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Fluctuation Dissipation Equation for Lattice Gas with Energy

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In this paper we introduce a "lattice gas with energy," and obtain the "fluctuation dissipation equation" for it. The system has two conserved quantities, the number of particles and the total energy. Once the "fluctuation dissipation equation" is established, the hydrodynamic limit is easily deduced from it by using the methods found in ref. 1 for this model.

KEY WORDS: Fluctuation dissipation equation; lattice gas; hydrodynamic limit.

1. INTRODUCTION

In this paper we introduce a Markov process of a system of many particles which carry "energies" and move on a large cubic lattice, exchanging their energies with other particles. We investigate its hydrodynamic scaling limit; in particular we derive the "fluctuation dissipation equation" for it.

In this Markov process a particle moves to a nearest neighbor site obeying the exclusion rule at a rate which depends only on the energy carried by the particle. One unit of energy is transfered from a particle to another particle located in a nearest neighbor site of the particle with the generalized exclusion law which is introduced by Kipnis *et al.*[2] The dynamics has two conserved quantities, the number of particles and total energy. This model is of "non gradient type."

The hydrodynamic limit for systems of non gradient type have been obtained for various models (cf. refs. 1–4; see also refs. 5 and 6 for asymmetric models where a similar method is used), where it is a crucial step to derive the "fluctuation dissipation equation." The equation is essentially

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introduced and verified by Varadhan[4] for a "non-gradient" Ginzburg–Landau model.

In this paper we establish the fluctuation dissipation equation for the model we introduce. The framework of our proof is similar to that originally devised in ref. 4 and developed by others. We study a quadratic form of central limit theorem variance for the time evolution of a finite system and its limit as the size of the system tends to infinity. This limiting quadratic form naturally defines a Hilbert space of functions of configurations on the infinite lattice. This Hilbert space contains all functions of the form Lf, local functions f acted by the formal generator L of the associated infinite particle system. Our main task is to identify the orthogonal complement of the subspace of $\{Lf\}$ in the Hilbert space with the $2d$-dimensional space of the "gradients" of two conserved "quantities."

Adapting the method of ref. 1 we can deduce from the "fluctuation dissipation equation" that the hydrodynamic limit holds true for the model in the sense that the sequence of empirical density fields for our process is tight and any of its limit density field is a weak solution of a system of diffusion equations of two components. Since the jump of particles and the transfer of energy is allowed only between neighboring sites, the model is mirror symmetric with respect to each coordinate axis. From this it will be inferred that the system of diffusion equations is in a diagonal form with respect to the coordinates of the space variable, namely all the diffusion coefficients of the partial derivatives that involve two coordinates of a spatial point vanish.

This paper is organized as follows: In Section 2 we introduce our model and state the main results. In Section 3 we give a spectral gap estimate and related ones. In Section 4 we characterize the class of closed forms. In Section 5 we compute some variances. Finally in Section 6 we prove the main results.

2. MODEL AND RESULTS

Let Λ_N be a d-dimensional cube in $\mathbf{Z}^d$ with width $2N+1$, centered at origin. Let $\eta = (\eta_x)_{x \in \Lambda_N}$ denote a configuration of the lattice gas with energy where for each x, $\eta_x \in \{0, 1, 2,..., k\}$. Let us define $\xi_x := 1_{\{\eta_x \neq 0\}}$. We regard that if $\xi_x = 0$, then the site x is vacant, and if $\xi_x = 1$, then there exists a particle at site x; furthermore if there exists a particle at site x, then this particle has the energy η_x.

For a point $x \in \mathbf{Z}^d$ we use the norm

$$|x| := \sum_{i=1}^{d} |x_i|,$$

and for a directed bond $b = (x, y)$, $x, y \in \mathbf{Z}^d$ we define

$$|b| := |x - y|.$$

We consider the two types of jump: firstly a particle jumps to one of its neighboring vacant sites and secondly one unit of the energy on an occupied site is transfered to one of its neighboring occupied sites if any according to a generalized exclusion law.

Let $\eta^{(x,y)}$ and $\eta^{x \to y}$ be the configurations defined by

$$(\eta^{(x,y)})_z = \begin{cases} \eta_y, & \text{if} \quad z = x, \\ \eta_x, & \text{if} \quad z = y, \\ \eta_z, & \text{otherwise,} \end{cases}$$

$$(\eta^{x \to y})_z = \begin{cases} \eta_x - 1, & \text{if} \quad z = x, \\ \eta_y + 1, & \text{if} \quad z = y, \\ \eta_z, & \text{otherwise.} \end{cases}$$

Let $\pi^{(x,y)}$ and $\pi^{x \to y}$ be the operators defined by

$$\pi^{(x,y)} f(\eta) := f(\eta^{(x,y)}) - f(\eta),$$

$$\pi^{x \to y} f(\eta) := f(\eta^{x \to y}) - f(\eta),$$

for any local function f. Let $c_{\mathrm{ex}}(r)$, $c_{\mathrm{ge}}(r)$ be functions of $r = 0, 1, 2, \ldots, k$ such that $c_{\mathrm{ex}}(0) = 0$ and $c_{\mathrm{ex}}(l) > 0$ for all $1 \leqslant l \leqslant k$, and $c_{\mathrm{ge}}(0) = c_{\mathrm{ge}}(1) = 0$ and $c_{\mathrm{ge}}(l) > 0$ for all $2 \leqslant l \leqslant k$.

For a directed bond $b = (x, y)$, let L_b and $\mathscr{L}_b$ be the operators defined by

$$L_b f(\eta) := c_{\mathrm{ex}}(\eta_x)(1 - \xi_y)\, \pi^{(x,y)} f(\eta) + c_{\mathrm{ge}}(\eta_x)\, 1_{\{1 \leqslant \eta_y \leqslant k-1\}} \pi^{x \to y} f(\eta),$$

$$\mathscr{L}_b f(\eta) := \xi_x (1 - \xi_y)\, \pi^{(x,y)} f(\eta) + 1_{\{\eta_x \geqslant 2\}} 1_{\{1 \leqslant \eta_y \leqslant k-1\}} \pi^{x \to y} f(\eta),$$

for any local function f. For any directed bond $b = (x, y)$, let $c_b(\eta)$ be a function defined by

$$c_b(\eta) := c_{\mathrm{ex}}(\eta_x)(1 - \xi_y) + c_{\mathrm{ge}}(\eta_x)\, 1_{\{1 \leqslant \eta_y \leqslant k-1\}}.$$

Then

$$L_b f(\eta) = c_b(\eta)\, \mathscr{L}_b f(\eta)$$

for all local functions f. Let L_N be the Markov operator defined by

$$L_N := \sum_{b \in \Lambda_N,\, |b|=1} L_b.$$

Since for each local function f there exists n_0 such that for any $n > n_0$

$$L_n f = L_{n_0} f,$$

we simply write Lf for $L_n f$ if n is large enough.

We regard the process as a gas of particles with energy. A particle at site x moves to neighboring site y at rate $c_{\mathrm{ex}}(\eta_x)$, which depends only on the value of the energy of the particle, if y is vacant. Between two neighboring particles the energies are exchanged by the same stochastic rule as the $(k-1)$-generalized exclusion process, which is introduced by Kipnis *et al.*[2]

Consider the family of product measures on the product space $\{0, 1, 2,..., k\}^{\Lambda_N}$ with the marginal distribution

$$\bar{P}_{p,\rho}(\{\eta : \eta_x = l\}) := \begin{cases} 1-p & \text{if } \; l=0, \\ p\,\dfrac{1}{Z_{\alpha(p,\rho)}} & \text{if } \; l=1, \\ p\,\dfrac{1}{Z_{\alpha(p,\rho)}}\,\dfrac{(\alpha(p,\rho))^{l-1}}{c_{\mathrm{ge}}(2)\,c_{\mathrm{ge}}(3)\cdots c_{\mathrm{ge}}(l)} & \text{if } \; 2 \leqslant l \leqslant k \end{cases}$$

for all $x \in \Lambda_N$, $0 \leqslant p \leqslant 1$ and $p \leqslant \rho \leqslant kp$, where $Z_{\alpha(p,\rho)}$ is the normalization constant and $\alpha(p,\rho)$ is a positive constant depending on p and ρ and uniquely determined by the relation

$$\bar{E}_{p,\rho}[\eta_x] = \rho.$$

From the definition, we have reversibility, or what is the same thing, our model satisfies detailed balance condition, namely

$$\begin{aligned} &c_{\mathrm{ge}}(\eta_x)\, 1_{\{1 \leqslant \eta_w \leqslant k-1\}} \bar{P}_{p,\rho}(\{\eta\}) \\ &\qquad = c_{\mathrm{ge}}((\eta^{x\to w})_w)\, 1_{\{1 \leqslant (\eta^{x\to w})_x \leqslant k-1\}} \bar{P}_{p,\rho}(\{\eta^{x\to w}\}), \qquad (1) \\ &\bar{P}_{p,\rho}(\{\eta\}) = \bar{P}_{p,\rho}(\{\eta^{(x,w)}\}) \end{aligned}$$

for any $p, \rho, x, w \in \Lambda_N$, $x \neq w$ and $\eta \in \{0, 1, 2,..., k\}^{\Lambda_N}$, which means that L_{Λ_n} is symmetric with respect to $\bar{P}_{p,\rho}$.

For any directed bond $b = (x, y)$ and for any local function f, g let us define $\mathscr{D}_b(f; p, \rho)$, $\mathscr{D}_b(f, g; p, \rho)$ by

$$\mathscr{D}_b(f; p, \rho) := \mathscr{D}_b(f, f; p, \rho),$$
$$\mathscr{D}_b(f, g; p, \rho) := -\bar{E}_{p,\rho}[f(L_b + L_{b'})\, g],$$

where $b' = (y, x)$. Using the reversibility (1) we have

$$\mathscr{D}_b(f, g; p, \rho) = \bar{E}_{p,\rho}[c_b(\mathscr{L}_b f)(\mathscr{L}_b g)] \tag{2}$$

for all local functions f, g, and for all directed bonds $b = (x, y)$.

