Electronic Journal of Differential Equations, Vol. 2008(2008), No. 83, pp. 1–36. ISSN: 1072-6691. URL: http://ejde.math.txstate.edu or http://ejde.math.unt.edu ftp ejde.math.txstate.edu (login: ftp)

ON HOMOGENIZATION OF A DIFFUSION PERTURBED BY A PERIODIC REFLECTION INVARIANT VECTOR FIELD

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ABSTRACT. In this paper the author studies the problem of the homogenization of a diffusion perturbed by a periodic reflection invariant vector field. The vector field is assumed to have fixed direction but varying amplitude. The existence of a homogenized limit is proven and formulas for the effective diffusion constant are given. In dimension d=1 the effective diffusion constant is always less than the constant for the pure diffusion. In d>1 this property no longer holds in general.

1. Introduction

We consider the problem of the homogenization of a diffusion perturbed by a reflection invariant vector field. The general set up we have in mind is to understand the limit as $\varepsilon \to 0$ of the solutions u_{ε} to an elliptic equation,

$$-\frac{1}{2d}\Delta u_{\varepsilon}(x,\omega) - 2b_{\varepsilon}(x,\omega)\partial u_{\varepsilon}(x,\omega)/\partial x_{1} + u_{\varepsilon}(x,\omega) = f(x),$$

$$x = (x_{1},\dots,x_{d}) \in \mathbb{R}^{d}, \quad \omega \in \Omega.$$
(1.1)

Here the function $f: \mathbb{R}^d \to \mathbb{R}$ is smooth of compact support and Ω is a probability space. For simplicity we have assumed that the vector field is always in the x_1 direction and hence can be described by the scalar function b_{ε} . As $\varepsilon \to 0$ the field becomes rapidly oscillatory and therefore one might expect that $u_{\varepsilon}(x,\omega)$ converges with probability 1 as $\varepsilon \to 0$ to a homogenized limit u(x) which is the solution to a constant coefficient elliptic equation,

$$-q(b)\frac{\partial^2 u}{\partial x_1^2} - \sum_{i=2}^d \frac{1}{2d} \frac{\partial^2 u}{\partial x_i^2} + u(x) = f(x), \quad x \in \mathbb{R}^d.$$
 (1.2)

The effect of the rapidly oscillating vector field b_{ε} is contained in the coefficient q(b) in (1.2).

In order for a limit u(x) satisfying (1.2) to exist it is necessary to make assumptions concerning the rapidly oscillating field b_{ε} . These are primarily that the distribution functions of the variables $b_{\varepsilon}(x,\cdot)$, $x \in \mathbb{R}^d$, are translation and reflection invariant. To be specific, we assume that there are translation operators

²⁰⁰⁰ Mathematics Subject Classification. 35R60, 60H30, 60J60.

Key words and phrases. PDE with periodic coefficients; homogenization.

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Submitted March 26, 2007. Published May 30, 2008.

 $\tau_x: \Omega \to \Omega, \ x \in \mathbb{R}^d$, which are measure preserving and satisfy the group properties $\tau_x \tau_y = \tau_{x+y}, \ x, y \in \mathbb{R}^d$, τ_0 =identity. Suppose $b: \Omega \to \mathbb{R}$ is a bounded function. We then set $b_{\varepsilon}(x,\omega) = \varepsilon^{-1}b(\tau_{x/\varepsilon}\ \omega), \ x \in \mathbb{R}^d, \ \omega \in \Omega, \ \varepsilon > 0$. Such a b_{ε} has translation invariant distribution functions and is rapidly oscillating as $\varepsilon \to 0$. For b_{ε} to satisfy reflection invariance we let $R: \mathbb{R}^d \to \mathbb{R}^d$ be the reflection operator $R(x_1, \ldots, x_d) = (-x_1, x_2, \ldots, x_d), \ x = (x_1, \ldots, x_d) \in \mathbb{R}^d$. We then require $b: \Omega \to \mathbb{R}$ to satisfy the identities,

$$\left\langle \prod_{i=1}^{n} b(\tau_{x_i} \cdot) \right\rangle = (-1)^n \left\langle \prod_{i=1}^{n} b(\tau_{Rx_i} \cdot) \right\rangle, \quad x_i \in \mathbb{R}^d, \ 1 \le i \le n, \ n \ge 1,$$
 (1.3)

where $\langle \cdot \rangle$ denotes expectation on Ω . Evidently (1.3) implies that $\langle b(\cdot) \rangle = 0$, so the vector field has no net drift.

A concrete example of an Ω and a $b: \Omega \to \mathbb{R}$ which satisfies (1.3) is given by taking Ω to be a torus, $\Omega = \prod_{i=1}^{d} [0, L_i]$ with periodic boundary conditions and uniform measure. The operators $\tau_x: \Omega \to \Omega$, $x \in \mathbb{R}^d$, are just translation on Ω and reflection invariance of (1.3) is guaranteed by the condition,

$$b(x_1, x_2, \dots, x_d) = -b(L_1 - x_1, x_2, \dots, x_d), \quad x = (x_1, \dots, x_d) \in \Omega.$$
 (1.4)

We shall show that for a discrete version of a periodic Ω with b satisfying (1.4) a homogenized limit exists with q(b) satisfying $0 < q(b) < \infty$. For d = 1 one has $q(b) \le q(0) = 1/2$. For d > 1 it is no longer the case that $q(b) \le q(0) = 1/2d$ in general although this does hold for L_1 sufficiently small. One might wish to understand this difference between d = 1 and d > 1 by observing that only in d > 1 can one construct nontrivial divergence free vector fields. The homogenized limit of diffusion perturbed by a divergence free vector field necessarily yields an effective diffusion constant which is larger than the constant for the pure diffusion [10].

The homogenization problem considered here appears to have only been studied in the case where Ω is an infinite space for which the variables $b(\tau_x \cdot)$, $x \in \mathbb{R}$, are uncorrelated on a scale larger than O(1). The problem was introduced by Sinai [18] in a discrete setting. He proved that in dimension d=1 a scaling limit of the random walk corresponding to a finite difference approximation to (1.1) exists with probability 1 in Ω . The limiting process is strongly subdiffusive. In a subsequent paper Kesten [12] obtained an explicit formula for the distribution of the scaling limit. For dimension $d \geq 3$ Fisher [11] and Derrida-Lück [9] predicted that a homogenized limit exists as in (1.2) with $0 < q(b) < \infty$. This was proved for sufficiently small b by Bricmont-Kupiainen [4] and Sznitman-Zeitouni [21] using a very difficult induction argument. A formal perturbation expansion for q(b) was obtained in [5, 6] where it was shown that each term of the expansion is finite if $d \geq 3$. One does not expect the series to converge however. For d=1,2 there are individual terms in the perturbation expansion which diverge.

A main difficulty in the homogenization problem (1.1), (1.2) is that when Ω is infinite, good a-priori estimates on the solution to (1.1) do not hold for all configurations of $b(\cdot)$. In contrast such estimates do hold for divergence form equations with zero drift. The proof of homogenization in these cases is therefore considerably simpler than for the problem (1.1), (1.2). The first proofs of homogenization for divergence form equations were obtained by Kozlov [13] and Papanicolaou-Varadhan [16] in the continuous case. Künneman [14] proved a corresponding result for the discrete case. For non-divergence form equations with zero drift the

first proofs in the continuous case were given by Papanicolaou-Varadhan [17] and Zhikov-Sirazhudinov [23]. Lawler [15] and Anshelevich et al [1] proved homogenization for a discrete version. See the books of Bolthausen-Sznitman [3] for an account of the theory in a discrete setting and of Zhikov et al [22] for the continuous case.

In this paper we shall be concerned with a discrete version of the homogenization problem described by (1.1), (1.2), (1.3). Thus the probability space Ω is acted upon by translation operators $\tau_x : \Omega \to \Omega$ where now $x \in \mathbb{Z}^d$, the integer lattice in \mathbb{R}^d , and satisfy the group properties $\tau_x \ \tau_y = \tau_{x+y}, \ \tau_0 = \text{identity}$. For $i = 1, \ldots, d$ let $\mathbf{e}_i \in \mathbb{Z}^d$ be the element with entry 1 in the ith position and 0 in the other positions. the discrete equation corresponding to (1.1) is given by

$$u_{\varepsilon}(x,\omega) - \sum_{i=1}^{d} \frac{1}{2d} \left[u_{\varepsilon}(x + \varepsilon \mathbf{e}_{i}, \omega) + u_{\varepsilon}(x - \varepsilon \mathbf{e}_{i}, \omega) \right]$$

$$- b(\tau_{x/\varepsilon}\omega) \left[u_{\varepsilon}(x + \varepsilon \mathbf{e}_{1}, \omega) - u_{\varepsilon}(x - \varepsilon \mathbf{e}_{1}, \omega) \right] + \varepsilon^{2} u_{\varepsilon}(x,\omega)$$

$$= \varepsilon^{2} f(x), \quad x \in \mathbb{Z}^{d} = \varepsilon \mathbb{Z}^{d}, \quad \omega \in \Omega.$$

$$(1.5)$$

We assume that $b:\Omega\to\mathbb{R}$ satisfies $\sup_{\omega}|b(\omega)|<1/2d$, in which case (1.5) is an equation for the expectation value of a function of an asymmetric random walk. Hence (1.5) has a unique bounded solution. We assume that b satisfies the reflection invariant condition (1.3) (with $x_i\in\mathbb{Z}^d, 1\leq i\leq n$, now). We also assume that Ω is finite, in which case one can see (Lemma 2.4) that Ω is isomorphic to the integer points on a torus and b has the reflection invariance property (1.4). In §2 we prove the following theorem (with $|\cdot|$ denoting the integer part):

Theorem 1.1. Assume Ω is a finite probability space and the translation operators $\tau_x: \Omega \to \Omega$ are ergodic, $x \in \mathbb{Z}^d$. Then there exists q(b), $0 < q(b) < \infty$ such that with u_{ε} the solution to (1.5) and u the solution to (1.2),

$$\lim_{\varepsilon \to 0} \sup_{x \in \mathbb{R}^d, \omega \in \Omega} |u_{\varepsilon}(\varepsilon \lfloor x/\varepsilon \rfloor, \omega) - u(x)| = 0.$$

One should note here that Theorem 1.1 may be obtained from a homogenization theorem for divergence form operators. This follows from the representation

$$\mathcal{L} = \Delta + b.\nabla = (1/\phi^*)\operatorname{div}(\phi^*(I+H)\nabla\cdot), \tag{1.6}$$

where ϕ^* is the invariant measure for \mathcal{L} on Ω and H is an antisymmetric matrix. This follows since (1.3) implies that $\langle b(\cdot)\phi^*(\cdot)\rangle = 0$.

Suppose now that Ω consists of the integer points on the torus $\prod_{i=1}^d [0, L_i] \subset \mathbb{R}^d$ with periodic boundary conditions. The reflection invariant condition corresponding to (1.4) is given by

$$b(x_1, x_2, \dots, x_d) = -b(L_1 - 1 - x_1, x_2, \dots, x_d), \quad x = (x_1, x_2, \dots, x_d) \in \Omega.$$
 (1.7)

For b satisfying (1.7) we prove in §2, §3 the following results concerning the coefficient q(b) of the homogenized equation (1.2):

Theorem 1.2. (a) For d = 1 one has $q(b) \le 1/2$.

- (b) If $d \ge 1$ and $L_1 = 2$ one has $q(b) \le 1/2d$.
- (c) If d = 2 and $L_1 = 4$ one has $q(b) \le 1/4$.
- (d) If $d \ge 2$ and $L_1 \ge 6$ is even then there exists b with q(b) > 1/2d.

The proofs of (a), (b), (c) are given in $\S 3$ and are based on applications of the Schwarz inequality to certain representations of q(b) obtained in $\S 2$. The proof

of (c) is quite lengthy. Basically one shows that $q(b) \leq 1/4$ provided a quadratic form corresponding to a fourth order difference operator is non-negative definite. The non-negative definiteness of the quadratic form depends crucially on actual numerical values for a Green's function associated with standard random walk on the integers. The proof of (d) is given in §2. One observes that perturbation theory yields $q(b) = 1/2d + O(|b|^2)$ and that the term $O(|b|^2)$ can be positive.

In the proof of Theorem 1.2 we use a representation for q(b) in terms of invariant measures for random walk on Ω with drift b. Let Ω_{d-1} consist of the integer points on the d-1 dimensional torus $\prod_{i=2}^d [0,L_i] \subset \mathbb{R}^{d-1}$ with periodic boundary conditions. Setting $L_1 = 2L$ with L an integer we define $\hat{\Omega}$ by

$$\hat{\Omega} = \{(n, y) : 1 \le n \le L, y \in \Omega_{d-1}\},\$$

whence Ω is the double of $\hat{\Omega}$. Observe that the boundary of $\partial \hat{\Omega}$ is given by

$$\partial \hat{\Omega} = \{(1, y), (L, y) : y \in \Omega_{d-1}\}.$$

Let φ^* be the invariant measure for random walk on $\hat{\Omega}$ with drift $b(\cdot)$ in the \mathbf{e}_1 direction and reflecting boundary conditions on $\partial \hat{\Omega}$. The normalization of φ^* is chosen so that $\langle \varphi^* \rangle_{\hat{\Omega}} = 1$ where $\langle \cdot \rangle_{\hat{\Omega}}$ is the uniform probability measure on $\hat{\Omega}$. We define $\psi: \Omega_{d-1} \to \mathbb{R}$ by

$$\psi(y) = [1/2d - b(1, y)] \varphi^*(1, y), y \in \Omega_{d-1},$$

Then q(b) is given by the formula,

$$q(b) = 8d\langle \psi \left[-\Delta_{d-1} + 4 \right]^{-1} \psi_R \rangle_{\Omega_{d-1}},$$
 (1.8)

where ψ_R is defined exactly as ψ but with b replaced by -b. In (1.8) the expectation $\langle \cdot \rangle_{\Omega_{d-1}}$ is the uniform probability measure on Ω_{d-1} and Δ_{d-1} is the d-1 dimensional finite difference Laplacian on functions with domain Ω_{d-1} . The general formula (1.8) is proven in §4.

2. Proof of Theorem 1.1

We follow the method introduced in [8] to obtain homogenized limits. Thus in (1.5) we put $u_{\varepsilon}(x,\omega) = v_{\varepsilon}(x,\tau_{x/\varepsilon} \omega)$ whence (1.5) becomes

$$v_{\varepsilon}(x,\omega) - \sum_{i=1}^{2d} \frac{1}{2d} \left[v_{\varepsilon}(x + \varepsilon \mathbf{e}_{i}, \tau_{\mathbf{e}_{i}} \ \omega) + v_{\varepsilon}(x - \varepsilon \mathbf{e}_{i}, \tau_{-\mathbf{e}_{i}} \ \omega) \right]$$

$$- b(\omega) \left[v_{\varepsilon}(x + \varepsilon \mathbf{e}_{1}, \tau_{\mathbf{e}_{1}} \ \omega) - v_{\varepsilon}(x - \varepsilon \mathbf{e}_{1}, \tau_{-\mathbf{e}_{1}} \ \omega) \right]$$

$$+ \varepsilon^{2} v_{\varepsilon}(x,\omega)$$

$$= \varepsilon^{2} f(x), \quad x \in \mathbb{Z}_{\varepsilon}^{d} = \varepsilon \mathbb{Z}^{d}, \quad \omega \in \Omega.$$

$$(2.1)$$

Next we wish to take the Fourier transform of (2.1). To show that this is legitimate we first show that the solution $u_{\varepsilon}(x,\omega)$ of (1.5) decreases exponentially as $x\to\infty$.

Lemma 2.1. Suppose $f: \mathbb{Z}^d_{\varepsilon} \to \mathbb{R}$ has finite support in the set $\{x = (x_1, \dots, x_d) \in \mathbb{Z}^d_{\varepsilon} : |x| < R\}$. Let $u_{\varepsilon}(x, \omega)$ be a bounded solution to (1.5). Then there are constants $C, K(\varepsilon) > 0$ such that

$$|u_{\varepsilon}(x,\omega)| \le C \exp[K(\varepsilon)(R-|x|)] ||f||_{\infty}, \quad x \in \mathbb{Z}_{\varepsilon}^{d}.$$
 (2.2)

Proof. We write $u_{\varepsilon}(x,\omega) = e^{-kx_1} u_{\varepsilon,k}(x,\omega)$. Then from (1.5) the function $u_{\varepsilon,k}$ satisfies

$$\frac{1}{2d} \sum_{i=2}^{d} \left[2u_{\varepsilon,k}(x,\omega) - u_{\varepsilon,k}(x + \varepsilon \mathbf{e}_{i},\omega) - u_{\varepsilon,k}(x - \varepsilon \mathbf{e}_{i},\omega) \right] / \varepsilon^{2}
+ e^{-k\varepsilon} \left[\frac{1}{2d} + b(\tau_{x/\varepsilon}\omega) \right] \left\{ u_{\varepsilon,k}(x,\omega) - u_{\varepsilon,k}(x + \varepsilon \mathbf{e}_{1},\omega) \right\} / \varepsilon^{2}
+ e^{k\varepsilon} \left[\frac{1}{2d} - b(\tau_{x/\varepsilon}\omega) \right] \left\{ u_{\varepsilon,k}(x,\omega) - u_{\varepsilon,k}(x - \varepsilon \mathbf{e}_{1},\omega) \right\} / \varepsilon^{2}
+ \left\{ 1 - \left[\cosh k\varepsilon - 1 \right] / d\varepsilon^{2} + 2b(\tau_{x/\varepsilon}\omega) \sinh k\varepsilon / \varepsilon^{2} \right\} u_{\varepsilon,k}(x,\omega)
= e^{kx_{1}} f(x), \quad x \in \mathbb{Z}_{c}^{d}.$$
(2.3)

We may assume without loss of generality (wlog) that f is nonnegative, whence $u_{\varepsilon,k}$ is also nonnegative. Suppose $u_{\varepsilon,k}$ attains its maximum at a point $\bar{x} \in \mathbb{Z}_{\varepsilon}^d$. Then we have that

$$\left\{1 - \left[\cosh k\varepsilon - 1\right]/d\varepsilon^2 + 2b(\tau_{\bar{x}/\varepsilon} \omega) \sinh k\varepsilon/\varepsilon^2\right\} u_{\varepsilon,k}(\bar{x},\omega)
\leq \exp\left[k(\bar{x} \cdot \mathbf{e}_1)\right] ||f||_{\infty}, \quad |\bar{x}| < R.$$
(2.4)

Observe that the coefficient of $u_{\varepsilon,k}(\bar{x},\omega)$ on the LHS of (2.4) is positive if k is sufficiently small. Hence it follows that

$$u_{\varepsilon}(x,\omega) \le C \exp\left[k(\bar{x}-x) \cdot \mathbf{e}_1\right] \|f\|_{\infty}, \ x \in \mathbb{Z}_{\varepsilon}^d.$$
 (2.5)

We need to show that the point \bar{x} exists for sufficiently small k. To see this assume for contradiction that it does not exist. Then (2.3) implies that $a_N = \sup_{|x| \le N} u_{\varepsilon,k}(x,\omega)$ grows exponentially in N as $N \to \infty$. This follows since we see from (2.3) that if N > R then there is a positive α such that $a_{N+1} \ge (1+\alpha)a_N$. The rate of exponential growth remains bounded away from 0 as $k \to 0$. Hence, taking k sufficiently small, we conclude that the function u_{ε} is unbounded, contradicting our assumption on u_{ε} . The inequality (2.2) now follows from (2.4), (2.5) on generalizing to all directions \mathbf{e}_j , $1 \le j \le d$.

