A Quantum Crystal with Multidimensional Anharmonic Oscillators

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The quantum anharmonic crystal is made up of a large number of multidimensional anharmonic oscillators arranged in a periodic spatial lattice with a nearest neighbor coupling. If the coupling coefficient is sufficiently small, then there is a convergent expansion for the ground state of the crystal. The estimates on the convergence are independent of the size of the crystal. The proof uses the path integral representation of the ground state in terms of diffusion processes. The convergence of the cluster expansion depends on the ergodicity properties of these processes.

1. THE QUANTUM CRYSTAL

This note is an extension of work of Minlos, Verbeure, and Zagrebnov.[1] The problem is to describe the ground state of a quantum anharmonic crystal. The crystal is made of a large number of anharmonic oscillators with a nearest neighbor coupling. The new feature of this note is that the oscillators are multi-dimensional. The main result is the same as before: if the coupling coefficient is sufficiently small, then there is a convergent expansion for the ground state of the crystal. The estimates on the convergence are independent of the size of the crystal.

Each anharmonic oscillator individually is described by a quantum mechanical Hamiltonian which is a Schrödinger operator of the form

$$H_0 = -\tfrac{1}{2}\nabla^2 + V(x) \tag{1.1}$$

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acting in $L^2(\mathbf{R}^\nu, d^\nu x)$. We shall assume that $V(x) \approx |x|^{2s}$ for large $|x|$. We take this to mean that $V(x)$ is bounded both above and below by functions of the form $C_1 + C_2 |x|^{2s}$, with possibly different constants in the two bounds. In the following $s > 1$, so this is an anharmonic oscillator.

The quantum crystal itself consists of some large number N of oscillators associated to points in d-dimensional space. The points are those belonging to a finite subset $\Lambda \subset \mathbf{Z}^d$. Thus N is the number of points in Λ. For each $i \in \Lambda$ the corresponding oscillator coordinate x_i ranges over $\mathbf{R}^\nu$. The configuration of all the oscillators is a point x in $\mathbf{R}^{N\nu}$. The corresponding Hilbert space describing the quantum states is $L^2(\mathbf{R}^{N\nu}, d^{N\nu}x)$.

The Hamiltonian is the sum of two parts. The first is

$$H_0^\Lambda = \sum_{i \in \Lambda} H_0^{(i)} \tag{1.2}$$

where the operator $H_0^{(i)}$ is the oscillator Hamiltonian depending on the ith coordinate. The other part of the Hamiltonian is a multiplication operator. It is specified by a fixed symmetric bilinear form Q on $\mathbf{R}^\nu \times \mathbf{R}^\nu$ and a real parameter α. It is

$$W^\Lambda = \alpha \sum_{\substack{i,\,j \in \Lambda \\ |i-j|=1}} x_i Q x_j \tag{1.3}$$

The sum is over nearest neighbor sites in Λ. The parameter α is merely a convenient coupling constant for keeping track of the strength of the interaction. The total Hamiltonian of interest is

$$H^\Lambda = H_0^\Lambda + W^\Lambda \tag{1.4}$$

This is of course a Schrödinger operator in a high dimensional space, so by known properties of such operators,[2] it has a ground state $\psi^\Lambda > 0$ satisfying

$$H^\Lambda \psi^\Lambda = E^\Lambda \psi^\Lambda \tag{1.5}$$

We are interested in the case when the crystal Λ approaches the entire space $\mathbf{Z}^d$. Thus the number of points N in the crystal approaches infinity, and in the limit there are infinitely many coordinates.

Let A a bounded real function that depends on some fixed finite family of coordinates. The expectation of this function is

$$G^\Lambda(A) = \langle \psi^\Lambda, A\psi^\Lambda \rangle \tag{1.6}$$

The following is the main result.

Theorem 1.1. Consider the quantum crystal consisting of anharmonic oscillators at each site together with quadratic coupling with coupling constant α. There exists α_0 such that for $|\alpha| < \alpha_0$ the ground state expectation of each local coordinate observable A exists in the limit

$$G(A) = \lim_{\Lambda \to \mathbf{Z}^d} G^\Lambda(A) \tag{1.7}$$

of an infinite crystal and is given by a convergent power series expansion in the coupling constant α.

The meaning of this limit, of course, is that for every $\varepsilon > 0$ there exists a Λ_0 such that $\Lambda \supset \Lambda_0$ implies $G_\Lambda(A)$ is within ε of $G(A)$. The existence of the limit shows that the configuration probabilities associated with the quantum state are defined in the limit of the infinite crystal.

Remark 1. The regime in which the theorem applies may be regarded as one of small mass rather than of small coupling constant.

The small mass interpretation gives a more physical interpretation of this parameter region. To see how this comes about, begin with the Hamiltonian

$$H = \sum_i \left(-\frac{1}{2m} \nabla_i^2 + V(x_i) \right) + \sum_{i,j} x_i Q x_j \tag{1.8}$$

Recall that $V(x)$ grows at infinity like $|x|^{2s}$ with $s > 1$. Make a scale change in the Hamiltonian where x_i is replaced by γx_i. The Hamiltonian becomes

$$H = \gamma^{2s} \left[\sum_i \left(-\frac{1}{2m\gamma^{2(s+1)}} \nabla_i^2 + \frac{V(\gamma x_i)}{\gamma^{2s}} \right) + \frac{1}{\gamma^{2(s-1)}} \sum_{i,j} x_i Q x_j \right] \tag{1.9}$$

Take $m\gamma^{2(s+1)} = 1$ and set $\alpha = 1/\gamma^{2(s-1)}$. Then for small m the corresponding γ becomes large, and so in the anharmonic regime $s > 1$ the effective coupling constant α becomes small.

Remark 2. While the discussion here is limited for simplicity to the ground state, the same techniques may be used to construct equilibrium states at non-zero temperature.[1]

Remark 3. A somewhat more complicated argument involving other more general local observables[1] would show that the quantum state

itself is well-defined in the limit. That is, one can prove existence of the limiting state on the whole quasilocal algebra, not only on its commutative part.

The theorem will be proved later in Section 6. The proof depends on looking at the system in a number of different ways. The original quantum crystal is given by a Hamiltonian which is the sum of independent quantum oscillators (indexed by sites in the crystal) and interaction terms. The Feynman-Kac formula represents this in terms of a system of independent diffusion processes (again indexed by sites in the crystal). This reduces the quantum mechanics problem to a probability problem.

This problem is in turn transformed into a system of independent random variables (indexed by sites and discrete time instants). This allows the use of the factorization property of expectations of products of independent random variables.

Finally, the cluster expansion reduces the problem to the setting of a Banach space of functions of subsets of the index set. The function of interest is defined on each set as an expectation of variables associated with the complement of the set. The factorization property is used to show that the dependence of local quantities on distant parts of the crystal is very weak.