We write $\Lambda \subset\subset \mathbf{Z}^d$ if $\Lambda \subset \mathbf{Z}^d$ and $|\Lambda| < \infty$. Let us consider canonical measures $P_{\Lambda, y, E}$ defined by

$$P_{\Lambda, y, E}(\cdot) := \bar{P}_{p,\rho}\left(\cdot \,\middle|\, \sum_{x \in \Lambda} \xi_x = y,\ \sum_{x \in \Lambda} \eta_x = E\right)$$

for $\Lambda \subset\subset \mathbf{Z}^d$, $0 \leqslant y \leqslant |\Lambda|$ and $y \leqslant E \leqslant ky$. Then reversibility similar to (1) hold for the canonical measures. For $\Lambda \subset \mathbf{Z}^d$ define

$$\mathscr{F}_\Lambda = \sigma\text{-algebra generated by } \{\eta_x : x \in \Lambda\}.$$

We also define

$$\tilde{\mathscr{D}}_b(f; \Lambda, y, E) := \tilde{\mathscr{D}}_b(f, f; \Lambda, y, E),$$
$$\tilde{\mathscr{D}}_b(f, g; \Lambda, y, E) := -E_{\Lambda, y, E}[f(L_b + L_{b'})\, g]$$

for all $\Lambda \subset\subset \mathbf{Z}^d$, $0 \leqslant y \leqslant |\Lambda|$, $y \leqslant E \leqslant ky$, $b = (x, y) \in \Lambda$ and $\mathscr{F}_\Lambda$ measurable functions f, g, where $b' = (y, x)$. We have the formulas for $\tilde{\mathscr{D}}$ similar to (2).

Following ref. 1, we introduce the "fluctuation dissipation equation" for this model. Let us define

$$\mathscr{G} := \{h : h \text{ is a local function and satisfies } E_{\Lambda_n, y, E}[h] = 0$$
$$\text{for some } n \text{ and for all } y, E\}.$$

Let τ_x be the shift operator which acts on all $A \subset \mathbf{Z}^d$ and all local functions h as well as configurations η as follows:

$$\tau_x A := x + A,$$
$$\tau_x h(\eta) := h(\tau_x \eta),$$
$$(\tau_x \eta)_z := \eta_{z-x}.$$

Let us introduce the spatial averaging operator defined by

$$\operatorname*{Av}_{x\in\Lambda} := \frac{1}{|\Lambda|}\sum_{x\in\Lambda}$$

for $\Lambda \subset\subset \mathbf{Z}^d$. For any $h, g \in \mathscr{G}$ we can define, for all sufficiently large l,

$$V^{(l)}(h; y, E) := V^{(l)}(h, h; y, E)$$
$$V^{(l)}(h, g; y, E) := E_{\Lambda_l, y, E}[\operatorname*{Av}_{x\in\Lambda_{l_1}} \tau_x h(-L^{(l)})^{-1} \operatorname*{Av}_{x\in\Lambda_{l_1}} \tau_x g],$$

where $l_1 = l - \sqrt{l}$, $L^{(l)} = \mathrm{Av}_{b\in\Lambda_l, |b|=1} L_b$.

Lemma 2.1. For any $g \in \mathscr{G}$ there exists a limit

$$\lim_{l\to\infty, (\frac{y}{|\Lambda_l|}, \frac{E}{|\Lambda_l|})\to(p,\rho)} [V^{(l)}(g; y, E)].$$

We will prove Lemma 2.1 in Section 5. Let us define $V(g; p, \rho)$ by

$$V(g; p, \rho) := \lim_{l\to\infty, (\frac{y}{|\Lambda_l|}, \frac{E}{|\Lambda_l|})\to(p,\rho)} [V^{(l)}(g; y, E)].$$

Let us define the current ${}^t w = ({}^t w^E, {}^t w^P)$ by

$$w_e^E := -(L_{(0,e)} + L_{(e,0)})\,\eta_0,$$
$$w_e^P := -(L_{(0,e)} + L_{(e,0)})\,\xi_0.$$

We also define the density gradients ${}^t(\nabla\vec{\eta}) = ({}^t\nabla\eta, {}^t\nabla\xi)$ by

$$(\nabla\eta)_e := \eta_e - \eta_0,$$
$$(\nabla\xi)_e := \xi_e - \xi_0.$$

For $a, b \in \mathbf{R}^k$, denote by $(a\cdot b)$ the standard inner product on $\mathbf{R}^k$. Let h be a local function. For any directed bond b we can define $\sum_{x\in\mathbf{Z}^d} \mathscr{L}_b \tau_x h$, for which we write $\mathscr{L}_b \sum_{x\in\mathbf{Z}^d} \tau_x h$ although the infinite sum $\sum_{x\in\mathbf{Z}^d} \tau_x h$ does not make sense. Similarly we write

$$\mathscr{D}_b\left(\sum_{x\in\mathbf{Z}^d} \tau_x h; p, \rho\right) = \bar{E}_{p,\rho}\left[c_b\left(\mathscr{L}_b \sum_{x\in\mathbf{Z}^d} \tau_x h\right)^2\right]$$

and so on. With these notations our main theorem in this paper is stated as follows:

Theorem 2.2 (Fluctuation Dissipation Equation). Fix densities p and ρ. Then for any $2d$ dimensional unit vector α,

$$\inf_g V((\alpha \cdot (w + D\,\nabla \vec{\eta} + Lg)); p, \rho) = 0,$$

where the infimum is taken over $g = {}^t(g_1, \dots, g_{2d})$ such that all components are local functions, $Lg = {}^t(Lg_1, \dots, Lg_{2d})$ and $D = D(p, \rho)$ is a $2d \times 2d$ matrix defined as follows.

Let $\tilde{D}(p, \rho) = (\tilde{D}_{i,j}(p, \rho))_{i,j \in \{E, P\}}$ be a 2×2 matrix defined by the variational formula: for any 2-dimensional vector α,

$$\begin{aligned}(\alpha \cdot \tilde{D}(p, \rho)\, \alpha) &= \sum_{i,j \in \{E, P\}} \alpha_i \tilde{D}_{i,j}(p, \rho)\, \alpha_j \\ &:= \inf_u \mathscr{D}_{(0,e)} \left((\alpha \cdot {}^t(\eta_0, \xi_0)) + \sum_{x \in \mathbf{Z}^d} \tau_x u; p, \rho \right)\end{aligned}$$

where $\inf_u$ is taken over all local functions. (Here E, P are two indices, suggesting energy and particle, respectively.) Put

$$\begin{aligned}\chi(p, \rho) &:= \begin{pmatrix} \bar{E}_{p,\rho}[\eta_0^2] - \rho^2 & (1-p)\,\rho \\ (1-p)\,\rho & p(1-p) \end{pmatrix}, \\ D_1(p, \rho) &= \tilde{D}(p, \rho)\, \chi^{-1}(p, \rho).\end{aligned}$$

($\chi^{-1}(p, \rho)$ denotes the inverse matrix of $\chi(p, \rho)$.) Then for the case $d = 1$,

$$D := D_1(p, \rho)$$

and for the case $d \geqslant 2$, the $((i, e), (j, e'))$ component of $D(p, \rho)$ is given by

$$(D(p, \rho))_{i,e,j,e'} := \begin{cases} 0 & \text{if } \; e \neq e' \\ (D_1(p, \rho))_{i,j} & \text{if } \; e = e' \end{cases}$$

for all $i, j \in \{E, P\}$.

Remark. Let p be a finite range, translation invariant, irreducible, symmetric transition probability on $\mathbf{Z}^d$. Then we generalize our generator to

$$L_N := \sum_{x, y \in \Lambda_N} p(x-y)\, L_{(x,y)},$$

and accordingly extend Theorem 2.2, but in general it seems that

$$(D(p, \rho))_{i, e, j, e'} \neq 0$$

for $i, j \in \{E, P\}$ if $e \neq e'$. But if p is mirror symmetric with respect to each axis, then if $e \neq e'$

$$(D(p, \rho))_{i, e, j, e'} = 0$$

for $i, j \in \{E, P\}$. In our model p is mirror symmetric since it is given by the transition probability of the simple random walk on $\mathbf{Z}^d$.

Remark. Adapting the method of ref. 1 we can deduce from Theorem 2.2 the hydrodynamic limit for the present model in the sense that the sequence of empirical density fields for our process is tight and any of its limit density field is a weak solution of the following system of diffusion equations

$$\frac{\partial}{\partial t} \rho^E(t, \theta) = \sum_{i=1}^{d} \frac{\partial}{\partial \theta_i} \left(D_{E, e_i, E, e_i}(\boldsymbol{\rho}) \frac{\partial}{\partial \theta_i} \rho^E(t, \theta) + D_{E, e_i, P, e_i}(\boldsymbol{\rho}) \frac{\partial}{\partial \theta_i} \rho^P(t, \theta) \right)$$

$$\frac{\partial}{\partial t} \rho^P(t, \theta) = \sum_{i=1}^{d} \frac{\partial}{\partial \theta_i} \left(D_{P, e_i, E, e_i}(\boldsymbol{\rho}) \frac{\partial}{\partial \theta_i} \rho^E(t, \theta) + D_{P, e_i, P, e_i}(\boldsymbol{\rho}) \frac{\partial}{\partial \theta_i} \rho^P(t, \theta) \right)$$

under the periodic boundary condition in the space variable $\theta \in [0, 1]^d$ where D is the diffusion coefficient matrix given in Theorem 2.2 and ρ^E and ρ^P are densities corresponding to η and ξ respectively. The problem for the uniqueness of the weak solution to the Cauchy problem for such a system of diffusion equations seems unsolved in the existing literatures. In ref. 7, however, the present author proves that if $d \geqslant 3$ then $D(\boldsymbol{\rho})$ is smooth in $\boldsymbol{\rho}$, from which the uniqueness would be obtained. Hence for $d \geqslant 3$ the hydrodynamic limit is established in the usual sense.