For $\xi \in [-\pi/\varepsilon, \pi/\varepsilon]^d$ we put

$$\hat{v}_{\varepsilon}(\xi,\omega) = \int_{\mathbb{Z}_{\varepsilon}^{d}} v_{\varepsilon}(x,\omega) e^{ix\cdot\xi} dx = \sum_{x\in\mathbb{Z}_{\varepsilon}^{d}} \varepsilon^{d} v_{\varepsilon}(x,\omega) e^{ix\cdot\xi}. \tag{2.6}$$

Then from (2.1) we have that

$$\hat{v}_{\varepsilon}(\xi,\omega) - \sum_{j=1}^{d} \frac{1}{2d} \left[e^{-i\varepsilon\xi_{j}} \hat{v}_{\varepsilon}(\xi,\tau_{\mathbf{e}_{j}}\omega) + e^{i\varepsilon\xi_{j}} \hat{v}_{\varepsilon}(\xi,\tau_{-\mathbf{e}_{j}}\omega) \right] - b(\omega) \left[e^{-i\varepsilon\xi_{1}} \hat{v}_{\varepsilon}(\xi,\tau_{\mathbf{e}_{1}}\omega) - e^{i\varepsilon\xi_{1}} \hat{v}_{\varepsilon}(\xi,\tau_{-\mathbf{e}_{1}}\omega) \right] + \varepsilon^{2} \hat{v}_{\varepsilon}(\xi,\omega) = \varepsilon^{2} \hat{f}_{\varepsilon}(\xi), \quad \xi \in [-\pi/\varepsilon,\pi/\varepsilon]^{d}, \ \omega \in \Omega,$$

$$(2.7)$$

where \hat{f}_{ε} denotes the discrete Fourier transform (2.6) of f. To solve (2.7) we define for $\zeta \in [-\pi, \pi]^d$ an operator \mathcal{L}_{ζ} on functions $\Psi : \Omega \to \mathbb{C}$ defined by

$$\mathcal{L}_{\zeta}\Psi(\omega) = \Psi(\omega) - \sum_{j=1}^{d} \frac{1}{2d} \left[e^{-i\zeta_{j}} \Psi(\tau_{\mathbf{e}_{j}}\omega) + e^{i\zeta_{j}} \Psi(\tau_{-\mathbf{e}_{j}}\omega) \right] - b(\omega) \left[e^{-i\zeta_{1}} \Psi(\tau_{\mathbf{e}_{1}}\omega) - e^{i\zeta_{1}} \Psi(\tau_{-\mathbf{e}_{1}}\omega) \right].$$
(2.8)

Next we define an operator $T_{\eta,\zeta}, \ \eta > 0, \ \zeta \in [-\pi,\pi]^d$ on $L^{\infty}(\Omega)$ by

$$T_{\eta,\zeta} \varphi(\omega) = \eta \left[\mathcal{L}_{\zeta} + \eta \right]^{-1} \varphi(\omega), \quad \omega \in \Omega.$$
 (2.9)

It is easy to see that $T_{\eta,\zeta}$ is a bounded operator on $L^{\infty}(\Omega)$ with norm at most 1. In fact the RHS of (2.9) is the expectation for a continuous time random walk on $\Omega \times \mathbb{Z}^d$. The walk is defined as follows:

- (a) The waiting time at $(\omega, x) \in \Omega \times \mathbb{Z}^d$ is exponential with parameter 1.
- (b) For j = 2, ..., d the particle jumps from (ω, x) to $(\tau_{\mathbf{e}_j} \omega, x + \mathbf{e}_j)$ with probability 1/2d and to $(\tau_{-\mathbf{e}_j} \omega, x \mathbf{e}_j)$ with probability 1/2d.
- (c) The particle jumps from (ω, x) to $(\tau_{\mathbf{e}_1}\omega, x + \mathbf{e}_1)$ with probability $1/2d + b(\omega)$, and to $(\tau_{-\mathbf{e}_1}\omega, x \mathbf{e}_1)$ with probability $1/2d b(\omega)$.

If $[\omega(t), X(t)] \in \Omega \times \mathbb{Z}^d$ is the position of the walk at time t then

$$T_{\eta,\zeta}\varphi(\omega) = \eta E \left[\int_0^\infty dt \ e^{-\eta t} \varphi(\omega(t)) \exp[-iX(t) \cdot \zeta] \middle| \omega(0) = \omega, \ X(0) = 0 \right]. \quad (2.10)$$

It is clear from the representation (2.10) that $||T_{\eta,\zeta}||_{\infty} \leq 1$. We conclude from this that (2.7) is solvable with solution given by

$$\hat{v}_{\varepsilon}(\xi,\omega) = \hat{f}_{\varepsilon}(\xi) \ T_{\varepsilon^{2},\varepsilon\xi}(1)(\omega), \ \omega \in \Omega, \ \xi \in [-\pi/\varepsilon,\pi/\varepsilon]^{d}.$$
 (2.11)

To obtain the homogenization theorem we need then to obtain the limit of the RHS of (2.11) as $\varepsilon \to 0$. To facilitate this we observe from (2.8) that

$$[\mathcal{L}_{\zeta} + \eta] 1 = 1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_j + 2ib(\omega) \sin \zeta_1.$$
 (2.12)

It follows therefore that

$$T_{\eta,\zeta}(1)(\omega) = \eta / \left[1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_j \right] - \left\{ 2i \sin \zeta_1 / \left[1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_j \right] \right\} T_{\eta,\zeta} b(\omega).$$

$$(2.13)$$

Setting $\eta = \varepsilon^2$, $\zeta = \varepsilon \xi$ for some fixed $\xi \in \mathbb{R}^d$ we see from (2.13) that

$$\lim_{\varepsilon \to 0} T_{\varepsilon^2, \varepsilon\xi}(1)(\omega) = 1 / \left[1 + \frac{1}{2d} \sum_{j=1}^d \xi_j^2 \right] - \left\{ 2i\xi_1 / \left[1 + \frac{1}{2d} \sum_{j=1}^d \xi_j^2 \right] \right\} \lim_{\varepsilon \to 0} \varepsilon^{-1} T_{\varepsilon^2, \varepsilon\xi} b(\omega). \tag{2.14}$$

We shall show that under the assumption of (1.3) the limit on the RHS of (2.14) exists. To do this we define two subspaces of the space $L^{\infty}(\Omega)$. We define $L_{R}^{\infty}(\Omega)$ as all functions $\Phi \in L^{\infty}(\Omega)$ such that

$$\left\langle \Phi(\tau_x \cdot) \prod_{i=1}^n b(\tau_{x_i} \cdot) \right\rangle = (-1)^{n+1} \left\langle \Phi(\tau_{Rx} \cdot) \prod_{i=1}^n b(\tau_{Rx_i} \cdot) \right\rangle,$$

with $x, x_i \in \mathbb{Z}^d$, $1 \leq i \leq n$, $n = 0, 1, 2, \ldots$ Evidently (1.3) implies that $b \in L^\infty_R(\Omega)$. We also see that if $\Phi \in L^\infty_R(\Omega)$ then $\Phi(\tau_{\mathbf{e_j}}\cdot)$ and $\Phi(\tau_{-\mathbf{e_j}}\cdot)$ are also in $L^\infty_R(\Omega)$, $j = 2, \ldots, d$. For j = 1 one has that $\Phi \in L^\infty_R(\Omega)$ implies both $[\Phi(\tau_{\mathbf{e_1}}\cdot) + \Phi(\tau_{-\mathbf{e_1}}\cdot)]$ and $b(\cdot)[\Phi(\tau_{\mathbf{e_1}}\cdot) - \Phi(\tau_{-\mathbf{e_1}}\cdot)]$ are in $L^\infty_R(\Omega)$. The space $\hat{L}^\infty_R(\Omega)$ is defined similarly as all functions $\Phi \in L^\infty(\Omega)$ such that

$$\left\langle \Phi(\tau_x \cdot) \prod_{i=1}^n b(\tau_{x_i} \cdot) \right\rangle = (-1)^n \left\langle \Phi(\tau_{Rx} \cdot) \prod_{i=1}^n b(\tau_{Rx_i} \cdot) \right\rangle,$$

with $x, x_i \in \mathbb{Z}^d$, $1 \leq i \leq n$, $n = 0, 1, 2, \ldots$ ¿From (1.3) we see that the function $\Phi \equiv 1$ is in $\hat{L}_R^{\infty}(\Omega)$. As for the space $L_R^{\infty}(\Omega)$, if $\Phi \in \hat{L}_R^{\infty}(\Omega)$ then $\Phi(\tau_{\mathbf{e_j}}\cdot)$ and $\Phi(\tau_{-\mathbf{e_j}}\cdot)$ are also in $\hat{L}_R^{\infty}(\Omega), j = 2, \ldots, d$. Similarly both $[\Phi(\tau_{\mathbf{e_1}}\cdot) + \Phi(\tau_{-\mathbf{e_1}}\cdot)]$ and $b(\cdot)[\Phi(\tau_{\mathbf{e_1}}\cdot) - \Phi(\tau_{-\mathbf{e_1}}\cdot)]$ are in $\hat{L}_R^{\infty}(\Omega)$. We note that the mapping $\Phi(\cdot) \to b(\cdot)\Phi(\cdot)$ maps $L_R^{\infty}(\Omega)$ into $\hat{L}_R^{\infty}(\Omega)$ and vice-versa.

We denote the operator \mathcal{L}_{ζ} of (2.8) for $\zeta=0$ by \mathcal{L} . It is evident that \mathcal{L} is the generator of a random walk on Ω . Hence the kernel of the operator \mathcal{L} is just the constant function. Furthermore \mathcal{L} leaves the space $L_R^{\infty}(\Omega)$ invariant. Since the constant function is not in $L_R^{\infty}(\Omega)$ it follows that there is a unique function $\varphi \in L_R^{\infty}(\Omega)$ such that

$$\mathcal{L}\varphi = b. \tag{2.15}$$

Let φ^* be the invariant measure for the walk on Ω generated by \mathcal{L} . Thus $\varphi^* > 0$,

$$\mathcal{L}^* \varphi^* = 0, \quad \langle \varphi^* \rangle = 1, \tag{2.16}$$

where \mathcal{L}^* is the adjoint of \mathcal{L} . Since \mathcal{L} is non singular on the space $L_R^{\infty}(\Omega)$ it follows that φ^* is orthogonal to $L_R^{\infty}(\Omega)$. We can also see that $\varphi^* \in \hat{L}_R^{\infty}(\Omega)$. One simply notes that both \mathcal{L} and \mathcal{L}^* leave the space $\hat{L}_R^{\infty}(\Omega)$ invariant and that the constant function is in $\hat{L}_R^{\infty}(\Omega)$. We obtain the limit on the RHS of (2.14) in terms of the functions φ, φ^* defined by (2.15), (2.16).

Lemma 2.2. Let $\psi \in L^{\infty}(\Omega)$ be defined by

$$\psi(\cdot) = \left\{ \frac{1}{2d} + b(\cdot) \right\} \varphi(\tau_{\mathbf{e}_1} \cdot) - \left\{ \frac{1}{2d} - b(\cdot) \right\} \varphi(\tau_{-\mathbf{e}_1} \cdot), \tag{2.17}$$

where φ is given by (2.15). Then if φ^* is as in (2.16) there is the limit,

$$\lim_{\varepsilon \to 0} \varepsilon^{-1} T_{\varepsilon^2, \varepsilon \xi} b(\omega) = -i\xi_1 < \varphi^* \psi > / \left[1 + \frac{1}{2d} \sum_{j=1}^d \xi_j^2 + 2\xi_1^2 < \varphi^* \psi > \right], \quad (2.18)$$

for all $\omega \in \Omega$, provided ξ_1 is sufficiently small.

Proof. For $\eta > 0$, $\zeta \in [-\pi, \pi]^d$, let $\varphi(\eta, \zeta)$ be the unique solution to the equation

$$[\mathcal{L}_{\zeta} + \eta]\varphi(\eta, \zeta) = b. \tag{2.19}$$

It is clear then that

$$\varepsilon^{-1} T_{\varepsilon^2, \varepsilon \xi} b = \varepsilon \varphi(\varepsilon^2, \varepsilon \xi). \tag{2.20}$$

We define operators A_{ζ}, B_{ζ} by $A_{\zeta} = [\mathcal{L}_{\zeta} + \mathcal{L}_{R\zeta}]/2$, $B_{\zeta} = [\mathcal{L}_{\zeta} - \mathcal{L}_{R\zeta}]/2$, where $R(\zeta_1, \ldots, \zeta_d) = (-\zeta_1, \zeta_2, \ldots, \zeta_d)$. The operator A_{ζ} leaves the spaces $L_R^{\infty}(\Omega), \hat{L}_R^{\infty}(\Omega)$ invariant whereas B_{ζ} takes $L_R^{\infty}(\Omega)$ into $\hat{L}_R^{\infty}(\Omega)$ and vice versa. Equation (2.19) is now equivalent to

$$[(A_{\zeta} + \eta) + B_{\zeta}] \varphi(\eta, \zeta) = b , \qquad (2.21)$$

and we may write the solution of this formally as a power series,

$$\varphi(\eta,\zeta) = \sum_{n=0}^{\infty} \left\{ -(A_{\zeta} + \eta)^{-1} B_{\zeta} \right\}^{n} (A_{\zeta} + \eta)^{-1} b.$$
 (2.22)

The operators B_{ζ} , $(A_{\zeta} + \eta)^{-1}$ on $L^{\infty}(\Omega)$ have norms satisfying $||B_{\zeta}|| \leq C_2 |\zeta_1|$, $||(A_{\zeta} + \eta)^{-1}|| \leq 1/\eta$, for some constant C_2 . Since $A_0 = \mathcal{L}$ is invertible on $L_R^{\infty}(\Omega)$ it follows that for (η, ζ) sufficiently small the operator norm of $(A_{\zeta} + \eta)^{-1}$ acting on

 $L_R^{\infty}(\Omega)$ satisfies $||(A_{\zeta} + \eta)^{-1}|| \leq C_1$ for some constant C_1 . We conclude therefore for (η, ζ) sufficiently small that

$$\|\{(A_{\zeta} + \eta)^{-1}B_{\zeta}\}^{n}(A_{\zeta} + \eta)^{-1}b\|_{\infty} \le C_{2}^{n}|\zeta_{1}|^{n}C_{1}^{n+1-r}\eta^{-r}\|b\|_{\infty}, \qquad (2.23)$$

where r = n/2 if n is even, r = (n+1)/2 if n is odd. Hence if (η, ζ) and $|\zeta_1|^2/\eta$ are small then the series in (2.22) converges in $L^{\infty}(\Omega)$ to the solution of (2.21). It follows that for $\xi \in \mathbb{R}^d$ fixed with ξ_1 sufficiently small we may construct the function $\varphi(\varepsilon^2, \varepsilon\xi)$ by means of (2.22) as $\varepsilon \to 0$.

To obtain the limit in (2.18) we write

$$\varphi(\eta,\zeta) = \varphi_1(\eta,\zeta) + \varphi_2(\eta,\zeta) \tag{2.24}$$

where $\varphi_1(\eta,\zeta)$ is the sum on the RHS of (2.22) over odd powers of n. It is evident from (2.23) that for $|\xi_1| < 1/C_2\sqrt{C_1}$ one has

$$\lim_{\varepsilon \to 0} \varepsilon \varphi_2(\varepsilon^2, \varepsilon \xi) = 0. \tag{2.25}$$

We consider the first term in the sum for φ_1 . Setting $\eta = \varepsilon^2$, $\zeta = \varepsilon \xi$ and multiplying the term by ε as in (2.20) we see that

$$-\lim_{\varepsilon \to 0} \varepsilon \left(A_{\varepsilon\xi} + \varepsilon^2 \right)^{-1} B_{\varepsilon\xi} \left(A_{\varepsilon\xi} + \varepsilon^2 \right)^{-1} b$$

$$= -\lim_{\varepsilon \to 0} i \varepsilon^2 \xi_1 \left(A_{\varepsilon\xi} + \varepsilon^2 \right)^{-1} \left[\left\{ \frac{1}{2d} + b(\cdot) \right\} \varphi(\tau_{\mathbf{e}_1} \cdot) - \left\{ \frac{1}{2d} - b(\cdot) \right\} \varphi(\tau_{-\mathbf{e}_1} \cdot) \right],$$

where φ is the solution of (2.15). Observe now that for any $\psi \in L^{\infty}(\Omega)$ we have

$$-\lim_{\varepsilon \to 0} i\varepsilon^2 \xi_1 \left(A_{\varepsilon\xi} + \varepsilon^2 \right)^{-1} \psi = -i\xi_1 \langle \varphi^* \psi \rangle \lim_{\varepsilon \to 0} \varepsilon^2 \left(A_{\varepsilon\xi} + \varepsilon^2 \right)^{-1} 1,$$

where φ^* is the solution of (2.16). From (2.12) we have that

$$\varepsilon^2 \left(A_{\varepsilon \xi} + \varepsilon^2 \right)^{-1} 1 = \varepsilon^2 / \left[1 + \varepsilon^2 - \frac{1}{d} \sum_{i=1}^d \cos \varepsilon \xi_i \right],$$

whence we conclude that

$$\lim_{\varepsilon \to 0} \varepsilon^2 \left(A_{\varepsilon \xi} + \varepsilon^2 \right)^{-1} = 1 / \left[1 + \frac{1}{2d} \sum_{i=1}^d \xi_j^2 \right].$$

We have therefore obtained a formula for the limit as $\varepsilon \to 0$ of the first term in the series representation of $\varepsilon \varphi_1(\varepsilon^2, \varepsilon \xi)$. Using the same argument we can obtain a formula for all the terms. For the rth term corresponding to r = (n+1)/2 with n as in (2.22) we see that the limit is given by the formula

$$\frac{i}{2\xi_1} \left\{ -2\xi_1^2 \left\langle \varphi^* \psi \right\rangle \middle/ \left[1 + \frac{1}{2d} \sum_{j=1}^d \xi_j^2 \right] \right\}^r, \tag{2.26}$$

where ψ is the function (2.17). Evidently $\psi \in \hat{L}_R^{\infty}(\Omega)$. We have already observed that φ^* is also in $\hat{L}_R^{\infty}(\Omega)$. We conclude that

$$\lim_{\varepsilon \to 0} \varepsilon \varphi_1(\varepsilon^2, \varepsilon \xi) = -i\xi_1 \langle \varphi^* \psi \rangle / \left[1 + \frac{1}{2d} \sum_{j=1}^d \xi_j^2 + 2\xi_1^2 \langle \varphi^* \psi \rangle \right].$$

Then (2.18) follows from this and (2.25).

