Continuous Model for Homopolymers

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Abstract

We consider the model for the distribution of a long homopolymer in a potential field. The typical shape of the polymer depends on the temperature parameter. We show that at a critical value of the temperature the transition occurs from a globular to an extended phase. For various values of the temperature, including those at or near the critical value, we consider the limiting behavior of the polymer when its size tends to infinity.

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1 Introduction

The goal of this paper is to analyze various critical phenomena for a model of long homogeneous polymer chains in an attracting potential field. The model exhibited here demonstrates a phase transition from a densely packed globular phase at low temperatures to an extended phase at higher temperatures. In the latter phase, the thermal fluctuations overcome the attraction between monomers and the chain takes on the shape of a $3d$ random walk or Brownian motion with a typical scale $O(\sqrt{T})$ where T is the length of the polymer. A real life example of this phenomenon is that of albumen (egg white). We describe a rough picture of this situation. The physical reality is more complex as there are present several types of protein with different critical points. However in a simplified version, at room temperature the albumen is in the globular state and as a result, it forms a viscous, translucent liquid. However, at higher temperatures (around $60-65^o$ C) there is a transition of the albumen to a diffusive (extended) state resulting in an opaque semi-solid material. While this transition may be reversible for an individual polymer, in the aggregate, the polymer strands in the diffusive state become interwoven and form chemical bonds with each other and can not return to the globular state when the temperature is decreased.

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It is worthwhile recalling Gibbs' philosophy of phase transitions. Start with a system of finite size T. The configuration space $\Sigma_T = \{x(\cdot)\}$ denotes all possible states $x(\cdot)$ of the system. The space Σ_T is equipped with a reference measure $\mathrm{P}_{0,T}$ which corresponds to infinite absolute temperature (in our case, the inverse temperature $\beta = 0$). The configurations satisfy boundary conditions which reflect the interaction of the finite system with its environment. This system is endowed with a Hamiltonian H_T giving the energy $H_T(x)$ of the state x. For $\beta > 0$, the Gibbs measure $\mathrm{P}_{\beta,T}$ is given by the density

$$\frac{d\mathrm{P}_{\beta,T}}{d\mathrm{P}_{0,T}}(x) = \frac{\exp(-\beta H_T(x))}{Z_{\beta,T}}, \tag{1}$$

where

$$Z_{\beta,T} = \int_{\Sigma_T} \exp(-\beta H_T(x)) dP_{0,T}. \tag{2}$$

When $T < \infty$, the measure $\mathrm{P}_{\beta,T}$ and the thermodynamic quantities associated to $\mathrm{P}_{\beta,T}$ are analytic functions of β.

Now let $T \to \infty$. In typical situations, there is a critical value β_{cr} such that for $\beta > \beta_{cr}$, there exists a unique limiting measure P_β on Σ, the space of infinite configurations, and this limiting measure is independent of the boundary conditions on Σ_T. Moreover, P_β and its relevant thermodynamic quantities are still analytic functions of β for $\beta > \beta_{cr}$. One manifestation of the phase transition is the non-uniqueness for $\beta < \beta_{cr}$ of the limiting measure as $T \to \infty$ as it has dependence on the boundary conditions on Σ_T. Another is the non-analyticity of thermodynamic quantities associated to P_β as a function of β. The mathematical characterization of the phase transition in terms of non-uniqueness of the limiting Gibbs measure traces its history to the works of Dobrushin [2] and Ruelle [7].

Modern physical theories predict that near the critical point $\beta = \beta_{cr}$ the limiting Gibbs measure P_β must be invariant with respect to renormalizations of the system (self-similarity). This idea is related to the two-parametric scaling by Fisher [3] for β near β_{cr}. Another important fact is that critical behavior as $\beta \to \beta_{cr}$ of the physical system demonstrates universality, that is the same behavior holds for a wide class of Hamiltonians.

The most essential part of the present paper is the detailed description of the polymer chain near the critical point and the establishment of the physical ideas of universality and self-similarity for our particular model of homopolymers.

2 Description of the Model and Results

A continuous function $x : [0, T] \to \mathbb{R}^d$, $x(0) = 0$, will be thought of as a realization of the polymer. The parameter $t \in [0, T]$ can be intuitively understood as the length along the polymer (although the functions $x = x(t)$ are not differentiable and the genuine notion of length can not be defined).

We assume that for $\beta = 0$, the polymer is distributed according to the Wiener measure $\mathrm{P}_{0,T}$ on $\Sigma_T = C([0,T],\mathbb{R}^d)$. For an infinitely smooth compactly supported potential $v \in C_0^\infty(\mathbb{R}^d)$ and a coupling constant $\beta \geq 0$, the polymer is distributed according to the Gibbs measure $\mathrm{P}_{\beta,T}$, whose density with respect to $\mathrm{P}_{0,T}$ is

$$\frac{d\mathrm{P}_{\beta,T}}{d\mathrm{P}_{0,T}}(x) = \frac{\exp(\beta \int_0^T v(x(t))dt)}{Z_{\beta,T}}, \quad x \in C([0,T],\mathbb{R}^d),$$

In other words, the Hamiltonian H_T is given by $H_T = -\int_0^T v(x(s)ds$. The normalizing factor $Z_{\beta,T}$, called the partition function, is given by

$$Z_{\beta,T} = \int_{C([0,T],\mathbb{R}^d)} \exp(\beta \int_0^T v(x(t))dt)d\mathrm{P}_{0,T}(x) = \mathrm{E}_{0,T} e^{-\beta H_T}. \tag{3}$$

It will be usually assumed that the potential is nonnegative and not identically equal to zero. We shall be interested in the prevalent behavior of the polymer with respect to the measure $\mathrm{P}_{0,T}$ as $T \to \infty$.

We shall see that there are two qualitatively different cases corresponding to different values of β. Namely, for all sufficiently large values of β there is a limiting distribution for $x(T)$ with respect to $\mathrm{P}_{0,T}$. Moreover, for each positive constant s and each function $S(T)$ such that $S(T) \to \infty$ and $T - S(T) \to \infty$ as $T \to \infty$, the family of processes $x(S(T)+t)$, $t \in [0,s]$, with respect to either measure $\mathrm{P}_{\beta,T}$ or $\mathrm{P}_{\beta,T}(\cdot|x(T)=0)$, converges to a Markov process as $T \to \infty$. The generator of the limiting Markov process and its invariant measure are written out explicitly in Theorem 8.3. Since $x(S(T))$ and $x(T)$ converge to limiting distributions and thus typically remain bounded as $T \to \infty$, we shall say that the polymer is in the globular state.

If $\beta > 0$ is sufficiently small and $d \geq 3$, then the family of processes $x(tT)/\sqrt{T}$, $0 \leq t \leq 1$, defined on $(C([0,T],\mathbb{R}^d),\mathrm{P}_{\beta,T})$, converges to a Brownian motion on the interval $[0,1]$ (Theorem 9.2). In this case we shall say that the polymer is in the diffusive state. Similarly, the family of processes $x(tT)/\sqrt{T}$, $0 \leq t \leq 1$, defined on $((C([0,T],\mathbb{R}^d),\mathrm{P}_{\beta,T}(\cdot|x(T)=0))$, converges to a Brownian bridge on the interval $[0,1]$.

We shall see that there is a number β_{cr} (called the critical value of the coupling constant) such that the polymer is in the diffusive state for $\beta < \beta_{cr}$ and in the globular state for $\beta > \beta_{cr}$. The value of β_{cr} and the behavior of the polymer when β is near β_{cr} depend on the dimension d and on the potential. In particular, we shall see that $\beta_{cr} = 0$ for $d = 1,2$ and $\beta_{cr} > 0$ for $d \geq 3$.

Of particular interest is the behavior of the polymer when $\beta = \beta_{cr}$. In this case the appropriate scaling is the same as in the diffusive case, that is we study the family of processes $x(tT)/\sqrt{T}$, $0 \leq t \leq 1$. We shall find the limit of this family as $T \to \infty$. It turns out to be a Markov process with a non-Gaussian, spherically symmetric transition function (Theorem 10.6). The transition function of the limiting Markov process will be written out explicitly.

In order to determine whether the polymer is in the globular or diffusive state for a given β, we shall look at the rate of growth of the partition function $Z_{\beta,T}$. Namely, let

$$\lambda_0(\beta) = \lim_{T\to\infty} \frac{\ln Z_{\beta,T}}{T}.$$

It will be demonstrated that the limit exists and is equal to the supremum of the spectrum of the operator $H_\beta = \frac{1}{2}\Delta + \beta v : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$. The infimum of the set of β for which $\lambda_0(\beta) > 0$ is equal to β_{cr}. It will be seen that $\lambda_0(\beta_{cr}) = 0$ is an eigenvalue of $H_{\beta_{cr}}$ in dimensions $d \geq 5$, and corresponds to a ground state of $H_{\beta_{cr}}$ in dimensions $d = 3, 4$.

The paper is organized as follows.

In Section 3 we consider finite T and show that $\{x(t), 0 \leq t \leq T\}$ is a time-inhomogeneous Markov process with respect to the measures $\mathrm{P}_{\beta,T}$ and $\mathrm{P}_{\beta,T}(\cdot|x(T) = 0)$.

In Section 4 we prove the existence of the critical value of the coupling constant. In Section 5 we analyze the properties of the resolvent of the operator H_β which, in particular, will be needed to study the asymptotic properties of the partition function.

In Section 6 we shall examine the asymptotics of $\lambda_0(\beta)$ when $\beta \downarrow \beta_{cr}$ and show it has the following asymptotic behavior as $\beta \downarrow \beta_{cr}$,

$$\lambda_0(\beta) \sim \begin{cases} c_3(\beta - \beta_{cr})^2, \ d = 3, \\ c_4(\beta - \beta_{cr})/\ln(1/(\beta - \beta_{cr})), \ d = 4, \\ c_d(\beta - \beta_{cr}), \ d \geq 5. \end{cases}$$

These asymptotics demonstrate universality in that they depend only on dimension. The constants c_d, $d \geq 3$, are not universal however. In Section 7 we find the asymptotics, as $T \to \infty$, of $Z_{\beta,T}$. In particular, when $\beta > \beta_{cr}$, we shall find that $Z_{\beta,T} \sim k_\beta e^{\lambda_0(\beta)T}$ for some constant k_β, while for $\beta < \beta_{cr}$, $Z_{\beta,T}$ has a finite limit as $T \to \infty$. Finally, when $\beta = \beta_{cr}$, it turns out that $Z_{\beta,T} \sim k_3 T^{1/2}$ for $d = 3$, $Z_{\beta,T} \sim k_4 T/\ln T$ for $d = 4$, while $Z_{\beta,T} \sim k_d T$ for $d \geq 5$. We also give asymptotics of the solutions to the parabolic equation $\partial u/\partial t = H_\beta u$.

In Sections 8, 9 and 10, we describe the behavior of the polymer for $\beta > \beta_{cr}$, $\beta < \beta_{cr}$ and $\beta = \beta_{cr}$, respectively, establishing the convergence results mentioned above.

Some of the results presented above have been obtained by Cranston and Molchanov in [1] for the discrete model with the potential concentrated at one point. The analysis was based on explicit formulas for the solution of the parabolic equation with such a potential. The current results demonstrate that the behavior of the polymer is "universal" with respect to the choice of the potential. Another essential feature of this paper is the detailed analysis of the behavior of the polymer when $\beta = \beta_{cr}$. We refer the reader to the review of Lifschitz, Grosberg and Khokhlov [5] for a wealth of information and ideas on polymer chains.

3 Time-inhomogeneous Markov Property

First we define p_β as the fundamental solution of the heat equation

$$\begin{aligned}\frac{\partial p_\beta}{\partial t}(t,y,x) =& \frac{1}{2}\Delta_x p_\beta(t,y,x) + \beta v(x) p_\beta(t,y,x),\\ p_\beta(0,y,x) =& \delta(x-y).\end{aligned} \tag{4}$$

In this section we shall prove that with respect to the measure $P_{\beta,T}$, the process $\{x(t), 0 \le t \le T\}$ is a time-inhomogeneous Markov process. Since we shall point out the link between non-uniqueness of Gibbs measures and phase transitions it will be necessary to also consider the transition mechanism for the process $\{x(t), 0 \le t \le T\}$ under the conditional measure $\mathrm{P}_{\beta,T}(\cdot|x(T)=0)$. Namely, we will show that the free boundary condition corresponding to the measure $\mathrm{P}_{\beta,T}$ and the pinned boundary condition corresponding to the measure $\mathrm{P}_{\beta,T}(\cdot|x(T)=0)$ lead to different Gibbs measures in the limit.

Let $Z_{\beta,t}(x) = \mathrm{E}^x \exp(\beta \int_0^t v(x_s)ds)$, where E^x is the expectation with respect to the measure induced by the Brownian motion starting at x. Thus $Z_{\beta,t}(0) = Z_{\beta,t}$, where $Z_{\beta,t}$ is the partition function introduced in the previous section.

Theorem 3.1. *The process $\{x(t), 0 \le t \le T\}$ is a time-inhomogeneous Markov process with respect to the measures $\mathrm{P}_{\beta,T}$. Its transition density is given by*

$$q_\beta^T((s,y),(t,x)) = p_\beta(t-s,y,x) Z_{\beta,T-t}(x) (Z_{\beta,T-s}(y))^{-1},. \tag{5}$$

The transition density $q_\beta^T((s,y),(t,x))$ solves the parabolic equation

$$\frac{\partial}{\partial s} q_\beta^T((s,y),(t,x)) + \ \tfrac{1}{2}\Delta_y q_\beta^T((s,y),(t,x)) + \nabla_y \ln Z_{\beta,T-s}(y) \nabla_y q_\beta^T((s,y),(t,x)) = 0. \tag{6}$$

With respect to the conditional measure $\mathrm{P}_{\beta,T}(\cdot\ |x(T)=0)$, the process $\{x(t), 0 \le t \le T\}$ is a time-inhomogeneous Markov process with transition density

$$q_\beta^{(T,0)}((s,y),(t,x)) = \ p_\beta(t-s,y,x) p_\beta(T-t,x,0)(p_\beta(T-s,y,0))^{-1}. \tag{7}$$

While this result is not used directly in later sections, it provides some intuition on the nature of the limiting processes when we consider the limit $T \to \infty$.