3. A SPECTRAL GAP ESTIMATE AND RELATED RESULTS

Main results of this section are Lemmas 3.1 and 3.3 later. Adapting the methods of refs. 8 or 9, we get a spectral gap estimate under the measure conditioned on the particle number and the total energy.

From here to the end of the paper we fix the parameter of the product measure p, ρ, and omit them from the notations $\bar{P}$, $\bar{E}$, V, $\mathscr{D}$ unless stated otherwise. In this section all the estimates are understood to hold uniformly in parameters of product measures. Let us define $S^{(x,y)}$ and $S^{x\to y}$ by

$$S^{(x,y)}\eta := \eta^{(x,y)},$$
$$S^{x\to y}\eta := \eta^{x\to y}.$$

Let $\gamma(x, y)$ denote the canonical path from x to y, namely, $\gamma(x, y)$ is the nearest neighbor path that goes from x to y, moving successively as far as it has to do in each of the coordinate directions, following the natural order for the different coordinate directions. It is formally defined by

$$\gamma(x, y) := \{z(i)\colon 0 \leqslant i \leqslant |x-y|\}, \tag{3}$$

where $z(i) = (z(i)_1,..., z(i)_d)$ are given as follows:

$$z(i)_j = x_j \qquad \text{for} \quad i \leqslant \sum_{k=1}^{j-1} |x_k - y_k|,$$
$$z(i)_j = y_j \qquad \text{for} \quad i \geqslant \sum_{k=1}^{j} |x_k - y_k|,$$
$$z(i)_j = x_j + \left(i - \sum_{k=1}^{j-1} |x_k - y_k|\right)\frac{y_j - x_j}{|y_j - x_j|}$$
$$\text{for} \quad \sum_{k=1}^{j-1} |x_k - y_k| < i < \sum_{k=1}^{j} |x_k - y_k|.$$

Let us define $\mathscr{D}^{x\to y}(f)$ and $\mathscr{D}^{(x,y)}(f)$ by

$$\mathscr{D}^{x\to y}(f) := \bar{E}[c_{\text{ge}}(\eta_x)\, 1_{\{1 \leqslant \eta_y \leqslant k-1\}}((\pi^{x\to y} f)(\eta))^2]$$
$$\mathscr{D}^{(x,y)}(f) := \bar{E}[c_{\text{ex}}(\eta_x)(1-\xi_y)((\pi^{(x,y)} f)(\eta))^2],$$

for a local function f.

Lemma 3.1. There exists a constant C such that for any local function f, we have

$$\mathscr{D}^{x\to y}(f) \leqslant C\,|x-y| \sum_{b\in\gamma(x,y),\,|b|=1} \mathscr{D}_b(f), \tag{4}$$

$$\mathscr{D}^{(x,y)}(f) \leqslant C\,|x-y| \sum_{b\in\gamma(x,y),\,|b|=1} \mathscr{D}_b(f), \tag{5}$$

where $\gamma(x, y)$ is the canonical path from x to y.

In the proof of Lemma 3.1, the next lemma plays an important role.

Lemma 3.2. There exists a constant C such that for any local function f, we have

$$\bar{E}[(\pi^{(0,e)} f)^2] \leqslant C\mathscr{D}_{(0,e)}(f).$$

The Dirichlet forms $\mathscr{D}^{x\to y}$, $\mathscr{D}_b$ etc are defined by means of grand canonical measures. Note that the same statements as Lemmas 3.1 and 3.2 hold for the corresponding Dirichlet forms for the canonical measures.

Proof of Lemma 3.2. Lemma 3.2 is essentially proved in ref. 8. We have and only have to show that

$$\bar{E}[1_{\{0<\eta_0<\eta_e\}}((\pi^{(0,e)} f)(\eta))^2] \leqslant C_1 k^2 \mathscr{D}_{(0,e)}(f). \tag{6}$$

Fix $1 \leqslant a < b \leqslant k$, consider the configuration η with $\eta_0 = a$ and $\eta_e = b$. For $0 \leqslant l \leqslant b-a$, let η^l be the configuration defined by

$$\eta^0 := \eta,$$
$$\eta^l := S^{e\to 0}\eta^{l-1}, \qquad \text{for} \quad 1 \leqslant l \leqslant b-a.$$

Using the Schwarz inequality and reversibility (1) we have

$$\bar{E}[1_{\{\eta_0=a,\,\eta_e=b\}}(\pi^{(0,e)} f)^2] \leqslant (b-a) \sum_{l=1}^{b-a} \sum_{\eta:\,\eta_0=a,\,\eta_e=b} \bar{P}(\{\eta^{l-1}\})$$
$$\times \frac{c_{\mathrm{ge}}(a+1)\cdots c_{\mathrm{ge}}(a+l-1)}{c_{\mathrm{ge}}(b)\cdots c_{\mathrm{ge}}(b-l)} (f(\eta^l)-f(\eta^{l-1}))^2.$$

Since $c_{\mathrm{ge}} > 0$ for $b \geqslant 2$, and the number of c_{ge} in the last line is at most $2k$, there exists a constant C such that

$$\bar{E}[1_{\{\eta_0=a,\,\eta_e=b\}}(\pi^{(0,e)} f)^2]$$
$$\leqslant C(b-a) \sum_{l=1}^{b-a} \sum_{\eta:\,\eta_0=a,\,\eta_e=b} c_{\mathrm{ge}}((\eta^{l-1})_e)\, \bar{P}(\{\eta^{l-1}\})(f(\eta^l)-f(\eta^{l-1}))^2.$$

Summing up over $1 \leqslant a < b \leqslant k$, we have (6) as required. ∎

Proof of Lemma 3.1. Let $z(i) := z_{x,y}(i)$ $(0 \leqslant i \leqslant |x-y|)$ be defined by (3), namely $z(i)$ is the ith point from x on the canonical path $\gamma(x, y)$. In order to estimate (4) we take a large jump corresponding to Dirichlet form to nearest neighbor jumps which are allowed in our model or used in Lemma 3.2. We can express a large jump from x to y as a composition of at most $2|x-y|-1$ nearest neighbor jumps. We write the configuration corresponding to the ith nearest neighbor jumps by $S_i\eta$ for $0 \leqslant i \leqslant 2\,|x-y|-1$. Formally we define $S_i\eta$ by $S_0\eta := \eta$,

$$S_i\eta = S^{(z(i-1),\, z(i))}S_{i-1}\eta$$

for $1 \leqslant i \leqslant |x-y|-1$, and

$$S_{|x-y|}\eta = S^{z(|x-y|-1) \to z(|x-y|)}S_{|x-y|-1}\eta$$

and

$$S_i\eta = S^{(z(2\,|x-y|-i-1),\, z(2\,|x-y|-i))}S_{i-1}\eta$$

for $|x-y|+1 \leqslant i \leqslant 2\,|x-y|-1$. Then we have $S_{2\,|x-y|-1} = \eta^{x \to y}$. Hence we have

$$\pi^{x \to y} f(\eta) = \sum_{i=1}^{2\,|x-y|-1} (f(S_i\eta) - f(S_{i-1}\eta)),$$

and

$$f(S_i\eta) - f(S_{i-1}\eta) = \pi^{(z(i-1),\, z(i))} f(S_{i-1}\eta)$$

for $1 \leqslant i \leqslant |x-y|-1$, and

$$f(S_{|x-y|}\eta) - f(S_{|x-y|-1}\eta) = \pi^{|x-y|-1 \to |x-y|} f(S_{|x-y|-1}\eta),$$

and

$$f(S_i\eta) - f(S_{i-1}\eta) = \pi^{(z(2\,|x-y|-i-1),\, z(2\,|x-y|-i))} f(S_{i-1}\eta),$$

for $|x-y|+1 \leqslant i \leqslant 2\,|x-y|-1$. Using the Schwarz inequality and Lemma 3.2, we have

$$\mathscr{D}^{x \to y}(f) \leqslant (2\,|x-y|-1)\, \bar{E}[c_{\mathrm{ge}}(\eta_x) \sum_{i=1}^{2\,|x-y|-1} (f(S_i\eta) - f(S_{i-1}\eta))^2]$$

$$\leqslant C\,|x-y| \sum_{b \in \gamma(x,\, y),\, |b|=1} \mathscr{D}_b(f).$$

We can obtain (5) in the same way. ∎

Lemma 3.3. Suppose $\Lambda, \Lambda' \subset\subset \mathbf{Z}^d$, $\Lambda \cap \Lambda' = \emptyset$, $\Lambda \neq \emptyset$ and $x \notin \Lambda \cup \Lambda'$. Then there exist constants C_1, C_2 such that for each $\mathscr{F}_{\Lambda \cup \Lambda' \cup \{x\}}$-measurable function f, and for all $z \in \Lambda$.

$$\bar{E}[(\mathscr{L}_{(x,z)} \bar{E}[f \mid \mathscr{F}_{\Lambda' \cup \{x\}}])^2 \mid \mathscr{F}_{\Lambda'}]$$
$$\leqslant \frac{C_1}{|\Lambda|} \bar{E}[(f - \bar{E}[f \mid \mathscr{F}_{\Lambda'}])^2 \mid \mathscr{F}_{\Lambda'}] + C_2 \operatorname*{Av}_{y \in \Lambda} \bar{E}[(\mathscr{L}_{(y,x)} f)^2 \mid \mathscr{F}_{\Lambda'}]. \quad (7)$$

Applying Lemma 3.1 we have the following corollary of Lemma 3.3.