Lemma 2.1 enables us to compute the limit (2.14) when ξ_1 is small. We have

$$\lim_{\varepsilon \to 0} T_{\varepsilon^2, \varepsilon \xi}(1)(\omega) = 1 / \left[1 + \frac{1}{2d} \sum_{j=1}^d \xi_j^2 + 2\xi_1^2 \langle \varphi^* \psi \rangle \right]. \tag{2.27}$$

We wish now to extend the identity (2.27) to all $\xi \in \mathbb{R}^d$.

Lemma 2.3. Let $K \subset \mathbb{R}^d$ be a compact set. Then the limit (2.18) is uniform for $\xi \in K$, $\omega \in \Omega$.

Proof. Since the LHS of (2.27) does not exceed 1 in absolute value we conclude that

$$\frac{1}{2d} + 2\langle \varphi^* \psi \rangle \ge 0. \tag{2.28}$$

The inequality (2.28) in turn implies that the expression (2.26) is the rth power of a number strictly less than 1 provided we also assume that

$$2\left\langle \varphi^*\psi\right\rangle \le 1/2d. \tag{2.29}$$

We show that the power series methods of Lemma 2.1 apply to prove the result under the additional assumption (2.29). We shall see in §3 that $\langle \varphi^* \psi \rangle \leq 0$ for dimension d=1, in which case (2.29) certainly holds. Since the constant function is the unique eigenvector of $A_0 = \mathcal{L}$ with eigenvalue 0 and it is also an eigenvector of A_{ζ} it follows that there exists $\delta > 0$ such that if $|\zeta| < \delta$ then the adjoint A_{ζ}^* of A_{ζ} has a unique eigenvector φ_{ζ}^* with eigenvalue equal to the eigenvalue of A_{ζ} for the constant function. Normalizing φ_{ζ}^* so that $\langle \varphi_{\zeta}^* \rangle = 1$, it is easy to see that there is a constant C_1 such that

$$\|\varphi_{\zeta}^* - \varphi^*\|_{\infty} \le C_1|\zeta|, \quad |\zeta| < \delta. \tag{2.30}$$

For $|\zeta| < \delta$, $\eta > 0$ we define a projection $P_{n,\zeta}$ by

$$P_{\eta,\zeta} \psi = \langle \bar{\varphi}_{\zeta}^* \psi \rangle (A_{\zeta} + \eta)^{-1} 1, \quad \psi \in L^{\infty}(\Omega).$$

Then there is a constant C_2 such that

$$\|(A_{\zeta} + \eta)^{-1} - P_{\eta,\zeta}\| \le C_2, \ |\zeta| < \delta. \tag{2.31}$$

The uniform convergence of (2.18) for $\xi \in K$ follows now from (2.30), (2.31) just as in Lemma 2.1.

Finally we consider the situation where (2.29) is violated. As in Lemma 2.1 we decompose the solution $\varphi(\eta,\zeta)$ of (2.19) into a sum (2.24). The function $\varphi_1(\eta,\zeta)$ is a solution to the equation,

$$\[A_{\zeta} + \eta - B_{\zeta} (A_{\zeta} + \eta)^{-1} B_{\zeta} \] \varphi_{1}(\eta, \zeta) = -B_{\zeta} (A_{\zeta} + \eta)^{-1} b. \tag{2.32}$$

The function $\varphi_2(\eta,\zeta)$ is a solution to the equation,

$$\left[A_{\zeta} + \eta - B_{\zeta} \left(A_{\zeta} + \eta \right)^{-1} B_{\zeta} \right] \varphi_{2}(\eta, \zeta) = b.$$
 (2.33)

It is easy to see that if $\varphi_2(\eta,\zeta)$ is a solution of (2.33) then the function $\varphi_1(\eta,\zeta) = \varphi(\eta,\zeta) - \varphi_2(\eta,\zeta)$, where $\varphi(\eta,\zeta)$ solves (2.19), is a solution to (2.32). Hence if (2.32),(2.33) have unique solutions $\varphi_1(\eta,\zeta), \varphi_2(\eta,\zeta)$ then the identity (2.24) holds.

We show that (2.33) has a unique solution in $L_R^{\infty}(\Omega)$ provided $\eta > 0$ and (η, ζ) are sufficiently small. To see this we write (2.33) as

$$[A_{\zeta} + \eta - L_{n,\zeta} - B_{\zeta} P_{n,\zeta} B_{\zeta}] \varphi_2(\eta,\zeta) = b, \tag{2.34}$$

where by (2.31) the operator $L_{\eta,\zeta}$ is invariant on $L_R^{\infty}(\Omega)$ and satisfies $||L_{\eta,\zeta}|| \leq C|\zeta|^2$ for some constant C. Next let $\varphi_3(\eta,\zeta)$ be the solution to

$$[A_{\zeta} + \eta - L_{n,\zeta}] \varphi_3(\eta,\zeta) = b. \tag{2.35}$$

For (η,ζ) small there is a unique solution to (2.35) in $L_R^{\infty}(\Omega)$ which satisfies

$$\|\varphi - \varphi_3(\eta, \zeta)\|_{\infty} \le C[|\eta| + |\zeta|^2], \tag{2.36}$$

for some constant C, where φ is the solution of (2.15). Now it is easy to see that the solution $\varphi_2(\eta,\zeta)$ of (2.34) is given in terms of $\varphi_3(\eta,\zeta)$ by the formula

$$\varphi_{2}(\eta,\zeta) = \left[1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_{j}\right] \varphi_{3}(\eta,\zeta)
\div \left[1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_{j} + 2\left\langle \bar{\varphi}_{\zeta}^{*} B \varphi_{3}(\eta,\zeta) \right\rangle \sin^{2} \zeta_{1}\right],$$
(2.37)

where the operator B is defined by $B_{\zeta} = i \sin \zeta_1 B$. In view of (2.36) and the fact that $B\varphi = \psi$ and we are assuming (2.29) is violated, it follows that the denominator in (2.37) is positive for (η, ζ) sufficiently small. We have shown a solution $\varphi_2(\eta, \zeta)$ of (2.34) exists in $L_R^{\infty}(\Omega)$. The uniqueness of the solution follows from the uniqueness of the solution to (2.35). Evidently the limit (2.25) follows from (2.36), (2.37) for all ξ and is uniform for ξ restricted to a compact subset of \mathbb{R}^d .

Next we show that (2.32) has a unique solution in $L_R^{\infty}(\Omega)$ provided $\eta > 0$ and (η, ζ) are sufficiently small. First note that for (η, ζ) small the operator $B_{\zeta}(A_{\zeta} + \eta)^{-1}B_{\zeta}$ leaves $\hat{L}_R^{\infty}(\Omega)$ invariant and there is a constant C such that

$$||B_{\zeta}(A_{\zeta} + \eta)^{-1}B_{\zeta}|| \le C|\zeta|^{2}.$$
 (2.38)

We define the subspace \mathcal{E}_{ζ} of $\hat{L}_{R}^{\infty}(\Omega)$ by

$$\mathcal{E}_{\zeta} = \left\{ \psi \in \hat{L}_{R}^{\infty}(\Omega) : \left\langle \psi \ \bar{\varphi}_{\zeta}^{*} \right\rangle = 0 \right\}.$$

Let P_{ζ} be the projection operator on $\hat{L}_{R}^{\infty}(\Omega)$ orthogonal to \mathcal{E}_{ζ} , whence

$$P_{\zeta}\psi = \langle \psi \; \bar{\varphi}_{\zeta}^* \rangle, \quad \psi \in \hat{L}_R^{\infty}(\Omega).$$

Consider now the equation related to (2.32) given by

$$\left[A_{\zeta} + \eta - (I - P_{\zeta}) B_{\zeta} (A_{\zeta} + \eta)^{-1} B_{\zeta} \right] \varphi_{4}(\eta, \zeta) = -(I - P_{\zeta}) B_{\zeta} (A_{\zeta} + \eta)^{-1} b. \quad (2.39)$$

In view of (2.38) it is clear that for (η, ζ) sufficiently small the equation (2.39) has a unique solution $\varphi_4(\eta, \zeta)$ in \mathcal{E}_{ζ} . Furthermore, if we define $\varphi_1(\eta, \zeta)$ by

$$\varphi_{1}(\eta,\zeta) = \left\{ \left[1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_{j} \right] \varphi_{4}(\eta,\zeta) - i \sin \zeta_{1} \left\langle \bar{\varphi}_{\zeta}^{*} B (A_{\zeta} + \eta)^{-1} b \right\rangle \right. \\
\left. - \sin^{2} \zeta_{1} \left\langle \bar{\varphi}_{\zeta}^{*} B (A_{\zeta} + \eta)^{-1} B \varphi_{4}(\eta,\zeta) \right\rangle \right\} \\
\left. \div \left\{ 1 + \eta - \frac{1}{d} \sum_{j=1}^{d} \cos \zeta_{j} + 2 \sin^{2} \zeta_{1} \left\langle \bar{\varphi}_{\zeta}^{*} B (A_{\zeta} + \eta)^{-1} b \right\rangle \right. \\
\left. - 2i \sin^{3} \zeta_{1} \left\langle \bar{\varphi}_{\zeta}^{*} B (A_{\zeta} + \eta)^{-1} B \varphi_{4} \right\rangle \right\}, \tag{2.40}$$

then one sees that the formula (2.40) yields a solution to (2.32). Conversely, since we are assuming (2.29) is violated, it follows that for (η, ζ) small (2.40) is the unique solution in $\hat{L}_R^{\infty}(\Omega)$ to (2.32). It is easy to see now from (2.40) that the limit $\lim_{\varepsilon \to 0} \varepsilon \varphi_1(\varepsilon^2, \varepsilon \xi)$ exists and is uniform for ξ in a compact subset of \mathbb{R}^d . Furthermore, the limit is given by the RHS of (2.18).

Finally we show that if $\varphi_1(\eta, \zeta)$, $\varphi_2(\eta, \zeta)$ are solutions to (2.32), (2.33) then (2.24) holds. To see this we put $\varphi(\eta, \zeta) = \varphi_1(\eta, \zeta) + \varphi_2(\eta, \zeta)$ and note that (2.32), (2.33) imply that $\varphi(\eta, \zeta)$ satisfies the equation

$$[A_{\zeta} + \eta - B_{\zeta}(A_{\zeta} + \eta)^{-1}B_{\zeta}]\varphi(\eta, \zeta) = b - B_{\zeta}(A_{\zeta} + \eta)^{-1}b.$$

We can rewrite this equation as

$$[A_{\zeta} + B_{\zeta} + \eta - B_{\zeta}(A_{\zeta} + \eta)^{-1}(A_{\zeta} + B_{\zeta} + \eta)]\varphi(\eta, \zeta) = b - B_{\zeta}(A_{\zeta} + \eta)^{-1}b,$$

which is the same as

$$[\mathcal{L}_{R\zeta} + \eta](A_{\zeta} + \eta)^{-1}[\mathcal{L}_{\zeta} + \eta]\varphi(\eta, \zeta) = [\mathcal{L}_{R\zeta} + \eta](A_{\zeta} + \eta)^{-1} b.$$

Now using the fact that the operator $\mathcal{L}_{R\zeta} + \eta$ is invertible we obtain (2.19).

Next we show that there is strict inequality in (2.28). In order to do this we shall first obtain a concrete representation of spaces Ω which satisfy (1.2).

Lemma 2.4. Let Ω be a finite probability space and $b: \Omega \to \mathbb{R}$ satisfy (1.3). Then Ω may be identified with a rectangle in \mathbb{Z}^d with periodic boundary conditions. The operators τ_x , $x \in \mathbb{Z}^d$, act on Ω by translation and the measure $\langle \cdot \rangle$ is simple averaging. Let $R: \Omega \to \Omega$ be the reflection operator defined as reflection in the hyperplane through the center of Ω with normal \mathbf{e}_1 . Then there is the identity $b(\omega) = -b(R\omega), \ \omega \in \Omega$.

Proof. Since Ω has no nontrivial invariant subsets under the action of the $\tau_{\mathbf{e}_j}$, $1 \leq j \leq d$, it is isomorphic to a rectangle in \mathbb{Z}^d with periodic boundary conditions. Thus we may assume Ω is given by

$$\Omega = \{x = (x_1, \dots, x_d) \in \mathbb{Z}^d : 0 \le x_i \le L_i - 1, \ 1 \le i \le d\},$$
 (2.41)

where L_1, \ldots, L_d are positive integers. The action of the $\tau_{\mathbf{e}_j}$ is translation, $\tau_{\mathbf{e}_j} x = x + \mathbf{e}_j$ with periodic boundary conditions. The measure on Ω is averaging,

$$\langle \Psi(\cdot) \rangle = \frac{1}{L_1 L_2 \dots L_d} \sum_{0 \le x_i \le L_i - 1, \ 1 \le i \le d} \Psi(x_1, \dots, x_d).$$
 (2.42)

Functions $\Psi: \Omega \to \mathbb{R}$ are isomorphic to periodic functions $\Psi: \mathbb{Z}^d \to \mathbb{R}$.

Next we consider the condition (1.3). We define a function $b^R: \Omega \to \mathbb{R}$ by $b^R(\omega) = -b(R\omega)$, $\omega \in \Omega$. It is easy to see that $b^R(\tau_x\omega) = -b(R\tau_x\omega) = -b(\tau_{Rx}R\omega)$, $\omega \in \Omega$. Since R leaves the measure (2.42) invariant (1.3) implies that for any $\theta_1, \ldots, \theta_k \in \mathbb{R}$, $x_1, \ldots, x_k \in \mathbb{Z}^d$, there is the identity,

$$\left\langle \exp\left[\sum_{j=1}^{k} \theta_{j} \ b(\tau_{x_{j}} \cdot)\right] \right\rangle = \left\langle \exp\left[\sum_{j=1}^{k} \theta_{j} \ b^{R}(\tau_{x_{j}} \cdot)\right] \right\rangle.$$

We conclude that $b \equiv b^R$.

Next we wish to construct the solutions φ, φ^* of (2.15), (2.16) on the domain Ω defined by (2.41). First observe that since Ω is the fundamental region for the homogenization problem we can assume that L_1 is an even integer by simply doubling Ω if L_1 is odd. In that case the function b is determined by its values $b(x), x \in \Omega, 0 \le x_1 \le L_1/2 - 1$. Hence we define a new fundamental region $\hat{\Omega}$ by

$$\hat{\Omega} = \{ x \in \Omega : 0 \le x_1 \le L_1/2 - 1 \}. \tag{2.43}$$

We can extend functions $\Psi: \hat{\Omega} \to \mathbb{R}$ to Ω by either symmetric or antisymmetric extension. For a symmetric extension we define Ψ on $\Omega - \hat{\Omega}$ by

$$\Psi(x_1, \dots, x_d) = \Psi(L_1 - 1 - x_1, x_2, \dots, x_d), \ L_1/2 \le x_1 \le L_1 - 1.$$
 (2.44)

For an antisymmetric extension we define Ψ by

$$\Psi(x_1, \dots, x_d) = -\Psi(L_1 - 1 - x_1, x_2, \dots, x_d), \ L_1/2 \le x_1 \le L_1 - 1.$$
 (2.45)

Lemma 2.5. The solution $\varphi: \Omega \to \mathbb{R}$ of (2.15) is an antisymmetric extension of its restriction to $\hat{\Omega}$. The solution $\varphi^*: \Omega \to \mathbb{R}$ of (2.16) is a symmetric extension of its restriction to $\hat{\Omega}$.