We begin with a description of a single quantum oscillator and the associated diffusion process. The usual quantum harmonic oscillator corresponds to a stationary diffusion process with a linear drift term that maintains equilibrium against the diffusion. The anharmonic oscillator under consideration here corresponds to a diffusion processes with a drift that grows faster than linear, so that the equilibrium is reached extremely rapidly.

2. A SINGLE OSCILLATOR

The Hamiltonian H_0 given above defines a single quantum anharmonic oscillator. The Feynman–Kac formula for the associated semigroup is

$$\exp(-tH_0)\,f(x) = E_x\left[\exp\left(-\int_0^t V(\omega(\tau))\,d\tau\right)f(\omega(t))\right] \qquad (2.1)$$

The expectation is over all Wiener process paths ω with $\omega(0) = x$. Let $H_0\psi_0 = \lambda_0\psi_0$, where $\psi_0 > 0$ is the ground state. Then $\exp(-tH_0)\,\psi_0 = \exp(-t\lambda_0)\,\psi_0$. This may be written with the aid of the Feynman–Kac formula as

$$\psi_0(x) = e^{\lambda_0 t}E_x\left[\exp\left(-\int_0^t V(\omega(\tau))\,d\tau\right)\psi_0(\omega(t))\right] \qquad (2.2)$$

This formula involves the ground state wave function on both sides of the equation. Nevertheless, it gives rather precise information about the ground state of the Schrödinger operator. This is the work of several authors, especially Carmona. The book of Simon[3] has a useful exposition. In this section we summarize the part of this material that we need to get estimates for the cluster expansion.

In the following we will assume $V(x) \approx |x|^{2s}$, where $s > 1$. We take this to mean that we have both a lower bound and an upper bound of this form, with suitable multiplicative and additive constants.

We will need a standard lemma about the Wiener process, the reflection principle. Since we need the perhaps less familiar multi-dimensional form, for convenience we state it as the first lemma.

Lemma 2.1. The probability that the Wiener process path ever leaves a ball of radius a in the time interval from 0 to t is bounded by twice the probability that it is outside the ball at time t. Thus

$$P_x[\exists \tau \, 0 \leqslant \tau \leqslant t, |\omega(\tau) - x| \geqslant a] \leqslant 2P_x[|\omega(t) - x| \geqslant a] \tag{2.3}$$

Note. The random variable $\omega(t)$ in the reflection principle is Gaussian in $\mathbf{R}^v$ with mean x and variance equal to $1/t$ times the identity matrix. It follows that the right hand side is bounded above by $p(a/\sqrt{t}) \exp(-a^2/(2t))$. The coefficient $p(z)$ is a constant in dimensions one and two and a polynomial of degree $v - 2$ in higher dimensions.

Proof. Define the random escape time $T = \min_\tau |\omega(\tau) - x| \geqslant a$. Define the reflected path for $\tau \leqslant T$ by $\tilde{\omega}(\tau) = \omega(\tau)$ and for $\tau \geqslant T$ by $\tilde{\omega}(\tau) = \omega(T) - (\omega(\tau) - \omega(T))$. Then by the strong Markov property the reflected path is also a Wiener process. Furthermore, $T \leqslant t$ implies $|\omega(t) - x| \geqslant a$ or $|\tilde{\omega}(t) - x| \geqslant a$. Hence $P_x[T \leqslant t] \leqslant P_x[|\omega(t) - x| \geqslant a] + P_x[|\tilde{\omega}(t) - x| \geqslant a]$. Since $\omega(t)$ and $\tilde{\omega}(t)$ have the same distribution, this translates to the desired bound.

Lemma 2.2. Suppose that the potential energy function V of the Schrödinger operator satisfies $V(x) \geqslant C_1 + C_2 |x|^{2s}$ with $s > 1$. The ground state wave function has an upper bound of the form $A \exp(-C |x|^{s+1})$.

Proof. The argument for the upper bound is in two stages. All we know a priori is that ψ_0 is in L^2. Since V is bounded below by C_1, we can use the Feynman–Kac formula to bound $|\psi_0(x)|$ by $\exp(\lambda_0 t) \exp(-C_1 t) E_x[|\psi_0(\omega(t)|]$. For fixed $t > 0$ the Wiener integral is given by convolution by a Gaussian. Since the Gaussian is also in L^2, we conclude that ψ_0 in L^∞.

Now use the Feynman–Kac formula again, taking the integral over paths starting at x. Break the integral into two parts, one in which the path up to time t stays in a ball of radius $|x|/2$ about x, and the other in which it leaves the ball. Take t proportional to $1/|x|^{s-1}$. Thus for the large values of $|x|$ of interest to us, the value of t is small.

If the path stays in the ball, then in particular it stays outside of the ball of radius $|x|/2$ centered at 0. Thus $V(\omega(\tau))$ is bounded below $C_1 + C_2 |x/2|^{2s}$. So the exponential in the integrand is bounded by a constant times $\exp(-C|x|^{2s}t) = \exp(-C|x|^{s+1})$. This gives the desired bound for this part.

If the path ever leaves the ball, then by the reflection principle we have a bound proportional to $\exp(-C|x|^2/t) = \exp(-C|x|^{s+1})$. This gives the desired bound for the other part.

The importance of this upper bound is that it controls the expectations involving exponentials of quadratic expressions of the type that occur in the interaction term. The following corollary illustrates this control.

Corollary 2.3. The function

$$\langle \psi_0, \exp(zx^2)\,\psi_0 \rangle = \int \exp(zx^2)\,\psi_0^2(x)\,d^\nu x \tag{2.4}$$

is an entire analytic function of z of order $(s+1)/(s-1)$.

The proof that this is an entire function of order $(s+1)/(s-1)$ may be carried out by adapting the argument in ref. 1.

Lemma 2.4. Suppose that the potential energy function V in the Schrödinger operator satisfies $V(x) \leqslant C_1 + C_2 |x|^{2s}$. Then the ground state wave function $\psi_0(x)$ has a lower bound of the form $A \exp(-C|x|^{s+1})$.

Proof. The argument for the lower bound is also in two stages. In both stages it uses the general fact that the probabilty of the intersection $A \cap B$ of two events is bounded below by the probability of A minus the probability of the complement of B.