Corollary 3.4. Suppose that $z \in \Lambda_n$ and $z + e \notin \Lambda_n$. There exist constants C_1, C_2 such that for each $\mathscr{F}_{\Lambda_{3n}}$-measurable function f,

$$\bar{E}[(\mathscr{L}_{(z,z+e)} \bar{E}[f \mid \mathscr{F}_{\Lambda_n}])^2]$$
$$\leqslant \frac{C_1}{|\Lambda_n|} \bar{E}[(f - \bar{E}[f])^2] + C_2 n \operatorname*{Av}_{y \in \Lambda_{n,z,e}} \sum_{b \in \gamma(y,z)} \bar{E}[(\mathscr{L}_b f)^2], \quad (8)$$

where $\gamma(y, z)$ denotes the canonical path from y to z defined by (3), and $\Lambda_{n,z,e} = \tau_{z+ne} \Lambda_n$.

Adapting the methods of refs. 8 or 9, we can easily deduce the following spectral gap estimate from Lemmas 3.1 and 3.3.

Corollary 3.5 (Spectral Gap Estimate). There exists a constant C such that for any positive integer n, y, E satisfying $y \leqslant |\Lambda_n|$, $y \leqslant E \leqslant ky$

$$E_{\Lambda_n, y, E}[(f - E_{\Lambda_n, y, E}[f])^2] \leqslant C n^2 \sum_{b \in \Lambda_n : |b| = 1} \tilde{\mathscr{D}}_b(f; \Lambda_n, y, E).$$

Proof of Lemma 3.3. We adapt the method of ref. 9. We only prove the case $\Lambda' = \emptyset$, since the proof of the case $\Lambda' \neq \emptyset$ is similar to that of the case $\Lambda' = \emptyset$. Without risk of confusion, we simply write $\bar{E}[\cdot \mid r]$ for $\bar{E}[\cdot \mid \{\eta_x = r\}]$, $\bar{P}(\eta)$ for $\bar{P}(\{\eta\})$, $\bar{P}(\eta_x = r)$ for $\bar{P}(\{\eta : \eta_x = r\})$ and so on. By the definition

$$\mathscr{L}_{(x,z)} \bar{E}[f \mid r] = 1_{\{r \geqslant 1\}} (1 - \xi_z) \{\bar{E}[f \mid 0] - \bar{E}[f \mid r]\}$$
$$+ 1_{\{r \geqslant 2\}} 1_{\{1 \leqslant \eta_z \leqslant k-1\}} \{\bar{E}[f \mid r-1] - \bar{E}[f \mid r]\}. \quad (9)$$

Denote a covariance of f, g with respect to $\bar{E}$ by

$$\bar{E}[f; g] := \bar{E}[fg] - \bar{E}[f]\, \bar{E}[g].$$

Let us define $f^{(x,y)}$ and $f^{y\to x}$ by

$$f^{(x,y)}(\eta) := \xi_x(1-\xi_y)\, f(\eta^{(x,y)}),$$

$$f^{y\to x}(\eta) := 1_{\{2\leqslant \eta_y\leqslant k\}} 1_{\{1\leqslant \eta_x \leqslant k-1\}}\, f(\eta^{y\to x}),$$

for $y\in\Lambda$. For $1\leqslant r\leqslant k$ we define $M_\Lambda^{\mathrm{ex},r}(\eta)$ by

$$M_\Lambda^{\mathrm{ex},r}(\eta) := \frac{1}{\bar{E}[1_{\{\eta_y=r\}}]} \operatorname*{Av}_{y\in\Lambda} 1_{\{\eta_y=r\}}.$$

Note that $\bar{E}[M_\Lambda^{\mathrm{ex},r}\,|\,0]=1$. We have

$$\bar{E}[f\,|\,r]-\bar{E}[f\,|\,0] = \operatorname*{Av}_{y\in\Lambda} \frac{1}{\bar{P}[\xi_z=0\,|\,r]}\, \bar{E}[(1-\xi_y)(f-f^{(x,y)})\,|\,r]$$

$$+\bar{E}[f;\, M_\Lambda^{\mathrm{ex},r}\,|\,0] - \frac{1}{\bar{E}[(1-\xi_z)\,|\,r]}\,\bar{E}[f;\, \operatorname*{Av}_{y\in\Lambda}(1-\xi_y)\,|\,r], \tag{10}$$

for $1\leqslant r\leqslant k$.

Similarly let us define $M_\Lambda^{\mathrm{ge},r}(\eta)$ by

$$M_\Lambda^{\mathrm{ge},r}(\eta) := \frac{\bar{P}[\eta_y=r]}{c_{\mathrm{ge}}(r+1)\,\bar{P}[\eta_y=r+1]} \operatorname*{Av}_{y\in\Lambda} c(\eta_y).$$

From reversibility (1), we have

$$\bar{E}[M_\Lambda^{\mathrm{ge},r}\,|\,r] = \bar{E}[1_{\{1\leqslant\eta_y\leqslant k-1\}}\,|\,r],$$

for $1\leqslant r\leqslant k-1$. We have

$$\bar{E}[f\,|\,r+1]-\bar{E}[f\,|\,r] = \operatorname*{Av}_{y\in\Lambda}\frac{1}{\bar{E}[c_{\mathrm{ge}}]}\,\bar{E}[c_{\mathrm{ge}}(\eta_y)(f^{y\to x}-f)\,|\,r]$$

$$-\frac{1}{\bar{E}[1_{\{1\leqslant\eta_z\leqslant k-1\}}\,|\,r+1]}\,\bar{E}[f;\,\operatorname*{Av}_{y\in\Lambda} 1_{\{1\leqslant\eta_y\leqslant k-1\}}\,|\,r+1]$$

$$+\bar{E}[f;\, M_\Lambda^{\mathrm{ge},r}\,|\,r]. \tag{11}$$

for $1\leqslant r\leqslant k-1$.

Using (9)–(11) and the Schwarz inequality we get

$$
\begin{aligned}
&\bar{E}[(\mathscr{L}_{(x,z)}\bar{E}[f \mid \mathscr{F}_{\{x\}}])^2] \\
&\quad \leqslant C\bar{P}(\xi_z = 0)\sum_{r=1}^{k}\bar{P}(\zeta_x = r) \\
&\quad \times\left\{\left(\operatorname*{Av}_{y\in\Lambda}\frac{1}{\bar{P}[\xi_z = 0 \mid r]}\bar{E}[(1-\xi_y)(f - f^{(x,y)}) \mid r]\right)^2\right. \\
&\quad + (\bar{E}[f; M_\Lambda^{\mathrm{ex},r} \mid 0])^2 \\
&\quad \left.+\left(\frac{1}{\bar{E}[(1-\xi_{z+e}) \mid r]}\bar{E}[f; \operatorname*{Av}_{y\in\Lambda}(1-\xi_y) \mid r]\right)^2\right\} \\
&\quad + C\bar{P}(1 \leqslant \eta_z \leqslant k-1)\sum_{r=1}^{k-1}\bar{P}(\zeta_z = r+1) \\
&\quad \times\left\{\left(\operatorname*{Av}_{y\in\Lambda}\frac{1}{\bar{E}[c_{\mathrm{ge}}]}\bar{E}[c_{\mathrm{ge}}(\eta_y)(f^{y\to x} - f) \mid r]\right)^2\right. \\
&\quad +\left(\frac{1}{\bar{E}[1_{\{1\leqslant \eta_z \leqslant k-1\}} \mid r+1]}\bar{E}[f; \operatorname*{Av}_{y\in\Lambda}1_{\{1\leqslant \eta_y \leqslant k-1\}} \mid r+1]\right)^2 \\
&\quad \left.+ (\bar{E}[f; M_\Lambda^{\mathrm{ge},r} \mid r])^2\right\}.
\end{aligned}
$$

We calculate to see

$$
\bar{E}[(M_\Lambda^{\mathrm{ex},r} - \bar{E}[M_\Lambda^{\mathrm{ex},r} \mid 0])^2 \mid 0] = \frac{1}{|\Lambda|}\frac{1-\bar{P}(\eta_x = r)}{\bar{P}(\eta_x = r)}
$$

for all $1 \leqslant r \leqslant k$, and

$$
\bar{E}[(M_\Lambda^{\mathrm{ge},r} - \bar{E}[M_\Lambda^{\mathrm{ge},r} \mid r])^2 \mid r] = \frac{1}{|\Lambda|}\frac{\bar{E}[(c_{\mathrm{ge}} - \bar{E}[c_{\mathrm{ge}}])^2]}{\bar{E}[c_{\mathrm{ge}}]}\bar{P}(1 \leqslant \eta_x \leqslant k-1).
$$

for all r. Using these results and the inequality

$$
\bar{E}[f; g] \leqslant (\bar{E}[f; f]\,\bar{E}[g; g])^{1/2}
$$

valid for all local functions f, g, we conclude that

$$
\bar{E}[(\mathscr{L}_{(x,z)}\bar{E}[f \mid \mathscr{F}_{\{x\}}])^2] \leqslant \frac{C_1}{|\Lambda|}\bar{E}[(f - \bar{E}[f])^2] + C_2\operatorname*{Av}_{y\in\Lambda}\bar{E}[(\mathscr{L}_{(y,x)}f)^2]. \quad \blacksquare
$$

4. STRUCTURE OF THE SPACE OF CLOSED FORMS

In this section firstly we introduce and characterize the space of translation covariant closed forms for our model, and secondly we show that any limit point of functions of the form $\mathscr{L}_{(0,e)}\mathrm{Av}_{x\in\Lambda_k}[\tau_x u]$ with certain moment conditions is essentially in this space.