Proof. The Feynman-Kac formula gives that for $0 < t \le T$,

$$\mathrm{P}_{\beta,T}(x(t) \in dx) = \frac{p_\beta(t,0,x)\mathrm{E}^x \exp(\beta \int_0^{T-t} v(x_s)ds)}{Z_{\beta,T}} dx. \tag{8}$$

Similarly, for $0 = t_0 < t_1 < t_2 < ... < t_n \le T$ and $x_0 = 0$,

$$\mathrm{P}_{\beta,T}(x(t_1) \in dx_1, ..., x(t_n) \in dx_n) =$$

$$\frac{\prod_{i=0}^{n-1} p_\beta(t_{i+1}-t_i,x_i,x_{i+1})\mathrm{E}^{x_n}\exp(\beta\int_0^{T-t_n} v(x_s)ds)}{Z_{\beta,T}}dx_1dx_2...dx_n.$$

So, if we set for $0\le s<t\le T$,

$$q_\beta^T((s,y),(t,x)) = p_\beta(t-s,y,x)Z_{\beta,T-t}(x)(Z_{\beta,T-s}(y))^{-1},$$

then

$$\mathrm{P}_{\beta,T}\left(x(t_1)\in dx_1,...,x(t_n)\in dx_n\right) = \prod_{i=0}^{n-1} q_\beta^T((t_i,x_i),(t_{i+1},x_{i+1})).$$

Since $q_\beta^T((s,y),(t,x))>0$ and

$$\int_{\mathbb{R}^d} q_\beta^T((s,y),(t,x))dx = 1,$$

this means that $\{x(t),0\le t\le T\}$ under the measure $P_{\beta,T}$ is a time-inhomogeneous Markov process with transition probabilities q^T. Turning the equation for q_β^T around and solving for p_β yields

$$p_\beta(t-s,y,x) = \frac{q_\beta^T((s,y),(t,x))Z_{\beta,T-s}(y)}{Z_{\beta,T-t}(x)}.$$

Using the fact that

$$\frac{\partial}{\partial s}p_\beta(t-s,y,x)+\frac{1}{2}\Delta_y p_\beta(t-s,y,x)+\beta v(y)p_\beta(t-s,y,x)=0,$$

we derive that q_β^T satisfies the equation

$$\begin{aligned}&\frac{\partial}{\partial s}q_\beta^T((s,y),(t,x))\frac{Z_{\beta,T-s}(y)}{Z_{\beta,T-t}(x)}+q_\beta^T((s,y),(t,x))\frac{\frac{\partial}{\partial s}Z_{\beta,T-s}(y)}{Z_{\beta,T-t}(x)}\\ &+\frac{1}{2}\Delta_y q_\beta^T((s,y),(t,x))\frac{Z_{\beta,T-s}(y)}{Z_{\beta,T-t}(x)}+\beta v(y)q_\beta^T((s,y),(t,x))\frac{Z_{\beta,T-s}(y)}{Z_{\beta,T-t}(x)}\\ &+\frac{1}{2}\frac{q_\beta^T((s,y),(t,x))}{Z_{\beta,T-t}(x)}\Delta_y Z_{\beta,T-s}(y)+\nabla_y q_\beta^T((s,y),(t,x))\frac{\nabla_y Z_{\beta,T-s}(y)}{Z_{\beta,T-t}(x)}\\ &=0.\end{aligned} \tag{9}$$

Simplifying this leads to the following parabolic equation for q_β^T,

$$\frac{\partial}{\partial s}q_\beta^T((s,y),(t,x))+\ \tfrac{1}{2}\Delta_y q_\beta^T((s,y),(t,x))+\nabla_y\ln Z_{\beta,T-s}(y)\nabla_y q_\beta^T((s,y),(t,x))=0. \tag{10}$$

Next we consider the pinned case, for $0 = t_0 < t_1 < ... < t_n < t_{n+1} = T$ and $x_0 = x_{n+1} = 0$. Then,

$$\begin{aligned}\mathrm{P}_{\beta,T}\left(x(t_1) \in dx_1, ..., x(t_n) \in dx_n | x(T) = 0\right) =& \frac{\mathrm{P}_{\beta,T}\left(x(t_1) \in dx_1, ..., x(t_n) \in dx_n, x(T) = 0\right)}{\mathrm{P}_{\beta,T}\left(x(T) = 0\right)} \\ =& \frac{\prod_{i=0}^{n-1} p_\beta(t_{i+1} - t_i, x_i, x_{i+1})}{p_\beta(T, 0, 0)} dx_1 ... dx_n.\end{aligned} \tag{11}$$

Now set for $0 \leq s < t \leq T$,

$$q_\beta^{(T,0)}((s, y), (t, x)) = \quad p_\beta(t - s, y, x) p_\beta(T - t, x, 0)(p_\beta(T - s, y, 0))^{-1}. \tag{12}$$

Then

$$\mathrm{P}_{\beta,T}\left(x(t_1) \in dx_1, ..., x(t_n) \in dx_n | x(T) = 0\right) = \prod_{i=0}^{n-1} q_\beta^{(T,0)}((t_i, x_i), (t_{i+1}, x_{i+1})). \tag{13}$$

Since $q_\beta^{(T,0)}((s, y), (t, x)) > 0$ and

$$\int_{\mathbb{R}^d} q_\beta^T((s, y), (t, x)) dx = 1,$$

this means that $\{x(t), 0 \leq t \leq T\}$ under the conditional measure $\mathrm{P}_{\beta,T}\left(\cdot | x(T) = 0\right)$ is a time-inhomogeneous Markov process with transition densities $q_\beta^{(T,0)}$. □

We shall see below in that in the globular phase $\beta > \beta_{cr}$ the drift term $\nabla_x \ln Z_{\beta,T-s}(x)$ has a non-trivial limit as $T \to \infty$. This means that for $\beta > \beta_{cr}$, the Gibbs measure corresponds to a stationary Markov process in the $T \to \infty$ limit. On the other hand, this limit will vanish for $\beta < \beta_{cr}$. This explains the nature of the diffusive state for high temperature.

4 Critical Value of the Coupling Constant

Let

$$H_\beta = \frac{1}{2}\Delta + \beta v : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d), \quad v = v(x) \in C_0^\infty(\mathbb{R}^d), \quad \beta \geq 0.$$

We shall always assume that $v(x)$ is non-negative and compactly supported, although many results do not require these restrictions or can be modified to be valid without these restrictions. We shall also assume that v is not identically equal to zero. It is well-known that the spectrum of H_β consists of the absolutely continuous part $(-\infty, 0]$ and at most a finite number of non-negative eigenvalues:

$$\sigma(H_\beta) = (-\infty, 0] \cup \{\lambda_j\}, \quad 0 \leq j \leq N, \quad \lambda_j = \lambda_j(\beta) \geq 0.$$

We enumerate the eigenvalues in the decreasing order. Thus, if $\{\lambda_j\} \neq \emptyset$, then $\lambda_0 = \max \lambda_j$.

Lemma 4.1. *There exists* $\beta_{cr} \geq 0$ *(which will be called the critical value of* β*) such that* $\sup \sigma(H_\beta) = 0$ *for* $\beta \leq \beta_{cr}$ *and* $\sup \sigma(H_\beta) = \lambda_0(\beta) > 0$ *for* $\beta > \beta_{cr}$*. For* $\beta > \beta_{cr}$ *the eigenvalue* $\lambda_0(\beta)$ *is a strictly increasing and continuous function of* β*. Moreover,* $\lim_{\beta \downarrow \beta_{cr}} \lambda(\beta) = 0$ *and* $\lim_{\beta \uparrow \infty} \lambda(\beta) = \infty$*.*

Proof. The form $(H_\beta \psi, \psi)$ is positive on a function ψ supported on $\mathrm{supp}(v)$ if β is large enough. Thus $\sup \sigma(H_\beta) > 0$ for sufficiently large β. On the other hand, $\sigma(H_\beta) = (-\infty, 0]$ when $\beta = 0$. Let $\beta_{cr} = \sup\{\beta : \sup \sigma(H_\beta) = 0\}$. It is clear that $\sup \sigma(H_\beta) = 0$ for $\beta < \beta_{cr}$ since the operator H_β depends monotonically on β.

Other statements easily follow from the fact that for each ψ the form $(H_\beta \psi, \psi)$ depends continuously and monotonically on β. □

Remark. As will be shown below, $\beta_{cr} = 0$ for $d = 1, 2$, and $\beta_{cr} \geq 0$ for $d \geq 3$. Thus we do not talk about phase transition for $d = 1, 2$ since we do not consider negative values of β.

For $d \geq 3$, by the Cwikel-Lieb-Rozenblum estimate [6],

$$\sharp\{\lambda_i(\beta) \geq 0\} \leq c_d \beta^{d/2} \int_{\mathbb{R}^d} |v(x)|^{d/2} dx.$$

This implies that there are no eigenvalues for sufficiently small values of β if $d \geq 3$, that is $\beta_{cr} > 0$. It is also well-know (see [6]) that $\sup \sigma(H_\beta) > 0$ for $d = 1, 2$ if $\beta > 0$, $v \geq 0$ and v is not identically zero. These statements will also be proved below without referring to the Cwikel-Lieb-Rozenblum estimate.

5 Analytic Properties of the Resolvent

The resolvent of the operator H_β will be considered in the spaces of square-integrable and continuous functions. The resolvent $R_\beta(\lambda) = (H_\beta - \lambda)^{-1} : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is a meromorphic operator valued function on $\mathbb{C}' = \mathbb{C} \backslash (-\infty, 0]$. Denote the kernel of $R_\beta(\lambda)$ by $R_\beta(\lambda, x, y)$. If $\beta = 0$, the kernel depends on the difference $x - y$ and will be denoted by $R_0(\lambda, x - y)$. The kernel $R_0(\lambda, x)$ can be expressed through the Hankel function $H_\nu^{(1)}$:

$$R_0(1, x) = c|x|^{1-\frac{d}{2}} H^{(1)}_{\frac{d}{2}-1}(i\sqrt{2}|x|), \tag{14}$$

and

$$R_0(\lambda, x) = c k^{d-2} (k|x|)^{1-\frac{d}{2}} H^{(1)}_{\frac{d}{2}-1}(i\sqrt{2}k|x|), \quad k = \sqrt{\lambda}, \quad \mathrm{Re} k > 0. \tag{15}$$

In particular,

$$R_0(\lambda, x) = \frac{e^{-\sqrt{2}k|x|}}{-\sqrt{2}k}, \quad d = 1; \quad R_0(\lambda, x) = \frac{e^{-\sqrt{2}k|x|}}{-2\pi|x|}, \quad d = 3.$$

We shall say that $f \in L^2_{\exp}(\mathbb{R}^d)$ if f is measurable and

$$||f||_{L^2_{\exp}(\mathbb{R}^d)} = (\int_{\mathbb{R}^d} f^2(x) e^{|x|^2} dx)^{\frac{1}{2}} < \infty.$$

Similarly, we shall say that $f \in C_{\exp}(\mathbb{R}^d)$ if f is continuous and

$$||f||_{C_{\exp}(\mathbb{R}^d)} = \sup_{x \in \mathbb{R}^d} (|f(x)| e^{|x|^2}) < \infty.$$

Note that $R_0(\lambda)$, $\lambda \in \mathbb{C}'$, is a bounded operator not only in $L^2(\mathbb{R}^d)$ but also from $C_{\exp}(\mathbb{R}^d)$ to $C(\mathbb{R}^d)$, where $C(\mathbb{R}^d)$ is the space of bounded continuous functions on $\mathbb{R}^d$. Denote

$$A(\lambda) = v(x) R_0(\lambda) : \ L^2_{\exp}(\mathbb{R}^d) \to L^2_{\exp}(\mathbb{R}^d) \ \ (\text{and} \ \ C_{\exp}(\mathbb{R}^d) \to C_{\exp}(\mathbb{R}^d)). \tag{16}$$

The well-known properties of the Hankel functions together with (14) and (15) imply the following lemma (see [8] for a similar statement for general elliptic operators).

Lemma 5.1. *Consider the operator $A(\lambda)$ in the spaces $L^2_{\exp}(\mathbb{R}^d)$ and $C_{\exp}(\mathbb{R}^d)$.*

(1) The operator $A(\lambda)$ is analytic in $\lambda \in \mathbb{C}'$. It admits an analytic extension as an entire function of $\sqrt{\lambda}$ if d is odd, except $d = 1$, when it has a pole (with respect to $\sqrt{\lambda}$) at the origin. The operator $A(\lambda)$ has the form $A(\lambda) = A_1(\lambda) + \ln \lambda A_2(\lambda)$ if d is even, where A_1 and A_2 are entire functions.

(2) $A_2(0) = 0$ if $d \geq 4$ (d is even), and therefore $A(0) = \lim_{\lambda \to 0, \lambda \in \mathbb{C}'} A(\lambda)$ exists and is a bounded operator for all $d \geq 3$.

(3) The operator $A(\lambda)$ is compact for all $\lambda \in \mathbb{C}' \cup \{0\}$ ($\lambda \neq 0$ if $d = 1$ or 2).

(4) For each $\varepsilon > 0$, we have $||A(\lambda)|| = O(1/|\lambda|)$ as $\lambda \to \infty$, $|\arg \lambda| \leq \pi - \varepsilon$.