First we need to argue that $\psi_0(x)$ is bounded below away from zero on each ball $|x| \leqslant \delta$. Fix $t > 0$ and use the Feynman–Kac formula with x in the ball and with this value of t. Consider an $\varepsilon > 0$ and a bounded set S with strictly positive measure such that $\psi_0 \geqslant \varepsilon$ on S. Consider the integral over the set of paths where $\omega(t)$ is in S and $|\omega(\tau)| \leqslant R$ for $0 \leqslant \tau \leqslant t$. On this set $V(\omega(\tau))$ is bounded above by $C_1 + C_2 R^{2s}$, so we need only estimate the probability of this set of paths. This is bounded below by the probability

that $\omega(t)$ is in S minus the probability that $|\omega(\tau)| > R$ for some τ with $0 \leqslant \tau \leqslant t$. The first probability is bounded below uniformly for $|x| \leqslant \delta$. The second probability goes to zero as R goes to infinity, uniformly for $|x| \leqslant \delta$, by the reflection principle. Take some fixed R sufficiently large so that the second probability is less than the first. This gives the desired lower bound.

For the second stage use the Feynman–Kac formula again. Consider the integral over paths starting at x. As in the previous lemma, choose t proportional to $1/|x|^{s-1}$. Restrict the integral to paths such that $|\omega(t)| \leqslant \delta$ and such that $|\omega(\tau) - x| \leqslant 2 |x|$ for $0 \leqslant \tau \leqslant t$. The second condition ensures that $|\omega(\tau)| \leqslant 3 |x|$ for the same range of τ. For such paths $V(\omega(\tau))$ is bounded above by $C_1 + C_2 |3x|^{2s}$. This gives a lower bound for the eigenfunction of the form of a constant times $\exp(- C |x|^{2s} t))$ times the probability of the event that the path satisfies these restrictions.

This probability is bounded below by the probability that $|\omega(t)| \leqslant \delta$ minus the probability that $|\omega(\tau) - x| > 2 |x|$ for some τ with $0 \leqslant \tau \leqslant t$. The first probability is bounded below by a constant times $1/t^{\nu/2} \exp(-(|x| + \delta)^2/(2t))$. The second probability can be bounded by the reflection principle: the bound is a polynomial factor times $\exp(- |2x|^2/(2t))$. When $|x|$ is large the first probability dominates the second probability. So the final estimate is a constant times $\exp(- C |x|^{2s} t) \exp(- C' |x|^2/t)$ for large $|x|$. This gives the desired lower bound for large $|x|$.

The conclusion of the discussion thus far may be summarized briefly. Assume that $V(x) \sim |x|^{2s}$ for some $s > 1$. Then $\log \psi_0(x) \sim |x|^{s+1}$. This says that when the potential grows faster than quadratic, the probability density $|\psi_0(x)|^2$ is more concentrated than Gaussian.

3. A SINGLE DIFFUSION PROCESS

There is a correspondence between quantum oscillators and diffusion processes. Start with the quantum oscillator Hamiltonian H_0. This is self-adjoint and has eigenvector ψ_0 with eigenvalue λ_0. Consider the operator $\hat{H}_0$ given by

$$\hat{H}_0 = \frac{1}{\psi_0} (H_0 - \lambda_0) \psi_0 = - \left(\frac{1}{2} \nabla^2 + u(x) \cdot \nabla \right) \qquad (3.1)$$

where $u(x) = \nabla \psi_0/\psi_0$. The operator $\hat{H}_0$ is a self-adjoint operator acting in a new Hilbert space $L^2(\mathbf{R}^\nu, |\psi_0(x)|^2 d^\nu x)$. It has eigenvector 1 with eigenvalue 0. From the definition we see that $\hat{H}_0$ is unitarily equivalent to the Schrödinger operator $H_0 - \lambda_0$ acting in the original Hilbert space.

The one-parameter semigroup of operators associated with the generator is $\exp(- t\hat{H}_0)$ defined for $t \geqslant 0$. Since it sends positive functions into

positive functions and since $\exp(-t\hat{H}_0)1 = 1$, the semigroup determines a Markov process according to a standard construction. Since it is self-adjoint with respect to a Hilbert space determined by a positive measure, the process may be taken to be a stationary time-reversible process with this measure as the invariant measure. The process is a probability measure on the space of all paths ω defined on the real time axis with values in $\mathbf{R}^\nu$.

For each t the random variable $\omega(t)$ has the distribution $|\psi_0(x)|^2 \, d^\nu x$ given by the invariant measure. The relation between the process and the semigroup is that the conditional expectation of $g(\omega(t))$ given $\omega(0) = x$ is

$$E[\,g(\omega(t)) \mid \omega(0) = x\,] = \exp(-t\hat{H}_0)\, g(x) = \int p_t(x, y)\, g(y)\, |\psi_0(y)|^2 \, d^\nu y \tag{3.2}$$

Here $p_t(x, y)\, |\psi_0(y)|^2 \, d^\nu y$ is the conditional probability given a starting point at x to make a transition to y in time t. It follows that the correlation at two different times is given by

$$E[\,f(\omega(0)\, g(\omega(t))\,]$$
$$= \langle f, \exp(-t\hat{H}_0)\, g \rangle = \iint f(x)\, p_t(x, y)\, g(y)\, |\psi_0(y)|^2 \, d^\nu y\, |\psi_0(x)|^2 \, d^\nu x \tag{3.3}$$

The quantity $p_t(x, y)$ is the joint density of $(\omega(0), \omega(t))$ with respect to the product measure $|\psi_0(x)|^2 \, d^\nu x\, |\psi_0(y)|^2 \, d^\nu y$. The fact that the process is time-reversible corresponds to the self-adjointness relation $p_t(x, y) = p_t(y, x)$.

A Markov process with a generator of this type is a diffusion process with continuous sample paths. The intuition is that its motion is a combination of symmetric diffusion and a systematic drift given by the $u(x)$. This drift inward compensates for the diffusion and makes the process have a stationary probability measure. When the drift is strong enough (growing faster than linear) the evolution of the process from a starting point x to the stationary distribution is extraordinarily rapid and uniform.

Lemma 3.1. Consider a diffusion process defined by a Schrödinger operator with potential V satisfying $V(x) \approx |x|^{2s}$ with parameter $s > 1$. Then the joint density with respect to the invariant measure satisfies $p_t(x, y) \to 1$ uniformly at an exponential rate as $t \to \infty$.

Proof. The result follows from the ultracontractive property of the semigroup and an elementary estimate on the Hilbert–Schmidt norm. The

ultracontractive property says that the semigroup maps L^2 into L^∞. This follows from Rosen's lemma as cited in Davies and Simon.[4]

Let H_0 be a Schrödinger operator as above. The hypothesis of Rosen's lemma is that for all $\delta > 0$

$$-\log \psi_0(x) \leqslant \delta H_0 + g(\delta) \tag{3.4}$$

where $g(\delta)$ is bounded by a polynomial in $1/\delta$. (The hypothesis could also be stated with H_0 replaced by $\hat{H}_0$, since it is invariant under the unitary equivalence that takes the Schrödinger operator into the diffusion operator.) The conclusion of Rosen's lemma is that for $t > 0$ the operator $\exp(-t\hat{H}_0)$ takes $L^2(\mathbf{R}^\nu, \psi_0(x)^2\, d^\nu x)$ into $L^\infty(\mathbf{R}^\nu, \psi_0(x)^2\, d^\nu x)$. This is the ultracontractive property.