For any directed bond $b=(x,y)$, we define T_b by

$$T_b\eta=\begin{cases}\eta^{x\to y} & \text{if} \quad \eta_x\geqslant 2 \quad \text{and} \quad 1\leqslant\eta_y\leqslant k-1,\\ \eta^{(x,y)} & \text{if} \quad \xi_x=1 \quad \text{and} \quad \xi_y=0,\\ \eta & \text{otherwise,}\end{cases}$$

so that

$$\mathscr{L}_b f(\eta)=f(T_b\eta)-f(\eta).$$

A set of functions $\{\Phi_b\}_b$ is said to be closed or a closed form if the following condition holds: for each finite sequence of directed bonds $b_1, b_2,..., b_n$ and each configuration η, such that $\eta^n=\eta$, if we define η^i, $0\leqslant i\leqslant n$, by $\eta^0=\eta$ and $\eta^i=T_{b_i}\eta^{i-1}$, then

$$\sum_{i=1}^{n}\Phi_{b_i}(\eta^{i-1})=0.$$

We consider the special cases. If a pair of a directed bond b and a configuration η satisfies $T_b\eta=\eta$, then from the defining relation in the case $n=1$ we have

$$\Phi_b(\eta)=0, \tag{12}$$

for all closed forms $\{\Phi_b\}_b$. If a pair of a directed bond $b=(x,y)$ and a configuration η satisfies $T_b\eta\neq\eta$, then $T_{(y,x)}T_{(x,y)}\eta=\eta$. Hence in the case $n=2$ we have

$$\Phi_{(x,y)}(\eta)=-\Phi_{(y,x)}(T_b\eta) \tag{13}$$

for all closed forms $\{\Phi_b\}_b$, if $T_{(x,y)}\eta\neq\eta$.

A closed form is said to be translation covariant if it holds that $\Phi_b=\tau_x\Phi_{\tau_x b}$ for all sites x and all bonds b. From (12) and (13), we can represent the translation covariant closed form by $\{\Phi_{(0,e)}\}_e$, where e varies over positive unit vectors on the lattice. We consider the set of the representatives of translation covariant and square integrable closed forms $\mathcal{G}_c$, which is formally defined as follows. Given $\{\Phi_{(0,e)}\}_e$ let us define $\{\Phi_{(0,-e)}\}_e$ by

$$\Phi_{(0,-e)}(\eta) := \begin{cases} 0, & \text{if} \quad T_{(0,-e)}\eta = \eta, \\ -\tau_{-e}\Phi_{(0,e)}(T_{(e,0)}\eta), & \text{otherwise} \end{cases} \tag{14}$$

and for all $|x-y| = 1$, let us define $\{\Phi_{(x,y)}\}_{(x,y)}$ by

$$\Phi_{(x,y)} := \tau_x \Phi_{(0,y-x)}. \tag{15}$$

Using these notations we define $\mathcal{G}_c$ by

$$\mathcal{G}_c := \{\{\Phi_{(0,e)}\}_e : \{\Phi_b\}_b \text{ defined by (14) and (15) is closed and } \bar{E}[\Phi^2_{(0,e)}] < \infty\}. \tag{16}$$

Given a finite box Λ_n, we decompose $\{0, 1,..., k\}^{\Lambda_n}$ into ergodic classes. Two configurations $\eta, \omega \in \{0, 1,..., k\}^{\Lambda_n}$ are in the same class if and only if there exist a positive integer l and a sequence of bonds $\{b_1, b_2,..., b_l\}$ where $b_i \in \Lambda_n$ for all $1 \leqslant i \leqslant l$ such that

$$\eta = T_{b_l} \circ T_{b_{l-1}} \circ \cdots \circ T_{b_1} \omega.$$

Each ergodic class is determined by the conserved quantities $\sum_{x \in \Lambda_n} \xi_x$, $\sum_{x \in \Lambda_n} \eta_x$. We pick up arbitrarily a pair of integers y, E satisfying $0 \leqslant y \leqslant |\Lambda_n|$, $y \leqslant E \leqslant ky$. For each pair of integers y, E, we write $\mathcal{E}^n_{y,E}$ for the ergodic class determined by $\sum_{x \in \Lambda_n} \xi_x = y$, and $\sum_{x \in \Lambda_n} \eta_x = E$. Furthermore for each $\mathcal{E}^n_{y,E}$ we pick up an element of it and denote it by $\eta^n_{y,E}$. If $\eta \in \mathcal{E}^n_{y,E}$, then we can find a sequence of bonds $\{b_1, b_2,..., b_l\}$ such that

$$\eta = T_{b_l} \circ T_{b_{l-1}} \circ \cdots \circ T_{b_1} \eta^n_{y,E}.$$

Given a closed form $\{\Phi_b\}_{b \in \Lambda_n}$, we put

$$\tilde{G}^n(\eta) := -\sum_{i=1}^{l} \Phi_{b_i}(T_{b_i} \circ T_{b_{i-1}} \circ \cdots \circ T_{b_1} \eta^n_{y,E}),$$

for $\eta \in \mathcal{E}^n_{y,E}$. In view of the definition of the closed form, it is not difficult to see that $\tilde{G}^n$ does not depend on the choice of the sequence of bonds. Therefore $\tilde{G}^n$ is well-defined for $\eta \in \mathcal{E}^n_{y,E}$ and for any $c \in \mathbf{R}$, it holds that

$$\mathcal{L}_b(\tilde{G}^n(\eta) + c) = \Phi_b(\eta),$$

for all $\eta \in \mathscr{E}^n_{y,E}$ and $b \in \Lambda_n$. Put

$$G^n(\eta) := \tilde{G}^n(\eta) - E_{\Lambda_n, y, E}[\tilde{G}^n]$$

for $\eta \in \mathscr{E}^n_{y,E}$. Carrying out such constructions for all y, E, we get the $\mathscr{F}_{\Lambda_n}$-measurable function satisfying

$$\mathscr{L}_b G^n(\eta) = \Phi_b$$

$$E_{\Lambda_n, y, E}[G^n] = 0$$

for $b \in \Lambda_n$ and for all y, E. G^n is an normalized "integral" of the closed form $\{\Phi_b\}$.

Lemma 4.1. We have $\mathscr{G}_c \subset \overline{\mathscr{G}_0 + \mathscr{G}_E}$ where $\mathscr{G}_0, \mathscr{G}_E$ are defined by

$\mathscr{G}_0 :=$ the linear subspace of functions spanned by $\{\mathscr{L}_{(0,e)}\eta_0, \mathscr{L}_{(0,e)}\xi_0\}_e$,

$$\mathscr{G}_E := \left\{\left\{\mathscr{L}_{(0,e)} \sum_y \tau_y g\right\}_e : g \text{ is a local function}\right\},$$

and $\overline{\mathscr{G}_0 + \mathscr{G}_E}$ is the closure of $\mathscr{G}_0 + \mathscr{G}_E$ in the Hilbert space $L^2(\bar{P})$.

Proof. We adapt the strategy found in ref. 8. Since $\mathscr{L}_b$ and the conditional expectation $\bar{E}[\,\cdot \mid \mathscr{F}_{\Lambda_n}]$ commute if $b \subset \Lambda_n$, $\{\bar{E}[\Phi_b \mid \mathscr{F}_{\Lambda_{3n}}]\}_{b \in \Lambda_{3n}}$ is closed on Λ_{3n}. We can "integrate" and construct an $\mathscr{F}_{\Lambda_{3n}}$ measurable function G^{3n} such that

$$\mathscr{L}_b G^{3n}(\eta) = \bar{E}[\Phi_b \mid \mathscr{F}_{\Lambda_{3n}}],$$

$$E_{\Lambda_{3n}, y, E}[G^{3n}] = 0,$$

for all y, E. We define h^n and Ψ^n_b by

$$h^n := \bar{E}[G^{3n} \mid \mathscr{F}_{\Lambda_n}],$$

$$\Psi^n_b := \frac{1}{(2n+1)^d} \mathscr{L}_b \sum_{x \in \mathbf{Z}^d} \tau_x h^n.$$

Since $\{\Psi^n_b\}_b$ are translation covariant, we only consider $\{\Psi^n_{(0,e)}\}_e$ where e varies over all positive unit vectors on the lattice. Throughout the rest of this section we fix a positive unit vector e. Without risk of confusion we simply write Ψ^n for $\Psi^n_{(0,e)}$. Noticing that h^n is $\mathscr{F}_{\Lambda_n}$ measurable, we decompose Ψ^n as the sum of the interior part Ω_1^n and the boundary part Ω_2^n, where Ω_1^n and Ω_2^n are defined by

$$\Omega_1^n := \frac{1}{(2n+1)^d} \mathscr{L}_{(0,e)} \sum_{y:\, y,\, y+e \in \Lambda_n} \tau_y h^n,$$

$$\Omega_2^n := \frac{1}{(2n+1)^d} \mathscr{L}_{(0,e)} \sum_{y:\, y \in \Lambda_n,\, y+e \notin \Lambda_n} \tau_y h^n + \frac{1}{(2n+1)^d} \mathscr{L}_{(0,e)} \sum_{y:\, y \notin \Lambda_n,\, y+e \in \Lambda_n} \tau_y h^n.$$

It holds that

$$\bar{E}[|\Phi_{(0,e)} - \Omega_1^n|^2] \to 0$$

as $n \to \infty$. Indeed, since $\mathscr{L}_b$ and conditional expectation $\bar{E}[\,\cdot \mid \mathscr{F}_{\Lambda_n}]$ commute for $b \in \Lambda_n$, we have

$$\Omega_1^n = \frac{1}{(2n+1)^d} \sum_{y:\, y,\, y+e \in \Lambda_n} \bar{E}[\Phi_{(0,e)} \mid \mathscr{F}_{\tau_y \Lambda_n}],$$

and since we have

$$\lim_{n \to \infty} \bar{E}[|\Phi_{(0,e)} - \bar{E}[\Phi_{(0,e)} \mid \mathscr{F}_{\tau_y \Lambda_n}]|^2] = 0$$

for all y satisfying $y,\, y+e \in \Lambda_n$.