Proof. This follows easily from the fact that $b: \Omega \to \mathbb{R}$ is an antisymmetric extension of its restriction to $\hat{\Omega}$ and the uniqueness of the solution to (2.15), (2.16). \square

Lemma 2.4 implies that we can find the functions φ, φ^* by solving (2.15), (2.16) on $\hat{\Omega}$ with antisymmetric and symmetric boundary conditions respectively. Thus \mathcal{L} acting on functions $\Psi: \hat{\Omega} \to \mathbb{R}$ with antisymmetric boundary conditions is defined by

$$\mathcal{L}\Psi(x) = \Psi(x) - \sum_{j=1}^{d} \frac{1}{2d} \left[\Psi(x + \mathbf{e}_j) + \Psi(x - \mathbf{e}_j) \right]$$

$$-b(x) \left[\Psi(x + \mathbf{e}_1) - \Psi(x - \mathbf{e}_1) \right], \quad x \in \hat{\Omega},$$

$$(2.46)$$

where the boundary conditions are

$$\Psi(-1, x_2, \dots, x_d) = -\Psi(0, x_2, \dots, x_d),
\Psi(L_1/2, x_2, \dots, x_d) = -\Psi(L_1/2 - 1, x_2, \dots, x_d),$$
(2.47)

where $0 \le x_j \le L_j - 1$, j = 2, ..., d; and periodic boundary conditions in the directions \mathbf{e}_j , $2 \le j \le d$. Evidently (2.47) is derived from (2.45). It is easy to see that the operator \mathcal{L} is invertible on the space $L^{\infty}(\hat{\Omega})$ if the boundary conditions (2.47) are imposed. In fact the solution to the equation

$$\mathcal{L}\Psi(x) = f(x), \quad x \in \hat{\Omega}, \tag{2.48}$$

with boundary conditions (2.47) can be represented as an expectation for a continuous time Markov chain $X(t), t \geq 0$, on $\hat{\Omega}$. For the chain the transition probabilities at a site $x \in \hat{\Omega}$ satisfying $0 < x_1 < L_1/2 - 1$ are given by $x \to x + \mathbf{e}_j, x \to x - \mathbf{e}_j, 2 \leq j \leq d$, each with probability 1/2d, with periodic boundary conditions in direction $\mathbf{e}_j, 2 \leq j \leq d$. In the direction \mathbf{e}_1 then $x \to x + \mathbf{e}_1$ with probability 1/2d + b(x) and $x \to x - \mathbf{e}_1$ with probability 1/2d - b(x). The waiting time at site x is exponential with parameter 1. If $x_1 = 0$ then $x \to x \pm \mathbf{e}_j, 2 \leq j \leq d$, with probability 1/2d[1 + 1/2d - b(x)] < 1/2d, and $x \to x + \mathbf{e}_1$ with probability 1/2d[1 + 1/2d - b(x)] < 1/d. The waiting time is exponential with parameter [1 + 1/2d - b(x)]. Note that there is a positive probability that the walk

will be killed at a site x with $x_1 = 0$. A similar situation occurs at a site x with $x_1 = L_1/2 - 1$. Now $x \to x - \mathbf{e}_1$ with probability [1/2d - b(x)]/[1+1/2d + b(x)] < 1/d and the waiting time is exponential with parameter [1 + 1/2d + b(x)]. The solution Ψ of (2.48) with boundary conditions (2.47) has the representation

$$\Psi(x) = E\left[\int_0^\tau f(X(t))dt | X(0) = x\right], \quad x \in \hat{\Omega}, \tag{2.49}$$

where τ is the killing time for the chain.

We may also consider the operator \mathcal{L} of (2.46) with symmetric boundary conditions,

$$\Psi(-1, x_2, \dots, x_d) = \Psi(0, x_2, \dots, x_d),
\Psi(L_1/2, x_2, \dots, x_d) = \Psi(L_1/2 - 1, x_2, \dots, x_d)$$
(2.50)

where $0 \le x_j \le L_j - 1$, $j = 2, \ldots, d$, corresponding to (2.44). This is also associated with a continuous time Markov chain X(t) on $\hat{\Omega}$. The transition probabilities and waiting time at a site $x \in \hat{\Omega}$ with $0 < x_1 < L_1/2 - 1$ are as for the chain defined in the previous paragraph. For $x \in \hat{\Omega}$ with $x_1 = 0$ reflecting boundary conditions corresponding to (2.50) are imposed. Thus the waiting time at x is exponential with parameter $[1-1/2d+b(x)], x \to x \pm \mathbf{e}_j, 2 \le j \le d$, with probability 1/2d[1-1/2d+b(x)] and $x \to x + \mathbf{e}_1$ with probability [1/2d+b(x)]/[1-1/2d+b(x)]. A similar situation occurs at $x \in \hat{\Omega}$ with $x_1 = L_1/2 - 1$. The formal adjoint \mathcal{L}^* of the operator \mathcal{L} of (2.46) is given by

$$\mathcal{L}^*\Psi(x) = \Psi(x) - \sum_{j=1}^d \frac{1}{2d} \left[\Psi(x + \mathbf{e}_j) + \Psi(x - \mathbf{e}_j) \right]$$

$$-b(x - \mathbf{e}_1)\Psi(x - \mathbf{e}_1) + b(x + \mathbf{e}_1)\Psi(x + \mathbf{e}_1), \quad x \in \hat{\Omega}.$$

$$(2.51)$$

It is easy to see that for functions Φ, Ψ on $\hat{\Omega}$ satisfying the symmetric boundary conditions (2.50) there is the identity

$$\langle \Phi \mathcal{L}^* \Psi \rangle_{\hat{\Omega}} = \langle \Psi \mathcal{L} \Phi \rangle_{\hat{\Omega}},$$
 (2.52)

where $\langle \cdot \rangle_{\hat{\Omega}}$ is the uniform probability measure on $\hat{\Omega}$. Note that to show (2.52) one has to use the fact that the function b satisfies the antisymmetric conditions (2.47). Hence the adjoint of the operator \mathcal{L} acting on functions $\Psi: \hat{\Omega} \to \mathbb{R}$ with symmetric boundary conditions (2.50) is the operator \mathcal{L}^* of (2.51) also acting on functions with symmetric boundary conditions. In particular, it follows from Lemma 2.4 that the solution φ^* of (2.16), restricted to $\hat{\Omega}$, is the unique invariant measure for the Markov chain X(t).

Next let $\psi_0: \hat{\Omega} \to \mathbb{R}$ be the solution of the homogeneous equation (2.48) i.e. $f \equiv 0$, with the non-homogeneous antisymmetric boundary conditions

$$\psi_0(-1, x_2, \dots, x_d) = -\psi_0(0, x_2, \dots, x_d),$$

$$\psi_0(L_1/2, x_2, \dots, x_d) = 1 - \psi_0(L_1/2 - 1, x_2, \dots, x_d)$$
(2.53)

where $0 \le x_j \le L_j - 1$, j = 2, ..., d. One can see that ψ_0 is a positive function since it has a representation given by (2.49), where f is the function

$$f(x) = \begin{cases} \frac{1}{2d} + b(x), & x \in \hat{\Omega}, \ x_1 = L_1/2 - 1, \\ 0, & \text{otherwise.} \end{cases}$$

The following lemma now shows that there is strict inequality in (2.28).

Lemma 2.6. Let φ^* be the solution of (2.16) and ψ be given by (2.17). Then there is the identity,

$$\frac{1}{2d} + 2\langle \varphi^* \psi \rangle = L_1^2 \langle \varphi^* (\cdot) \left[\frac{1}{2d} - b(\cdot) \right] \psi_0(\cdot) \chi_0(\cdot) \rangle_{\hat{\Omega}}, \tag{2.54}$$

where $\chi_0: \hat{\Omega} \to \mathbb{R}$ is defined by $\chi_0(x) = 1$ if $x_1 = 0$, $\chi_0(x) = 0$, otherwise.

Proof. Since both φ^* and ψ are symmetric on Ω in the sense of (2.44) we may regard them as functions on $\hat{\Omega}$ with symmetric boundary conditions (2.50). We define a function $\psi_1: \hat{\Omega} \to \mathbb{R}$ by $\psi_1(x) = [L_1/2 - 1/2 - x_1]\varphi(x), \ x \in \hat{\Omega}$, where φ is the solution to (2.15). It is easy to see that

$$\mathcal{L}\psi_1(x) = [L_1/2 - 1/2 - x_1]b(x) + \psi(x), \quad x \in \hat{\Omega}, \ 0 < x_1 < L_1/2 - 1. \tag{2.55}$$

We impose now symmetric boundary conditions on ψ_1 at $x_1 = 0$, $x_1 = L_1/2 - 1$. One sees that (2.55) continues to hold at $x_1 = L_1/2 - 1$ but at $x_1 = 0$ there is the formula

$$\mathcal{L}\psi_1(x) = [L_1/2 - 1/2]b(x) + \psi(x) - L_1[1/2d - b(x)]\varphi(x). \tag{2.56}$$

In deriving (2.56) we have used the fact that φ satisfies antisymmetric boundary conditions at $x_1 = 0$. Now from (2.16), (2.52), (2.55), (2.56) we have that

$$2 \langle \varphi^* \psi \rangle = 2 \langle \varphi^* \psi \rangle_{\hat{\Omega}}$$

$$= 2L_1 \langle \varphi^*(\cdot) \left[\frac{1}{2d} - b(\cdot) \right] \varphi(\cdot) \chi_0(\cdot) \rangle_{\hat{\Omega}} - \langle \varphi^*(\cdot) \left[L_1 - 1 - 2x_1 \right] b(\cdot) \rangle_{\hat{\Omega}}.$$
(2.57)

Next we define a function $\psi_2: \hat{\Omega} \to \mathbb{R}$ by $\psi_2(x) = (L_1 - 1 - 2x_1)^2, x \in \hat{\Omega}$. Then we have

$$\mathcal{L}\psi_2(x) = 8[L_1 - 1 - 2x_1]b(x) - 4/d, \quad x \in \hat{\Omega}, \ 0 < x_1 < L_1/2 - 1. \tag{2.58}$$

Again we impose symmetric boundary conditions on ψ_2 at $x_1 = 0$, $x_1 = L_1/2 - 1$, in which case (2.58) continues to hold at $x_1 = L_1/2 - 1$. At $x_1 = 0$ there is the formula

$$\mathcal{L}\psi_2(x) = 8[L_1 - 1 - 2x_1]b(x) - 4/d + 4L_1[1/2d - b(x)]. \tag{2.59}$$

It follows now from (2.16), (2.52), (2.58), (2.59) that

$$-\langle \varphi^*(\cdot) \left[L_1 - 1 - 2x_1 \right] b(\cdot) \rangle_{\hat{\Omega}} = -1/2d + \frac{L_1}{2} \langle \varphi^*(\cdot) \left[\frac{1}{2d} - b(\cdot) \right] \chi_0(\cdot) \rangle_{\hat{\Omega}}, \quad (2.60)$$

where we have used the fact that $\langle \varphi^* \rangle_{\hat{\Omega}} = 1$. It follows now from (2.57), (2.59) that

$$1/2d + 2\langle \varphi^* \psi \rangle = \frac{L_1}{2} \langle \varphi^* (\cdot) \left[\frac{1}{2d} - b(\cdot) \right] [1 + 4\varphi(\cdot)] \chi_0(\cdot) \rangle_{\hat{\Omega}}. \tag{2.61}$$

We put now $\psi_0(x) = [2x_1 + 1 + 4\varphi(x)]/2L_1$, and it is easy to verify that ψ_0 satisfies the homogenous equation (2.48) with the boundary conditions (2.53). The result follows then from (2.61).

Proof of Theorem 1.1. The proof proceeds identically to the proof of [7, Theorem 1.1], on using lemmas 2.1-2.4.

Finally we wish to show that Theorem 1.2 holds to leading order in perturbation theory (see [2] for an introduction to perturbation theory).

Theorem 2.7. There exists $\delta > 0$ such that if $b: \Omega \to \mathbb{R}$ satisfies

$$0 < \sup_{\omega \in \Omega} |b(\omega)| < \delta$$

then q(b) < 1/2d, provided d = 1, or d > 1 and $L_1 \le 4$. If $d \ge 2$ and $L_1 \ge 6$ then there exists arbitrarily small b with q(b) > 1/2d.

Proof. We shall use the LHS of (2.54) as an expression for q(b). If $b \equiv 0$ then $\varphi^* \equiv 1, \varphi \equiv 0 \Rightarrow \psi \equiv 0$. Thus to obtain an expression for q(b) which is correct to second order in perturbation theory we need to expand φ^* to first order in b and φ to second order. We consider first φ^* which is the solution to (2.16). Letting Δ be the finite difference Laplacian acting on functions $\Psi: \Omega \to \mathbb{R}$ with periodic boundary conditions,

$$\Delta\Psi(x) = \sum_{j=1}^{d} \left[\Psi(x + \mathbf{e}_j) + \Psi(x - \mathbf{e}_j) - 2\Psi(x) \right], \ x \in \Omega,$$

we have from (2.51) that (2.16) is given by

$$-\frac{\Delta}{2d}\varphi^*(x) + b(x+\mathbf{e}_1)\varphi^*(x+\mathbf{e}_1) - b(x-\mathbf{e}_1)\varphi^*(x-\mathbf{e}_1) = 0, \quad x \in \Omega, \ \langle \varphi^* \rangle = 1. \ (2.62)$$

Since $\langle [\tau_{-\mathbf{e}_1} - \tau_{\mathbf{e}_1}] b \rangle = 0$ the solution to (2.62) is to first order in perturbation theory given by

$$\varphi^* = 1 + (-\Delta/2d)^{-1} \left[\tau_{-\mathbf{e}_1} - \tau_{\mathbf{e}_1} \right] b. \tag{2.63}$$

From (2.46) equation (2.15) is the same as

$$-\frac{\Delta}{2d}\varphi(x) - b(x)\left[\tau_{\mathbf{e}_1} - \tau_{-\mathbf{e}_1}\right]\varphi(x) = b(x), \quad x \in \Omega.$$
 (2.64)

Using the fact that

$$\langle b \rangle = \langle b \left[\tau_{\mathbf{e}_1} - \tau_{-\mathbf{e}_1} \right] (-\Delta/2d)^{-1} b \rangle = 0,$$

we see that the solution to (2.64) correct to second order in b is given by

$$\varphi = (-\Delta/2d)^{-1}b + (-\Delta/2d)^{-1}b \left[\tau_{\mathbf{e}_1} - \tau_{-\mathbf{e}_1}\right] (-\Delta/2d)^{-1}b. \tag{2.65}$$

From (2.17) and (2.65) we can obtain an expression for ψ which is correct to second order in b,

$$\psi = \frac{1}{2d} \left[\tau_{\mathbf{e}_{1}} - \tau_{-\mathbf{e}_{1}} \right] (-\Delta/2d)^{-1} b + b \left[\tau_{\mathbf{e}_{1}} + \tau_{-\mathbf{e}_{1}} \right] (-\Delta/2d)^{-1} b + \frac{1}{2d} \left[\tau_{\mathbf{e}_{1}} - \tau_{-\mathbf{e}_{1}} \right] (-\Delta/2d)^{-1} b \left[\tau_{\mathbf{e}_{1}} - \tau_{-\mathbf{e}_{1}} \right] (-\Delta/2d)^{-1} b.$$
(2.66)

From (2.63), (2.66) we see that the lowest order term in the expansion of $\langle \varphi^* \psi \rangle$ in powers of b is second order. Thus correct to second order we have

$$\langle \varphi^* \psi \rangle = \langle b \left[\tau_{\mathbf{e}_1} + \tau_{-\mathbf{e}_1} \right] (-\Delta/2d)^{-1} b \rangle + \frac{1}{2d} \langle b \left[\tau_{\mathbf{e}_1} - \tau_{-\mathbf{e}_1} \right] (-\Delta/2d)^{-1} \left[\tau_{\mathbf{e}_1} - \tau_{-\mathbf{e}_1} \right] (-\Delta/2d)^{-1} b \rangle.$$
(2.67)

The RHS of this equation is a translation invariant quadratic form, whence it has eigenvectors $\exp[i\xi \cdot x]$, $x \in \Omega$, with corresponding eigenvalue given by the formula,

$$2d\left\{\cos\xi_{1} - \frac{\sin^{2}\xi_{1}}{\sum_{i=1}^{d}(1-\cos\xi_{i})}\right\} / \sum_{i=1}^{d}(1-\cos\xi_{i}).$$
 (2.68)

We obtain an expression for the quadratic form (2.67) by doing an eigenvector decomposition in the x_1 direction. Putting $L = L_1/2$ we have that $\xi_1 = \pi k/L$, $k = 0, \pm 1, \ldots, \pm (L-1), L$. The function b then has a representation,

$$b(x_1) = \sum_{\xi_1} e^{i\xi_1 x_1} \left(\frac{1}{2L} \sum_{y=0}^{2L-1} b(y) e^{-i\xi_1 y} \right).$$

If we use the antisymmetry property of b, b(y) = -b(2L - 1 - y) then one has that

$$\sum_{y=0}^{2L-1} b(y)e^{-i\xi_1 y} = -2ie^{i\xi_1/2} \sum_{y=0}^{L-1} b(y)\sin\xi_1(y+1/2).$$

We conclude from this and (2.68) that the expression (2.67) is the same as

$$\langle \varphi^* \psi \rangle = -\frac{4d}{L^2} \left\langle \left(\sum_{y=0}^{L-1} (-1)^y b(y) \right) [-\Delta_{d-1} + 4]^{-1} \left(\sum_{y=0}^{L-1} (-1)^y b(y) \right) \right\rangle$$

$$+ \frac{8d}{L^2} \sum_{k=1}^{L-1} \left\langle \left(\sum_{y=0}^{L-1} b(y) \sin \pi k (y + \frac{1}{2}) / L \right) \right.$$

$$\times \left\{ \cos \frac{\pi k}{L} - 2 \sin^2 \frac{\pi k}{L} \left[-\Delta_{d-1} + 2 \left(1 - \cos(\pi k / L) \right) \right]^{-1} \right\}$$

$$\times \left[-\Delta_{d-1} + 2 \left(1 - \cos(\pi k / L) \right) \right]^{-1} \left(\sum_{y=0}^{L-1} b(y) \sin \pi k (y + \frac{1}{2}) / L \right) \right\rangle,$$
(2.69)

where Δ_{d-1} denotes the d-1 dimensional Laplacian acting on the space $\{x_1=0\}$. Observe now that the L dimensional vectors $\sin \pi k(y+1/2)/L$, $0 \le y \le L-1$, are mutually orthogonal, $k=1,\ldots,L$. This is a consequence of the fact that they are the eigenvectors of the second difference operator on the set $\{0 \le y \le L-1\}$ with antisymmetric boundary conditions. It follows that the quadratic form (2.69) is negative definite if and only if all the eigenvalues (2.68) are negative. This is the case for d=1. For d>1 it is still true provided $L\le 2$, but already for L=3 it is false. Thus for L=3 one can find a b such that the homogenized limit has an effective diffusion constant which is larger than the $b\equiv 0$ case.

3. Proof of Theorem 1.2

We shall use the representation for the effective diffusion constant given by the RHS of (2.54). We consider first the d=1 case.