This lemma applies immediately to Schrödinger operators with potential satisfying $V(x) \sim |x|^{2s}$ with $s > 1$. For such a potential we have $-\log \psi_0(x) \sim |x|^{s+1}$. There is an inequality

$$|x|^{s+1} \leqslant \delta\, |x|^{2s} + \left(\frac{1}{\delta}\right)^{(s+1)/(s-1)} \tag{3.5}$$

The inequality is obvious both when $1/|x|^{s-1} \leqslant \delta$ and when $|x|^{s-1} \leqslant 1/\delta$, and these cover all cases. Since the negative Laplacian is a positive operator, this gives the hypothesis of Rosen's lemma for such anharmonic potentials.

Suppose that the norm of $\exp(-a\hat{H}_0)$ from L^2 to L^∞ is C_a. Ultracontractivity says that $C_a < \infty$ for $a > 0$. From the semigroup property $\exp(-t\hat{H}_0) = \exp(-a\hat{H}_0)\exp(-(t-2a)\,\hat{H}_0)\exp(-a\hat{H}_0)$ we have

$$p_t(x, y) - 1 = \iint p_a(x, z)(p_{t-2a}(z, w) - 1)\,\psi_0(z)^2\, d^\nu z\, p_a(w, y)\,\psi_0(w)^2\, d^\nu w \tag{3.6}$$

Estimating the norm twice gives the uniform bound

$$|p_t(x, y) - 1| \leqslant C_a^2 \sqrt{\iint (p_{t-2a}(z, w) - 1)^2\,\psi_0(z)^2\, d^\nu z\,\psi_0(w)^2\, d^\nu w} \tag{3.7}$$

The lowest eigenvalue of $\hat{H}_0$ is 0 with corresponding eigenvector 1. Let P_0 be the projection onto 1. The right hand side of the inequality is C_a^2 times the Hilbert–Schmidt norm

$$\|\exp(-(t-2a)\,\hat{H}_0) - P_0\|_2 = \sqrt{\sum_{n=1}^{\infty} e^{-2(\lambda_n - \lambda_0)(t-2a)}} \tag{3.8}$$

This goes to zero exponentially fast as t tends to infinity. This completes the proof.

The lemma shows that the process that arises from the anharmonic oscillator has a very strong ergodicity property. The intuitive reason for this is that the inward drift is so strong that the time to reach a bounded region is bounded independent of the starting point.

By contrast, a harmonic oscillator does not have this ergodicity property. If $V(x) = x^2/2$ is the harmonic oscillator potential, then the drift is $u(x) = -x$. The corresponding random process ω is the Ornstein–Uhlenbeck velocity process. The joint density of $\omega(0)$ and $\omega(t)$ with respect to Lebesgue measure is Gaussian and is given by

$$p_t(x, y) \exp(-x^2) \exp(-y^2) = \exp\left(-\frac{1}{1 - e^{-2t}}(x^2 - 2e^{-t}xy + y^2)\right) \quad (3.9)$$

It is evident that $p_t(x, y)$ approaches 1 pointwise but not uniformly as $t \to \infty$.

4. INDEPENDENT DIFFUSION PROCESSES

Since each quantum oscillator corresponds to a diffusion process, the entire quantum crystal may be represented as a collection of independent diffusion processes. This is just the standard reduction of quantum statistical mechanics to classical statistical mechanics in one higher dimension.

Let $\Lambda \subset \mathbf{Z}^d$ with N points. The Hilbert space for the quantum crystal is $L^2(\mathbf{R}^{Nv}, d^{Nv})$. The independent quantum anharmonic oscillators in the crystal have Hamiltonian

$$H_0^\Lambda = \sum_{i \in \Lambda} H_0^{(i)} = \sum_{i \in \Lambda} (\tfrac{1}{2}\nabla_i^2 + V(x_i)) \quad (4.1)$$

The ground state for the system of independent oscillators is given by the wave function ψ_0^Λ with

$$H_0^\Lambda \psi_0^\Lambda = \lambda_0^\Lambda \psi_0^\Lambda \quad (4.2)$$

Here $\psi_0(x)$ is the product of the $\psi_0(x_i)$ over i, and $\lambda_0^\Lambda = N\lambda_0$.

Let the corresponding diffusion generator be defined by

$$\hat{H}_0^\Lambda = \frac{1}{\psi_0^\Lambda}(H_0^\Lambda - \lambda_0^\Lambda)\psi_0^\Lambda = \sum_{i \in \Lambda} \hat{H}_0^{(i)} \quad (4.3)$$

This acts in $L^2(\mathbf{R}^{Nv}, |\psi_0^A(x)|^2 \, d^{Nv}x)$. The stationary diffusion process with this generator consists of independent diffusion processes ω_i for $i \in \Lambda$. We now use ω to denote the system of all these processes taken together. The invariant probability measure is given by $|\psi_0^A(x)|^2 \, d^{Nv}x$, and the correlation is determined by

$$\langle f, \exp(-t\hat{H}_0^A) \, g \rangle = E[f(\omega(0) \, g(\omega(t)))] \tag{4.4}$$

The ultimate purpose is to represent the quantum crystal with interaction. Let $H^A = H_0^A + W^A$ be the total Hamiltonian for the crystal. If we transform it to the independent diffusion process setting we get an operator

$$\hat{H}^A = \frac{1}{\psi_0^A} (H^A - \lambda_0^A) \, \psi_0^A = \hat{H}_0^A + W^A \tag{4.5}$$

The semigroup generated by this may be represented by another variant of the Feynman–Kac formula. This is

$$\langle f, \exp(-t\hat{H}^A) \, g \rangle = E\left[f(\omega(0) \exp\left(-\int_0^t W^A(\omega(\tau)) \, d\tau \right) g(\omega(t)) \right] \tag{4.6}$$

This Feynman–Kac representation may be used to determine the ground state. In fact, the ground state ψ^A should be obtained by applying the operator $\exp(-TH^A)$ to a suitable initial state, say ψ_0^A, normalizing, and letting $T \to \infty$. Equivalently, in the diffusion representation it should be obtained by applying $\exp(-T\hat{H}^A)$ to the function 1, normalizing, and letting $T \to \infty$. Let

$$G^{A, T}(A) = \frac{1}{Z_{A, T}} \langle \exp(-T\hat{H}^A) \, 1, A \exp(-T\hat{H}^A) \, 1 \rangle \tag{4.7}$$

where $Z_{A, T}$ is a normalization factor that makes $G^{A, T}(1) = 1$.