(5) The operator $A(\lambda)$ has the following asymptotic behavior as $\lambda \to 0$, $\lambda \in \mathbb{C}'$:

$$A(\lambda) = -vP_1/\sqrt{\lambda} + O(1), \quad d = 1,$$
$$A(\lambda) = -vP_2 \ln(1/\lambda) + O(1), \quad d = 2,$$
$$A(\lambda) = -v(P_3 + Q_3\sqrt{\lambda}) + O(|\lambda|), \quad d = 3,$$
$$A(\lambda) = -v(P_4 + Q_4 \lambda \ln(1/\lambda)) + O(|\lambda|), \quad d = 4,$$
$$A(\lambda) = -v(P_d + Q_d \lambda) + O(|\lambda|^{3/2}), \quad d \geq 5,$$

where the operators P_d, $d \geq 1$, Q_d, $d \geq 3$, have the following kernels:

$$P_1(x,y) = \frac{1}{\sqrt{2}}, \quad P_2(x,y) = \frac{1}{\pi},$$
$$P_3(x,y) = \frac{1}{2\pi|x-y|}, \quad Q_3(x,y) = -\frac{1}{\sqrt{2}\pi},$$
$$P_4(x,y) = \frac{1}{\pi^2|x-y|^2}, \quad Q_4(x,y) = -\frac{1}{2\pi^2},$$
$$P_d(x,y) = \frac{a_d}{|x-y|^{d-2}}, \quad Q_d(x,y) = \frac{-a_d}{(d-4)|x-y|^{d-4}}, \quad a_d > 0, \ d \geq 5.$$

Proof. Let d be odd. From (14), (15) and (16) it follows that the kernel $A(\lambda, x, y) = v(x)R_0(\lambda, x - y)$ of the operator $A(\lambda)$ is an entire function of $k = \sqrt{\lambda}$ if $d \geq 3$ (but has a pole at $k = 0$ if $d = 1$). The kernel has a weak singularity at $x = y$ and an exponential estimate at infinity. To be more exact,

$$|A(k^2, x, y)| + |\frac{\partial A(k^2, x, y)}{\partial k}| \leq C(d, k)|v(x)|e^{|k(x-y)|}(|x - y| + |x - y|^{-(d-1)}), \tag{17}$$

were $C(d, k)$ has a singularity at $k = 0$ if $d = 1$. Since

$$||A(k^2)||_{C_{\exp}(\mathbb{R}^d)} \leq \sup_{x\in\mathbb{R}^d} \int e^{|x|^2-|y|^2}|A(k^2, x, y)|dy,$$

$$||\frac{d}{dk}A(k^2)||_{C_{\exp}(\mathbb{R}^d)} \leq \sup_{x\in\mathbb{R}^d} \int e^{|x|^2-|y|^2}|\frac{\partial A(k^2, x, y)}{\partial k}|dy,$$

the estimate (17) immediately leads to the analyticity in $k = \sqrt{\lambda}$ of the operator $A(\lambda)$ in the space $C_{\exp}(\mathbb{R}^d)$. In order to get the same result in the space $L^2_{\exp}(\mathbb{R}^d)$, we represent $A(\lambda)$ in the form $B_1 + B_2$ were the kernel $B_1(\lambda, x, y)$ of the operator B_1 is equal to $\chi(x - y)A(\lambda, x, y)$. Here χ is the indicator function of the unit ball. Since

$$|\chi(x)R_0(k^2, x)| + |\frac{d}{dk}\chi(x)R_0(k^2, x)| \in L^1(\mathbb{R}^d), \tag{18}$$

the convolution with $\chi(x)R_0(k^2, x)$ is an analytic in k operator in the space $L^2(\mathbb{R}^d)$. Then B_1 (which is the convolution followed by multiplication by $v(x)$) is an analytic operator in the space $L^2_{\exp}(\mathbb{R}^d)$. The product of the kernel of the operator B_2 and $e^{|x|^2-|y|^2}$ is square integrable in (x, y). The same is true for the derivative in k of the kernel of B_2 multiplied by $e^{|x|^2-|y|^2}$. Thus B_2 is also analytic in k. This completes the proof of the analyticity of $A(\lambda)$ when d is odd. The case of even d is similar. One needs only to take into account that $R_0(\lambda, x)$ has a logarithmic branching point at $\lambda = 0$ in this case. The second statement of the lemma follows immediately from (14), (15) and (16).

To prove the compactness of $A(\lambda)$, we note that the estimate (17) is valid not only for $A(k^2, x, y)$ and $\partial A(k^2, x, y)/\partial k$, but also for $\nabla_x A(k^2, x, y)$. Thus the arguments above lead to the boundedness of the operators $\frac{\partial}{\partial x_i}A(\lambda)$ (the composition of $A(\lambda)$ with the differentiation). Since the supports of functions $A(\lambda)f$ belong to the support of v, the standard Sobolev embedding theorems imply the compactness of the operator $A(\lambda)$ in both the spaces $L^2_{\exp}(\mathbb{R}^d)$ and $C_{\exp}(\mathbb{R}^d)$.

In order to prove the fourth statement of the lemma, we observe that the $L^2(\mathbb{R}^d)$ norm of the resolvent $R_0(\lambda)$ does not exceed $1/|\mathrm{Im}\lambda|$ (the inverse distance from the spectrum). Since $A(\lambda)$ is obtained from $R_0(\lambda)$ after multiplying it by a bounded function with compact support, the $L^2_{\exp}(\mathbb{R}^d)$ norm of $A(\lambda)$ does not exceed $c/|\mathrm{Im}\lambda|$, where c is a positive constant which depends on v. The norm of $A(\lambda)$ in the space $C_{\exp}(\mathbb{R}^d)$ can be estimated by $\sup_{x\in\mathbb{R}^d} |v(x)e^{|x|^2}| \int_{\mathbb{R}^d} |R_0(\lambda, x)|dx$, which is of order $O(1/|\lambda|)$ as $\lambda \to \infty$, $|\arg\lambda| \leq \pi - \varepsilon$, due to (15).

The remaining statements also easily follow from (14) and (15). $\square$

Note that for $d \geq 3$, there exists the limit

$$R_0(0, x-y) := \lim_{\lambda \to 0, \lambda \in \mathbb{C}'} R_0(\lambda, x-y) = -a_d |x-y|^{2-d},$$

which is a fundamental solution of the operator $\frac{1}{2}\Delta$. The operator with this kernel will be denoted by $R_0(0)$. While $R_0(\lambda)$, $\lambda \in \mathbb{C}'$, acts in $L^2(\mathbb{R}^d)$ and $C(\mathbb{R}^d)$, the operator $R_0(0)$ only maps $C_{\exp}(\mathbb{R}^d)$ to $C(\mathbb{R}^d)$ if $d < 5$. The following lemma follows from formulas (14) and (15) similarly to Lemma 5.1.

Lemma 5.2. *For $d \geq 3$, the operator $R_0(\lambda)$ considered as an operator from $C_{\exp}(\mathbb{R}^d)$ to $C(\mathbb{R}^d)$ is analytic in $\lambda \in \mathbb{C}'$. It is uniformly bounded in $\mathbb{C}'$. For each $\varepsilon > 0$, it is of order $O(1/|\lambda|)$ as $\lambda \to \infty$, $|\arg\lambda| \leq \pi - \varepsilon$. It has the following asymptotic behavior as $\lambda \to 0$, $\lambda \in \mathbb{C}'$:*

$$R_0(\lambda) = R_0(0) + O(\sqrt{|\lambda|}), \quad d = 3,$$

$$R_0(\lambda) = R_0(0) + O(|\lambda \ln \lambda|), \quad d = 4,$$

$$R_0(\lambda) = R_0(0) + O(|\lambda|), \quad d \geq 5.$$

The following lemma is simply a resolvent identity. It plays an important role in our future analysis.

Lemma 5.3. *For $\lambda \in \mathbb{C}'$, we have the following relation between the meromorphic operator-valued functions*

$$R_\beta(\lambda) = R_0(\lambda) - R_0(\lambda)(I + \beta v(x) R_0(\lambda))^{-1}[\beta v(x) R_0(\lambda)] \tag{19}$$

Remark. Note that (19) can be written as

$$R_\beta(\lambda) = R_0(\lambda) - R_0(\lambda)(I + \beta A(\lambda))^{-1}[\beta v(x) R_0(\lambda)]. \tag{20}$$

From here it also follows that

$$R_\beta(\lambda) = R_0(\lambda)(I + \beta A(\lambda))^{-1}, \tag{21}$$

which should be understood as an identity between meromorphic in λ operators acting from $L^2_{\exp}(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$ and from $C_{\exp}(\mathbb{R}^d)$ to $C(\mathbb{R}^d)$. In the lattice case considered in [1], the operator $A(\lambda)$ has rank one and

$$R_\beta(\lambda, x, y) = R_0(\lambda, x, y)/(1 - \beta I(\lambda)),$$

where $I(\lambda)$ is an analytic function of $\sqrt{\lambda}$ related to $A(\lambda)$. This exact formula is the key to all the results in [1].

The kernels of the operators $I + \beta A(\lambda)$ (both in spaces $L^2_{\exp}(\mathbb{R}^d)$ and $C_{\exp}(\mathbb{R}^d)$) are described by the following lemma.

Lemma 5.4. *(1) The operator-valued function* $(I + \beta A(\lambda))^{-1}$ *is meromorphic in* $\mathbb{C}'$*. It has a pole at* $\lambda \in \mathbb{C}'$ *if and only if* λ *is an eigenvalue of* H_β*. These poles are of the first order.*

(2) Let $\lambda_i(\beta)$ *be a positive eigenvalue of* H_β*. There is a one-to-one correspondence between the kernel of the operator* $I + \beta A(\lambda_i)$ *and the eigenspace of the operator* H_β *corresponding to the eigenvalue* λ_i*. Namely, if* $(I + \beta A(\lambda_i))h = 0$*, then* $\psi = -R_0(\lambda_i)h$ *is an eigenfunction of* H_β *and* $h = \beta v \psi$*.*

(3) If $d \geq 3$*, there is a one-to-one correspondence between the kernel of the operator* $I + \beta A(0)$ *and solution space of the problem*

$$H_\beta(\psi) = \frac{1}{2}\Delta\psi + \beta v(x)\psi = 0, \quad \psi(x) = O(|x|^{2-d}), \quad \frac{\partial \psi}{\partial r}(x) = O(|x|^{1-d}) \ \ as \ \ r = |x| \to \infty. \tag{22}$$

Namely, if $(I + \beta A(0))h = 0$ *for* $h \in L^2_{\exp}(\mathbb{R}^d)$*, then* $h \in C_{\exp}(\mathbb{R}^d)$*,* $\psi = -R_0(0)h$ *is a solution of (22) and* $h = \beta v \psi$*.*

Remark. The relations (22) are an analogue of the eigenvalue problem for zero eigenvalue and the eigenfunction ψ which does not necessarily belong to $L^2(\mathbb{R}^d)$ (see Lemma 5.6 below). We shall call a non-zero solution of (22) a ground state.

Proof. The operator $A(\lambda)$, $\lambda \in \mathbb{C}'$, is analytic, compact, and tends to zero as $\lambda \to +\infty$ by Lemma 5.1. Therefore $(I+\beta A(\lambda))^{-1}$ is meromorphic by the Analytic Fredholm Theorem.

If $\lambda \in \mathbb{C}'$ is a pole of $(I + \beta A(\lambda))^{-1}$, then it is also a pole of the same order of $R_\beta(\lambda)$ as follows from (21) since the kernel of $R_0(\lambda)$ is trivial. Therefore the pole is simple and coincides with one of the eigenvalues λ_i. Note that λ is a pole of $(I+\beta A(\lambda))^{-1}$ if and only if the kernel of $I + \beta A(\lambda)$ is non-trivial. Let $h \in L^2_{\exp}(\mathbb{R}^d)$ be such that $||h||_{L^2_{\exp}(\mathbb{R}^d)} \neq 0$ and $(I + \beta v R_0(\lambda))h = 0$. Then $\psi := -R_0(\lambda)h \in L^2(\mathbb{R}^d)$ and $(\frac{1}{2}\Delta - \lambda + \beta v)\psi = 0$, that is ψ is an eigenfunction of H_β.

Conversely, let $\psi \in L^2(\mathbb{R}^d)$ be an eigenfunction corresponding to an eigenvalue λ_i, that is

$$(\frac{1}{2}\Delta - \lambda_i)\psi + \beta v \psi = 0. \tag{23}$$

Denote $h = \beta v \psi$. Then $(\frac{1}{2}\Delta - \lambda_i)\psi = -h$. Thus $\psi = -R_0(\lambda_i)h$ and (23) implies that h satisfies $(I + \beta v R_0(\lambda_i))h = 0$. Note that $h \in C^\infty(\mathbb{R}^d)$, h vanishes outside supp(v), and therefore belongs to the kernel of $I + \beta A(\lambda_i)$. This completes the proof of the first two statements.

Similar arguments can be used to prove the last statement. If $h \in L^2_{\exp}(\mathbb{R}^d)$ is such that $||h||_{L^2_{\exp}(\mathbb{R}^d)} \neq 0$ and $(I + \beta A(0))h = 0$, then h has compact support and the integral operator $R_0(0)$ can be applied to h. It is clear that $\psi := -R_0(0)h$ satisfies (22) and, since h has compact support, $h \in C_{\exp}(\mathbb{R}^d)$.

In order to prove that any solution of (22) corresponds to an eigenvector of $I+\beta A(0)$, one only needs to show that the solution ψ of the problem (22) can be represented in the form $\psi = -R_0(0)h$ with $h = \beta v \psi$. The latter follows from the Green formula

$$\psi(x) = -(R_0(0)(\beta v \psi))(x) + \int_{|y|=a} [R_0(0, x-y)\psi_r'(y) - \frac{\partial}{\partial r} R_0(0, x-y)\psi(y)]ds, \qquad |x| < a,$$

after passing to the limit as $a \to \infty$. □

Lemma 5.4 can be improved for $\lambda = \lambda_0(\beta)$. Due to the monotonicity and continuity of $\lambda = \lambda_0(\beta)$ for $\beta > \beta_{cr}$, we can define the inverse function

$$\beta = \beta(\lambda) : [0, \infty) \to [\beta_{cr}, \infty). \tag{24}$$

We shall prove that the operator $-A(\lambda)$, $\lambda > 0$, has a non-negative kernel and has a positive simple eigenvalue such that all the other eigenvalues are smaller in absolute value. Such an eigenvalue is called the principal eigenvalue.

Lemma 5.5. *The operator $-A(\lambda)$, $\lambda > 0$, (in the spaces $L^2_{\exp}(\mathbb{R}^d)$ and $C_{\exp}(\mathbb{R}^d)$) has the principal eigenvalue. This eigenvalue is equal to $1/\beta(\lambda)$ and the corresponding eigenfunction can be taken to be positive in the interior of* supp(v) *and equal to zero outside of* supp(v)*. If $d \geq 3$, then the same is true for the operator $-A(0)$ (in particular, $\beta_{cr} > 0$).*

Remark 1. Let $d \geq 3$. Lemmas 5.4 and 5.5 imply that the ground state of the operator H_β for $\beta = \beta_{cr}$ (defined by (22)) is defined uniquely up to a multiplicative constant and corresponds to the principal eigenvalue of $A(0)$. The ground state (with $\lambda = 0$) does not exist if $\beta < \beta_{cr}$.