Lemma 3.1. Let $\hat{\Omega}$ be the space $\hat{\Omega} = \{x \in \mathbb{Z} : 1 \leq x \leq L\}$. If $\varphi^* : \Omega \to \mathbb{R}$ is the solution to (2.16) then $\varphi^*(1)$ is given by the formula,

$$\varphi^*(1)\delta_1 = L \prod_{k=1}^L \delta_k / \sum_{r=1}^L \prod_{j=1}^{r-1} \bar{\delta}_j \prod_{j=r+1}^L \delta_j,$$
 (3.1)

where the $\delta_j, \bar{\delta}_j, 1 \leq j \leq L$, are given by

$$\delta_j = 1/2 - b(j), \quad \bar{\delta}_j = 1/2 + b(j).$$
 (3.2)

Proof. From (2.51) we see that $\varphi^* : \hat{\Omega} \to \mathbb{R}$ satisfies the equation

$$\varphi^*(x) - \frac{1}{2} \Big[\varphi^*(x+1) + \varphi^*(x-1) \Big]$$

$$-b(x-1)\varphi^*(x-1) + b(x+1)\varphi^*(x+1)$$

$$= 0, \quad 1 < x < L,$$
(3.3)

with the symmetric boundary conditions and normalization given by

$$\varphi^*(0) = \varphi^*(1), \ \varphi^*(L+1) = \varphi^*(L), \langle \varphi^* \rangle_{\hat{\Omega}} = 1.$$
(3.4)

We can solve (3.3), (3.4) uniquely by standard methods. Thus putting $D\varphi^*(x) = \varphi^*(x) - \varphi^*(x-1)$, $1 \le x \le L$, then we may write (3.3) as

$$\frac{1}{2} \left[D\varphi^*(x) - D\varphi^*(x+1) \right] - b(x-1)\varphi^*(x-1) + b(x+1)\varphi^*(x+1) = 0, \quad 1 \le x \le L.$$
(3.5)

If we sum (3.5) over the set $\{1 \le x \le y\}$ we obtain the equation,

$$\frac{1}{2} \left[D\varphi^*(1) - D\varphi^*(y+1) \right] - b(0)\varphi^*(0) - b(1)\varphi^*(1) + b(y)\varphi^*(y) + b(y+1)\varphi^*(y+1) = 0, \quad 1 \le y \le L.$$

Then, using the fact that $\varphi^*(1) = \varphi^*(0)$, b(1) = -b(0), we conclude that

$$\varphi^*(y+1) = \bar{\delta}_y \varphi^*(y) / \delta_{y+1}, \quad 1 \le y \le L,$$

whence we have

$$\varphi^*(y) = \varphi^*(1) \prod_{j=1}^{y-1} \bar{\delta}_j / \delta_{j+1}, \quad 1 \le y \le L.$$
 (3.6)

Formula (3.1) follows from (3.6) and the normalization condition in (3.4).

Lemma 3.2. Let $\hat{\Omega}$ be the space $\hat{\Omega} = \{x \in \mathbb{Z} : 1 \leq x \leq L\}$. If $\psi_0 : \hat{\Omega} \to \mathbb{R}$ is the solution to the homogeneous equation (2.48) with the boundary conditions (2.53) then $\psi_0(1)$ is given by the formula

$$2\psi_0(1) = \prod_{k=1}^L \bar{\delta}_k / \sum_{r=1}^L \prod_{j=1}^{r-1} \delta_j \prod_{j=r+1}^L \bar{\delta}_j,$$
 (3.7)

where $\delta_j, \bar{\delta}_j, 1 \leq j \leq L$, are as in (3.2).

Proof. ¿From (2.46), (2.48), (2.53), we see that $\psi_0(x)$ satisfies the equation

$$\psi_0(x) - \frac{1}{2} \left[\psi_0(x+1) + \psi_0(x-1) \right] - b(x) \left[\psi_0(x+1) - \psi_0(x-1) \right] = 0, \quad 1 \le x \le L, \quad (3.8)$$

with the boundary conditions,

$$\psi_0(0) = -\psi_0(1), \quad \psi_0(L+1) = 1 - \psi_0(L).$$
 (3.9)

We can solve (3.8), (3.9) by standard methods. Thus putting $D\psi_0(x) = \psi_0(x) - \psi_0(x-1)$ equation (3.8) implies

$$D\psi_0(x+1) = \delta_x D\psi_0(x)/\bar{\delta}_x, \quad 1 \le x \le L. \tag{3.10}$$

Observing from (3.9) that $D\psi_0(1) = 2\psi_0(1)$ we see from (3.10) that

$$D\psi_0(y+1) = 2\psi_0(1) \prod_{j=1}^y \delta_j / \bar{\delta}_j, \quad 1 \le y \le L.$$
 (3.11)

If we sum (3.11) we obtain a formula for $\psi_0(y)$ given by

$$\psi_0(y) = 2\psi_0(1) \left\{ 1/2 + \sum_{r=2}^y \prod_{j=1}^{r-1} \delta_j / \bar{\delta}_j \right\}, \quad 1 \le y \le L.$$
 (3.12)

Since $D\psi_0(L+1) = 1 - 2\psi_0(L)$ from (3.9) it follows that if we add (3.11) to twice (3.12) when y = L we obtain a formula for $\psi_0(1)$ given by

$$2\psi_0(1) = \prod_{k=1}^L \bar{\delta}_k / \left\{ \prod_{j=1}^L \bar{\delta}_j + 2 \sum_{r=2}^L \prod_{j=1}^{r-1} \delta_j \prod_{j=r}^L \bar{\delta}_j + \prod_{j=1}^L \delta_j \right\}.$$
 (3.13)

One can easily see that the denominator of the expression in (3.13) can be rewritten as in (3.7).

Remark 3.3. Observe from (3.1), (3.7) that under the reflection $b \to -b$ the expression $\varphi^*(1)\delta_1/L$ becomes $2\psi_0(1)$.

Lemma 3.4. There is the inequality $\varphi^*(1)\delta_1\psi_0(1) \leq 1/8L$.

Proof. For $1 \le r \le L$ define a_r by

$$a_r = \prod_{j=1}^{r-1} \bar{\delta}_j \prod_{j=r+1}^L \delta_j,$$

and \bar{a}_r the corresponding value of a_r under the reflection $b \to -b$. From Lemma 3.1, 3.2 we see that we need to prove that

$$4L^2 \prod_{k=1}^{L} \delta_k \bar{\delta}_k \le \left\{ \sum_{r=1}^{L} a_r \right\} \left\{ \sum_{r=1}^{L} \bar{a}_r \right\}.$$

Using the fact that for $1 \le r, s \le L$,

$$(a_r \bar{a}_s + a_s \bar{a}_r)/2 \ge (a_r \bar{a}_r a_s \bar{a}_s)^{1/2}$$

we see that

$$\left\{ \sum_{r=1}^{L} a_r \right\} \left\{ \sum_{r=1}^{L} \bar{a}_r \right\} \ge \sum_{r,s=1}^{L} (a_r \bar{a}_r a_s \bar{a}_s)^{1/2} \ge \sum_{r,s=1}^{L} 4 \prod_{k=1}^{L} \delta_k \bar{\delta}_k = 4L^2 \prod_{k=1}^{L} \delta_k \bar{\delta}_k,$$

where we have used the fact that for $1 \leq j \leq L$, one has $\delta_j \bar{\delta}_j \leq 1/4$.

Proof of Theorem 1.2 (d=1). This follows from Lemmas 3.1–3.4 and Lemma 2.5, using the RHS of (2.54) as the representation for q(b).

Next we turn to the d > 1 case with $L_1 = 2$. Then we can write $\Omega = \{(0, y) : y \in \Omega_{d-1}\}$ where $\Omega_{d-1} \subset \mathbb{Z}^{d-1}$ is a d-1 dimensional rectangle. It is easy to see now from (2.62), on using the anti-symmetry of b and the symmetry of ϕ^* , that $\phi^* \equiv 1$. Also from (2.64), on using the anti-symmetry of b and ϕ , we have that

$$\varphi(0,y) = 2d \left[-\Delta_{d-1} + 4 \right]^{-1} b(0,y), \tag{3.14}$$

where in (3.14) the operator Δ_{d-1} is the discrete Laplacian acting on functions $\Psi: \Omega_{d-1} \to \mathbb{R}$. We have then from (2.17) that $\psi(0,y) = -2b(0,y)\varphi(0,y)$, and so we get the formula for the effective diffusion constant,

$$1/2d + 2\langle \phi^* \psi \rangle = 1/2d - 8d\langle b(\cdot) \left[-\Delta_{d-1} + 4 \right]^{-1} b \rangle_{\Omega_{d-1}}.$$
 (3.15)

It is clear that the RHS of (3.15) is smaller than 1/2d. We can alternatively derive the effective diffusion constant formula by using the expression on the RHS of (2.54). Thus we have

$$\psi_0(0,y) = 2d \left[-\Delta_{d-1} + 4 \right]^{-1} \left[1/2d + b(0,y) \right],$$

whence the effective diffusion constant is given by the formula

$$L_{1}^{2} \langle \phi^{*}(\cdot) \left[1/2d - b(\cdot) \right] \psi_{0}(\cdot) \chi_{0}(\cdot) \rangle_{\hat{\Omega}}$$

$$= 8d \left\langle \left[1/2d - b(\cdot) \right] \left[-\Delta_{d-1} + 4 \right]^{-1} \left[1/2d + b(\cdot) \right] \right\rangle_{\Omega_{d-1}}.$$
(3.16)

We shall use the formula on the LHS of (3.16) to obtain an expression for the effective diffusion constant in the case $L_1=4$. Here $\hat{\Omega}$ is the space $\hat{\Omega}=\{(n,y):n=0,1,\ y\in\Omega_{d-1}\}$. For $y\in\Omega_{d-1}$ we define δ_y , $\bar{\delta}_y$, ε_y , $\bar{\varepsilon}_y$ by

$$\delta_y = 1/2d - b(0, y), \ \bar{\delta}_y = 1/2d + b(0, y),
\varepsilon_y = 1/2d + b(1, y), \ \bar{\varepsilon}_y = 1/2d - b(1, y).$$
(3.17)

We see then from (2.62), (3.17) that φ^* satisfies the system of equations,

$$\left(\frac{-\Delta_{d-1}+2}{2d}\right)\varphi^{*}(0,y) - \bar{\varepsilon}_{y} \varphi^{*}(1,y) - \delta_{y}\varphi^{*}(0,y) = 0,
\left(\frac{-\Delta_{d-1}+2}{2d}\right)\varphi^{*}(1,y) - \varepsilon_{y} \varphi^{*}(1,y) - \bar{\delta}_{y}\varphi^{*}(0,y) = 0.$$
(3.18)

Adding the two equations above we conclude that $-\Delta_{d-1}[\varphi^*(0,y) + \varphi^*(1,y)] = 0$, $y \in \Omega_{d-1}$, whence on using the normalization $\langle \varphi^* \rangle_{\hat{\Omega}} = 1$ we conclude that $\varphi^*(0,y) + \varphi^*(1,y) = 2$, $y \in \Omega_{d-1}$. Hence from (3.18) we have that $\varphi^*(0,y)$ satisfies the equation,

$$\left[-\Delta_{d-1}/2d + \bar{\varepsilon}_y + \bar{\delta}_y\right] \varphi^*(0,y) = 2\bar{\varepsilon}_y, \ y \in \Omega_{d-1}. \tag{3.19}$$

Evidently (3.19) has a unique positive solution.

We proceed similarly to obtain a formula for ψ_0 . Thus ψ_0 satisfies the system of equations

$$\left(\frac{-\Delta_{d-1}+2}{2d}\right)\psi_{0}(0,y) - \bar{\delta}_{y} \psi_{0}(1,y) + \delta_{y}\psi_{0}(0,y) = 0,
\left(\frac{-\Delta_{d-1}+2}{2d}\right)\psi_{0}(1,y) + \varepsilon_{y}\psi_{0}(1,y) - \bar{\varepsilon}_{y}\psi_{0}(0,y) = \varepsilon_{y}, \quad y \in \Omega_{d-1}.$$
(3.20)

Adding the two equations in (3.20) we get

$$[-\Delta_{d-1}/2d + \varepsilon_y + \delta_y] \{ \psi_0(0, y) + \psi_0(1, y) \} = \varepsilon_y, \quad y \in \Omega_{d-1}.$$
 (3.21)

We may also rewrite the first equation of (3.20) as,

$$\left(\frac{-\Delta_{d-1}+4}{2d}\right)\psi_0(0,y) = \bar{\delta}_y\{\psi_0(0,y) + \psi_0(1,y)\}, \quad y \in \Omega_{d-1}.$$
 (3.22)

We conclude from (3.19), (3.21), (3.22), and the formula on the LHS of (3.16) that the effective diffusion constant is

$$q(b) = 2^{7} d^{3} \left\langle \left\{ \delta \left[-\Delta_{d-1} + 2 - V \right]^{-1} \bar{\varepsilon} \right\} \right. \\ \left. \times \left[-\Delta_{d-1} + 4 \right]^{-1} \left\{ \bar{\delta} \left[-\Delta_{d-1} + 2 + V \right]^{-1} \varepsilon \right\} \right\rangle_{\Omega_{d-1}},$$
(3.23)

where $V: \Omega_{d-1} \to \mathbb{R}$ is given by $V(y) = 2d[b(1,y) - b(0,y)], y \in \Omega_{d-1}$. We first show that $q(b) \le 1/2d$ in the case where V is constant.

Lemma 3.5. Let q(b) be given by (3.23) and assume V is constant. Then there is the inequality, $q(b) \leq 1/2d$.

Proof. Since $\varepsilon + \delta = (2+V)/2d$ there is an $f: \Omega_{d-1} \to \mathbb{R}$ such that

$$\varepsilon = (2+V)/4d + f, \quad \delta = (2+V)/4d - f,$$

 $\bar{\varepsilon} = (2-V)/4d - f, \quad \bar{\delta} = (2-V)/4d + f.$ (3.24)

We rewrite the expression on the RHS of (3.23) in terms of f. To do this we let w_+, w_- be solutions to the equations

$$[-\Delta_{d-1} + 2 + V] w_{+} = f, \quad [-\Delta_{d-1} + 2 - V] w_{-} = f. \tag{3.25}$$

It follows that

$$[-\Delta_{d-1} + 2 + V]^{-1} \varepsilon = 1/4d + w_+,$$

$$[-\Delta_{d-1} + 2 - V]^{-1} \bar{\varepsilon} = 1/4d - w_-.$$

Hence from (3.23) q(b) is given by the expression,

$$\begin{split} q(b) &= 2^7 d^3 \Big\langle \Big\{ \Big[\frac{2+V}{4d} - f \Big] \Big[\frac{1}{4d} - w_- \Big] \Big\} \\ & \Big[-\Delta_{d-1} + 4 \Big]^{-1} \Big\{ \Big[\frac{2-V}{4d} + f \Big] \Big[\frac{1}{4d} + w_+ \Big] \Big\} \Big\rangle_{\Omega_{d-1}}. \end{split}$$

This is a quartic expression in f and the zeroth order term is given by,

zeroth order
$$=\frac{1}{2d}\left\langle (2+V)\left[-\Delta_{d-1}+4\right]^{-1}(2-V)\right\rangle_{\Omega_{d-1}}$$
. (3.26)

Observe that the expression in (3.26) is identical to the RHS of (3.16) if $\varepsilon = \delta$. For the first order term we have the expression

$$= 2 \left\langle (2+V) \left[-\Delta_{d-1} + 4 \right]^{-1} f \right\rangle_{\Omega_{d-1}} - 2 \left\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V) \right\rangle_{\Omega_{d-1}}$$

$$+ 2 \left\langle (2+V) \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V) w_{+} \right\rangle_{\Omega_{d-1}}$$

$$- 2 \left\langle (2+V) w_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V) \right\rangle_{\Omega_{d-1}}.$$

$$(3.27)$$

Now from (3.25) we have

$$(2-V)w_{+} = [-\Delta_{d-1} + 4] w_{+} - f,$$

$$(2+V)w_{-} = [-\Delta_{d-1} + 4] w_{-} - f.$$
(3.28)

From this we conclude that the expression in (3.27) is the same as

$$2\langle (2+V)w_{+}\rangle_{\Omega_{+}}$$
, $-2\langle (2-V)w_{-}\rangle_{\Omega_{+}}$, $=0$.

The second order term in (3.23) is given by

$$-2^{3}d \left\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} f \right\rangle_{\Omega_{d-1}}$$

$$-2^{3}d \left\langle (2+V)w_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V)w_{+} \right\rangle_{\Omega_{d-1}}$$

$$-2^{3}d \left\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V)w_{+} \right\rangle_{\Omega_{d-1}}$$

$$-2^{3}d \left\langle (2+V)w_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} f \right\rangle_{\Omega_{d-1}}$$

$$+2^{3}d \left\langle (2+V) \left[-\Delta_{d-1} + 4 \right]^{-1} f w_{+} \right\rangle_{\Omega_{d-1}}$$

$$+2^{3}d \left\langle f w_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V) \right\rangle_{\Omega_{d-1}}.$$
(3.29)

Observe from (3.28) that there is the identity,

$$\left\langle (2+V)w_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V)w_{+} \right\rangle_{\Omega_{d-1}}
= \left\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} f \right\rangle_{\Omega_{d-1}} + \left\langle w_{-} \left[-\Delta_{d-1} + 4 \right] w_{+} \right\rangle_{\Omega_{d-1}}
- \left\langle f w_{+} \right\rangle_{\Omega_{d-1}} - \left\langle f w_{-} \right\rangle_{\Omega_{d-1}}.$$
(3.30)

Similarly, we have

$$\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} (2 - V) w_{+} \rangle_{\Omega_{d-1}} = -\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} f \rangle_{\Omega_{d-1}} + \langle f w_{+} \rangle_{\Omega_{d-1}},$$

$$\langle (2 + V) w_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} f \rangle_{\Omega_{d-1}} = -\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} f \rangle_{\Omega_{d-1}} + \langle f w_{-} \rangle_{\Omega_{d-1}}.$$

$$(3.31)$$

Define now $U: \Omega_{d-1} \to \mathbb{R}$ as the solution to the equation,

$$[-\Delta_{d-1} + 4] U = V. (3.32)$$

Then from equations (3.29) - (3.32) we see that the second order term in (3.23) is given by

second order =
$$2^{3}d\left\{-\langle w_{-}[-\Delta_{d-1}+4]w_{+}\rangle_{\Omega_{d-1}} + \frac{1}{2}\langle f[w_{+}+w_{-}]\rangle_{\Omega_{d-1}} + \langle fU[w_{+}-w_{-}]\rangle_{\Omega_{d-1}}\right\}.$$
 (3.33)

The term of third order is given by

$$2^{5}d^{2} \left\langle fw_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} f \right\rangle_{\Omega_{d-1}} + 2^{5}d^{2} \left\langle fw_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} (2 - V)w_{+} \right\rangle_{\Omega_{d-1}} - 2^{5}d^{2} \left\langle f \left[-\Delta_{d-1} + 4 \right]^{-1} fw_{+} \right\rangle_{\Omega_{d-1}} \cdot (3.34)$$

Using (3.28) again we see that the expression (3.34) is the same as

$$2^5 d^2 \left\langle f w_- w_+ \right\rangle_{\Omega_{d-1}} - 2^5 d^2 \left\langle f w_- w_+ \right\rangle_{\Omega_{d-1}} = 0.$$