By using the Feynman–Kac representation we can write this as a functional integral of the form given in the following lemma.

Lemma 4.1. Consider the diffusion process ω consisting of N independent diffusion process each with values in $\mathbf{R}^v$. Let A be a function of oscillator coordinates each of which is in $\mathbf{R}^v$. Then the expectation of A in the oscillator ground state is

$$G^A(A) = \lim_{T \to \infty} G^{A, T}(A) \tag{4.8}$$

where

$$G^{A,\,T}(A) = \frac{1}{Z_{A,\,T}} E\left[A(\omega(0)) \exp\left(-\int_{-T}^{T} W^{A}(\omega(\tau))\, d\tau \right) \right] \qquad (4.9)$$

5. INDEPENDENT RANDOM VARIABLES

It is useful to replace the representation by independent diffusion processes by a representation in terms of independent random variables. This is done by discretizing the time index. Fix a time interval $a > 0$. Let $T = na$. From now on the discrete space-time will be indexed by integer pairs (i, k) with $i \in \Lambda$ and $|k| \leqslant n$. Introduce corresponding variables $q_{ik} = \omega_i(ka)$. These are not independent for the same i. However when a is large enough they are very close to being independent. In fact, the joint distribution of the q_{ik} is given by the measure

$$\prod_{e} p_e(q) \prod_{i} \prod_{k} |\psi_0(q_{ik})|^2\, dq_{ik} \qquad (5.1)$$

where

$$p_e(q) = p_a(q_{ik}, q_{i(k+1)}) \qquad (5.2)$$

is the transition density corresponding to the edge e consisting of the two points (i, k) and $(i, k + 1)$. Furthermore, the factors $p_e(q)$ are uniformly close to one for large a.

We can look at another measure on the q in which the q_{ik} are independent random variables each with the distribution $|\psi_0(q_{ik})|^2\, dq_{ik}$. We write E_0 for the expectation with respect to this product measure. The relation between the two measures is given by

$$E[F(q)] = E_0\left[F(q) \prod_{e} p_e(q) \right] \qquad (5.3)$$

Note that the factors $p_e(q)$ are independent with respect to the product measure when the edges e do not overlap.

Let

$$W(\omega) = \int_{-T}^{T} W^{A}(\omega(\tau))\, d\tau \qquad (5.4)$$

Write

$$W(\omega) = \sum_r W_r(\omega) \tag{5.5}$$

where

$$W_r(\omega) = \alpha \int_{ka}^{(k+1)\,a} \omega_i(\tau)\, Q\omega_j(\tau)\, d\tau \tag{5.6}$$

and r is the rectangle consisting of the four points (i, k), $(i, k+1)$, (j, k), $(j, k+1)$ with i and j nearest neighbors. Note that W_r only depends on the process ω_i restricted to the time interval $[ka, (k+1)\,a]$ and on the process ω_j restricted to the same interval. The only other quantity in the representation is A regarded as a function of $\omega(0)$. The expectation of interest is

$$G^{\Lambda'}(A) = \frac{1}{Z_{\Lambda'}} E[A \exp(-W)] = \frac{1}{Z_{\Lambda'}} E\left[A \prod_r \exp(-W_r) \right] \tag{5.7}$$

In this formula and in subsequent calculations we denote the space-time index set consisting of points (i, k) with $i \in \Lambda$ and $|k| \leqslant n$ by Λ'. The interest is in estimates that are independent of the size of this region.

We may write the expectation as the expectation of the conditional expectation given the q_{ik} and then express the integral in terms of independent random variables. This gives

$$G^{\Lambda'}(A) = \frac{1}{Z_{\Lambda'}} E\left[E\left[A \prod_r \exp(-W_r) \,\bigg|\, q \right] \right]$$

$$= \frac{1}{Z_{\Lambda'}} E_0\left[E\left[A \prod_r \exp(-W_r) \,\bigg|\, q \right] \prod_e p_e \right] \tag{5.8}$$

The function A depends on the $q_{i0} = \omega_i(0)$ for i in some fixed finite set. In the following we let u be the set of corresponding points $(i, 0)$. It is convenient to abbreviate the iterated expectation $E_0[E[\cdot \,|\, q]]$ by E_1. The calculation may be stated in terms of the following lemma.

Lemma 5.1. Consider the approximation to the expectation of A in the oscillator ground state corresponding to the space-time indices in Λ'. This is given by an expectation of a product, suitably normalized, in the form

$$G^{\Lambda'}(A) = \frac{1}{Z_{\Lambda'}} E_1\left[A \prod_r \exp(-W_r) \prod_e p_e \right] \tag{5.9}$$

The expectation E_1 is a conditional expectation followed by an expectation of a function of independent random variables q indexed by discrete space-time points. The factor A is a function of the variables associated with a set u of space-time indices at time zero. Each factor W_r is associated with a set r of four adjacent space-time index points and depends on the two diffusion processes and the time interval associated with r. Each factor p_e depends on the two variables associated with a set e consisting of a pair of successive space-time index points.

6. FUNCTIONS OF SUBSETS

The last stage of the argument is to show that even though the system is large, the dependence over long distances is small. There is sufficient locality so that the interaction may be estimated in terms of products of small factors. These are so small that they more than compensate for the combinatorial factors that result from the multi-dimensional geometry. It is at this stage that the estimates on the properties of the diffusion processes play an essential role. The general analysis is given in the appendix; here we sketch the particular application.

Recall that the random variables p_e are associated to two-point sets e, and the random variables W_r are associated to four point sets r. Furthermore the random variable A is associated to a finite set u. We call such sets u, r, and e elementary sets. Each elementary set is a finite subset of the index set. Define $A = \varepsilon_u$ and $\exp(-W_r) = 1 + \varepsilon_r$ and $p_e = 1 + \varepsilon_e$. Then the expectation is

$$G^{A'}(A) = \frac{1}{Z_{A'}} E_1 \left[\varepsilon_u \prod_r (1 + \varepsilon_r) \prod_e (1 + \varepsilon_e) \right] \tag{6.1}$$

We can write this as

$$G^{A'}(A) = \frac{1}{Z_{A'}} E_1 \left[\varepsilon_u \prod_{b \neq u} (1 + \varepsilon_b) \right] \tag{6.2}$$

A set Δ of elementary sets is called a cluster. For each cluster Δ define the cluster coefficient as the expectation

$$k_\Delta = E_1 \left[\prod_{b \in \Delta} \varepsilon_b \right] \tag{6.3}$$

We can expand the product and get

$$G^{A'}(A) = \frac{1}{Z_{A'}} \sum_{u \in \Delta} k_\Delta \tag{6.4}$$

where the sum is over all clusters with underlying set in Λ' that contain u. The denominator is defined so that $G^{\Lambda'}(1) = 1$. Thus

$$Z_{\Lambda'} = \sum_{u \notin \Delta} k_\Delta \tag{6.5}$$

where the sum is over all clusters with underlying set in Λ' not containing u.