Remark 2. Let $d \geq 3$. From Lemma 5.1 it follows that

$$\lim_{\lambda \to 0, \lambda \in \mathbb{C}'} A(\lambda) = A(0).$$

Therefore for all $\lambda \in \mathbb{C}'$ with $|\lambda|$ sufficiently small, the operator $-A(\lambda)$ has a simple eigenvalue whose real part is larger than the absolute values of the other eigenvalues. We shall denote this eigenvalue by $1/\beta(\lambda)$, thus extending the domain of the function $\beta(\lambda)$ (see (24)) from $[0, \infty)$ to $[0, \infty) \cup (U \cap \mathbb{C}')$, where U is a sufficiently small neighborhood of zero.

Proof of Lemma 5.5. By Lemma 5.4 it is sufficient to consider the case of $L^2_{\exp}(\mathbb{R}^d)$. The maximum principle for the operator $(\frac{1}{2}\Delta - \lambda)$, $\lambda > 0$, implies that the kernel of the operator $R_0(\lambda)$, $\lambda > 0$, is negative. Thus, by (16), for all y the kernel of $-A(\lambda)$ is positive when x is in the interior of supp(v) and zero otherwise. Thus $-A(\lambda)$, $\lambda > 0$, has the principal eigenvalue (see [4]). On the other hand, by Lemma 5.4, $1/\beta(\lambda)$ is a positive eigenvalue of $-A(\lambda)$. Note that this is the largest positive eigenvalue of $-A(\lambda)$. Indeed, if $\mu = 1/\beta' > 1/\beta(\lambda)$ is an eigenvalue of $-A(\lambda)$, then λ is one of the eigenvalues λ_i of $H_{\beta'}$ by Lemma 5.4. Therefore, $\lambda_i(\beta') = \lambda_0(\beta)$ for $\beta' < \beta$. This contradicts the monotonicity of $\lambda_0(\beta)$. Hence the statement of the lemma concerning the case $\lambda > 0$ holds.

For $d \geq 3$, the kernel of $-A(0)$ is equal to vP_d and has the same properties as the kernel of $-A(\lambda)$, $\lambda > 0$. Thus $-A(0)$ has the principal eigenvalue. Since $A(\lambda) \to A(0)$

as $\lambda \downarrow 0$, the principal eigenvalue $1/\beta(\lambda)$ converges to the principal eigenvalue $\mu < \infty$ of $-A(0)$. On the other hand, $\beta(\lambda)$ is a continuous function, and therefore $\mu = 1/\beta_{cr}$, which proves the statement concerning the case $\lambda = 0$. $\square$

The relationship between ground states and eigenfunctions of H_β is explained by the following lemma.

Lemma 5.6. *Let $\beta = \beta_{cr}$. If $d = 3$ or $d = 4$, then H_β has a unique ground state (up to a multiplicative constant), but $\lambda = 0$ is not an eigenvalue. If $d \geq 5$, then $\lambda = 0$ is a simple eigenvalue of H_β and the sets of ground states and eigenfunctions coincide.*

Proof. The ground states belong to $L^2(\mathbb{R}^d)$ if and only if $d \geq 5$. In order to complete the proof of the lemma, it remains to show that any eigenfunction of H_β with zero eigenvalue satisfies (22). Thus, it is enough to prove that if $\frac{1}{2}\Delta\psi + \beta v(x)\psi = 0$ and $\psi \in L^2(\mathbb{R}^d)$, then $\psi = -R_0(0)h$ with $h = \beta v \psi$. From $\frac{1}{2}\Delta\psi + \beta v(x)\psi - \lambda\psi = -\lambda\psi$ we obtain $\psi = -R_0(\lambda)(h + \lambda\psi)$. Obviously $R_0(\lambda)h \to R_0(0)h$ in $L^2(\mathbb{R}^d)$ as $\lambda \downarrow 0$ since $h \in L^2_{\exp}(\mathbb{R}^d)$. Now the lemma will be proved if we show that

$$||\lambda R_0(\lambda)\psi||^2_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} (\frac{2\lambda|\widetilde{\psi}(\sigma)|}{\sigma^2 + 2\lambda})^2 d\sigma \to 0 \quad \text{as} \quad \lambda \downarrow 0.$$

The latter follows from the dominated convergence theorem. $\square$

The following lemma summarizes some facts about the operator $(I + \beta A(\lambda))^{-1}$ proved above. It also describes the structure of the singularity of the operator $(I + \beta A(\lambda))^{-1}$ for λ and β in a neighborhood of $\lambda = 0$, $\beta = \beta_{cr}$.

Lemma 5.7. *Let $d \geq 3$ and $\beta \geq 0$. The operator $(I + \beta A(\lambda))^{-1}$ (considered in $L^2_{\exp}(\mathbb{R}^d)$ and $C_{\exp}(\mathbb{R}^d)$) is meromorphic in $\lambda \in \mathbb{C}'$ and has poles of the first order at eigenvalues of the operator H_β. For each $\varepsilon > 0$ and some $\Lambda = \Lambda(\beta)$, the operator is uniformly bounded in $\lambda \in \mathbb{C}'$, $|\arg\lambda| \leq \pi - \varepsilon$, $|\lambda| \geq \Lambda$.*

If $\beta = \beta_{cr}$, then the operator $(I + \beta A(\lambda))^{-1}$ is analytic in $\lambda \in \mathbb{C}'$ and uniformly bounded in $\lambda \in \mathbb{C}'$, $|\arg\lambda| \leq \pi - \varepsilon$, $|\lambda| \geq \varepsilon$.

If $\beta < \beta_{cr}$, then the operator $(I + \beta A(\lambda))^{-1}$ is analytic in $\lambda \in \mathbb{C}'$ and uniformly bounded in $\lambda \in \mathbb{C}'$, $|\arg\lambda| \leq \pi - \varepsilon$.

There are $\lambda_0 > 0$ and $\delta_0 > 0$ such that for $\lambda \in \mathbb{C}' \cup \{0\}$, $|\lambda| \leq \lambda_0$, $|\beta - \beta_{cr}| \leq \delta_0$, $\beta \neq \beta(\lambda)$, we have the representation

$$(I + \beta A(\lambda))^{-1} = \frac{\beta(\lambda)}{\beta(\lambda) - \beta}(B + S_d(\lambda)) + C(\lambda, \beta). \tag{25}$$

Here $\beta(\lambda)$ is defined in Remark 2 following Lemma 5.5, B is the one dimensional operator with the kernel

$$B(x, y) = \frac{v(x)\psi(x)\psi(y)}{\int_{\mathbb{R}^d} v(x)\psi^2(x)dx}, \tag{26}$$

where ψ is a ground state defined in the Remark following Lemma 5.4, and

$$S_3(\lambda) = O(\sqrt{|\lambda|}), \quad S_4(\lambda) = O(|\lambda \ln(\lambda)|), \quad S_d(\lambda) = O(|\lambda|), \quad d \geq 5, \quad \text{as} \quad \lambda \to 0, \quad \lambda \in \mathbb{C}', \tag{27}$$

$S_d(0) = 0$, $d \geq 3$, and $C(\lambda, \beta)$ is bounded uniformly in λ and β.

Proof. The analytic properties of $(I + \beta A(\lambda))^{-1}$ follow from Lemma 5.4. By Lemma 5.1, the norm of $A(\lambda)$ decays at infinity when $\lambda \to \infty$, $|\arg\lambda| \leq \pi - \varepsilon$. Therefore there is $\Lambda > 0$ such that the operator $(I + \beta A(\lambda))^{-1}$ is bounded for $|\arg\lambda| \leq \pi - \varepsilon$, $|\lambda| \geq \Lambda$.

If $\beta \leq \beta_{cr}$, then $(I + \beta A(\lambda))^{-1}$ does not have poles in $\lambda \in \mathbb{C}'$, and therefore Λ can be taken to be arbitrarily small.

If $\beta < \beta_{cr}$, then $(I + \beta A(0))$ is invertible by Lemma 5.5. By Lemma 5.1, the operators $A(\lambda)$ tend to $A(0)$ when $\lambda \to 0$, $\lambda \in \mathbb{C}'$. Therefore $(I + \beta A(\lambda))^{-1}$, $\lambda \in \mathbb{C}'$, are bounded in a neighborhood of zero. It remains to justify (25).

For $d \geq 3$, let h_λ be an eigenvector corresponding to the eigenvalue $1/\beta(\lambda)$ of the operator $-A(\lambda)$, $\lambda \in [0, \infty) \cup (U \cap \mathbb{C}')$. By Lemma 5.5 and the second remark following it, this eigenvector is defined up to a multiplicative constant. Let $A^*(\lambda)$ be the operator in $L^2_{\exp}(\mathbb{R}^d)$ or $C_{\exp}(\mathbb{R}^d)$ with the kernel $A^*(\lambda, x, y) = A(\lambda, y, x)e^{|y|^2 - |x|^2}$. Similarly to Lemma 5.5, it is not difficult to show that $1/\beta(\lambda)$ is an eigenvalue for the operator $-A^*(\lambda)$ and that its real part exceeds the absolute values of the other eigenvalues. The corresponding eigenvector h^*_λ is uniquely defined up to a multiplicative constant. Moreover, we can take h_λ and h^*_λ such that

$$v(x)e^{|x|^2} h^*_\lambda(x) = h_\lambda(x). \tag{28}$$

Note that h_λ and h^*_λ can be chosen in such a way that

$$||h_\lambda - h_0||, ||h^*_\lambda - h^*_0|| \leq k||A(\lambda) - A(0)|| \tag{29}$$

for some $k > 0$ and all sufficiently small $|\lambda|$, where the norms on both sides of (29) are either in the space $L^2_{\exp}(\mathbb{R}^d)$ or $C_{\exp}(\mathbb{R}^d)$.

Recall that $A(\lambda) \to A(0)$ as $\lambda \to 0$, $\lambda \in \mathbb{C}'$, by Lemma 5.1. Using this and the fact that $1/\beta_{cr}$ is the principal eigenvalue for $-A(0)$, it is easy to show that there are $\lambda_1 > 0$ and $\delta_1 > 0$ such that for $\lambda \in \mathbb{C}' \cup \{0\}$, $|\lambda| \leq \lambda_1$, the eigenvalue $1/\beta(\lambda)$ of the operator $-A(\lambda)$ is the unique eigenvalue whose distance from $1/\beta_{cr}$ does not exceed δ_1. Take $0 < \lambda_0 < \lambda_1$ and $0 < \delta_0 < \delta_1$ such that for $\lambda \in \mathbb{C}' \cup \{0\}$, $|\lambda| \leq \lambda_0$, the distance between $1/\beta(\lambda)$ and $1/\beta_{cr}$ does not exceed δ_0.

Then for $\lambda \in \mathbb{C}' \cup \{0\}$, $|\lambda| \leq \lambda_0$ and β such that $|1/\beta - 1/\beta_{cr}| \leq \delta_0$, the operator valued function

$$F(z) = \frac{(A(\lambda) + zI)^{-1}}{z - (1/\beta)}$$

is meromorphic inside the circle $\gamma = \{z : |z - 1/\beta_{cr}| = \delta_1\}$. It has two poles: one at $z = 1/\beta$ and the other at $z = 1/\beta(\lambda)$. The residue at the first pole is equal to $(A(\lambda) + I/\beta)^{-1}$. In order to find the residue at the second pole, recall that it is a simple pole for $(A(\lambda)+zI)^{-1}$, and therefore

$$(A(\lambda)+zI)^{-1}=T_{-1}(\lambda)(z-\frac{1}{\beta(\lambda)})^{-1}+T_0(\lambda)+T_1(\lambda)(z-\frac{1}{\beta(\lambda)})+...$$

for some operators $T_{-1},T_0,T_1,...$ and all z in a neighborhood of $1/\beta(\lambda)$. From here and the fact that the kernels of $A(\lambda)+I/\beta(\lambda)$ and $A^*(\lambda)+I/\beta(\lambda)$ are one-dimensional and coincide with span$\{h_\lambda\}$ and span$\{h^*_\lambda\}$, respectively, it easily follows that

$$T_{-1}(\lambda)f=\frac{h_\lambda\langle f,h^*_\lambda\rangle_{L^2_{\rm exp}(\mathbb{R}^d)}}{\langle h_\lambda,h^*_\lambda\rangle_{L^2_{\rm exp}(\mathbb{R}^d)}},\quad f\in L^2_{\rm exp}(\mathbb{R}^d)\ \ \text{(in particular if } f\in C_{\rm exp}(\mathbb{R}^d)).$$

From (29) and Lemma 5.1 it follows that $S_d(\lambda):=T_{-1}(\lambda)-T_{-1}(0)$ satisfies (27). The residue of $F(z)$ at $z=1/\beta(\lambda)$ is equal to

$$\frac{\beta(\lambda)\beta}{\beta-\beta(\lambda)}(T_{-1}(0)+S_d(\lambda)).$$

Integrating $F(z)$ over the contour γ, we obtain

$$(A(\lambda)+I/\beta)^{-1}+\frac{\beta(\lambda)\beta}{\beta-\beta(\lambda)}(T_{-1}(0)+S_d(\lambda))=\frac{1}{2\pi i}\int_\gamma\frac{(A(\lambda)+zI)^{-1}}{z-(1/\beta)}dz.$$

The right hand side of this formula is uniformly bounded, which completes the proof of the lemma if we show that $T_{-1}(0)=B$. Thus it remains to prove that

$$\frac{h_0(x)e^{|y|^2}h^*_0(y)}{\langle h_0,h^*_0\rangle_{L^2_{\rm exp}(\mathbb{R}^d)}}=\frac{v(x)\psi(x)\psi(y)}{\int_{\mathbb{R}^d}v(x)\psi^2(x)dx}.$$

The latter follows from the relation $h_0=\beta v\psi$ (see Lemma 5.4) and (28). □

Formula (21) and Lemmas 5.2 and 5.7 imply the following result.