To deal with Ω_2^n we show that the boundary term is bounded in $L^2(\bar{P})$. We decompose Ω_2^n into two parts B_n^+, B_n^- defined by

$$B_n^+ := \frac{1}{(2n+1)^d} \mathscr{L}_{(0,e)} \sum_{y:\, y \in \Lambda_n,\, y+e \notin \Lambda_n} \tau_y h^n$$

$$B_n^- := \frac{1}{(2n+1)^d} \mathscr{L}_{(0,e)} \sum_{y:\, y \notin \Lambda_n,\, y+e \in \Lambda_n} \tau_y h^n.$$

Lemma 4.2. It holds that

$$\sup_n \bar{E}[|B_n^\pm|^2] < \infty. \tag{17}$$

Proof. Using Corollary 3.4, we have only to estimate those quantities which correspond to two terms appearing on the right hand side of (8). By the definition of G^{3n}, $\bar{E}[G^{3n}] = 0$ and $E_{\Lambda_{3n}, y, E}[G^{3n}] = 0$ for all y, E. Therefore

$$\bar{E}[(G^{3n} - \bar{E}[G^{3n}])^2] = \bar{E}[E_{\Lambda_{3n}, y, E}[(G^{3n} - E_{\Lambda_{3n}, y, E}[G^{3n}])^2]].$$

According to Corollary 3.5 the right hand side of the last equality is less than or equal to

$$C(3n)^2 \sum_{b \in \Lambda_{3n}} \bar{E}[\Phi_b] \leqslant C' n^{d+2}.$$

we also have $\bar{E}[(\mathscr{L}_b G^{3n})^2] \leqslant C\bar{E}[\Phi_b^2] \leqslant C'$. Hence an application of (8) shows (17). ▮

Since the boundary terms $B_n^{\pm}$ are bounded in $L^2(\bar{P})$, we can take a weak limit of each. We write $B^{\pm}$ for each of them respectively.

Lemma 4.3. The limit points $B^{\pm}$ depend only on η_0 and η_e.

Proof. We show that B^- depends only on η_0 and η_e. By the construction, B_n^- is measurable with respect to the σ-algebra generated by $\{\eta_e, \eta_x : x \in \mathbf{Z}^d, (e \cdot x) \leqslant 0\}$. The weak limit B^- inherits this property.

We claim that if the bond $b = (z, y)$ satisfies

$$|z - y| = 1, \quad (e \cdot z) \leqslant 0, \quad (e \cdot y) \leqslant 0 \qquad \text{and} \qquad z, y \neq 0, \tag{18}$$

then $\mathscr{L}_{(z,y)} B^- = 0$. This implies that B^- is an exchangeable function of $\{\eta_x, x \neq 0, (e \cdot x) \leqslant 0\}$. Using the Hewitt–Savage 0-1 law, we conclude the proof of the lemma. To see the claim above let us consider a part of boundary of Λ_n

$$\Gamma_n = \Gamma_{e,-,n} := \{x \in \Lambda_n : (e \cdot x) = -n\}.$$

Then for each bond $b = (z, y)$ satisfying the condition (18), there exists $n_0 = n_0(z)$ such that for any $n \geqslant n_0$ we have

$$\begin{aligned} &\#\{x \in \Gamma_n : z \in \tau_x \Lambda_n, \ y \notin \tau_x \Lambda_n \text{ or } z \notin \tau_x \Lambda_n, \ y \in \tau_x \Lambda_n\} \\ &\leqslant \begin{cases} 0 & d = 1, \\ 2 & d = 2, \\ 2(2n+1)^{d-2} & d \geqslant 3. \end{cases} \end{aligned} \tag{19}$$

By simple computation we have

$$\mathscr{L}_b \tau_x h^n = \mathscr{L}_b \tau_x \bar{E}[G^{3n} \mid \mathscr{F}_n] = \begin{cases} \tau_x \bar{E}[\mathscr{L}_{\tau_{-x} b} G^{3n} | \mathscr{F}_n] & \text{if both} \quad z, y \in \tau_x \Lambda_n \\ 0 & \text{if both} \quad z, y \notin \tau_x \Lambda_n. \end{cases} \tag{20}$$

On using (19) and (20), Lemma 3.3, and the Schwarz inequality, there exists a constant C such that

$$\bar{E}[(\mathscr{L}_b B_n^-)^2] \leqslant \frac{C}{n^2}.$$

Hence we conclude that $\mathscr{L}_{(z,\, y)} B^- = 0$ as required. ∎

We derive certain equations for B^-, which specify the function form of B^-. We can rewrite $B_n^- = \mathscr{L}_{(0,\, e)} H_n$ where $H_n := \sum_{x \in \Gamma_n} \tau_x h^n$. By the definition of Γ_n and h^n, H_n does not depend on η_e. By this fact some terms vanish on special configurations;

$$\begin{aligned}
\mathscr{L}_{(2e,\, e)} B_n^-(\eta) &= \mathscr{L}_{(2e,\, e)}(\mathscr{L}_{(0,\, e)} H_n)(\eta) \\
&= -\{1_{\{\eta_0 = 1\}} 1_{\{\eta_e = 0\}} 1_{\{1 \leqslant \eta_{2e} \leqslant k-1\}} + 1_{\{\eta_0 \geqslant 2\}} 1_{\{\eta_e = 0\}} 1_{\{\eta_{2e} = k\}} \\
&\quad + 1_{\{\eta_0 \geqslant 2\}} 1_{\{\eta_e = k-1\}} 1_{\{\eta_{2e} \geqslant 2\}}\}\, B_n^-(\eta) \\
&\quad + 1_{\{\eta_0 \geqslant 2\}} 1_{\{\eta_e = 0\}} 1_{\{1 \leqslant \eta_{2e} \leqslant k-1\}} \mathscr{L}_{(2e,\, e)} B_n^-(\eta).
\end{aligned}$$

Since B^- is a weak limit of B_n^-, this equality holds for B^-.

Similarly we have

$$\begin{aligned}
\mathscr{L}_{(0,\, -e)} B_n^-(\eta) &= \mathscr{L}_{(0,\, -e)}(\mathscr{L}_{(0,\, e)} H_n)(\eta) \\
&= -\{1_{\{\eta_{-e} = 0\}} 1_{\{\eta_0 > 0\}} 1_{\{\eta_e = 0\}} + 1_{\{\eta_{-e} = 0\}} 1_{\{\eta_0 \geqslant 2\}} 1_{\{1 \leqslant \eta_e \leqslant k-1\}} \\
&\quad + 1_{\{1 \leqslant \eta_{-e} \leqslant k-1\}} 1_{\{\eta_0 = 2\}} 1_{\{1 \leqslant \eta_e \leqslant k-1\}}\}\, B^-(\eta) \\
&\quad + \{1_{\{1 \leqslant \eta_{-e} \leqslant k-1\}} 1_{\{\eta_0 \geqslant 2\}} 1_{\{\eta_e = 0\}} + 1_{\{1 \leqslant \eta_{-e} \leqslant k-1\}} 1_{\{\eta_0 \geqslant 3\}} 1_{\{1 \leqslant \eta_e \leqslant k-1\}}\} \\
&\quad \times \{\mathscr{L}_{(0,\, -e)}(H_n(T_{(0,\, e)}\eta) - H_n(\eta))\}.
\end{aligned}$$

From the definition of H_n we have

$$\mathscr{L}_{(0,\, -e)} H_n(\eta) = \frac{1}{(2n+1)^d} \sum_{x \in \Gamma_n} \bar{E}[\Phi_{(0,\, -e)} \mid \mathscr{F}_{\tau_x \Lambda_n}].$$

Since $\{\Phi_b\}_b$ is shift covariant and bounded in $L^2(\bar{P})$, $\mathscr{L}_{(0,\, -e)} H_n(\eta)$ vanishes as $n \to \infty$.

If η satisfies

$$(T_{(0,\, e)} T_{(0,\, -e)} \eta)_0 + (T_{(0,\, e)} T_{(0,\, -e)} \eta)_{-e} = (T_{(0,\, e)} \eta)_0 + (T_{(0,\, e)} \eta)_{-e} \tag{21}$$

then we can apply the method which is applied to $\mathscr{L}_{(0,-e)}H_n(\eta)$ also to $\mathscr{L}_{(0,-e)}H_n(T_{(0,e)}\eta)$. On the set $\{\eta : 1 \leqslant \eta_{-e} \leqslant k-1, \eta_0 \geqslant 3, 1 \leqslant \eta_e \leqslant k-1\}$, we certainly have (21). Hence $1_{\{1 \leqslant \eta_{-e} \leqslant k-1\}} 1_{\{\eta_0 \geqslant 3\}} 1_{\{1 \leqslant \eta_e \leqslant k-1\}} \mathscr{L}_{(0,-e)}H_n(T_{(0,e)}\eta)$ vanishes as $n \to \infty$. But on the set $\{\eta : 1 \leqslant \eta_{-e} \leqslant k-1, \eta_0 \geqslant 3, \eta_e = 0\}$, (21) fails to hold. But on this set we have

$$\begin{aligned}\mathscr{L}_{(0,-e)}H_n(T_{(0,e)}\eta) = &\{H_n(T_{(0,e)}T_{(0,-e)}\eta) - H_n(T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta)\}\\ &+ \{H_n(T_{(-e,0)}T_{(0,e)}\eta) - H_n(T_{(0,e)}\eta)\}\\ &- \{H_n(T_{(-e,0)}T_{(0,e)}\eta) - H_n(T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta)\},\end{aligned} \tag{22}$$

and

$$T_{(-e,0)}T_{(0,e)}\eta = T_{(0,e)}T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta,$$

$$(T_{(0,e)}T_{(0,-e)}\eta)_0 + (T_{(0,e)}T_{(0,-e)}\eta)_{-e} = (T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta)_0 + (T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta)_{-e},$$

$$(T_{(-e,0)}T_{(0,e)}\eta)_0 + (T_{(-e,0)}T_{(0,e)}\eta)_{-e} = (T_{(0,e)}\eta)_0 + (T_{(0,e)}\eta)_{-e}.$$