If Δ is a cluster, then the union of the elementary sets belonging to Δ is called the *underlying set* of the cluster. The underlying set of Δ is denoted $\bar{\Delta}$. A cluster is disconnected if it is a union of non-empty sets whose underlying sets are disjoint; otherwise it is *connected*. Each non-empty cluster Δ is a union of connected components.

In the present application the variables ε_r corresponding to different connected components are conditionally independent given q. Furthermore, in the subsequent expectation E_0 the variables corresponding to different connected components are also independent. It follows that for each non-empty cluster Δ the cluster coefficient factors as

$$k_\Delta = \prod_\Gamma k_\Gamma \tag{6.6}$$

where the Γ are the connected components of the cluster Δ.

The expectation $G^{\Lambda'}(A)$ is thus a sum of products divided by another sum of products. The sum in the numerator is over clusters containing the distinguished elementary set; the sum in the denominator is over clusters not containing the distinguished elementary set. The products are over the connected components of the clusters. The cluster expansion is obtained by rewriting this quotient in such a way that the resulting expression may be estimated uniformly in the number of sites. This analysis is standard; it is briefly summarized in the appendix.

The essential hypothesis for the cluster expansion is a *cluster estimate*. This is a bound on the size of the coefficients associated with connected clusters. The bound is stated in terms of coefficients μ and λ. It requires that for each connected cluster Γ not containing u the estimate $|k_\Gamma| \leqslant \lambda^{|\Gamma|}$ holds. Furthermore, it requires that for each connected cluster Γ containing u the estimate $|k_\Gamma| \leqslant \mu \lambda^{|\Gamma| - 1}$ holds. (Here $|\Gamma|$ denotes the number of elementary sets in Γ.)

The series expansion for $G^{\Lambda'}(A)$ may be written in explicit form. It is shown in the appendix that each term in the sequence is determined by a *connected sequence* of connected clusters. This consists of a sequence $\Gamma_0, B_1, \Gamma_1, B_2, \Gamma_2, B_3, ..., \Gamma_p$, where the connected cluster Γ_0 contains u, and the other connected clusters Γ_i for $1 \leqslant i \leqslant p$ do not. The B_i for $1 \leqslant i \leqslant p$

are certain non-empty subsets of the index set that perform the connections between the different clusters, in the following sense. It is assumed that each non-empty subset contains a distinguished point. Each B_i for $1 \leqslant i \leqslant p$ is obtained by successively removing some number (possibly zero) of distinguished points from $B_{i-1} \cup \bar{\Gamma}_{i-1}$, where $B_0 = \varnothing$. Each connected cluster Γ_i for $1 \leqslant i \leqslant p$ is such that $\bar{\Gamma}_i$ intersects B_i in its distinguished point. The result of the analysis presented in the appendix is summarized in the following lemma.

Lemma 6.1. Suppose that the cluster estimate is satisfied with sufficiently small parameter λ. Consider a bounded function A of oscillator coordinates and the elementary set u corresponding to the fixed finite number of coordinates on which it depends. Then the expectation $G^{A'}(A)$ is a sum over connected sequences of connected clusters $\Gamma_0, B_1, \Gamma_1, B_2,..., \Gamma_p$, where the cluster Γ_0 contains u, and the other clusters Γ_i for $1 \leqslant i \leqslant p$ do not. The term corresponding to such a connected sequence is the product $(-1)^p k_{\Gamma_0} k_{\Gamma_1} \cdots k_{\Gamma_p}$. The expansion converges absolutely, independently of the size of the space-time region Λ'.

The remaining task is to obtain the cluster estimate on the expectation $k_\Gamma = E_1[\prod_{b \in \Gamma} \varepsilon_b]$. There are three kinds of factors in this expression. Since the function $\varepsilon_u(q) = A(q)$ satisfies a bound $|\varepsilon_b| \leqslant \mu$ and occurs at most once, it is not a problem. The following lemma is a restatement of the estimate on the diffusion process.

Lemma 6.2. For every $\lambda > 0$ there is a time separation a such that the factors $\varepsilon_e(q) = p_e(q) - 1$ associated with temporal edges e satisfy $|\varepsilon_e(q)| \leqslant \lambda$.

The major problem is with the expression $\varepsilon_r(\omega) = \exp(-W_r(\omega)) - 1$, since $W_r(\omega)$ is not a bounded function.

Lemma 6.3. Consider a range of coupling constants $|\alpha| \leqslant \alpha_0$ and corresponding interaction factors $\varepsilon_r = \exp(W_r) - 1$ associated with space-time rectangles r. For every $\lambda > 0$ there exists $\alpha_0 > 0$ such that the expectation $E_1[\prod_{r \in \Gamma} |\varepsilon_r|] \leqslant \lambda^{|\Gamma|}$.

Proof. It is useful to exploit the fact that $W_r(\omega)$ only depends on ω through ω_i and ω_j, each restricted to the time interval from ka to $(k+1)a$. Furthermore, the conditional expectation of a function of this quantity depends on q at the sites (i, k), $(i, k+1)$, (j, k), and $(j, k+1)$. This local dependence must be exploited in order to obtain the cluster estimate. For this, the following lemma is useful.

Lemma 6.4. Consider a probability space and let F_j be a collection of independent σ-fields. Fix n. Suppose that $X_1, ..., X_r$ are random variables. Assume that, for each j, the number of i such that X_i is not independent of F_j is bounded by n. Then the random variables satisfy the generalized Hölder inequality

$$|E[X_1 \cdots X_r]| \leqslant \|X_1\|_n \cdots \|X_r\|_n \qquad (6.7)$$

This lemma is indeed a generalization of the ordinary Hölder inequality, as may be seen by taking $r = n$. However it is of greater interest when n is a small fixed number determined by some sort of locality condition and r is very large. This is the case in the present application. Consider the σ-field generated by ω_j restricted to the interval from ka to $(k+1) a$. Then there are only $2d$ values of r such that $\varepsilon_r(\omega)$ depend on this σ-field. So the lemma can be applied to the conditional expectation given q, provided that n is taken larger than $2d$. This gives an estimate in terms of a product of factors of $E[|\varepsilon_r|^n \mid q]^{1/n}$. Furthermore, for each site (i, k) there are $4d$ values of r for which such a factor depends on q_{ik}. So the lemma can be applied to the expectation with respect to the independent random variables q_{ik}, provided that n is taken larger than $4d$. This gives an estimate in terms of a product of factors of the form $E_0[E[|\varepsilon_r|^n \mid q]]^{1/n}$. Now since the factors that related the E_0 and E expectations are uniformly close to 1, each such factor can be bounded above by a constant times $E[E[|\varepsilon_r|^n \mid q]]^{1/n} = E[|\varepsilon_r|^n]^{1/n}$. Thus the analysis reduces to showing this norm is small.