Lemma 5.8. *Let $d\geq 3$ and $\beta\geq 0$. The operator $R_\beta(\lambda)$ (considered as an operator from $C_{\rm exp}(\mathbb{R}^d)$ to $C(\mathbb{R}^d)$) is meromorphic in $\lambda\in\mathbb{C}'$ and has poles of the first order at eigenvalues of the operator H_β. For each $\varepsilon>0$ and some $\Lambda=\Lambda(\beta)$, the operator is uniformly bounded in $\lambda\in\mathbb{C}'$, $|\arg\lambda|\leq\pi-\varepsilon$, $|\lambda|\geq\Lambda$. It is of order $O(1/|\lambda|)$ as $\lambda\to\infty$, $|\arg\lambda|\leq\pi-\varepsilon$.*

If $\beta=\beta_{cr}$, then the operator $R_\beta(\lambda)$ is analytic in $\lambda\in\mathbb{C}'$ and uniformly bounded in $\lambda\in\mathbb{C}'$, $|\arg\lambda|\leq\pi-\varepsilon$, $|\lambda|\geq\varepsilon$.

If $\beta<\beta_{cr}$, then the operator $R_\beta(\lambda)$ is analytic in $\lambda\in\mathbb{C}'$ and uniformly bounded in $\lambda\in\mathbb{C}'$, $|\arg\lambda|\leq\pi-\varepsilon$.

There are $\lambda_0>0$ and $\delta_0>0$ such that for $\lambda\in\mathbb{C}'$, $0<|\lambda|\leq\lambda_0$, $|\beta-\beta_{cr}|\leq\delta_0$, $\beta\neq\beta(\lambda)$, we have the representation

$$R_\beta(\lambda)=\frac{\beta(\lambda)}{\beta(\lambda)-\beta}(R_0(0)B+S_d(\lambda))+C(\lambda,\beta),\tag{30}$$

where $\beta(\lambda)$ is defined in Remark 2 following Lemma 5.5 and B is given by (26), S_d, $d\geq 3$, satisfy (27), and $C(\lambda,\beta)$ is bounded uniformly in λ and β.

6 The Behavior of the Principal Eigenvalue for $\beta \downarrow \beta_{cr}$

In Lemma 5.5 we showed that $\beta_{cr} > 0$ for $d \geq 3$. The following theorem implies, in particular, that $\beta_{cr} = 0$ for $d = 1$ or 2.

Theorem 6.1. *For $d = 1, 2$ (when $\beta_{cr} = 0$) the eigenvalue $\lambda_0(\beta)$ has the following behavior as $\beta \downarrow \beta_{cr}$:*

$$\lambda_0(\beta) \sim \frac{1}{2} c_1^2 \beta^2, \quad c_1 = \int_{\mathbb{R}^d} v(x) dx, \quad d = 1, \tag{31}$$

$$\lambda_0(\beta) \sim \exp(-\frac{c_2}{\beta}), \quad c_2 = \frac{\pi}{c_1}, \quad d = 2. \tag{32}$$

In dimensions $d \geq 3$ the eigenvalue $\lambda_0(\beta)$ has the following behavior as $\beta \downarrow \beta_{cr}$:

$$\lambda_0(\beta) \sim c_3 (\beta - \beta_{cr})^2, \quad d = 3, \tag{33}$$

$$\lambda_0(\beta) \sim c_4 (\beta - \beta_{cr}) / \ln(1/(\beta - \beta_{cr})), \quad d = 4, \tag{34}$$

$$\lambda_0(\beta) \sim c_d (\beta - \beta_{cr}), \quad d \geq 5, \tag{35}$$

where $c_d \neq 0$, $d \geq 3$, depend on v and will be indicated in the proof.

Proof. Since we are interested in the behavior of $\lambda_0(\beta)$ for $\beta \downarrow \beta_{cr}$ and $\lambda_0(\beta) \downarrow 0$ when $\beta \downarrow \beta_{cr}$ by Lemma 4.1, we shall study the behavior of $\beta(\lambda)$ as $\lambda \downarrow 0$ (or, more generally, as $\lambda \to 0$, $\lambda \in \mathbb{C}'$). The arguments below are based on Lemma 5.1.

First consider the case $d = 1$. For $\lambda \to 0$, $\lambda \in \mathbb{C}'$, the eigenvalue problem for $-A(\lambda)$ can be written in the form

$$(vP_1 + O(\sqrt{\lambda}))h_\lambda = \frac{\sqrt{\lambda}}{\beta(\lambda)} h_\lambda. \tag{36}$$

Note that the kernel of vP_1 is positive when x is an interior point of $\mathrm{supp}(v)$. Therefore vP_1 has a principal eigenvalue. In fact, the operator vP_1 is one-dimensional and the eigenvalue is equal to $c_1/\sqrt{2}$ where $c_1 = \int_{\mathbb{R}^d} v(x)dx$. Since this eigenvalue is simple and the operator in the left-hand side of (36) is analytic in $\sqrt{\lambda}$, both h_λ and $\sqrt{\lambda}/\beta(\lambda)$ are analytic functions of $\sqrt{\lambda}$ in a neighborhood of the origin and

$$\lim_{\lambda \to 0, \lambda \in \mathbb{C}'} (\sqrt{\lambda}/\beta(\lambda)) = c_1/\sqrt{2}.$$

Therefore, $\beta_{cr} = 0$, $\beta(\lambda)$ is analytic in $\sqrt{\lambda}$, and $\beta(\lambda) \sim \sqrt{2\lambda}/c_1$ as $\lambda \to 0$, $\lambda \in \mathbb{C}'$, which proves (31).

The same arguments in the case $d = 2$ lead to the relation

$$\lim_{\lambda \to 0, \lambda \in \mathbb{C}'} (\frac{-1}{\beta(\lambda) \ln \lambda}) = c_1/\pi.$$

This implies that $\beta_{cr}=0$ and (32) holds.

In the case $d=3$ the eigenvalue problem for $-A(\lambda)$ takes the form

$$(-A(0)+\sqrt{\lambda}v(x)Q_3+O(\lambda))h_\lambda=\frac{1}{\beta(\lambda)}h_\lambda. \tag{37}$$

As in the one-dimensional case, $1/\beta(\lambda)$ and h_λ are analytic functions of $\sqrt{\lambda}$. Now $1/\beta_{cr}$ is equal to the principal eigenvalue of $-A(0)$. Recall that h_0 is the principal eigenfunction of $-A(0)$ and h_0^* is the principal eigenfunction of $-A^*(0)$. Standard perturbation arguments imply that

$$\frac{1}{\beta(\lambda)}=\frac{1}{\beta_{cr}}-\gamma\sqrt{\lambda}+O(\lambda),\quad \lambda\to 0,\ \lambda\in\mathbb{C}', \tag{38}$$

where

$$\gamma=\frac{-\langle vQ_3h_0,h_0^*\rangle_{L^2_{\exp}(\mathbb{R}^d)}}{\langle h_0,h_0^*\rangle_{L^2_{\exp}(\mathbb{R}^d)}}>0, \tag{39}$$

which implies (33) with $c_3=1/(\gamma^2\beta_{cr}^4)$. Note that $\gamma>0$ since the kernel of the operator vQ_3 is negative and principal eigenfunctions h_0, h_0^* can be chosen to be positive inside $\mathrm{supp}(v)$.

Formula for γ can be simplified. We choose $h_0=\beta v\psi$ (see Lemma 5.4) and h_0^* defined in (28). Then

$$\gamma=\frac{(\int_{\mathbb{R}^3}v(x)\psi(x)dx)^2}{\sqrt{2}\pi\int_{\mathbb{R}^3}v(x)\psi^2(x)dx},\quad d=3. \tag{40}$$

Let $d=4$. Then instead of (37) we get

$$(-A(0)+\lambda\ln(1/\lambda)vQ_4+O(\lambda))h_\lambda=\frac{1}{\beta(\lambda)}h_\lambda. \tag{41}$$

From here it follows that

$$\frac{1}{\beta(\lambda)}=\frac{1}{\beta_{cr}}-\gamma\lambda\ln(1/\lambda)+O(\lambda),\quad \lambda\to 0,\ \lambda\in\mathbb{C}', \tag{42}$$

where $1/\beta_{cr}$ is the principal eigenvalue of $-A(0)$ and γ is given by (39) with Q_3 replaced by Q_4. Thus (34) holds with $c_4=1/(\gamma\beta_{cr}^2)$.

For $d\geq 5$ we get

$$(-A(0)+\lambda vQ_d+O(\lambda^{3/2}))h_\lambda=\frac{1}{\beta(\lambda)}h_\lambda.$$

From here it follows that

$$\frac{1}{\beta(\lambda)}=\frac{1}{\beta_{cr}}-\gamma\lambda+O(\lambda^{3/2}),\quad \lambda\to 0,\ \lambda\in\mathbb{C}',$$

where $1/\beta_{cr}$ is the principal eigenvalue of $-A(0)$ and γ is given by (39) with Q_3 replaced by Q_d. Thus (35) holds with $c_d=1/(\gamma\beta_{cr}^2)$. □

7 Asymptotics of the Partition Function, Solutions, and Fundamental Solutions

We shall need the following notation. Recall from (4) that by $p_\beta(t,y,x)$ we denote the fundamental solution of the parabolic problem

$$\frac{\partial p_\beta(t,y,x)}{\partial t} = \frac{1}{2}\Delta_x p_\beta(t,y,x) + \beta v(x) p_\beta(t,y,x),$$
$$p_\beta(0,y,x) = \delta(x-y).$$

For a given $f \in L^2(\mathbb{R}^d)$, let

$$u_\beta(t,x) = \int_{\mathbb{R}^d} p_\beta(t,y,x) f(y) dy$$

be the solution of the Cauchy problem with the initial data f. The partition function is defined as the integral of the fundamental solution

$$Z_{\beta,t}(x) = \int_{\mathbb{R}^d} p_\beta(t,x,y)dy = \int_{\mathbb{R}^d} p_\beta(t,y,x)dy.$$

Note that the partition function defined in (3) is simply $Z_{\beta,T} = Z_{\beta,T}(0)$. Also note that $Z_{\beta,t}(x)$ is the solution of the Cauchy problem with initial data equal to one:

$$\frac{\partial Z_{\beta,t}(x)}{\partial t} = \frac{1}{2}\Delta Z_{\beta,t}(x) + \beta v(x) Z_{\beta,t}(x), \quad Z_{\beta,0}(x) \equiv 1.$$

For $\beta > \beta_{cr}$, let ψ_β be the positive eigenfunction for the operator H_β with eigenvalue $\lambda_0(\beta)$ normalized by the condition $||\psi_\beta||_{L^2(\mathbb{R})} = 1$. This function is defined uniquely by Lemma 5.4 and is equal to $-R_0(\lambda)h_\lambda$, where $\lambda = \lambda_0(\beta)$ and h_λ is the principal eigenfunction for the operator $-A(\lambda)$. Note that ψ_β decays exponentially at infinity.

For $a \in \mathbb{R}$, let $\Gamma(a)$ be the following contour in the complex plane

$$\Gamma(a) = \{a - s + is,\ s \geq 0\} \cup \{a - s - is,\ s \geq 0\}.$$

We choose the direction along $\Gamma(a)$ in such a way that the imaginary coordinate increases.

The following lemma is an important tool for investigating the asymptotics of $Z_{\beta,T}$.

Lemma 7.1. *Let $a > \lambda_0(\beta)$. Then for $f \in L^2(\mathbb{R}^d)$ (or $f \in C_{\exp}(\mathbb{R}^d)$) and $t > 0$,*

$$u_\beta(t,x) = \frac{-1}{2\pi i}\int_{\Gamma(a)} e^{\lambda t}(R_\beta(\lambda)f)(x)d\lambda, \tag{43}$$

which holds in $L^2(\mathbb{R}^d)$ (or $C(\mathbb{R}^d)$). This formula remains valid if the initial function f is identically equal to one and $R_\beta(\lambda)f$ is understood by substituting $f \equiv 1$ into (19) with $R_0(\lambda)1 = -1/\lambda$. More precisely,

$$Z_{\beta,t}(x) - 1 = \frac{-1}{2\pi i}\int_{\Gamma(a)} \frac{e^{\lambda t}}{\lambda}(R_\beta(\lambda)(\beta v))(x)d\lambda \tag{44}$$

in $L^2(\mathbb{R}^d)$ and $C(\mathbb{R}^d)$.

Proof. First, let $f \in L^2(\mathbb{R}^d)$. We solve the Cauchy problem for u_β using the Laplace transform with respect to t. This leads to (43) with $\Gamma(a)$ replaced by the line $\{\lambda : \mathrm{Re}\lambda = a\}$. The integral over this line is equal to the integral over $\Gamma(a)$ since the resolvent is analytic between these contours and its norm decays as $|\lambda|^{-1}$ when $|\lambda| \to \infty$.

Now let $f \equiv 1$. Then $w(t,x) = Z_{\beta,t}(x) - 1$ is the solution of the problem

$$\frac{\partial w(t,x)}{\partial t} = \frac{1}{2}\Delta w(t,x) + \beta v(x) w(t,x) + \beta v(x), \quad w(0,x) \equiv 0.$$

By the Duhamel formula and (43),

$$w(t,x) = \frac{-1}{2\pi i}\int_0^t \int_{\Gamma(a)} e^{\lambda(t-s)}(R_\beta(\lambda)\beta v)(x) d\lambda ds =$$

$$\frac{-1}{2\pi i}\int_{\Gamma(a)} \frac{e^{\lambda t}-1}{\lambda}(R_\beta(\lambda)\beta v)(x) d\lambda = \frac{-1}{2\pi i}\int_{\Gamma(a)} \frac{e^{\lambda t}}{\lambda}(R_\beta(\lambda)\beta v)(x) d\lambda,$$

since in the domain $\Gamma^+(a)$ to the right of the contour $\Gamma(a)$, the operator $R_\beta(\lambda) : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ is analytic and decays as $|\lambda|^{-1}$ at infinity. This justifies (44) in $L^2(\mathbb{R}^d)$ sense. It remains to show that the right-hand side of (43) is continuous for $f \in C_{\exp}(\mathbb{R}^d)$ and the right-hand side of (44) is continuous. Since $\beta v \in C_0^\infty$, the integrands are continuous in (t,x) for each $\lambda \in \Gamma_a$. It remains to note that the integrals converge uniformly when $x \in \mathbb{R}^n$, $t \ge t_0 > 0$. This is due to the fact that $||R_\beta(\lambda) f||_{C(\mathbb{R}^d)}, ||R_\beta(\lambda)\beta v||_{C(\mathbb{R}^d)} \le C_d(a)$, as follows from Lemma 5.8. □

In order to state the next theorem we shall need the following notation. As in part (3) of Lemma 5.4, it is not difficult to show that for $d \ge 3$, $0 \le \beta < \beta_{cr}$ and $f \in C_0^\infty(\mathbb{R}^d)$ there is a unique solution of the problem

$$H_\beta(\varphi) = \frac{1}{2}\Delta\varphi + \beta v(x)\varphi = f, \quad \varphi = O(|x|^{2-d}), \quad \frac{\partial\varphi}{\partial r}(x) = O(|x|^{1-d}) \;\; as \;\; r = |x| \to \infty. \tag{45}$$

This solution is given by $\varphi = R_0(0)(I + \beta A(0))^{-1} f$. For $f = -\beta v$, we denote this solution by φ_β.