In the same way as dealing with $\mathscr{L}_{(0,-e)}H_n(\eta)$ we therefore see that the first and second terms on the right hand side of (22) vanish in the limit. On this set the third term of (22) is equal to

$$-B_n^-(T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta).$$

We conclude that B^- satisfies the following equations:

$$\begin{aligned}\mathscr{L}_{(2e,e)}B^-(\eta) = &-\{1_{\{\eta_0=1\}}1_{\{\eta_e=0\}}1_{\{1\leqslant\eta_{2e}\leqslant k-1\}} + 1_{\{\eta_0\geqslant 2\}}1_{\{\eta_e=0\}}1_{\{\eta_{2e}=k\}}\\ &+ 1_{\{\eta_0\geqslant 2\}}1_{\{\eta_e=k-1\}}1_{\{\eta_{2e}\geqslant 2\}}\}\ B^-(\eta)\\ &+ 1_{\{\eta_0\geqslant 2\}}1_{\{\eta_e=0\}}1_{\{1\leqslant\eta_{2e}\leqslant k-1\}}\mathscr{L}_{(2e,e)}B^-(\eta),\end{aligned} \tag{23}$$

$$\begin{aligned}\mathscr{L}_{(0,-e)}B^-(\eta) = &-\{1_{\{\eta_{-e}=0\}}1_{\{\eta_0>0\}}1_{\{\eta_e=0\}} + 1_{\{\eta_{-e}=0\}}1_{\{\eta_0\geqslant 2\}}1_{\{1\leqslant\eta_e\leqslant k-1\}}\\ &+ 1_{\{1\leqslant\eta_{-e}\leqslant k-1\}}1_{\{\eta_0=2\}}1_{\{1\leqslant\eta_e\leqslant k-1\}}\}\ B^-(\eta)\\ &- 1_{\{1\leqslant\eta_{-e}\leqslant k-1\}}1_{\{\eta_0\geqslant 2\}}1_{\{\eta_e=0\}}B^-(T_{(-e,0)}T_{(0,e)}T_{(0,-e)}\eta).\end{aligned} \tag{24}$$

From Lemma 4.3 $B^-(\eta)$ depends only on η_0 and η_e, we write $B^-(\eta) = f(\eta_0, \eta_e)$ and solve f where f is a function from $\{0, 1, 2,..., k\} \times \{0, 1, 2,..., k\}$ into **R**. Substituting special configurations (for example $\eta_0 = 1, \eta_e = 0, \eta_{2e} = 1$) in (23) and (24), we get

$$
\begin{aligned}
f(1,l) &= 0, && \text{for} \quad l \geqslant 2,\\
f(l,k) &= 0, && \text{for} \quad l \geqslant 2,\\
f(0,l) &= f(0,0), && \text{for} \quad l \geqslant 1,\\
f(l,m) &= f(l,m+1), && \text{for} \quad l \geqslant 2, \quad 1 \leqslant m \leqslant k-1,\\
f(0,l) &= 0, && \text{for} \quad 0 \leqslant l \leqslant k-1,\\
f(1,l) &= 0, && \text{for} \quad 1 \leqslant l \leqslant k-1,\\
f(l-1,0) - f(l,0) &= -f(m+1,l-1), && \text{for} \quad l \geqslant 2, \quad 1 \leqslant m \leqslant k-1,\\
f(l-1,m) &= f(l,m), && \text{for} \quad l \geqslant 2, \quad 1 \leqslant m \leqslant k-1.
\end{aligned}
$$

The solutions of these equations are

$$
f(l,m) = \begin{cases} a & \text{if} \quad l \geqslant 2, \quad 1 \leqslant m \leqslant k-1 \\ al + b & \text{if} \quad l \geqslant 1, \quad m = 0 \\ 0 & \text{otherwise} \end{cases}
$$

where $a, b \in \mathbf{R}$ are parameters. We can easily check that $\mathscr{L}_{(0,e)}\eta_0$ and $\mathscr{L}_{(0,e)}\xi_0$ constitute a basis of these solutions.

We have shown that $\Phi_{(0,e)}$ is approximated by $\Psi^n_{(0,e)} - \Omega^n_2$ and all limit points of Ω^n_2 are elements of $\mathscr{G}_0$. This concludes that $\mathscr{G}_c \subset \overline{\mathscr{G}_0 + \mathscr{G}_E}$. ▮

The next lemma will be used to prove Lemma 5.2 in Section 5.

Lemma 4.4. Suppose that a sequence of functions $\{u_k\}_k$ satisfies the following: For each k, u_k is $\mathscr{F}_{\Lambda_k}$ measurable and there exists a constant C such that

$$
\operatorname*{Av}_{b \in \Lambda_k} \bar{E}[(\mathscr{L}_b u_k)^2] \leqslant C
$$

uniformly in k. Let us define a set of functions $\{\phi^k_b\}_b$ by

$$
\begin{aligned}
\phi^k_{(x,x+e)} &:= \tau_x \phi^k_{(0,e)}\\
\phi^k_{(0,e)} &:= \mathscr{L}_{(0,e)} \operatorname*{Av}_{y \in \Lambda_k} [\tau_y u_k],
\end{aligned}
$$

for all x and e with $|e| = 1$. Then each limit point of $\{\phi^k_b\}_b$ is a translation covariant closed form.

Proof. By the definition, $\{\phi^k_b\}_b$ is translation covariant. Hence we have only to prove that each limit point constitutes a closed form. But the proof of the fact is parallel to that of Lemma 4.1. We omit the details. ▮

5. CALCULATION OF V

We introduce two linear spaces of functions:

$$\mathscr{G}^w := \text{the linear space of functions spanned by } \{w_e^E, w_e^P\}_e,$$
$$L\mathscr{G} := \{Lg : g \text{ is a local function}\}.$$

Obviously these are subspaces of $\mathscr{G}$. In order to state a formula for $V(g)$ with $g \in \mathscr{G}^w + L\mathscr{G}$, we introduce some notations. For any local function h and any $g \in \mathscr{G}$, let

$$\langle g, h\rangle_0 = \langle g, h\rangle_0 \, (p, \rho) := \sum_x \bar{E}[g\tau_x h].$$

(Recall that p and ρ are omitted from the notations $\bar{P}$, $\bar{E}$ etc.) For any $g \in \mathscr{G}$, let

$$t_e(g) = t_e(g; p, \rho) := \sum_x (e \cdot x) \, \bar{E}[\eta_x g],$$

$$s_e(g) = s_e(g; p, \rho) := \sum_x (e \cdot x) \, \bar{E}[\xi_x g].$$

From the definition of $\mathscr{G}$, these are well-defined. From the definition of V we can easily get the following proposition.

Proposition 5.1. For any $2d$-dimensional vector α, any local function h and any $g \in \mathscr{G}$, we have

$$V\left(\sum_e (\alpha_e^E w_e^E + \alpha_e^P w_e^P) + Lh, g\right) = -\sum_e \{\alpha_e^E t_e(g) + \alpha_e^P s_e(g)\} - \langle g, h\rangle_0.$$

From the definitions of s_e, t_e, $\langle \cdot \rangle_0$, and $\mathscr{D}_{(0,e)}$ we get the following relations which will be used to prove the Theorem 2.2 in Section 6.

$$s_e(w_{e'}^P) = -\delta_{e,e'} \mathscr{D}_{(0,e)}(\xi_0), \tag{25}$$

$$t_e(w_{e'}^P) = -\delta_{e,e'} \mathscr{D}_{(0,e)}(\eta_0, \xi_0), \tag{26}$$

$$s_e(w_{e'}^E) = -\delta_{e,e'} \mathscr{D}_{(0,e)}(\eta_0, \xi_0), \tag{27}$$

$$t_e(w_{e'}^E) = -\delta_{e,e'} \mathscr{D}_{(0,e)}(\eta_0), \tag{28}$$

$$s_e(Lu) = \mathscr{D}_{(0,e)}\left(\xi_0, \sum_x \tau_x u\right), \tag{29}$$

$$t_e(Lu) = \mathscr{D}_{(0,e)}\left(\eta_0, \sum_x \tau_x u\right), \tag{30}$$

$$\langle Lu, v\rangle_0 = -\sum_{e\,:\,e>0,\,|e|=1} \mathscr{D}_{(0,e)}\left(\sum_x \tau_x u, \sum_x \tau_x v\right), \tag{31}$$

$$s_e(\nabla_{e'}\xi) = -\delta_{e,e'}\, p(1-p), \tag{32}$$

$$t_e(\nabla_{e'}\xi) = -\delta_{e,e'}(1-p)\,\rho, \tag{33}$$

$$\langle u, \nabla_{e'}\xi\rangle_0 = 0, \tag{34}$$

$$s_e(\nabla_{e'}\eta) = -\delta_{e,e'}(1-p)\,\rho, \tag{35}$$

$$t_e(\nabla_{e'}\eta) = -\delta_{e,e'}(\bar{E}[\eta_0^2]-\rho^2), \tag{36}$$

$$\langle u, \nabla_{e'}\eta\rangle_0 = 0, \tag{37}$$

where $\delta_{e,e'} = 1$ if $e = e'$ and 0 if $e \neq e'$ and $\mathscr{D}_{(0,e)}(\xi_0)$, e.g., denotes the value of $\mathscr{D}_{(0,e)}(h)$ for the function $h(\eta) = \xi_0$.

Lemma 5.2. For any $h \in \mathscr{G}$ we have the variational formula;

$$\begin{aligned}&\overline{\lim_{l\to\infty,\,(\frac{y}{|\Lambda_l|},\frac{E}{|\Lambda_l|})\to(p,\rho)}}\;[V^{(l)}(h;y,E)]\\ &\quad= \sup_{\alpha,u}\,\{2V(h,((\alpha\cdot w)+Lu))+V((\alpha\cdot w)+Lu)\}\end{aligned} \tag{38}$$

where supremum is taken over $2d$ dimensional vectors α and all local functions u.

Proof. Once Lemmas 4.1 and 4.4 are established the proof of Lemma 5.2 is the same as that of Theorem 4.1 of ref. 8, that of Theorem 5.2 of ref. 2, or that of Lemma 8.4 of ref. 1 since the proof does not depend on the specific form of $\mathscr{D}_b$. ▮

Let us consider the equivalence relation $\sim$ in $\mathscr{G}$ which is defined by

$$h \sim h' \qquad \text{if and only if} \quad V(h-h') = 0,$$

and the quotient set of $\mathscr{G}$ relative to the relation $\sim$. Since we always identify h and h' if $h \sim h'$ in what follows, without running a risk of confusion we denote the quotient set by the same letter $\mathscr{G}$.