Finally the fourth order term is given by

fourth order =
$$2^7 d^3 \left\langle f w_- \left[-\Delta_{d-1} + 4 \right]^{-1} f w_+ \right\rangle_{\Omega_{d-1}}$$
. (3.35)

Hence from (3.26), (3.33), (3.35) we have the formula

$$q(b) = \frac{1}{2d} \left\langle (2+V) \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V) \right\rangle_{\Omega_{d-1}}$$

$$- 2^{3} d \left\langle w_{-} \left[-\Delta_{d-1} + 4 \right] w_{+} \right\rangle_{\Omega_{d-1}}$$

$$+ 2^{2} d \left\langle f[w_{+} + w_{-}] \right\rangle_{\Omega_{d-1}} + 2^{3} d \left\langle fU[w_{+} - w_{-}] \right\rangle_{\Omega_{d-1}}$$

$$+ 2^{7} d^{3} \left\langle fw_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} fw_{+} \right\rangle_{\Omega_{d-1}} .$$

$$(3.36)$$

It is clear from the definitions of V, f that

$$|V(y)| < 2, |f(y)| < [2 - |V(y)|]/4d, \quad y \in \Omega_{d-1}.$$
 (3.37)

From (3.37) it follows that there is the inequality

$$2^{7}d^{3} \left\langle fw_{-} \left[-\Delta_{d-1} + 4 \right]^{-1} fw_{+} \right\rangle_{\Omega_{d-1}} \leq 2^{4}d^{3} \left\langle (fw_{-})^{2} \right\rangle_{\Omega_{d-1}} + 2^{4}d^{3} \left\langle (fw_{+})^{2} \right\rangle_{\Omega_{d-1}} \\ \leq d \left\langle [2 - |V|]^{2} [w_{-}^{2} + w_{+}^{2}] \right\rangle_{\Omega_{d-1}}.$$

$$(3.38)$$

We define now a quadratic form Q_V depending on V by

$$Q_{V}(f) = \langle w_{-} \left[-\Delta_{d-1} + 4 \right] w_{+} \rangle_{\Omega_{d-1}} - \frac{1}{2} \langle f[w_{+} + w_{-}] \rangle_{\Omega_{d-1}} - \langle fU[w_{+} - w_{-}] \rangle_{\Omega_{d-1}} - \frac{1}{8} \langle [2 - |V|]^{2} [w_{-}^{2} + w_{+}^{2}] \rangle_{\Omega_{d-1}}.$$

$$(3.39)$$

It is evident from (3.36), (3.38) that

$$q(b) \le \frac{1}{2d} \left\langle (2+V) \left[-\Delta_{d-1} + 4 \right]^{-1} (2-V) \right\rangle_{\Omega_{d-1}} - 2^3 dQ_V(f). \tag{3.40}$$

Thus to prove the result it will be sufficient to show that Q_V is nonnegative definite. Since V is constant we can compute the eigenvalues of Q_V explicitly. Thus if p^2 denotes the eigenvalue of $-\Delta_{d-1}$, corresponding to the eigenvector $\exp[i\xi \cdot x], x \in \Omega_{d-1}$, then the eigenvalue of Q_V is

$$\left\{2(4+V^2)(p^2+2+V)(p^2+2-V) - \frac{1}{2}(2-|V|)^2\left[(p^2+2+V)^2+(p^2+2-V)^2\right]\right\} / 4(p^2+2+V)^2(p^2+2-V)^2.$$
(3.41)

We can rewrite the numerator of (3.41) as

$${2(4+V^2)-(2-|V|)^2}[p^2+2]^2-V^2{2(4+V^2)+(2-|V|)^2}.$$
 (3.42)

Since |V| < 2 the expression in (3.42) is bounded below by its value for p = 0 which can be written as

$$(4+V^2)(2-|V|)[2+3|V|] \ge 0.$$

We proceed now to the general case which will follow from the fact that the quadratic form (3.39) is nonnegative definite for any V satisfying (3.37). From here on we shall denote $\Delta_{d-1}, \langle \cdot \rangle_{\Omega_{d-1}}$ simply as Δ and $\langle \cdot \rangle$ respectively. We first note that by using (3.25) we can obtain some alternate representations for Q_V . Thus if we write

$$\left\langle w_{-}\left[-\Delta_{d-1}+4\right]w_{+}\right\rangle =2\left\langle w_{-}w_{+}\right\rangle +\frac{1}{2}\left\langle f[w_{+}+w_{-}]\right\rangle ,$$

we see that Q_V is given by

$$Q_V(f) = 2 \langle w_- w_+ \rangle - \langle fU[w_+ - w_-] \rangle - \frac{1}{8} \langle [2 - |V|]^2 [w_-^2 + w_+^2] \rangle. \tag{3.43}$$

We also have

$$\langle fU[w_+ - w_-] \rangle = \langle \{U[-\Delta + 2 - V]w_-\} w_+ \rangle - \langle \{U[-\Delta + 2 + V]w_+\} w_- \rangle$$

$$= -2 \langle UVw_-w_+ \rangle - \langle Uw_+\Delta w_- \rangle + \langle Uw_-\Delta w_+ \rangle .$$

Hence from (3.43) we have

$$Q_{V}(f) = 2 \langle w_{-}w_{+}[1 + UV] \rangle + \langle Uw_{+}\Delta w_{-} \rangle - \langle Uw_{-}\Delta w_{+} \rangle - \frac{1}{8} \langle [2 - |V|]^{2} [w_{-}^{2} + w_{+}^{2}] \rangle.$$
 (3.44)

We first show that a simple quadratic form related to Q_V is nonnegative definite.

Lemma 3.6. Let V satisfy (3.37) and w_+, w_- be solutions to (3.25) for any $f: \Omega_{d-1} \to \mathbb{R}$. Then there is the inequality $\langle w_+ w_- \rangle \geq 0$.

Proof. Let w be the solution to the equation,

$$[-\Delta + 2 + V][-\Delta + 2 - V]w = f. \tag{3.45}$$

Then from (3.25) we see that $w_+ = [-\Delta + 2 - V]w$. Hence we have from (3.25), (3.45) that

$$\langle w_{+}w_{-}\rangle = \langle [-\Delta + 2 - V]w \ w_{-}\rangle$$

$$= \langle w[-\Delta + 2 - V]w_{-}\rangle = \langle w \ f\rangle$$

$$= \langle \{[-\Delta + 2 + V]w\} \{[-\Delta + 2 - V]w\}\rangle$$

$$= \langle \{(-\Delta + 2)w\}^{2}\rangle - \langle V^{2}w^{2}\rangle$$

$$\geq \langle (4 - V^{2})w^{2}\rangle \geq 0.$$

To proceed further we need to localize the quadratic form (3.44).

Lemma 3.7. Let $\mathcal{L}_+, \mathcal{L}_-$ be operators on functions $\Phi : \Omega_{d-1} \to \mathbb{R}$ defined by

$$\mathcal{L}_{+}\Phi = (-\Delta + 2)\Phi/V - \Phi,$$

$$\mathcal{L}_{-}\Phi = (-\Delta + 2)\Phi/V + \Phi,$$

where we assume V satisfies (3.37) and $V(y) \neq 0, y \in \Omega_{d-1}$. Then $\mathcal{L}_+, \mathcal{L}_-$ are invertible and there is the identity,

$$[-\Delta + 2 + V]\mathcal{L}_{+} = [-\Delta + 2 - V]\mathcal{L}_{-}. \tag{3.46}$$

The statement of the above lemma is easy to verify; we omit its proof.

It follows from Lemma 3.7 that we can choose f in (3.25), (3.44) as the operator (3.46) acting on a function $\Phi: \Omega_{d-1} \to \mathbb{R}$, in which case $w_+ = \mathcal{L}_+ \Phi$, $w_- = \mathcal{L}_- \Phi$. If we substitute into (3.44) we obtain a quadratic form $\tilde{Q}_V(\Phi)$ which is local in Φ , and it is this quadratic form which we will show is nonnegative definite. First we show that the quadratic form obtained from \tilde{Q}_V upon replacing U by V/4 is nonnegative definite.

Lemma 3.8. For $\Phi: \Omega_{d-1} \to \mathbb{R}$ and $w_+ = \mathcal{L}_+\Phi$, $w_- = \mathcal{L}_-\Phi$, there is for d=2 the inequality,

$$2\langle w_{-}w_{+}[4+V^{2}]\rangle + \langle Vw_{+}\Delta w_{-}\rangle - \langle Vw_{-}\Delta w_{+}\rangle - \frac{1}{2}\langle [2-|V|]^{2}[w_{-}^{2}+w_{+}^{2}]\rangle \ge 0.$$
(3.47)

Proof. We first note that the first term in (3.47) is nonnegative. Thus we have

$$\langle w_- w_+ [4+V^2] \rangle = \langle [(-\Delta+2)\Phi]^2 [4/V^2+1] \rangle - \langle \Phi^2 [4+V^2] \rangle$$

$$\geq 2 \langle [(-\Delta+2)\Phi]^2 \rangle - \langle \Phi^2 [4+V^2] \rangle \geq \langle \Phi^2 [4-V^2] \rangle \geq 0,$$

where we have used (3.37). The second and third terms of (3.47) are given by the formula

$$\begin{split} &\langle Vw_{+}\Delta w_{-}\rangle - \langle Vw_{-}\Delta w_{+}\rangle \\ &= 2\,\langle [(-\Delta+2)\Phi](\Delta\;\Phi)\rangle - 2\big\langle [\Delta(V\Phi)]\big[\frac{(-\Delta+2)\Phi}{V}\big]\big\rangle, \end{split}$$

on summation by parts. From the last two equations we therefore have that

$$2 \left\langle w_{-}w_{+}[4+V^{2}] \right\rangle + \left\langle Vw_{+}\Delta w_{-} \right\rangle - \left\langle Vw_{-}\Delta w_{+} \right\rangle$$

$$= 8 \left\langle \frac{[(-\Delta+2)\Phi]^{2}}{V^{2}} \right\rangle - 2 \left\langle V^{2}\Phi^{2} \right\rangle + 4 \left\langle (\nabla\Phi)^{2} \right\rangle - 2 \left\langle [\Delta(V\Phi)] \left[\frac{(-\Delta+2)\Phi]}{V} \right] \right\rangle. \tag{3.48}$$

Using the fact that

$$-\frac{1}{V(x)}\Delta(V\Phi)(x)$$

$$= 2(d-1)\Phi(x) - \sum_{j=2}^{d} \left[\frac{V(x+\mathbf{e}_{j})}{V(x)} \Phi(x+\mathbf{e}_{j}) + \frac{V(x-\mathbf{e}_{j})}{V(x)} \Phi(x-\mathbf{e}_{j}) \right],$$

we conclude from (3.48) that

$$\langle w_{-}w_{+}[4+V^{2}]\rangle + \frac{1}{2}\langle Vw_{+}\Delta w_{-}\rangle - \frac{1}{2}\langle Vw_{-}\Delta w_{+}\rangle$$

$$= 4\langle \frac{[(-\Delta+2)\Phi]^{2}}{V^{2}}\rangle + \langle [4(d-1)-V^{2}]\Phi^{2}\rangle + 2d\langle (\nabla\Phi)^{2}\rangle$$

$$-\langle [(-\Delta+2)\Phi(\cdot)]\sum_{j=2}^{d} \left[\frac{V(\cdot + \mathbf{e}_{j})}{V(\cdot)}\Phi(\cdot + \mathbf{e}_{j}) + \frac{V(\cdot - \mathbf{e}_{j})}{V(\cdot)}\Phi(\cdot - \mathbf{e}_{j}) \right]\rangle.$$
(3.49)

Now the Schwarz inequality yields

$$\left| \left[(-\Delta + 2)\Phi(x) \right] \frac{V(y)\Phi(y)}{V(x)} \right| \le V(y)^2 \left[\alpha \frac{\Phi(y)^2}{V(y)^2} + \frac{1}{4\alpha} \frac{\left[(-\Delta + 2)\Phi(x) \right]^2}{V(x)^2} \right]
\le \alpha \Phi(y)^2 + \frac{1}{\alpha} \frac{\left[(-\Delta + 2)\Phi(x) \right]^2}{V(x)^2}, \quad x, y \in \Omega_{d-1},$$

for any $\alpha > 0$. Hence there is from (3.49) the inequality,

$$\langle w_{-}w_{+}[4+V^{2}]\rangle + \frac{1}{2}\langle Vw_{+}\Delta w_{-}\rangle - \frac{1}{2}\langle Vw_{-}\Delta w_{+}\rangle$$

$$\geq \left[4 - \frac{2(d-1)}{\alpha}\right] \langle \frac{[(-\Delta+2)\Phi]^{2}}{V^{2}}\rangle$$

$$+ \langle \left[2(d-1)(2-\alpha) - V^{2}\right] \Phi^{2}\rangle + 2d\langle (\nabla\Phi)^{2}\rangle.$$
(3.50)

For d=3 and $\alpha=1$ the RHS of (3.50) is evidently nonnegative but this is no longer the case when d>3. For $\alpha=1, d=2$ the RHS of (3.50) is bounded below by the nonnegative quantity,

$$\frac{1}{2} \left\langle \left(\frac{4 - V^2}{V^2} \right) \left[(-\Delta + 2)\Phi \right]^2 \right\rangle + \left\langle (4 - V^2)\Phi^2 \right\rangle. \tag{3.51}$$

We consider now the last term in the expression (3.47). We have

$$\frac{1}{4} \langle [2 - |V|]^2 [w_-^2 + w_+^2] \rangle = \frac{1}{2} \langle [2 - |V|]^2 \{ \frac{[(-\Delta + 2)\Phi]^2}{V^2} + \Phi^2 \} \rangle.$$
 (3.52)

If we now use the inequality $[2 - |V|]^2 \le 4 - V^2$ we see that the expression (3.52) is less than (3.51). Hence the inequality (3.47) is established for d = 2.

Next we turn to showing that \tilde{Q}_V is nonnegative definite for d=2. To do this we write the solution U of (3.32) as

$$U(x) = \frac{1}{4} \sum_{y} G(y)V(x+y),$$
(3.53)

where G(y) is the Green's function for $[-\Delta/4+1]^{-1}$, whence G(y) is nonnegative for all y and

$$\sum_{y} G(y) = 1, \quad G(y) = G(-y), \quad y = 1, 2, \dots$$
 (3.54)

We consider the first three terms in the expression (3.44) for Q_V . Using Lemma 3.7 and setting $w_+ = \mathcal{L}_+ \Phi, w_- = \mathcal{L}_- \Phi$ we have that

$$\langle w_{-}w_{+}[1+UV]\rangle + \frac{1}{2}\langle Uw_{+}\Delta w_{-}\rangle - \frac{1}{2}\langle Uw_{-}\Delta w_{+}\rangle$$

$$= \langle \frac{1}{V^{2}} \left[(-\Delta+2)\Phi \right]^{2} \left[1+UV \right] \rangle - \langle \Phi^{2}[1+UV]\rangle$$

$$+ \langle \frac{U}{V} [\Delta\Phi] \left[(-\Delta+2)\Phi \right] \rangle - \langle \Delta(U\Phi) \frac{1}{V} [-\Delta+2]\Phi \rangle$$

$$= \langle \frac{1}{V^{2}} \left[(-\Delta+2)\Phi \right]^{2} \rangle - \langle \Phi^{2}\rangle - \langle \Phi^{2}UV \rangle$$

$$+ 2\langle \frac{U}{V}\Phi(-\Delta+2)\Phi \rangle - \langle \Delta(U\Phi) \frac{1}{V} [-\Delta+2]\Phi \rangle$$

$$= \langle \frac{1}{V^{2}} \left[(-\Delta+2)\Phi \right]^{2} \rangle - \langle \Phi^{2}\rangle - \langle \Phi^{2}UV \rangle$$

$$+ 4\langle \frac{U}{V}\Phi(-\Delta+2)\Phi \rangle - \langle (\tau_{1}U)(\tau_{1}\Phi) \frac{1}{V} [-\Delta+2]\Phi \rangle$$

$$- \langle (\tau_{-1}U)(\tau_{-1}\Phi) \frac{1}{V} [-\Delta+2]\Phi \rangle,$$

$$(3.55)$$

where $\tau_x \varphi(y) = \varphi(x+y)$, $y \in \mathbb{Z}$. We consider the last three terms in the previous expression. We write using (3.53),

$$\begin{split} 4 \Big\langle \frac{U}{V} \Phi(-\Delta + 2) \Phi \Big\rangle &= G(0) \left\langle (\nabla \Phi)^2 + 2 \Phi^2 \right\rangle + \sum_{y \neq 0} G(y) \Big\langle \frac{\tau_y V}{V} \Phi(-\Delta + 2) \Phi \Big\rangle, \\ \Big\langle (\tau_1 U)(\tau_1 \Phi) \frac{1}{V} [-\Delta + 2] \Phi \Big\rangle &= \frac{1}{4} G(-1) \left\{ \left\langle \nabla (\tau_1 \Phi) \nabla \Phi \right\rangle + 2 \left\langle (\tau_1 \Phi) \Phi \right\rangle \right\} \\ &+ \frac{1}{4} \sum_{y \neq 0} G(y - 1) \Big\langle \frac{\tau_y V}{V} \tau_1 \Phi(-\Delta + 2) \Phi \Big\rangle, \end{split}$$

with a similar expression for the last term in (3.55). We conclude from this that the last three terms of (3.55) are given by,

$$\begin{split} &4 \langle \frac{U}{V} \Phi(-\Delta + 2) \Phi \rangle - \langle (\tau_1 U)(\tau_1 \Phi) \frac{1}{V} [-\Delta + 2] \Phi \rangle - \langle (\tau_{-1} U)(\tau_{-1} \Phi) \frac{1}{V} [-\Delta + 2] \Phi \rangle \\ &= G(0) \left\langle (\nabla \Phi)^2 + 2 \Phi^2 \right\rangle - \frac{1}{4} G(-1) \left\{ \langle \nabla (\tau_1 \Phi) \nabla \Phi \rangle + 2 \left\langle (\tau_1 \Phi) \Phi \rangle \right\} \\ &- \frac{1}{4} G(1) \left\{ \langle \nabla (\tau_{-1} \Phi) \nabla \Phi \rangle + 2 \left\langle (\tau_{-1} \Phi) \Phi \rangle \right\} \\ &+ \sum_{y \geq 1} \left[G(y) - \frac{1}{4} G(y - 1) - \frac{1}{4} G(y + 1) \right] \left\langle \frac{\tau_y V}{V} \tau_1 \Phi(-\Delta + 2) \Phi \right\rangle \\ &+ \sum_{y \leq -1} \left[G(y) - \frac{1}{4} G(y - 1) - \frac{1}{4} G(y + 1) \right] \left\langle \frac{\tau_y V}{V} \tau_{-1} \Phi(-\Delta + 2) \Phi \right\rangle \\ &+ \sum_{y \geq 1} G(y) \left\langle \frac{\tau_y V}{V} \left[\Phi - \tau_1 \Phi \right] (-\Delta + 2) \Phi \right\rangle \\ &- \frac{1}{4} \sum_{y \geq 1} G(y + 1) \left\langle \frac{\tau_y V}{V} \left[\tau_{-1} \Phi - \tau_1 \Phi \right] (-\Delta + 2) \Phi \right\rangle \\ &+ \sum_{y \leq -1} G(y) \left\langle \frac{\tau_y V}{V} \left[\Phi - \tau_{-1} \Phi \right] (-\Delta + 2) \Phi \right\rangle \\ &- \frac{1}{4} \sum_{y \leq -1} G(y - 1) \left\langle \frac{\tau_y V}{V} \left[\tau_1 \Phi - \tau_{-1} \Phi \right] (-\Delta + 2) \Phi \right\rangle. \end{split}$$

We shall use the representation (3.56) to show that the quadratic form Q_V is non-negative definite.