Theorem 7.2. *(1) For $\beta > \beta_{cr}$ there is $\varepsilon > 0$ such that we have the following asymptotics for the partition function:*

$$Z_{\beta,t}(x) - 1 = \exp(\lambda_0(\beta)t)(||\psi_\beta||_{L^1(\mathbb{R}^d)}\psi_\beta(x) + O(\exp(-\varepsilon t))) \;\; as \;\; t \to \infty,$$

which holds in $L^2(\mathbb{R}^d)$ and in $C(\mathbb{R}^d)$, where ψ_β is the positive eigenfunction for the operator H_β with eigenvalue $\lambda_0(\beta)$ normalized by the condition $||\psi_\beta||_{L^2(\mathbb{R})} = 1$.

(2) For $\beta = \beta_{cr}$ we have the following asymptotics for the partition function:

$$Z_{\beta,t}(x) = k_3 t^{1/2}\psi(x) + O(1) \;\; as \;\; t \to \infty, \quad d = 3,$$

$$Z_{\beta,t}(x) = k_4 \frac{t}{\ln t}\psi(x) + O(\frac{t}{\ln^2 t}) \;\; as \;\; t \to \infty, \quad d = 4,$$

$$Z_{\beta,t}(x) = k_d t\psi(x) + O(\sqrt{t}) \quad as \quad t \to \infty, \quad d \geq 5,$$

which holds in $C(\mathbb{R}^d)$. *Here* k_d, $d \geq 3$, *are positive constants and* ψ *is the positive ground state for* $H_{\beta_{cr}}$ *normalized by the condition* $||\beta_{cr} v\psi||_{L^2_{\exp}(\mathbb{R}^d)} = 1$.

(3) If $0 \leq \beta < \beta_{cr}$, *then*

$$\lim_{t\to\infty} Z_{\beta,t}(x) = 1 + \varphi_\beta(x)$$

in $C(\mathbb{R}^d)$.

Proof. (1) Note that the resolvent $R_\beta(\lambda)$ has only one pole between the contours $\Gamma(a)$ and $\Gamma(\lambda_0(\beta) - \varepsilon)$ if ε is less than the distance from λ_0 to the rest of the spectrum. This pole is at the point $\lambda_0(\beta)$ and the residue is the integral operator with the kernel $-\psi_\beta(x)\psi_\beta(y)$. Therefore from (44) it follows that

$$Z_{\beta,t}(x) - 1 = \frac{e^{\lambda_0(\beta)t}}{\lambda_0(\beta)}\psi_\beta(x)\int_{\mathbb{R}^d} \beta v(y)\psi_\beta(y)dy - \frac{1}{2\pi i}\int_{\Gamma(\lambda_0(\beta)-\varepsilon)} \frac{e^{\lambda t}}{\lambda}(R_\beta(\lambda)\beta v)(x)d\lambda. \quad (46)$$

Since $(\frac{1}{2}\Delta + \beta v - \lambda_0(\beta))\psi_\beta = 0$, we have $\beta v\psi_\beta = (\lambda_0(\beta) - \frac{1}{2}\Delta)\psi_\beta$, and the integral in the first term of the right-hand side of (46) is equal to $\lambda_0(\beta)||\psi_\beta||_{L^1(\mathbb{R}^d)}$. Thus the first term on the right-hand side coincides with the main term of the asymptotics stated in the theorem.

It remains to show that the second term on the right-hand side of (46) is exponentially smaller than the first term. This is due to the fact that the norm of the operator $R_\beta(\lambda)$ is of order $1/|\lambda|$ at infinity for $\lambda \in \Gamma(\lambda_0(\beta) - \varepsilon)$.

(2) Let $d = 3$. First, let us analyze (30) when $\beta = \beta_{cr}$ and $\lambda \to 0$, $\lambda \in \mathbb{C}'$. By (38), the factor $\beta(\lambda)/(\beta(\lambda) - \beta)$ in the right hand side of (30) is equal to $(\beta_{cr}\gamma\sqrt{\lambda})^{-1} + O(1)$ as $\lambda \to 0$, $\lambda \in \mathbb{C}'$, where $\gamma > 0$ is given by (39).

We choose the same ground state ψ specified in the statement of Theorem 7.2. Then from (26) and Lemma 5.4 it follows that

$$R_0(0)B(\beta_{cr}v) = \frac{\int_{R^d} v(x)\psi(x)dx}{\int_{R^d} v(x)\psi^2(x)dx}R_0(0)(\beta_{cr}v\psi) = -\frac{\int_{R^d} v(x)\psi(x)dx}{\int_{R^d} v(x)\psi^2(x)dx}\psi. \quad (47)$$

Now, by Lemma 5.8 and (33), (38),

$$R_{\beta_{cr}}(\lambda)(\beta_{cr}v) = \frac{-\int_{R^d} v(x)\psi(x)dx}{\gamma\beta_{cr}\sqrt{\lambda}\int_{R^d} v(x)\psi^2(x)dx}\psi + D(\lambda) = \frac{-k_3'\psi}{\sqrt{\lambda}} + D(\lambda), \quad k_3' > 0, \quad (48)$$

where the remainder $D(\lambda)$ is of order $O(1)$ when $\lambda \to 0$, $\lambda \in \mathbb{C}'$. Note that $D(\lambda)$ is bounded on $\Gamma^+(0)$ since the left hand side and the first term on the right hand side of (48) are bounded on $\Gamma^+(0)$ outside a neighborhood of zero.

Next, we apply (44) with a replaced by $1/t$ and use the expression (48) to obtain

$$Z_{\beta,t}(x) - 1 = \frac{1}{2\pi i}\int_{\Gamma(1/t)} \frac{e^{\lambda t}}{\lambda}(\frac{k_3'\psi}{\sqrt{\lambda}} + D(\lambda))d\lambda. \quad (49)$$

Let us change the variables in the integral $\lambda t = z$. Thus

$$Z_{\beta,t}(x) - 1 = \frac{1}{2\pi i} \int_{\Gamma(1)} \frac{e^z}{z} (\frac{\sqrt{t} k_3' \psi}{\sqrt{z}} + D(\frac{z}{t})) dz.$$

The contribution to the integral from the term containing $D(z/t)$ is bounded, while the contribution from the first term is equal to $k_3 t^{1/2} \psi(x)$, as claimed in the lemma. One needs only to note that $k_3 > 0$ since

$$\frac{1}{2\pi i} \int_{\Gamma(1)} z^{-3/2} e^z dz = \frac{1}{\pi i} \int_{\Gamma(1)} z^{-1/2} e^z dz = \frac{2}{\pi} \int_0^\infty \sigma^{-1/2} e^{-\sigma} d\sigma = \frac{2}{\sqrt{\pi}} > 0.$$

If $d = 4$, then (34), (42) imply that $\beta(\lambda) - \beta_{cr} \sim \beta_{cr}^2 \gamma \lambda \ln(1/\lambda)$ as $\lambda \to 0, \lambda \in C'$. This leads to the following analog of (49)

$$Z_{\beta,t}(x) - 1 = \frac{1}{2\pi i} \int_{\Gamma(1/t)} \frac{e^{\lambda t}}{\lambda} (\frac{k_4' \psi(x)}{\lambda \ln(1/\lambda)} + D(\lambda)) d\lambda, \quad k_4' > 0,$$

where $D(\lambda)$ is of order $O(1/|\lambda \ln^2 \lambda|)$ when $\lambda \to 0$, $\lambda \in \mathbb{C}'$ and is bounded at infinity. After the change of variables $\lambda t = z$, we obtain

$$Z_{\beta,t}(x) - 1 = \frac{1}{2\pi i} \int_{\Gamma(1)} \frac{e^z}{z} (\frac{t k_4' \psi(x)}{z(\ln t - \ln z)} + D(\frac{z}{t})) dz,$$

which easily leads to the second part of the lemma in the case $d = 4$. The treatment of the case $d \geq 5$ is similar.

(3) We apply (44) with a replaced by $1/t$ to obtain

$$Z_{\beta,t}(x) - 1 = \frac{-1}{2\pi i} \int_{\Gamma(1/t)} \frac{e^{\lambda t}}{\lambda} (R_\beta(\lambda)(\beta v))(x) d\lambda = \frac{-1}{2\pi i} \int_{\Gamma(1)} \frac{e^z}{z} (R_\beta(\frac{z}{t})(\beta v))(x) dz. \quad (50)$$

Note that by Lemma 5.2 and since $1/\beta$ is not an eigenvalue of $A(0)$ we have

$$\lim_{\lambda \to 0, \lambda \in \mathbb{C}'} R_\beta(\lambda)(\beta v) = \lim_{\lambda \to 0, \lambda \in \mathbb{C}'} R_0(\lambda)(I + \beta A(\lambda))^{-1}(\beta v) = R_0(0)(I + \beta A(0))^{-1}(\beta v) = -\varphi_\beta.$$

Since the difference between $R_\beta(z/t)(\beta v)$ and $-\varphi_\beta$ is bounded on $\Gamma(1)$, one can pass to the limit $t \to \infty$ under the integral sign in (50), which leads to

$$\lim_{t \to \infty} Z_{\beta,t}(x) = 1 + \frac{\varphi_\beta(x)}{2\pi i} \int_{\Gamma(1)} \frac{e^z}{z} dz = 1 + \varphi_\beta(x).$$

□

The third part of Theorem 7.2 establishes the existence of $\lim_{t \to \infty} Z_{\beta,t}(x)$ for $\beta < \beta_{cr}$. Next we examine the behavior of this quantity as $\beta \uparrow \beta_{cr}$.

Lemma 7.3. *There are positive constant b_d, $d \geq 3$, such that*

$$\lim_{t\to\infty} Z_{\beta,t}(x) - 1 = \frac{b_d}{\beta_{cr} - \beta}\psi(x) + O(1) \quad as \quad \beta \uparrow \beta_{cr}$$

is valid in $C(\mathbb{R}^d)$, where ψ is the positive ground state for $H_{\beta_{cr}}$ normalized by the condition $||\beta_{cr} v\psi||_{L^2_{\exp}(\mathbb{R}^d)} = 1$.

Proof. By the third part of Theorem 7.2, we only need to find the asymptotics as $\beta \uparrow \beta_{cr}$ of $\varphi_\beta = -R_0(0)(I + \beta A(0))^{-1}(\beta v)$. From (25) with $\lambda = 0$ and $\beta(0) = \beta_{cr}$ and (47) it follows that

$$\varphi_\beta = -R_0(0)(I + \beta A(0))^{-1}(\beta v) = \frac{-\beta_{cr}}{\beta_{cr} - \beta} R_0(0)B(\beta_{cr} v) + O(1) = \frac{b_d}{\beta_{cr} - \beta}\psi + O(1)$$

for some positive constant b_d. □

8 Behavior of the Polymer for $\beta > \beta_{cr}$

In this section we shall assume that $\beta > \beta_{cr}$ is fixed. A result similar to the first part of Theorem 7.2 is valid for the solution of the Cauchy problem and for the fundamental solution.

Theorem 8.1. *Let $f \in L^2(\mathbb{R}^d)$ (or $f \in C_{\exp}(\mathbb{R}^d)$). For $\beta > \beta_{cr}$ there is $\varepsilon > 0$ such that we have the following asymptotics for the solution u_β of the Cauchy problem with the initial data f:*

$$u_\beta(t) = \exp(\lambda_0(\beta)t)(\langle \psi_\beta, f\rangle_{L^2(\mathbb{R}^d)}\psi_\beta + q_f(t)), \tag{51}$$

which holds in $L^2(\mathbb{R}^d)$ (or in $C(\mathbb{R}^d)$), where $||q_f(t)|| \leq c||f|| \exp(-\varepsilon t)$ for some c and all sufficiently large t.

We have the following asymptotics for the fundamental solution of the parabolic equation:

$$p_\beta(t, y, x) = \exp(\lambda_0(\beta)t)(\psi_\beta(y)\psi_\beta(x) + q(t, y, x)), \tag{52}$$

where $\lim_{t\to\infty} ||q(t, y, x)|| = 0$, uniformly in y, and (52) holds in $L^2(\mathbb{R}^d)$ and in $C(\mathbb{R}^d)$ for each y fixed.

Proof. The proof of (51) is the same as the proof of the first part of Theorem 7.2, and therefore we omit it.

Let $f_\beta^{\delta,y}(x) = p_\beta(\delta, y, x)$ be the fundamental solution of the parabolic problem at time δ. Note that $f_\beta^{\delta,y} \in L^2(\mathbb{R}^d)$ for all $\delta > 0$ and all y, and $f_\beta^{\delta,y} \in C_{\exp}(\mathbb{R}^d)$ for all sufficiently small $\delta > 0$ and all y. Denote the solution of the parabolic equation with the initial data $f_\beta^{\delta,y}$ by $u_\beta^{\delta,y}(t, x)$. Then

$$p_\beta(t, y, x) = u_\beta^{\delta,y}(t - \delta, x) = \exp(\lambda_0(\beta)(t - \delta))(\langle \psi_\beta, f_\beta^{\delta,y}\rangle_{L^2(\mathbb{R}^d)}\psi_\beta(x) + q^\delta(t, y, x)),$$

where $||q^\delta(t,y,x)|| \leq c||f_\beta^{\delta,y}|| \exp(-\varepsilon(t-\delta))$ for some c and all sufficiently large t.

