k$. As these functions are also nearly orthogonal, we get

$$(5.32) \quad \mathbb{P}_\varepsilon \left(A_{k,\varepsilon} \ \& \ \left\| |\tilde{g}_{k, \xi}^\varepsilon| - |\varphi_D^{(k)}| \right\|_{L^2(D)} > \delta \right) \xrightarrow{\varepsilon \downarrow 0} 0$$

for any $\delta > 0$. As both $|\tilde{g}_{k, \xi}^\varepsilon|$ and $|\varphi_D^{(k)}|$ are uniformly bounded, this implies

$$(5.33) \quad \int_{\mathbb{R}^d} dy \mathbb{E} \left(\left| |\varphi_D^{(k)}(y)|^2 - |\tilde{g}_{k, \xi}^\varepsilon(y)|^2 \mathbf{1}_{A_{k,\varepsilon}} \right| \right) \xrightarrow{\varepsilon \downarrow 0} 0$$

with the help of (5.24). But (3.14) gives

$$(5.34) \quad \sum_{m=1}^{|D_\varepsilon|} \int_{B_\varepsilon(x_m)} dy \mathbb{E} \left(\left| \tilde{g}_{k,\xi}^\varepsilon(y) - \varepsilon^{-d/2} g_{D_\varepsilon,\xi}^{(k)}(x_m) \right|^2 \mathbf{1}_{A_{k,\varepsilon}} \right) \leq C(d) \mathbb{E} \left(\|\nabla^{(d)} g_{D_\varepsilon,\xi}^{(k)}\|_2^2 \mathbf{1}_{A_{k,\varepsilon}} \right),$$

which tends to zero proportionally to ε^2 , due to boundedness of the kinetic energy. Combining (5.33–5.34), we get the claim. \square

Proof of Proposition 5.4. Combining Lemmas 5.5 and 5.6, and using that the conditional expectation is a contraction in L^2 , we get

$$(5.35) \quad \sum_{m=1}^{|D_\varepsilon|} \int_{B_\varepsilon(x_m)} dy \mathbb{E} \left(\left| \varepsilon^{-d} Z_m^{(k)} - (\xi(x_m) - U(\varepsilon x_m)) |\varphi_D^{(k)}(y)|^2 \right|^2 \right) \xrightarrow{\varepsilon \downarrow 0} 0.$$

for both $k = i, j$. The claim now reduces to

$$(5.36) \quad \sum_{m=1}^{|D_\varepsilon|} \int_{B_\varepsilon(x_m)} dy |V(y) - V(\varepsilon x_m)| |\varphi_D^{(i)}(y)|^2 |\varphi_D^{(j)}(y)|^2 \xrightarrow{\varepsilon \downarrow 0} 0,$$

which follows by uniform continuity of $y \mapsto V(y)$ and the boundedness of the eigenfunctions. \square

Proof of Theorem 1.4. Thanks to Proposition 5.4 and the fact that $|B_\varepsilon(x_m)| = \varepsilon^d$,

$$(5.37) \quad \varepsilon^{-d} \sum_{m=1}^{|D_\varepsilon|} \mathbb{E}(Z_m^{(k_i)} Z_m^{(k_j)} | \mathcal{F}_{m-1}) \xrightarrow{\varepsilon \downarrow 0} \int_D V(y) |\varphi_D^{(k_i)}(y)|^2 |\varphi_D^{(k_j)}(y)|^2 dy$$

in $L^1(\mathbb{P}_\varepsilon)$ and thus in probability. This verifies the (last yet unproved) condition (1) of the Martingale Central Limit Theorem and so the result follows. \square

Proof of Theorem 1.5. The relation (1.14) is a direct consequence of Lemma 5.6 and the boundedness of eigenfunctions. For (1.13) we again drop the suffixes on all quantities and write, on $A_{k,\varepsilon}$,

$$(5.38) \quad T^{(k)} - \mathbb{E}(T^{(k)} \mathbf{1}_{A_{k,\varepsilon}}) = \lambda^{(k)} - \mathbb{E}(\lambda^{(k)} \mathbf{1}_{A_{k,\varepsilon}}) - \sum_{x \in D_\varepsilon} (\xi(x) - U(x\varepsilon)) |g^{(k)}(x)|^2 \\ + \sum_{x \in D_\varepsilon} \left(U(x\varepsilon) |g^{(k)}(x)|^2 - \mathbb{E}(\xi(x) |g^{(k)}(x)|^2 \mathbf{1}_{A_{k,\varepsilon}}) \right)$$

Lemma 5.6 and the boundedness of eigenfunctions now allows us to replace the square of the discrete eigenfunction by $\varepsilon^d |\varphi_D^{(k)}(x\varepsilon)|^2$ up to an error that is negligible at overall scale ε^d . Using $Z_m := \mathbb{E}(\lambda^{(k)} | \mathcal{F}_m) - \mathbb{E}(\lambda^{(k)} | \mathcal{F}_{m-1})$, we thus get

$$(5.39) \quad \varepsilon^{-d/2} (T^{(k)} - \mathbb{E}(T^{(k)} \mathbf{1}_{A_{k,\varepsilon}})) = o(1) + \sum_{m=1}^{|D_\varepsilon|} \left(\varepsilon^{-d} Z_m - (\xi(x_m) - U(\varepsilon x_m)) |\varphi_D^{(k)}(\varepsilon x_m)|^2 \right),$$

where $o(1)$ represents a random variable whose variance vanishes as ε goes to zero. The sum on the right is a martingale and so its variance is estimated by sum of variances of individual terms. Using a slight modification of (5.35), the result tends to zero as $\varepsilon \downarrow 0$. \square

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