Lemma 3.9. Suppose the function G(y) of (3.53) is decreasing, non-negative for $y \ge 1$, satisfies (3.54) and the inequalities,

$$(-\Delta+2)G(y) \le 0$$
, $y \ge 1$; $1-G(0)-2G(1) < G(1)/2$; $G(2) < G(1)/5$. (3.57)

Then the quadratic form Q_V of (3.44) is nonnegative definite.

Proof. We estimate the terms in (3.56) by applying the Schwarz inequality. Before doing this we make one further simplification of terms in (3.56). We write

$$\sum_{y\geq 1} G(y) \left\langle \frac{\tau_y V}{V} \left[\Phi - \tau_1 \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle + \sum_{y\leq -1} G(y) \left\langle \frac{\tau_y V}{V} \left[\Phi - \tau_{-1} \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle
= \sum_{y\geq 2} G(y) \left\langle \frac{\tau_y V}{V} \left[\Phi - \tau_1 \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle + \sum_{y\leq -2} G(y) \left\langle \frac{\tau_y V}{V} \left[\Phi - \tau_{-1} \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle
+ G(1) \left\langle \tau_1 V \left[\frac{1}{V} - \frac{V}{4} \right] \left[\Phi - \tau_1 \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle
+ G(-1) \left\langle \tau_{-1} V \left[\frac{1}{V} - \frac{V}{4} \right] \left[\Phi - \tau_{-1} \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle
- \frac{G(1)}{4} \left\langle (\tau_1 V) V \left[\Phi - \tau_1 \Phi \right] \Delta \Phi \right\rangle - \frac{G(-1)}{4} \left\langle (\tau_{-1} V) V \left[\Phi - \tau_{-1} \Phi \right] \Delta \Phi \right\rangle
+ \frac{G(1)}{2} \left\langle (\tau_1 V) V (\nabla \Phi)^2 \right\rangle,$$
(3.58)

where we have used the fact that G(1) = G(-1). We also rewrite the first two terms on the RHS of (3.58) as

$$\sum_{y\geq 2} G(y) \left\langle \frac{(\tau_y V - V)}{V} \left[\Phi - \tau_1 \Phi \right] (-\Delta + 2) \Phi \right\rangle
+ \sum_{y\leq -2} G(y) \left\langle \frac{(\tau_y V - V)}{V} \left[\Phi - \tau_{-1} \Phi \right] (-\Delta + 2) \Phi \right\rangle
+ \sum_{y\geq 2} G(y) \left\langle (\Delta \Phi)^2 + 2(\nabla \Phi)^2 \right\rangle.$$
(3.59)

We similarly rewrite the sum of the last and third last terms of (3.56) as

$$-\frac{1}{4} \sum_{y \ge 1} G(y+1) \left\langle \frac{(\tau_y V - V)}{V} \left[\tau_{-1} \Phi - \tau_1 \Phi \right] (-\Delta + 2) \Phi \right\rangle$$

$$-\frac{1}{4} \sum_{y \le -1} G(y-1) \left\langle \frac{(\tau_y V - V)}{V} \left[\tau_1 \Phi - \tau_{-1} \Phi \right] (-\Delta + 2) \Phi \right\rangle.$$
(3.60)

Consider now the first three terms on the RHS of (3.55). These can be written as

$$\left\langle \left(\frac{1}{V^2} - \frac{1}{4}\right) \left[(-\Delta + 2)\Phi \right]^2 \right\rangle + \frac{1}{4} \left\langle \left(\Delta\Phi\right)^2 \right\rangle + \left\langle \left(\nabla\Phi\right)^2 \right\rangle \\
- \frac{1}{4} G(0) \left\langle V^2 \Phi^2 \right\rangle + \frac{1}{8} \sum_{y \neq 0} G(y) \left[\left\langle (\tau_y V - V)^2 \Phi^2 \right\rangle - \left\langle \left\{ (\tau_y V)^2 + V^2 \right\} \Phi^2 \right\rangle \right].$$
(3.61)

Next we apply the Schwarz inequality to terms in (3.56). Thus we estimate

$$\left| \left\langle \frac{\tau_y V}{V} \tau_1 \Phi(-\Delta + 2) \Phi \right\rangle \right| \le \left\langle \Phi^2 \right\rangle + \left\langle \frac{1}{V^2} [(-\Delta + 2) \Phi]^2 \right\rangle, \tag{3.62}$$

with a similar estimate when $\tau_1 \Phi$ is replace by $\tau_{-1} \Phi$.

Observe now that

$$\sum_{y>1} \left[G(y) - \frac{1}{4}G(y-1) - \frac{1}{4}G(y+1) \right] = -\frac{1}{4} [2G(0) - 1 - G(1)],$$

where we have used (3.54). Hence on using the fact that $[-\Delta + 2]G(y) < 0$, $y \ge 1$, we see from (3.62) that the sum of the first five terms on the RHS of (3.56) are bounded below by the expression,

$$[G(0) - \frac{1}{2} G(1)] \left\langle (\nabla \Phi)^2 + 2\Phi^2 \right\rangle - \left\{ \left\langle \Phi^2 \right\rangle + \left\langle \frac{1}{V^2} [(-\Delta + 2)\Phi]^2 \right\rangle \right\} [G(0) - \frac{1}{2} - \frac{1}{2} G(1)]. \tag{3.63}$$

If we combine the estimate (3.63) with (3.61) and use the fact that |V| < 2 we get a lower bound for the sum of the first three terms of (3.55) and the first five terms of (3.56). It is given by,

$$\left\langle \left(\frac{1}{V^2} - \frac{1}{4} \right) \left[(-\Delta + 2)\Phi \right]^2 \right\rangle \left\{ \frac{3}{2} + \frac{1}{2} G(1) - G(0) \right\}
+ \frac{1}{4} \left\langle (\Delta \Phi)^2 \right\rangle \left\{ \frac{3}{2} + \frac{1}{2} G(1) - G(0) \right\} + \frac{3}{2} \left\langle (\nabla \Phi)^2 \right\rangle + \frac{1}{4} G(0) \left\langle (4 - V^2)\Phi^2 \right\rangle
+ \frac{1}{8} \sum_{y \neq 0} G(y) \left\langle (\tau_y V - V)^2 \Phi^2 \right\rangle + \left[1 - G(0) \right] \left\langle \Phi^2 \right\rangle
- \frac{1}{8} \sum_{y \neq 0} G(y) \left\langle \left\{ (\tau_y V)^2 + V^2 \right\} \Phi^2 \right\rangle.$$
(3.64)

Observe that all terms in (3.64) except for the final one are nonnegative. Furthermore, the sum of the last two terms is nonnegative.

Next we estimate the terms on the RHS of (3.58) which involve G(1) and G(-1). To do this we use the Schwarz inequalities

$$\left| \left\langle \tau_{1} V \left[\frac{1}{V} - \frac{V}{4} \right] \left[\Phi - \tau_{1} \Phi \right] \left(-\Delta + 2 \right) \Phi \right\rangle \right|$$

$$\leq \alpha_{1} \left\langle \left[\frac{1}{V^{2}} - \frac{1}{4} \right] \left[\left(-\Delta + 2 \right) \Phi \right]^{2} \right\rangle + \frac{1}{\alpha_{1}} \left\langle (\nabla \Phi)^{2} \right\rangle,$$

$$\frac{1}{2} \left| \left\langle (\tau_{1} V) V \left[\Phi - \tau_{1} \Phi \right] \Delta \Phi \right\rangle \right| \leq \alpha_{2} \left\langle (\Delta \Phi)^{2} \right\rangle + \frac{1}{\alpha_{2}} \left\langle (\nabla \Phi)^{2} \right\rangle,$$

$$(3.65)$$

for any constants $\alpha_1, \alpha_2 > 0$. Hence on using the fact that |V| < 2 we see that the expression (3.64) plus the terms in G(1), G(-1) of (3.58) is bounded below by the expression,

$$\left\langle \left(\frac{1}{V^{2}} - \frac{1}{4}\right) \left[(-\Delta + 2)\Phi \right]^{2} \right\rangle \left\{ \frac{3}{2} + \frac{1}{2} G(1) - G(0) - 2\alpha_{1}G(1) \right\}
+ \frac{1}{4} \left\langle (\Delta\Phi)^{2} \right\rangle \left\{ \frac{3}{2} + \frac{1}{2}G(1) - G(0) - 4\alpha_{2}G(1) \right\}
+ \left\langle (\nabla\Phi)^{2} \right\rangle \left\{ \frac{3}{2} - 2G(1) - \frac{2}{\alpha_{1}}G(1) - \frac{1}{\alpha_{2}}G(1) \right\}
+ \frac{1}{4} G(0) \left\langle (4 - V^{2})\Phi^{2} \right\rangle + \frac{1}{8} \sum_{y \neq 0} G(y) \left\langle (\tau_{y}V - V)^{2}\Phi^{2} \right\rangle.$$
(3.66)

Let us assume for the moment that G(y)=0 for $y\geq 2$. Then (3.55) is bounded below by (3.66). We write $G(0)=1-\gamma$ whence $G(1)=\gamma/2$. Since $(-\Delta+2)G(y)\leq 0, y\geq 1$, we must have $\gamma<1/3$. We choose α_1 such that

$$\frac{3}{2} + \frac{1}{2}G(1) - G(0) - 2\alpha_1 G(1) = \frac{1}{2},$$
(3.67)

which yields $\alpha_1 = 5/4$. We choose α_2 so that

$$\frac{3}{2} + \frac{1}{2}G(1) - G(0) - 4\alpha_2 G(1) = 0, (3.68)$$

which yields $\alpha_2 = 5/8 + 1/4\gamma$. The coefficient of $<(\nabla \Phi)^2>$ in (3.66) is therefore bounded below by $1.5 - 2.6\gamma > 0$ since $\gamma < 1/3$. Hence from (3.52) the quadratic form $Q_V/2$ of (3.44) is bounded below by twice the expression,

$$\frac{1}{2} \left\langle \left(\frac{1}{V^2} - \frac{1}{4} \right) \left[(-\Delta + 2)\Phi \right]^2 \right\rangle + \frac{1}{4} G(0) \left\langle (4 - V^2)\Phi^2 \right\rangle
- \frac{1}{8} \left\langle [2 - |V|]^2 \left\{ \frac{\left[(-\Delta + 2)\Phi \right]^2}{V^2} + \Phi^2 \right\} \right\rangle.$$
(3.69)

If we now use the fact that $[2-|V|]^2 \le 4-V^2$ we see that (3.69) is nonnegative. To complete the proof of the lemma we need to estimate the sum of the terms in (3.59), (3.60). We rewrite these as

$$-\frac{1}{4}G(2)\left\langle \frac{(\tau_{1}V-V)}{V}\left[\tau_{-1}\Phi-\tau_{1}\Phi\right]\left(-\Delta+2\right)\Phi\right\rangle$$

$$-\frac{1}{4}G(-2)\left\langle \frac{(\tau_{-1}V-V)}{V}\left[\tau_{1}\Phi-\tau_{-1}\Phi\right]\left(-\Delta+2\right)\Phi\right\rangle$$

$$+\sum_{y\geq2}\left[G(y)-\frac{1}{4}G(y+1)\right]\left\langle \frac{(\tau_{y}V-V)}{V}\left[\Phi-\tau_{1}\Phi\right]\left(-\Delta+2\right)\Phi\right\rangle$$

$$+\frac{1}{4}\sum_{y\geq2}G(y+1)\left\langle \frac{(\tau_{y}V-V)}{V}\left[\Phi-\tau_{-1}\Phi\right]\left(-\Delta+2\right)\Phi\right\rangle$$

$$+\sum_{y\leq-2}\left[G(y)-\frac{1}{4}G(y-1)\right]\left\langle \left(\frac{\tau_{y}V-V}{V}\right)\left[\Phi-\tau_{-1}\Phi\right]\left(-\Delta+2\right)\Phi\right\rangle$$

$$+\frac{1}{4}\sum_{y\leq-2}G(y-1)\left\langle \frac{(\tau_{y}V-V)}{V}\left[\Phi-\tau_{1}\Phi\right]\left(-\Delta+2\right)\Phi\right\rangle$$

$$+\frac{1}{4}\left[1-G(0)-2G(1)\right]\left\langle (\Delta\Phi)^{2}+2(\nabla\Phi)^{2}\right\rangle.$$
(3.70)

We first estimate the third term in (3.70). Thus we write

$$\left\langle \frac{(\tau_{y}V - V)}{V} \left[\Phi - \tau_{1}\Phi \right] (-\Delta + 2)\Phi \right\rangle
= \left\langle (\tau_{y}V - V) \left[\frac{1}{V} - \frac{V}{4} \right] \left[\Phi - \tau_{1}\Phi \right] (-\Delta + 2)\Phi \right\rangle
- \frac{1}{4} \left\langle (\tau_{y}V - V)V \left[\Phi - \tau_{1}\Phi \right] \Delta \Phi \right\rangle + \frac{1}{2} \left\langle (\tau_{y}V - V)V \left[\Phi - \tau_{1}\Phi \right] \Phi \right\rangle.$$
(3.71)

We estimate the first two terms on the RHS of (3.71) similarly to (3.65). For the third term we use

$$|\langle (\tau_y \ V - V)V[\Phi - \tau_1 \Phi]\Phi \rangle| \le \alpha \langle (\nabla \Phi)^2 \rangle + \frac{1}{\alpha} \langle (\tau_y \ V - V)^2 \Phi^2 \rangle, \tag{3.72}$$

for any $\alpha > 0$. Choosing $\alpha = 4$ in (3.72) it follows that the sum of the third, fourth, fifth and sixth terms of (3.70) is bounded below by

$$-\sum_{|y|\geq 2} G(y) \left\{ 2\alpha_3 \left\langle \left(\frac{1}{V^2} - \frac{1}{4}\right) \left[(-\Delta + 2)\Phi \right]^2 \right\rangle + \alpha_4 \left\langle (\Delta\Phi)^2 \right\rangle + \left[\frac{2}{\alpha_3} + \frac{1}{\alpha_4} + 2 \right] \left\langle (\nabla\Phi)^2 \right\rangle + \frac{1}{8} \left\langle (\tau_y V - V)^2 \Phi^2 \right\rangle \right\},$$

$$(3.73)$$

for any $\alpha_3, \alpha_4 > 0$. We estimate the sum of the first two terms in (3.70) from below similarly. Choosing now $\alpha = 2G(2)/G(1)$ in (3.72) we obtain the lower bound,

$$-G(2)\left\{2\alpha_{5}\left\langle\left(\frac{1}{V^{2}}-\frac{1}{4}\right)\left[(-\Delta+2)\Phi\right]^{2}\right\rangle + \alpha_{6}\left\langle(\Delta\Phi)^{2}\right\rangle + \left[\frac{2}{\alpha_{5}}+\frac{1}{\alpha_{6}}+\frac{G(2)}{G(1)}\right]\left\langle(\nabla\Phi)^{2}\right\rangle\right\} - \frac{G(1)}{8}\left\langle(\tau_{1} V - V)^{2}\Phi^{2}\right\rangle - \frac{G(-1)}{8}\left\langle(\tau_{-1} V - V)^{2}\Phi^{2}\right\rangle,$$
(3.74)

for any $\alpha_5, \alpha_6 > 0$.