Note that $\langle \psi_\beta, f_\beta^{\delta,y}\rangle_{L^2(\mathbb{R}^d)}$ can be made arbitrarily close to $\psi_\beta(y)$ uniformly in y, by choosing a sufficiently small δ, and $||f_\beta^{\delta,y}||$ is uniformly bounded in y for any fixed δ . This justifies (52). $\square$

Next, let us study the distribution of the end of the polymer with respect to the measure $\mathrm{P}_{\beta,T}$ as $T \to \infty$.

Theorem 8.2. *The distribution of $x(T)$ with respect to the measure $\mathrm{P}_{\beta,T}$ converges, weakly, as $T \to \infty$, to the distribution with the density $\psi_\beta/||\psi_\beta||_{L^1(\mathbb{R}^d)}$.*

Proof. The density of $x(T)$ with respect to the Lebesgue measure is equal to

$$\frac{p_\beta(T,0,x)}{Z_{\beta,T}(0)} = \frac{\exp(\lambda_0(\beta)T)(\psi_\beta(0)\psi_\beta(x) + q(T,0,x))}{\exp(\lambda_0(\beta)T)(||\psi_\beta||_{L^1(\mathbb{R}^d)}\psi_\beta(0) + o(1))}, \tag{53}$$

where q is the same as in (52). When $T \to \infty$, the right hand side of (53) converges to $\psi_\beta(x)/||\psi_\beta||_{L^1(\mathbb{R}^d)}$ uniformly in x by Theorem 8.1. This justifies the weak convergence. $\square$

Now let us examine the behavior of the polymer in a region separated both from zero and T. Let $S(T)$ be such that

$$\lim_{T\to\infty} S(T) = \lim_{T\to\infty}(T - S(T)) = +\infty. \tag{54}$$

Let $s > 0$ be fixed. Consider the process $y^T(t) = x(S(T)+t)$, $0 \leq t \leq s$.

Theorem 8.3. *The distribution of the process $y^T(t)$ with respect to either of the measures $\mathrm{P}_{\beta,T}$ or $\mathrm{P}_{\beta,T}(\cdot|x(T)=0)$ converges as $T \to \infty$, weakly in the space $C([0,s],\mathbb{R}^d)$, to the distribution of a stationary Markov process with invariant density ψ_β^2 and the generator*

$$L_\beta g = \frac{1}{2}\Delta g + \frac{(\nabla\psi_\beta, \nabla g)}{\psi_\beta}.$$

Remark. Let

$$r_\beta(t,y,x) = \frac{p_\beta(t,y,x)\psi_\beta(x)}{\psi_\beta(y)}\exp(-\lambda_0(\beta)t). \tag{55}$$

Note that $r_\beta(t,y,x)$ is the fundamental solution for the operator $\partial/\partial t - L_\beta^*$, where L_β^* is the formal adjoint to L_β. Thus r_β is the transition density for the Markov process with the generator L_β. Also note that $L_\beta^*\psi_\beta^2 = 0$, and thus ψ_β^2 is the invariant density for the Markov process.

Proof of Theorem 8.3. We shall only consider the measure $\mathrm{P}_{\beta,T}$ since the arguments for the measure $\mathrm{P}_{\beta,T}(\cdot|x(T)=0)$ are completely analogous. First, let us prove the convergence of the finite-dimensional distributions. For $y \in \mathbb{R}^d$ and a Borel set $A \in \mathcal{B}(\mathbb{R}^d)$, let

$$R(t,y,A) = \int_A r_\beta(t,y,x)dx,$$

with r_β given by (55). Note that R is a Markov transition function since

$$\int_{\mathbb{R}^d} r_\beta(t,y,x)dx \equiv 1.$$

The generator of the corresponding Markov process is L_β and the invariant density is ψ_β^2. Let $0 \le t_1 < ... < t_n \le s$. The density of the random vector $(y^T(t_1),...,y^T(t_n))$ with respect to the Lebesgue measure on $\mathbb{R}^{dn}$ is equal to

$$\rho^T(x_1,...,x_n) =$$

$$p_\beta(S(T)+t_1,0,x_1)p_\beta(t_2-t_1,x_1,x_2)...p_\beta(t_n-t_{n-1},x_{n-1},x_n)Z_{\beta,T-t_n}(x_n)(Z_{\beta,T}(0))^{-1}.$$

We replace here all factors p_β, except the first one, by r_β using (55). We replace the first factor and the factors Z by their asymptotic expansions given in Theorems 8.1 and 7.2, respectively. This leads to

$$\rho^T(x_1,...,x_n) = \psi_\beta^2(x_1)r_\beta(t_2-t_1,x_1,x_2)...r_\beta(t_n-t_{n-1},x_{n-1},x_n) + o(1), \quad T \to \infty,$$

where the remainder tends to zero uniformly in $(x_1,...,x_n)$. By the remark made after the statement of the theorem, this justifies the convergence of the finite dimensional distributions of y^T to those of the Markov process. It remains to justify the tightness of the family of measures induced by the processes y^T.

From the convergence of the one-dimensional distributions it follows that for any $\eta > 0$ there is $a > 0$ such that

$$\mathrm{P}_{\beta,T}(|y^T(0)| > a) \le \eta. \tag{56}$$

for all sufficiently large T. For a continuous function $x : [0,T] \to \mathbb{R}^d$, $x(0) = 0$, let

$$m^T(x,\delta) = \sup_{|t_1-t_2|\le\delta,\ S(T)\le t_1,t_2\le S(T)+s} |x(t_1)-x(t_2)|.$$

Let us prove that for each $\varepsilon, \eta > 0$, there is $\delta > 0$ such that

$$\mathrm{P}_{\beta,T}(m^T(x,\delta) > \varepsilon) \le \eta \tag{57}$$

for all sufficiently large T. Observe that

$$\mathrm{P}_{\beta,T}(m^T(x,\delta) > \varepsilon) =$$

$$(Z_{\beta,T}(0))^{-1}\mathrm{E}_{0,T}(\exp(\int_0^{S(T)+s} \beta v(x(t))dt)\chi_{\{m^T(x,\delta)>\varepsilon\}} Z_{\beta,T-S(T)-s}(x(S(T)+s))) \le$$

$$(Z_{\beta,T}(0))^{-1} \sup_{x\in\mathbb{R}^d} Z_{\beta,T-S(T)-s}(x)\mathrm{E}_{0,T}(\exp(\int_0^{S(T)+s} \beta v(x(t))dt)\chi_{\{m^T(x,\delta)>\varepsilon\}}) \le$$

$$\exp(s\beta \sup_{x\in\mathbb{R}^d} v(x))(Z_{\beta,T}(0))^{-1} \sup_{x\in\mathbb{R}^d} Z_{\beta,T-S(T)-s}(x)\mathrm{E}_{0,T}(\exp(\int_0^{S(T)} \beta v(x(t))dt)\chi_{\{m^T(x,\delta)>\varepsilon\}})$$

$$\leq \exp(s\beta \sup_{x\in\mathbb{R}^d} v(x))(Z_{\beta,T}(0))^{-1} \sup_{x\in\mathbb{R}^d} Z_{\beta,T-S(T)-s}(x) \sup_{x\in\mathbb{R}^d} p_\beta(S(T),0,x)C(\delta,\varepsilon),$$

where $C(\delta,\varepsilon)$ is the probability that for a d-dimensional Brownian motion W_t, $0 \leq t \leq s$, we have

$$\sup_{|t_1-t_2|\leq\delta,\ 0\leq t_1,t_2\leq s} |W(t_1)-W(t_2)| > \varepsilon.$$

Note that

$$\exp(s\beta \sup_{x\in\mathbb{R}^d} v(x))(Z_{\beta,T}(0))^{-1} \sup_{x\in\mathbb{R}^d} Z_{\beta,T-S(T)-s}(x) \sup_{x\in\mathbb{R}^d} p_\beta(S(T),0,x)$$

is bounded, as follows from Theorems 7.2 and 8.1, while $C(\delta,\varepsilon)$ can be made arbitrarily small by selecting a sufficiently small δ. This justifies (57). Since the inequalities (56) and (57) hold for all sufficiently large T, by choosing different a and δ, we can make sure that they hold for all T. Thus the family of measures induced by the processes y^T is tight. □

Remark. If instead of (54) we assume that $S(T) = 0$, the result of Theorem 8.3 will hold with the only difference that the initial distribution for the limiting Markov process will now be concentrated at zero, instead of being the invariant distribution.

9 Behavior of the Polymer for $\beta < \beta_{cr}$

First, we shall study the asymptotic behavior of the solution $u_\beta(t,x)$ of the Cauchy problem and of the fundamental solution $p_\beta(t,y,x)$ when $t\to\infty$, $|y| \leq \varepsilon^{-1}$, $\varepsilon\sqrt{t} \leq |x| \leq \varepsilon^{-1}\sqrt{t}$, and $\varepsilon > 0$ is small but fixed. Recall that φ_β was defined before Theorem 7.2.

Lemma 9.1. *Let $d \geq 3$, $0 \leq \beta < \beta_{cr}$, $\varepsilon > 0$ and $f \in C_{\exp}(\mathbb{R}^d)$, $f \geq 0$. We have the following asymptotics for the solution u_β of the Cauchy problem with the initial data f:*

$$u_\beta(t,x) = (2\pi t)^{-d/2}\exp(-|x|^2/2t)(\langle 1+\varphi_\beta, f\rangle_{L^2(\mathbb{R}^3)} + q_f(t,x)), \tag{58}$$

where for some constant $C_\beta(\varepsilon)$ we have

$$\sup_{\varepsilon\sqrt{t}\leq|x|\leq\varepsilon^{-1}\sqrt{t}} |q_f(t,x)| \leq C_\beta(\varepsilon)t^{-1/2}||f||_{C_{\exp}(\mathbb{R}^3)}, \quad t\geq 1.$$

We have the following asymptotics for the fundamental solution of the parabolic equation:

$$p_\beta(t,y,x) = (2\pi t)^{-d/2}\exp(-|x|^2/2t)(1+\varphi_\beta(y)+q(t,y,x)), \tag{59}$$

where

$$\lim_{t\to\infty} \sup_{|y|\leq\varepsilon^{-1},\ \varepsilon\sqrt{t}\leq|x|\leq\varepsilon^{-1}\sqrt{t}} |q(t,y,x| = 0.$$

Proof. Note that (59) follows from (58) since the fundamental solution at time t is equal to the solution with the initial data $p_\beta(t, y, \delta)$ evaluated at time $t-\delta$ (the same argument was used in the proof of Theorem 8.1). Therefore it is sufficient to prove (58).

For the sake of transparency of exposition, we shall consider only the case $d = 3$. From Lemma 5.8 it follows that we can put $a = 0$ in (43) when $\beta < \beta_{cr}$. Thus using (21) and the explicit formula for $R_0(\lambda)$, we obtain

$$u_\beta(t,x) = \frac{-1}{2\pi i}\int_{\Gamma(0)} e^{\lambda t}(R_\beta(\lambda)f)(x)d\lambda = \frac{1}{2\pi i}\int_{\Gamma(0)}\int_{\mathbb{R}^3} e^{\lambda t}\frac{e^{-\sqrt{2\lambda}|x-y|}}{2\pi|x-y|}g(\lambda,y)dyd\lambda, \qquad (60)$$

where

$$g(\lambda) = (I + \beta A(\lambda))^{-1}f. \qquad (61)$$

By Lemma 5.1, $A(\lambda)$ is an entire function of $\sqrt{\lambda}$. By the Analytic Fredholm Theorem, $(I + \beta A(\lambda))^{-1}$ is a meromorphic function of $\sqrt{\lambda}$, since $A(\lambda)$ tends to zero as $\lambda \to +\infty$, $\mathrm{Im}(\lambda) = 0$. It does not have a pole at zero as follows from Lemma 5.4 and Remark 1 following Lemma 5.5. Therefore, by the Taylor formula, for all sufficiently small $|\lambda|$, $\lambda \in \Gamma(0)$, and some $c > 0$, we have

$$g(\lambda) = g_0 + g_1(\lambda), \quad ||g_1(\lambda)||_{C_{\exp}(\mathbb{R}^3)} \le c\sqrt{|\lambda|}||f||_{C_{\exp}(\mathbb{R}^3)}, \qquad (62)$$

where $g_0 = (I+\beta A(0))^{-1}f$. Since $||(I+\beta A(\lambda))^{-1}||_{C_{\exp}(\mathbb{R}^3)}$ is bounded on $\Gamma(0)$, formula (62) is valid for all $\lambda \in \Gamma(0)$, but not only in a neighborhood of zero.