Lemma 5.3. It holds that

$$\mathscr{G}^w + L\mathscr{G} \qquad \text{is dense in } \bar{\mathscr{G}} \tag{39}$$

where $\bar{\mathscr{G}}$ is the closure of $\mathscr{G}$ relative to the inner product V.

Proof of Lemmas 2.1 and 5.3. Let us define $V^+(h, g)$ and $V^-(h, g)$ by

$$V^+(h, g) = V^+(h, g; p, \rho) := \varlimsup_{l \to \infty, (\frac{y}{|\Lambda_l|}, \frac{E}{|\Lambda_l|}) \to (p, \rho)} [V^{(l)}(h, g; y, E)],$$

$$V^-(h, g) = V^-(h, g; p, \rho) := \varliminf_{l \to \infty, (\frac{y}{|\Lambda_l|}, \frac{E}{|\Lambda_l|}) \to (p, \rho)} [V^{(l)}(h, g; y, E)],$$

for all $h, g \in \mathscr{G}$. From the trivial identity

$$\begin{aligned} V^{(l)}(h, h; y, E) = {} & V^{(l)}(h - ((\alpha \cdot w) + Lu); y, E) \\ & + 2V^{(l)}(h - ((\alpha \cdot w) + Lu), ((\alpha \cdot w) + Lu); y, E) \\ & + V^{(l)}(((\alpha \cdot w) + Lu); y, E), \end{aligned}$$

neglecting the first line which is not negative and taking the inferior limit of the both sides, we deduce

$$V^-(h, h) \geqslant 2V(h - ((\alpha \cdot w) + Lu), ((\alpha \cdot w) + Lu)) + V((\alpha \cdot w) + Lu)$$

for all $2d$ dimensional vectors α and all local functions u. This combined with (38) yields

$$V^-(h, h) \geqslant V^+(h, h) \tag{40}$$

for all $h \in \mathscr{G}$. Lemmas 2.1 and 5.3 follows from (38) and (40). ∎

6. PROOF OF THEOREM 2.2

In this section we consider the Hilbert space $(\bar{\mathscr{G}}, V)$. Let us define $\mathscr{G}^{(0)}$ by

$$\mathscr{G}^{(0)} := \text{ the linear subspace of functions spanned by } \{(\nabla\eta)_e, (\nabla\xi)_e\}_e.$$

Fix densities p and ρ. From (34), (37) we have, $\mathscr{G}^{(0)} \perp \overline{L\mathscr{G}}$. From (32), (33), (35), (36) we see that the projection of the space $\mathscr{G}^w$ on $\mathscr{G}^{(0)}$ has rank $2d$; in particular the dimension of $\mathscr{G}^w$ is $2d$. Lemma 5.3 therefore shows that

$$\mathscr{G}^{(0)} + L\mathscr{G} \qquad \text{is dense in } \bar{\mathscr{G}}.$$

Hence there exists a matrix D such that

$$\inf_g V((\alpha \cdot (w + D\,\nabla\vec{\eta} + Lg))) = 0, \tag{41}$$

where the infimum is taken over $g = {}^t(g_1, g_2, \ldots, g_{2d})$ with g_i local functions, and $(Lg) = {}^t(Lg_1, Lg_2, \ldots, Lg_{2d})$.

We give a variational formula for D. First we consider the case $d = 1$. From (41) it follows that there exist $\zeta^E, \zeta^P \in \overline{L\mathscr{G}}$ such that

$$\begin{pmatrix} w^E \\ w^P \end{pmatrix} + \begin{pmatrix} \zeta^E \\ \zeta^P \end{pmatrix} = D \begin{pmatrix} \nabla\eta \\ \nabla\xi \end{pmatrix}. \tag{42}$$

Taking inner product with w^E and w^P for each element of (42), we have

$$\begin{pmatrix} V(w^E+\zeta^E, w^E) & V(w^E+\zeta^E, w^P) \\ V(w^P+\zeta^P, w^E) & V(w^P+\zeta^P, w^P) \end{pmatrix} = D \begin{pmatrix} -t_e(\nabla_e\eta) - s_e(\nabla_e\eta) \\ -t_e(\nabla_e\xi) - s_e(\nabla_e\xi) \end{pmatrix}.$$

Note that the last matrix is $-\chi$. Since $w^E + \zeta^E$ and $w^P + \zeta^P$ are elements of $\mathscr{G}^{(0)}$, the left hand side of the last equality is equal to

$$\begin{pmatrix} V(w^E+\zeta^E, w^E+\zeta^E) & V(w^E+\zeta^E, w^P+\zeta^P) \\ V(w^P+\zeta^P, w^E+\zeta^E) & V(w^P+\zeta^P, w^P+\zeta^P) \end{pmatrix}.$$

Denote this matrix by $\tilde{D}$. Since αw is in the space spanned by $\alpha\nabla\vec{\eta}$ and $L\mathscr{G}$, which are the orthogonal complements of each other, $V(\alpha(w+\zeta))^{1/2}$ is equal to the distance of αw to $L\mathscr{G}$. Applying Proposition 5.1, we therefore have the following variational formula for $\tilde{D}$: for ${}^t\alpha = (\alpha^E, \alpha^P)$,

$$(\alpha \cdot \tilde{D}\alpha) = \inf_{g^E, g^P} \mathscr{D}_{(0,e)}\left(\alpha^E\left(\eta_0 + \left(\sum_x \tau_x g^E\right)\right) + \alpha^P\left(\xi_0 + \left(\sum_x \tau_x g^P\right)\right)\right),$$

where the infimum is taken over all local functions.

For $d \geqslant 2$, the diffusion coefficient matrix $D = (D_{p, e_i, q, e_j})$ for $1 \leqslant i, j \leqslant d$, $p, q \in \{E, P\}$, is determined by

$$\begin{pmatrix} w^E_{e_1} \\ w^P_{e_1} \\ \vdots \\ w^E_{e_d} \\ w^P_{e_d} \end{pmatrix} = D \begin{pmatrix} \nabla_{e_1}\eta \\ \nabla_{e_1}\xi \\ \vdots \\ \nabla_{e_d}\eta \\ \nabla_{e_d}\xi \end{pmatrix} - \begin{pmatrix} \zeta^E_{e_1} \\ \zeta^P_{e_1} \\ \vdots \\ \zeta^E_{e_d} \\ \zeta^P_{e_d} \end{pmatrix},$$

where $\zeta^E_{e_1}, \eta^P_{e_1}, \ldots, \zeta^P_{e_d} \in \overline{L\mathscr{G}}$.

Lemma 6.1. For $d \geqslant 2$ if $e \neq e'$ then $D_{p, e, q, e'} = 0$, for all $p, q \in \{E, P\}$.

Proof. We have only to show that $D_{E, e, E, e'} = D_{E, e, P, e'} = 0$. Since we have

$$w_e^E = \sum_{e^*} D_{E, e, E, e^*} \nabla_{e^*} \eta + \sum_{e^*} D_{E, e, P, e^*} \nabla_{e^*} \xi + \zeta_e^E,$$

taking inner product with $\nabla_{e'} \eta$ and $\nabla_{e'} \xi$, we have

$$V(w_e^E, \nabla_{e'} \eta) = \sum_{e^*} D_{E, e, E, e^*} V(\nabla_{e^*} \eta, \nabla_{e'} \eta) + \sum_{e^*} D_{E, e, P, e^*} V(\nabla_{e^*} \xi, \nabla_{e'} \eta),$$

$$V(w_e^E, \nabla_{e'} \xi) = \sum_{e^*} D_{E, e, E, e^*} V(\nabla_{e^*} \eta, \nabla_{e'} \xi) + \sum_{e^*} D_{E, e, P, e^*} V(\nabla_{e^*} \xi, \nabla_{e'} \xi).$$

Since $V(w_e^E, \nabla_{e'} \eta)$ and $V(w_e^E, \nabla_{e'} \xi)$ are zero if $e \neq e'$, we have only to show that if $e^* \neq e'$ then both $V(\nabla_{e^*} \eta, \nabla_{e'} \eta)$ and $V(\nabla_{e^*} \xi, \nabla_{e'} \eta)$ vanish. Denote by θ_e the reflection operator with respect to the origin along the e direction formally

$$(\theta_e x)_{e'} = \begin{cases} x_{e'} & \text{if} \quad e \neq e' \\ -x_e & \text{if} \quad e = e'. \end{cases}$$

We may extend θ_e to the configuration space naturally by $(\theta_e \eta)_x = \eta_{\theta_e x}$ and $(\theta_e f)(\eta) = f(\theta_e \eta)$. Since our model is symmetric under θ_e, we have $V(f, g) = V(\theta_e f, \theta_e g)$. From the definition of V, V is shift invariant, namely $V(f, g) = V(f, \tau_e g)$ for all $f, g \in \mathcal{G}$. Since $\theta_e \nabla_{e'} \eta$ is equal to $\nabla_{e'} \eta$ if $e \neq e'$ and $-\tau_{e'} \nabla_{e'} \eta$ if $e = e'$, we have

$$V(\nabla_e \eta, \nabla_{e'} \eta) = -V(\tau_e \nabla_e \eta, \nabla_{e'} \eta) = -V(\nabla_e \eta, \nabla_{e'} \eta) = 0,$$

for all $e \neq e'$. In the same way we have

$$V(\nabla_e \eta, \nabla_{e'} \xi) = -V(\tau_e \nabla_e \eta, \nabla_{e'} \xi) = -V(\nabla_e \eta, \nabla_{e'} \xi) = 0,$$

for all $e \neq e'$. Hence we conclude the proof of the lemma. ∎

From Lemma 6.1 we get the variational formula for the diffusion coefficient matrix for $d \geqslant 2$ in the same way as in the case $d = 1$. ∎

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