We may now obtain a lower bound for (3.55) by adding (3.66) to the final term in (3.70) and the expressions of (3.73) and (3.74). We obtain the lower bound,

$$\left\langle \left(\frac{1}{V^2} - \frac{1}{4}\right) \left[(-\Delta + 2)\Phi \right]^2 \right\rangle \left\{ \frac{3}{2} + \frac{1}{2} G(1) - G(0) - 2\alpha_1 G(1) - 2\alpha_5 G(2) - 2\alpha_3 \left[1 - G(0) - 2G(1) \right] \right\}$$

$$+ \frac{1}{4} \left\langle (\Delta \Phi)^2 \right\rangle \left\{ \frac{3}{2} + \frac{1}{2} G(1) - G(0) - 4\alpha_2 G(1) - 4\alpha_6 G(2) - 4\alpha_4 \left[1 - G(0) - 2G(1) \right] + 2\left[1 - G(0) - 2G(1) \right] \right\}$$

$$+ \left\langle (\nabla \Phi)^2 \right\rangle \left\{ \frac{3}{2} - 2G(1) - \frac{2}{\alpha_1} G(1) - \frac{1}{\alpha_2} G(1) - G(2)^2 / G(1) - \left[\frac{2}{\alpha_5} + \frac{1}{\alpha_6} \right] G(2) - \left[\frac{2}{\alpha_3} + \frac{1}{\alpha_4} + 2 \right] \left[1 - G(0) - 2G(1) \right] \right\}$$

$$+ \left[1 - G(0) - 2G(1) \right] \right\} + \frac{1}{4} G(0) \left\langle (4 - V^2) \Phi^2 \right\rangle.$$

$$(3.75)$$

We may rewrite the coefficient of the first term in (3.75) as

$$\frac{3}{2} + \frac{1}{2}G(1) - G(0) - 2\alpha_1 G(1) - 2\alpha_5 G(2) - 2\alpha_3 [1 - G(0) - 2G(1)]
= \frac{1}{2} + (1 - 2\alpha_3)[1 - G(0) - 2G(1)] + \left[\frac{5}{2} - 2\alpha_1 - 2\alpha_5 \frac{G(2)}{G(1)}\right]G(1).$$
(3.76)

If we set now

$$\alpha_3 = 1/2, \quad \alpha_1 + \alpha_5 G(2)/G(1) = 5/4,$$
(3.77)

we see as in (3.67) that the coefficient of the first term in (3.75) is 1/2. We similarly rewrite the coefficient of the second term as

$$\frac{3}{2} + \frac{1}{2}G(1) - G(0) - 4\alpha_2 G(1) - 4\alpha_6 G(2)
- 4\alpha_4 [1 - G(0) - 2G(1)] + 2[1 - G(0) - 2G(1)]
= \frac{1}{2} + (3 - 4\alpha_4)[1 - G(0) - 2G(1)] + [\frac{5}{2} - 4\alpha_2 - 4\alpha_6 \frac{G(2)}{G(1)}]G(1).$$
(3.78)

Hence if we set

$$\alpha_2 = 5/8, \quad \alpha_4 = 3/4, \quad \alpha_6 = 1/8 G(2)$$
 (3.79)

then the second term in (3.75) is zero. We consider the third term in (3.75). This can be written as

$$\begin{split} &\frac{3}{2} - 2G(1) - \frac{2}{\alpha_1}G(1) - \frac{1}{\alpha_2}G(1) - G(2)^2/G(1) \\ &- \left[\frac{2}{\alpha_5} + \frac{1}{\alpha_6}\right]G(2) - \left[\frac{2}{\alpha_3} + \frac{1}{\alpha_4} + 1\right][1 - G(0) - 2G(1)] \\ &= -\frac{3}{2}(-\Delta + 2)G(1) + \left[\frac{1}{2} - \frac{2}{\alpha_3} - \frac{1}{\alpha_4}\right][1 - G(0) - 2G(1)] \\ &+ \left[7 - \frac{2}{\alpha_1} - \frac{1}{\alpha_2}\right]G(1) - G(2)^2/G(1) - \left[\frac{3}{2} + \frac{2}{\alpha_5} + \frac{1}{\alpha_6}\right]G(2). \end{split}$$
(3.80)

Using the inequalities (3.57) we see this is bounded below by the expression,

$$\left\{7 - \frac{2}{\alpha_1} - \frac{1}{\alpha_2} + \frac{1}{2} \left[\frac{1}{2} - \frac{2}{\alpha_3} - \frac{1}{\alpha_4} \right] - \frac{1}{25} - \frac{1}{5} \left[\frac{3}{2} + \frac{2}{\alpha_5} + \frac{1}{\alpha_6} \right] \right\} G(1)$$

$$= \left\{ 6.91 - \frac{2}{\alpha_1} - \frac{1}{\alpha_2} - \frac{1}{\alpha_3} - \frac{1}{2\alpha_4} - \frac{2}{5\alpha_5} - \frac{1}{5\alpha_6} \right\} G(1).$$
(3.81)

If we substitute the values (3.77), (3.79) for $\alpha_3, \alpha_4, \alpha_2, \alpha_6$ into (3.75) we see that the coefficient of G(1) is bounded below by

$$2.64 - 1.6 G(2) - g_a(\alpha_1), \quad a = G(2)/G(1),$$
 (3.82)

where the function $g_a(z)$ is defined by

$$g_a(z) = \frac{2}{z} + \frac{8a}{5[5-4z]}, \quad 0 < z < 5/4, \ a > 0.$$

We can easily compute the minimum of g_a to be

$$\inf_{0 < z < 5/4} g_a(z) = 8 \left[\sqrt{5} + \sqrt{a} \right]^2 / 25.$$

Using the fact that a < 1/5, G(2) < G(1)/5 < 1/10 we see that the quantity (3.82) is bounded below by 2.64 - .16 - 2.304 > 0.

Proof of Theorem 1.2 (d = 2, $L_1 = 4$). We need only verify that the function G defined by (3.32), (3.53) satisfies the inequalities (3.57). Since G(y), $y \ge 1$, decays exponentially one can verify these inequalities with aid of a computer. In particular we see that

$$G(0) = .7071, \quad G(1) = .1213, \quad G(2) = .0208,$$

correct to 4 decimal places, whence (3.57) holds.

4. Formula for Effective Diffusion Constant

In this section we obtain the formula (1.8) of §1 for the effective diffusion constant which generalizes the formulas obtained in §3. We take $L_1 = 2L$ with $L \geq 2$ in Lemma 2.6. Then $\hat{\Omega} = \{(n,y) : 1 \leq n \leq L, y \in \Omega_{d-1}\}$. For $y \in \Omega_{d-1}$, $1 \leq j \leq L$ we define $\delta_j(y), \bar{\delta}_j(y)$ by

$$\delta_j(y) = \frac{1}{2d} - b(j, y), \quad \bar{\delta}_j(y) = \frac{1}{2d} + b(j, y).$$
 (4.1)

We see from (2.62), (4.1) that φ^* satisfies the system of equations,

$$\frac{(-\Delta+2)}{2d}\varphi^{*}(1,y) - \delta_{2}(y)\varphi^{*}(2,y) - \delta_{1}(y)\varphi^{*}(1,y) = 0,$$

$$\frac{(-\Delta+2)}{2d}\varphi^{*}(2,y) - \delta_{3}(y)\varphi^{*}(3,y) - \bar{\delta}_{1}(y)\varphi^{*}(1,y) = 0,$$

$$\cdots - \cdots = 0,$$

$$\frac{(-\Delta+2)}{2d}\varphi^{*}(L-1,y) - \delta_{L}(y)\varphi^{*}(L,y) - \bar{\delta}_{L-2}(y)\varphi^{*}(L-2,y) = 0,$$

$$\frac{(-\Delta+2)}{2d}\varphi^{*}(L,y) - \bar{\delta}_{L}(y)\varphi^{*}(L,y) - \bar{\delta}_{L-1}(y)\varphi^{*}(L-1,y) = 0,$$

where $\Delta = \Delta_{d-1}$ is the d-1 dimensional Laplacian. If we add all the equations in (4.2) we obtain the equation

$$-\Delta \sum_{j=1}^{L} \varphi^*(j, y) = 0, \quad y \in \Omega_{d-1}.$$

On using the normalization $\langle \varphi^* \rangle_{\hat{\Omega}} = 1$ we conclude that

$$\sum_{j=1}^{L} \varphi^*(j, y) = L, \quad y \in \Omega_{d-1}. \tag{4.3}$$

Evidently we can rewrite the first equation of (4.2) as

$$\left[-\frac{\Delta}{2d} + \bar{\delta}_1(y)\right]\varphi^*(1,y) - \delta_2(y)\varphi^*(2,y) = 0. \tag{4.4}$$

If we add (4.4) to the second equation of (4.2) we obtain the equation

$$\left(-\frac{\Delta}{2d}\right)\varphi^*(1,y) + \left[-\frac{\Delta}{2d} + \bar{\delta}_2(y)\right]\varphi^*(2,y) - \delta_3(y)\varphi^*(3,y) = 0. \tag{4.5}$$

Adding (4.5) to the third equation of (4.2) and proceeding similarly with subsequent equations we obtain the system

$$\left(-\frac{\Delta}{2d}\right)\varphi^{*}(1,y) + \left(-\frac{\Delta}{2d}\right)\varphi^{*}(2,y)$$

$$+ \left[-\frac{\Delta}{2d} + \bar{\delta}_{3}(y)\right]\varphi^{*}(3,y) - \delta_{4}(y)\varphi^{*}(4,y) = 0,$$

$$\cdots$$

$$\left(-\frac{\Delta}{2d}\right)\varphi^{*}(1,y) + \cdots + \left(-\frac{\Delta}{2d}\right)\varphi^{*}(L-2,y)$$

$$+ \left[-\frac{\Delta}{2d} + \bar{\delta}_{L-1}(y)\right]\varphi^{*}(L-1,y) - \delta_{L}(y)\varphi^{*}(L,y) = 0,$$

$$(4.6)$$

where we have omitted the final equation of (4.2). From (4.4), (4.5), (4.6) we can write $\varphi^*(j,y)$, $2 \leq j \leq L$, in terms of $\varphi^*(1,y)$. Substituting these into (4.3) we obtain an equation for $\varphi^*(1,y)$ of the form

$$\mathcal{L}\ \varphi^*(1,y) = L, \quad y \in \Omega_{d-1},\tag{4.7}$$

where \mathcal{L} is an operator on functions on Ω_{d-1} .

Next we consider the equations (2.48), (2.53) for the function ψ_0 on $\hat{\Omega}$. Thus ψ_0 satisfies the system of equations,

$$\frac{(-\Delta+2)}{2d}\psi_{0}(1,y) - \bar{\delta}_{1}(y)\psi_{0}(2,y) + \delta_{1}(y)\psi_{0}(1,y) = 0,$$

$$\frac{(-\Delta+2)}{2d}\psi_{0}(2,y) - \bar{\delta}_{2}(y)\psi_{0}(3,y) - \delta_{2}(y)\psi_{0}(1,y) = 0,$$

$$\cdots - \cdots = 0,$$

$$\frac{(-\Delta+2)}{2d}\psi_{0}(L-1,y) - \bar{\delta}_{L-1}(y)\psi_{0}(L,y) - \delta_{L-1}(y)\psi_{0}(L-2,y) = 0,$$

$$\frac{(-\Delta+2)}{2d}\psi_{0}(L,y) + \bar{\delta}_{L}(y)\psi_{0}(L,y) - \delta_{L}(y)\psi_{0}(L-1,y) = \bar{\delta}_{L}(y).$$
(4.8)

We can rewrite the first equation of (4.8) as

$$\frac{(-\Delta+4)}{2d}\psi_0(1,y) = \bar{\delta}_1(y)\left[\psi_0(1,y) + \psi_0(2,y)\right] = \bar{\delta}_1(y)u(1,y), \quad y \in \Omega_{d-1}, \quad (4.9)$$

where $u(1) = \psi_0(1) + \psi_0(2)$. If we put now $u(2) = \psi_0(3) - \psi_0(1)$ then on using (4.9) we see that the second equation of (4.8) is the same as

$$\left[-\frac{\Delta}{2d} + \delta_1 \right] u(1) - \bar{\delta}_2 u(2) = 0. \tag{4.10}$$

Observe that (4.10) is identical to (4.4) under the reflection $b \to -b$. We can similarly obtain the reflection of the equations (4.5), (4.6) by defining the variables $u(j), j = 3, \ldots$ by

$$u(j) = \psi_0(j+1) - \psi_0(j-1), \quad j = 3, \dots, L-1.$$

Let us assume that the u(j), $j=1,\ldots,J-1$, satisfy the reflection of the first J-2 of the equations (4.4), (4.5), (4.6). We show that u(J) then satisfies the (J-1)st equation provided $J \leq L-1$. To see this we consider the Jth equation of (4.8) which we may write as

$$\left(\frac{-\Delta+2}{2d}\right)\psi_0(J) - \bar{\delta}_J \left[u(J) + \psi_0(J-1)\right] - \delta_J \psi_0(J-1) = 0. \tag{4.11}$$

We may rewrite (4.11) as

$$\left[-\frac{\Delta}{2d} + \delta_{J-1} \right] u(J-1) - \bar{\delta}_J u(J) + \bar{\delta}_{J-1} u(J-1)
+ \frac{(-\Delta+2)}{2d} \psi_0(J-2) - \frac{2}{2d} \psi_0(J-1) = 0.$$
(4.12)

If J=3, then

$$\begin{split} \bar{\delta}_{J-1}u(J-1) + \frac{(-\Delta+2)}{2d}\psi_0(J-2) - \frac{2}{2d}\psi_0(J-1) \\ &= \bar{\delta}_2 u(2) + \frac{(-\Delta+4)}{2d}\psi_0(1) - \frac{2}{2d}\left[\psi_0(1) + \psi_0(2)\right] \\ &= \bar{\delta}_2 u(2) + \bar{\delta}_1 u(1) - \frac{2}{2d}u(1) \\ &= \bar{\delta}_2 u(2) - \delta_1 u(1) \\ &= \left[-\frac{\Delta}{2d} + \delta_1 \right] u(1) - \delta_1 u(1) \\ &= -\frac{\Delta}{2d}u(1). \end{split}$$

We have shown that the result holds for J=3. More generally we have

$$\bar{\delta}_{J-1}u(J-1) + \frac{(-\Delta+2)}{2d}\psi_0(J-2) - \frac{2}{2d}\psi_0(J-1)
= \left[-\frac{\Delta}{2d} + \delta_{J-2} \right]u(J-2) + \sum_{j=1}^{J-3} -\frac{\Delta}{2d}u(j) + \frac{(-\Delta+2)}{2d}\psi_0(J-2) - \frac{2}{2d}\psi_0(J-1)
= \sum_{j=1}^{J-2} -\frac{\Delta}{2d}u(j) - \bar{\delta}_{J-2}u(J-2) - \frac{2}{2d}\psi_0(J-3) + \frac{(-\Delta+2)}{2d}\psi_0(J-2).$$

To complete the proof we need then to show that

$$-\bar{\delta}_{J-2} u(J-2) - \frac{2}{2d} \psi_0(J-3) + \frac{(-\Delta+2)}{2d} \psi_0(J-2) = 0.$$

This last equation is however simply the (J-2)nd equation of (4.8).

We have shown that u(j), j = 1, ..., L-1 satisfies the reflection of the first L-2 equations of (4.4), (4.5), (4.6). Define now $u(L) = 1 - \psi_0(L) - \psi_0(L-1)$, whence there is the identity

$$\sum_{j=1}^{L} u(j) = 1. (4.13)$$

We shall show that the u(j), j = 1, ..., L satisfy the reflection of the final equation of (4.6). To see this we write the final equation of (4.8) as

$$\left(\frac{-\Delta+2}{2d}\right)\psi_0(L) + \bar{\delta}_L \left[1 - u(L) - \psi_0(L-1)\right] - \delta_L \psi_0(L-1) = \bar{\delta}_L,$$

whence we have

$$\left(\frac{-\Delta+2}{2d}\right)\left[u(L-1)+\psi_0(L-2)\right] - \bar{\delta}_L u(L) - \frac{2}{2d}\psi_0(L-1) = 0.$$

We may rewrite the previous equation as

$$\left[-\frac{\Delta}{2d} + \delta_{L-1} \right] u(L-1) - \bar{\delta}_L u(L) + \bar{\delta}_{L-1} u(L-1) + \frac{(-\Delta+2)}{2d} \psi_0(L-2) - \frac{2}{2d} \psi_0(L-1) = 0.$$

Now if we use the identity already established,

$$\bar{\delta}_{L-1}u(L-1) = \left[-\frac{\Delta}{2d} + \delta_{L-2} \right] u(L-2) + \sum_{j=1}^{L-3} -\frac{\Delta}{2d} u(j),$$

we see that it is sufficient to show that

$$\delta_{L-2}u(L-2) + \frac{(-\Delta+2)}{2d}\psi_0(L-2) - \frac{2}{2d}\psi_0(L-1) = 0.$$

This last equation is just the (L-2)nd equation of (4.8).

Let \mathcal{L}_R be the reflection of the operator \mathcal{L} of (4.7) obtained by replacing b by -b. Then on comparing (4.3), (4.13) we see that u(1) satisfies the equation

$$\mathcal{L}_R \ u(1) = 1. \tag{4.14}$$

We are able now to come up with a new formula for the effective diffusion constant. On using (2.54), (4.7), (4.9), (4.14) we have that the effective diffusion constant is given by

$$8L^2d\left\langle \left[\delta_1\mathcal{L}^{-1}\ 1\right](-\Delta+4)^{-1}\left[\bar{\delta}_1\mathcal{L}_R^{-1}\ 1\right]\right\rangle,\tag{4.15}$$

where $\langle \cdot \rangle$ is the uniform probability measure on Ω_{d-1} . The formula (1.8) follows from (4.15). In order for (4.15) to be valid we need to show that \mathcal{L} is invertible.

Lemma 4.1. Let \mathcal{L} be the matrix defined by (4.7). Then \mathcal{L} is invertible and the matrix \mathcal{L}^{-1} has all positive entries.

Proof. We proceed by induction. For k = 2, 3..., let \mathcal{L}_k be the operator (4.7) when L = k. It is easy to see from (4.3) - (4.6) that the \mathcal{L}_k satisfy the recurrence relation,

$$\mathcal{L}_{k+1} = \frac{1}{\delta_{k+1}} \left[-\frac{\Delta}{2d} + \bar{\delta}_k + \delta_{k+1} \right] \mathcal{L}_k - \frac{\bar{\delta}_k}{\delta_{k+1}} \mathcal{L}_{k-1}, \quad k \ge 1; \ \mathcal{L}_0 = 0, \ \mathcal{L}_1 = 1. \ (4.16)$$

The result will follow by showing that the matrices $A_k = \mathcal{L}_{k-1}\mathcal{L}_k^{-1}$, $k \geq 2$, have all positive entries and principal eigenvalue strictly less than 1. Evidently this is the case for k = 2. Now from (4.16) we see that the A_k satisfy the recurrence relation,

$$A_{k+1} = \left\{ -\frac{\Delta}{2d} + \bar{\delta}_k + \delta_{k+1} - \bar{\delta}_k A_k \right\}^{-1} \delta_{k+1}. \tag{4.17}$$

If A_k has all positive entries with principal eigenvalue strictly less than 1 then the matrix $[-\Delta/2d + \bar{\delta}_k + \delta_{k+1}]^{-1}\bar{\delta}_k A_k$ has the same property and the matrix A_{k+1} defined by (4.17) has all positive entries. To conclude the induction step we need therefore to show that A_{k+1} has principal eigenvalue strictly less than 1. To see this note that if 1 denotes the vector with all entries 1 then

$$\left\{-\frac{\Delta}{2d} + \bar{\delta}_k + \delta_{k+1} - \bar{\delta}_k A_k\right\} 1 > \delta_{k+1},$$

whence we conclude that

$$\left\{-\frac{\Delta}{2d} + \bar{\delta}_k + \delta_{k+1} - \bar{\delta}_k A_k\right\}^{-1} \delta_{k+1}(1) < 1.$$

Acknowledgements. The author would like to thank the anonymous referee for bringing his attention to the formula (1.6). This research was partially supported by grant DMS-0500608 from the NSF.

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