The explicit form of this norm is

$$E[|\varepsilon_r|^n]^{1/n} = E\left[\left|\exp\left(-\alpha \int_{ka}^{(k+1)a} \omega_i(\tau) \, Q\omega_j(\tau) \, d\tau\right) - 1\right|^n\right]^{1/n} \qquad (6.8)$$

The technique of ref. 1 reduces the problem of bounding the norm to the result of Corollary 2.3. The resulting bound involves a factor of α. With a large but fixed, this bound may be made less or equal to λ by taking $|\alpha| \leqslant \alpha_0$ with α_0 sufficiently small. This gives the required cluster estimate.

The end result of the analysis is the following theorem.

Theorem 6.5. Consider the quantum crystal consisting of an anharmonic oscillator at each site in Λ and with quadratic nearest neighbor coupling with coupling constant α. Let A be a bounded function of the oscillator coordinates corresponding to a fixed finite subset of crystal sites. Let $G^\Lambda(A)$ be the expectation of A in the ground state of the quantum crystal. Then there is an $\alpha_0 > 0$ independent of Λ and A such that $G^\Lambda(A)$

is analytic in α for $|\alpha| < \alpha_0$. Furthermore, the infinite volume limit $G(A)$ exists and is also analytic in α in the same interval.

Proof. The bounds in the cluster estimate are independent of the number of points N in the region $\Lambda \subset \mathbf{Z}^d$ and of the number $2n + 1$ of time instants in the interval from $-T$ to T (with $T = na$). We want to consider the limits $n \to \infty$ and $N \to \infty$. For the limiting case the natural space-time index set is $\mathbf{Z}^{d+1}$. The analysis in the appendix also applies to such an infinite index set. The series expansion for the limiting $G^{\mathbf{Z}^{d+1}}(A)$ is well-defined and is given explicitly as an infinite series with terms indexed by connected sequences of connected clusters.

It is shown in the appendix that this series expansion is dominated in absolute value by a convergence series of positive terms. The finite region expansions are obtained by setting some of the terms in the expansion equal to zero, so they also are dominated by the same convergent series of positive terms. It follows from the dominated convergence theorem that the finite region sums converge to the infinite region sum. The convergence is uniform for $|\alpha| \leqslant \alpha_0$, so it preserves the analyticity property. This proves the theorem.

APPENDIX.   CLUSTER EXPANSIONS

This appendix is a brief summary of the facts about cluster expansions.[5] Consider a countable index set S. (This is thought of as indexing independent random variables.) Consider also a collection of *elementary sets* that are subsets of S. (The idea is that there is a random variable associated with each elementary set that depends on the independent random variables indexed by the elements of the set.) Assume that there are constants m and k such that the cardinality of each elementary set is bounded by m and such that for each point the cardinality of the number of elementary sets containing the point is bounded by k.

A *cluster* is a finite set of elementary sets. For each cluster Δ, there is an associated *cluster coefficient* k_Δ. (In an application this could be the expectation of the product of the random variables associated with the elementary sets in Δ.)

For the moment take the index set S to be finite, so that there are also finitely many elementary sets and finitely many clusters. Throughout there will be a fixed elementary set u. The goal is to estimate

$$G = \frac{1}{Z} \sum_{u \in \Delta} k_\Delta \tag{A.1}$$

The factor Z is determined by

$$Z = \sum_{u \notin \Delta} k_\Delta \tag{A.2}$$

Each non-empty cluster Δ is a union of connected components Γ. The fundamental assumption on the cluster coefficients is the factorization

$$k_\Delta = \prod_\Gamma k_\Gamma \tag{A.3}$$

where the Γ are the connected components of Δ. (This is intended to express the independence of random variables corresponding to disjoint elementary sets.) The procedure is to use this factorization to rewrite G in a form in which one can obtain estimates independent of the size of the index set S. The resulting expressions will be meaningful even when S is a countable infinite set.

For a subset B of the index set define the *excluded region factor* to be

$$g(B) = \frac{1}{Z} \sum_{B \cap \bar{\Delta} = \varnothing} k_\Delta \tag{A.4}$$

The sum is over all clusters Δ whose underlying set $\bar{\Delta}$ does not intersect the excluded region B. The quantity G may be expressed in terms of cluster coefficients and these excluded region factors. The device is to factor out the coefficients corresponding to connected clusters Γ containing u. The sum over remaining factors results in appropriate excluded region factors. The resulting expression is

$$G = \sum_{u \in \Gamma} k_\Gamma \, g(\bar{\Gamma}) \tag{7.5}$$

Here the excluded region $\bar{\Gamma}$ is the underlying set of the connected cluster Γ.

The equation for the excluded region factors is obtained by considering a non-empty subset B of the index set and a one point subset t of B. Then

$$g(B \backslash t) = g(B) + \sum_{B \cap \bar{\Gamma} = t} k_\Gamma \, g(B \cup \bar{\Gamma}) \tag{A.6}$$

Here the sum is over connected clusters Γ whose underlying sets intersect B in t. The boundary condition is $g(\varnothing) = 1$. The first term on the right comes from summing over the clusters whose underlying set does not intersect B. The second term comes from summing over the clusters whose

underlying set intersects B in t. Then one factors out the coefficients corresponding to the connected components Γ whose underlying set contains t. The remaining factors sum to the appropriate excluded region factors with excluded region consisting of the union of B with the underlying set $\bar{\Gamma}$ of the connected component.

The natural setting for this equation is the Banach space of all functions g defined on non-empty finite subsets of the index set. Let $M > 1$. Define the norm of g to be $\|g\| = \sup_B |g(B)|/M^{|B|}$. Thus the functions are allowed to grow exponentially in the cardinality of the set. From now on fix a function t defined on the non-empty finite subsets of the index set such that for each such subset B, t_B is a one-point subset of B.

The next task is to write the equation in terms of this Banach space and operators on it. Define the function δ by $\delta(B) = 0$ for $|B| \geqslant 2$, and $\delta(B) = 1$ for $|B| = 1$. This is an element of the Banach space. The shift operator R is defined by

$$Rg(B) = g(B \backslash t_B) \tag{A.7}$$

for $|B| \geqslant 2$, and by $Rg(B) = 0$ for $|B| = 1$. The summation operator K is defined by taking

$$Kg(B) = \sum_{B \cap \bar{\Gamma} = t_B} k_\Gamma \, g(B \cup \bar{\Gamma}) \tag{A.8}$$

where the sum is over connected clusters Γ not containing u whose underlying sets intersect B in t_B. The equation is then in the form

$$\delta + Rg = g + Kg \tag{A.9}$$

where δ is 1 on one-point sets, R is the generalized shift, and K is the summation operator defined by the cluster coefficients.

The estimate on the summation operator R is based on a combinatorial fact and on a cluster estimate. The combinatorial fact is that there are constants b and c (depending on m and k) such that the number s_n of connected clusters Γ of size n whose underlying set contains a given point satisfies $s_n \leqslant bc^n$.

Lemma A.1. Consider the Banach space of functions defined on finite non-empty subsets of the index set and with growth in the cardinality of the set limited by growth parameter M. Let R be the generalized shift and K be the summation operator defined by the k_Γ, where Γ ranges over

connected clusters. Then there is a $\lambda > 0$ such that the cluster estimate $|k_\Gamma| \leqslant \lambda^{|\Gamma|}$ implies that the equation

$$g = \delta + Rg - Kg \tag{A.10}$$

may be solved by iteration.

Proof. The norm of R is bounded by $1/M < 1$. Furthermore, each connected cluster with n elements satisfies the cluster estimate $|k_\Gamma| \leqslant \lambda^n$. Since each elementary set has at most m elements, the underlying set of Γ has at most mn elements. From this it is easy to see that the norm of K is bounded by $(1/M) \sum_{n \geqslant 1} s_n \lambda^n M^{mn}$ which in turn is dominated by $(b/M) \sum_{n \geqslant 1} c^n \lambda^n M^{mn}$. It follows that if λ is sufficiently small, then the norm of K is correspondingly small. If λ is chosen so small that the sum of the norms of R and K are less than one, then the equation may be solved by iteration.

Let L be the linear functional on the Banach space defined by

$$Lg = \sum_{u \in \Gamma} k_\Gamma \, g(\bar{\Gamma}) \tag{A.11}$$

where the sum is over connected clusters Γ containing the distinguished elementary set u, and $\bar{\Gamma}$ denotes the underlying set of Γ.

Lemma A.2. Let L be the functional on the Banach space defined by the k_Γ, where Γ ranges over connected clusters containing the distinguished elementary set u. There exists $\lambda > 0$ such that for every $\mu < \infty$ the cluster estimate $k_\Gamma \leqslant \mu \lambda^{|\Gamma| - 1}$ implies that L is a bounded functional.

Proof. The norm of L is bounded by $\mu \sum_{n \geqslant 1} s_n \lambda^{n-1} M^{mn}$ which is dominated by the sum $b\mu \sum_{n \geqslant 1} c^n \lambda^{n-1} M^{mn}$. This converges for sufficiently small λ. This proves the lemma.

Since the equation $\delta + Rg = g + Kg$ has a solution, the quantity $G = Lg$ is well-defined. There is an explicit expansion for this quantity. The term of pth order in K in the expansion of Lg is the sum over all $m_i \geqslant 0$ of $(-1)^p \, LR^{m_1}KR^{m_2}K \cdots R^{m_p}KR^{m_{p+1}}\delta$. Since L and K are each given by a sum over connected clusters, this is a sum of terms corresponding to certain sequences of connected clusters, called connected sequences. A *connected sequence* is a sequence of the form $\Gamma_0, B_1, \Gamma_1, B_2, \Gamma_2, ..., B_p, \Gamma_p$, where $p = 0, 1, 2, 3, ...$ Here the Γ_i are connected clusters. The first connected cluster Γ_0 containing the distinguished element u. Each Γ_i for $i \geqslant 1$ is chosen so that $B_i \cap \bar{\Gamma}_i = t_{B_i}$, where t is the distinguished one-point subset of B_i. For $i \geqslant 1$ each B_i is a non-empty set and is obtained by applying the

operation of removing the distinguished one-point subset some number $m_i \geqslant 0$ times to $B_{i-1} \cup \bar{\Gamma}_{i-1}$. It is natural to define $B_0 = \varnothing$ and to define a B_{p+1} with the additional requirement that it be a one-point set. The expansion indexed by such connected sequences is given by the following lemma.

Lemma A.3. Suppose the cluster estimates are satisfied, and let g be the solution that gives the excluded region factors. Let $\delta + Rg = g + Kg$. Then $G = Lg$ is given by a sum indexed by connected sequences of the form $\Gamma_0, B_1, \Gamma_1, B_2, \Gamma_2, ..., B_p, \Gamma_p$, where $p = 0, 1, 2, 3, ...$ The coefficient associated with each sequence is the product of cluster coefficients $(-1)^p k_{\Gamma_0} k_{\Gamma_1} \cdots k_{\Gamma_p}$.

Up to this point the goal has been to find estimates that are uniform in the size of the index set S. However even though the original expressions do not make sense in the limit of a countably infinite index set, the equations that they satisfy remain meaningful. Thus one has the following theorem.

Theorem A.4. Consider a countably infinite index set S and cluster coefficients satisfying the appropriate cluster estimates. For each finite subset S_0 of S containing the fixed subset u there is a corresponding G^{S_0}. Then the G^{S_0} converge to a limit G^S associated with the infinite set S as the finite sets S_0 increase to S. Furthermore, the limiting G^S is given by the series expansion described in the preceding lemma.

Proof. The bounds in the cluster estimate are independent of the number of points in the index set S. Thus the expansions make sense when S is infinite. The appropriate Banach space consists of functions defined on the set of all finite subsets B of S set with norm $\|g\| = \sup_B |g(B)|/M^{|B|}$. The equation $g = \delta + Rg - Kg$ for the excluded region factor makes sense and has a unique solution obtained by iteration. The expression $G = Lg$ for the expectation in terms of this solution is also well-defined and is given explicitly as a series with terms indexed by connected sequences of connected clusters.

Let λ be the constant in the cluster estimate. Let K_1 be the same as the operator K, but with each $-k_\Gamma$ replaced by its majorant $\lambda^{|\Gamma|}$. Similarly, let L_1 be the same as the operator L, but with each k_Γ replaced by its majorant $\mu \lambda^{|\Gamma|-1}$. The equation $g = \delta + Rg - K_1 g$ also has a solution g_1 obtained by iteration, and each term in the resulting sum is greater than or equal to zero. Furthermore, the expression for $L_1 g_1$ also converges, and again each term in the sum is greater than or equal to zero. Each term in the series expansion of $L_1 g_1$ dominates the absolute value of the corresponding term in Lg. The corresponding terms for the expansion of the G^{S_0}

for a finite subset S_0 of S are obtained by setting some of the terms in Lg equal to zero, so the terms in $L_1 g_1$ also dominate the absolute values of the terms in the expansion of G^{S_0}. It follows from the dominated convergence theorem that G^{S_0} converges to G^S as S_0 approaches S. This proves the theorem.

ACKNOWLEDGMENTS

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