Let $u_\beta^{(1)}(x)$ be given by (60) with g replaced by g_1. Then

$$u_\beta^{(1)}(t,x) = \frac{1}{2\pi i}\int_{\Gamma(0)}\int_{|y|\le\varepsilon\sqrt{t}/2} e^{\lambda t}\frac{e^{-\sqrt{2\lambda}|x-y|}}{2\pi|x-y|}g_1(\lambda,y)dyd\lambda +$$

$$\frac{1}{2\pi i}\int_{\Gamma(0)}\int_{|y|>\varepsilon\sqrt{t}/2} e^{\lambda t}\frac{e^{-\sqrt{2\lambda}|x-y|}}{2\pi|x-y|}g_1(\lambda,y)dyd\lambda = I_1 + I_2.$$

We change the variable $\lambda t = \zeta$ and use the estimate $1/|x-y| < 2/(\varepsilon\sqrt{t})$ in I_1. This implies

$$|I_1| \le \frac{c||f||_{C_{\exp}(\mathbb{R}^3)}}{2\pi^2\varepsilon t^2}\int_{\Gamma(0)}\int_{|y|\le\varepsilon\sqrt{t}/2}|\sqrt{|\zeta|}e^{\zeta-\sqrt{2\zeta}\frac{|x-y|}{\sqrt{t}}}e^{-y^2}|dyd\zeta \le$$

$$\frac{C(\varepsilon)||f||_{C_{\exp}(\mathbb{R}^3)}}{t^2}, \quad \varepsilon\sqrt{t} \le |x| \le \varepsilon^{-1}\sqrt{t}.$$

In I_2 we change the variables $\lambda t = \zeta$, $x = \sqrt{t}z$, $y = \sqrt{t}u$ and use the estimate $e^{-y^2} \le e^{-(\varepsilon t/2)^2}$. This leads to the exponential decay of $|I_2|$ as $t \to \infty$. Hence

$$u_\beta(t,x) = \frac{1}{2\pi i}\int_{\mathbb{R}^3}\int_{\Gamma(0)} e^{\lambda t}\frac{e^{-\sqrt{2\lambda}|x-y|}}{2\pi|x-y|}g_0(y)d\lambda dy + r_1(t,x), \qquad (63)$$

where the remainder $r_1(t,x)$ satisfies

$$\sup_{\varepsilon\sqrt{t}\le|x|\le\varepsilon^{-1}\sqrt{t}}|r_1(t,x)|=||f||_{C_{\exp}(\mathbb{R}^3)}O(t^{-2})\ \text{ as }\ t\to\infty. \tag{64}$$

The integral over $\Gamma(0)$ in (63) can be evaluated, and we obtain

$$u_\beta(t,x)=\frac{1}{(2\pi t)^{3/2}}\int_{\mathbb{R}^3}e^{-\frac{|x-y|^2}{2t}}g_0(y)dy+r_1(t,x).$$

Since $||g_0||_{C_{\exp}(\mathbb{R}^3)}\le C||f||_{C_{\exp}(\mathbb{R}^3)}$ for some constant C, we have

$$u_\beta(t,x)=\frac{1}{(2\pi t)^{3/2}}e^{-\frac{|x|^2}{2t}}\int_{\mathbb{R}^3}g_0(y)dy+r_2(t,x),$$

where r_2 satisfies (64) with r_1 replaced by r_2. In order to prove (58), it remains to show that

$$\int_{\mathbb{R}^3}g_0(x)dx=\int_{\mathbb{R}^3}(1+\varphi_\beta(x))f(x)dx. \tag{65}$$

Since $(I+\beta vR_0(0))g_0=f$, we have $g_0=f-\beta vR_0(0)g_0$. Recall that φ_β is the solution of (45) with $f=-\beta v$. Thus

$$\int_{\mathbb{R}^3}g_0(x)dx=\int_{\mathbb{R}^3}f(x)dx+\int_{\mathbb{R}^3}[\frac{1}{2}\Delta\varphi_\beta+\beta v\varphi_\beta]R_0(0)g_0dx.$$

Since $\varphi_\beta, R_0(0)g_0=O(1/|x|)$ and their derivatives are of order $O(|x|^{-2})$ as $|x|\to\infty$, the Green formula implies

$$\int_{\mathbb{R}^3}\frac{1}{2}\Delta\varphi_\beta R_0(0)g_0dx=\int_{\mathbb{R}^3}\varphi_\beta\frac{1}{2}\Delta R_0(0)g_0dx=\int_{\mathbb{R}^3}\varphi_\beta g_0dx.$$

Hence

$$\int_{\mathbb{R}^3}g_0(x)dx=\int_{\mathbb{R}^3}f(x)dx+\int_{\mathbb{R}^3}\varphi_\beta(I+\beta vR_0(0))g_0dx,$$

which implies (65.) □

Next, let us study the distribution of the polymer with respect to the measure $\mathrm{P}_{\beta,T}$ as $T\to\infty$. Consider the process $y^T(t)=x(tT)/\sqrt{T}$, $0\le t\le 1$.

Theorem 9.2. *Let $d\ge 3$ and $0\le\beta<\beta_{cr}$. With respect to $\mathrm{P}_{\beta,T}$, the distribution of the process $y^T(t)$ converges as $T\to\infty$, weakly in the space $C([0,1],\mathbb{R}^d)$, to the distribution of the d-dimensional Brownian motion. With respect to $\mathrm{P}_{\beta,T}(\cdot|x(T)=0)$, the distribution of the process $y^T(t)$ converges as $T\to\infty$, weakly in the space $C([0,1],\mathbb{R}^d)$, to the distribution of the d-dimensional Brownian bridge.*

Proof. We shall only prove the first statement since the proof of the second one is completely similar. First, let us prove the convergence of the finite-dimensional distributions. Clearly $\mathrm{P}_{\beta,T}(y^T(0)=0)=1$. Let $0<t_1<...<t_n\le 1$. The density of the random vector $(y^T(t_1),...,y^T(t_n))$ with respect to the Lebesgue measure on $\mathbb{R}^{dn}$ is equal to

$$\rho^T(x_1,...,x_n)=$$

$$T^{\frac{dn}{2}}p_\beta(t_1T,0,x_1T^{\frac{1}{2}})p_\beta((t_2-t_1)T,x_1T^{\frac{1}{2}},x_2T^{\frac{1}{2}})...p_\beta((t_n-t_{n-1})T,x_{n-1}T^{\frac{1}{2}},x_nT^{\frac{1}{2}})(Z_{\beta,T}(0))^{-1}.$$

By Lemma 9.1,

$$p_\beta(t_1T,0,x_1T^{\frac{1}{2}})=T^{-d/2}(2\pi t_1)^{-d/2}(1+\varphi_\beta(0))\exp(-|x_1|^2/2t_1)(1+r(T,x_1)),$$

where

$$\lim_{T\to\infty}\sup_{\varepsilon\le|x_1|\le\varepsilon^{-1}}(|r(T,x_1|)=0. \tag{66}$$

Note that $p_\beta\ge p_0$ since v is non-negative, and $\lim_{T\to\infty}(Z_{\beta,T}(0))=(1+\varphi_\beta(0))$ by Theorem 7.2. Therefore,

$$\rho^T(x_1,...,x_n)\ge$$

$$(2\pi t_1)^{-\frac{d}{2}}e^{-\frac{|x_1|^2}{2t_1}}(1+r(T,x_1))(2\pi(t_2-t_1))^{-\frac{d}{2}}e^{-\frac{|x_2-x_1|^2}{2(t_2-t_1)}}...(2\pi(t_n-t_{n-1}))^{-\frac{d}{2}}e^{-\frac{|x_n-x_{n-1}|^2}{2(t_n-t_{n-1})}} \tag{67}$$
$$=\rho^W_{t_1,...,t_n}(x_1,...,x_n)(1+r(T,x_1)),$$

where $\rho^W_{t_1,...,t_n}(x_1,...,x_n)$ is the density of the Gaussian vector $(W(t_1),...,W(t_n))$, where W is a d-dimensional Brownian motion, and $q(T,x_1)$ satisfies (66) with q instead of r. Since ε was an arbitrary positive number, this implies the convergence of the finite-dimensional distributions of y^T to the finite-dimensional distributions of the Brownian motion. Indeed, the estimate from below for $\rho^T(x_1,...,x_n)$ in (67) is sufficient since we know a priori that $\rho^W_{t_1,...,t_n}(x_1,...,x_n)$ is the density of a probability measure.

It remains to prove tightness of the family of processes y^T, $T\ge 1$.

For a continuous function $x:[0,T]\to\mathbb{R}^d$, let

$$m(x,\delta)=\sup_{|t_1-t_2|\le\delta T,\ 0\le t_1,t_2\le T}|x(t_1)-x(t_2)|/\sqrt{T},$$

$$\widetilde{m}(x,\delta,\varepsilon)=\sup_{|t_1-t_2|\le\delta T,\ 0\le t_1,t_2\le T,\ |x(t_1)|\ge\varepsilon\sqrt{T}}|x(t_1)-x(t_2)|/\sqrt{T}.$$

The tightness will follow if we show that for each $\varepsilon,\eta>0$ there is $\delta>0$ such that

$$\mathrm{P}_{\beta,T}(m(x,\delta)>\varepsilon)\le\eta$$

for all sufficiently large T. Note that $m(x,\delta)>\varepsilon$ implies that $\widetilde{m}(x,\delta,\varepsilon/4)>\varepsilon/4$. Therefore, it is sufficient to show that

$$\mathrm{P}_{\beta,T}(\widetilde{m}(x,\delta,\varepsilon/4)>\varepsilon/4)\le\eta. \tag{68}$$

Fix $\varepsilon > 0$. For a continuous function $x : [0, T] \to \mathbb{R}^d$, let

$$\tau = \min(T, \inf\{t \geq 0 : |x(t)| = \varepsilon\sqrt{T}/4\}),$$

Let $\mathcal{E}_\delta$ be the event that $m(x, \delta) > \varepsilon/4$ and $\widetilde{\mathcal{E}}_\delta$ the event that $\widetilde{m}(x, \delta, \varepsilon/4) > \varepsilon/4$. For $0 \leq s \leq T$, let $\mathcal{E}_\delta^s$ be the event that a continuous function $x : [0, T - s] \to \mathbb{R}^d$ satisfies

$$\sup_{|t_1 - t_2| \leq \delta T,\ 0 \leq t_1, t_2 \leq T - s} |x(t_1) - x(t_2)|/\sqrt{T} > \varepsilon/4.$$

Then

$$\mathrm{P}_{\beta,T}(\widetilde{\mathcal{E}}_\delta) = (Z_{\beta,T}(0))^{-1}\mathrm{E}_{0,T}(\exp(\int_0^T \beta v(x(t))dt)\chi_{\widetilde{\mathcal{E}}_\delta}) \leq$$

$$(Z_{\beta,T}(0))^{-1}\mathrm{E}_{0,T}\left(\exp(\int_0^\tau \beta v(x(t))dt)\mathrm{E}_{0,T-\tau}^{x(\tau)}(\chi_{\mathcal{E}_\delta^\tau} \exp(\int_0^{T-\tau} \beta v(x(t))dt))\right),$$

where $\mathrm{E}_{0,T}^x$ denotes the expectation with respect to the measure induced by the Brownian motion starting at the point x. Since

$$\mathrm{E}_{0,T} \exp(\int_0^\tau \beta v(x(t))dt) \leq Z_{\beta,T}(0)$$

and

$$\mathrm{E}_{0,T-\tau}^{x(\tau)}(\chi_{\mathcal{E}_\delta^\tau} \exp(\int_0^{T-\tau} \beta v(x(t))dt)) \leq \sup_{x \in \mathbb{R}^d, |x| = \varepsilon\sqrt{T}/4} \mathrm{E}_{0,T}^x(\chi_{\mathcal{E}_\delta} \exp(\int_0^T \beta v(x(t))dt)),$$

it is sufficient to estimate

$$\sup_{x \in \mathbb{R}^d, |x| = \varepsilon\sqrt{T}/4} \mathrm{E}_{0,T}^x(\chi_{\mathcal{E}_\delta} \exp(\int_0^T \beta v(x(t))dt)). \tag{69}$$

Let $\mathcal{E}'$ be the event that a trajectory starting at x reaches the support of v before time T. Note that

$$\lim_{T \to \infty} \sup_{x \in \mathbb{R}^d, |x| = \varepsilon\sqrt{T}/4} \mathrm{P}_{0,T}^x(\mathcal{E}') = 0$$

since $d \geq 3$. The expression in (69) is estimated form above by

$$\sup_{x \in \mathbb{R}^d, |x| = \varepsilon\sqrt{T}/4} (\mathrm{E}_{0,T}^x(\chi_{\mathcal{E}'} \exp(\int_0^T \beta v(x(t))dt)) + \mathrm{P}_{0,T}^x(\mathcal{E}_\delta)).$$

The second term does not depend on T due to the scaling invariance of the Brownian motion, and can be made arbitrarily small by selecting a sufficiently small δ. Due to the Markov property of the Brownian motion, the first term is estimated from above by

$$\sup_{x \in \mathbb{R}^d, |x| = \varepsilon T/4} \mathrm{P}_{0,T}^x(\mathcal{E}') \cdot \sup_{x \in \mathrm{supp}(v)} Z_{\beta,T}(x),$$

and thus tends to zero when $T \to \infty$. □

10 Behavior of the Polymer for $\beta = \beta_{cr}$

In this section we assume that $d = 3$. Again, we start with the asymptotic behavior of the solution $u_\beta(t,x)$ of the Cauchy problem and of the fundamental solution $p_\beta(t,y,x)$ when $t \to \infty$, $|y| \le \varepsilon^{-1}$, $\varepsilon\sqrt{t} \le |x| \le \varepsilon^{-1}\sqrt{t}$, and $\varepsilon > 0$ is small but fixed.

Recall that ψ is the positive ground state for $H_{\beta_{cr}}$ normalized by the condition $||\beta_{cr} v\psi||_{L^2_{\exp}(\mathbb{R}^3)} = 1$ (see the remark following Lemma 5.4 and Theorem 7.2). For $f \in C_{\exp}(\mathbb{R}^3)$, define

$$\alpha(f) = \varkappa \int_{\mathbb{R}^3} \psi(x) f(x) dx, \quad \varkappa = \frac{1}{\sqrt{2\pi}\beta_{cr} \int_{\mathbb{R}^3} v(x)\psi(x)dx}.$$

We can formally apply this to f being the δ-function centered at a point y, and thus define

$$\alpha(\delta_y(x)) = \varkappa\psi(y).$$

Theorem 10.1. *Let $d = 3$, $\beta = \beta_{cr}$, $\varepsilon > 0$ and $f \in C_{\exp}(\mathbb{R}^3)$, $f \ge 0$. We have the following asymptotics for the solution u_β of the Cauchy problem with the initial data f:*

$$u_\beta(t,x) = \frac{1}{|x|\sqrt{t}} \exp(-|x|^2/2t)(\alpha(f) + q_f(t,x)), \tag{70}$$

where for some constant $C_\beta(\varepsilon)$ we have

$$\sup_{\varepsilon\sqrt{t} \le |x| \le \varepsilon^{-1}\sqrt{t}} |q_f(t,x)| \le C_\beta(\varepsilon) t^{-1/2} ||f||_{C_{\exp}(\mathbb{R}^3)}, \quad t \ge 1.$$

We have the following asymptotics for the fundamental solution of the parabolic equation:

$$p_\beta(t,y,x) = \frac{\varkappa}{|x|\sqrt{t}} \exp(-|x|^2/2t)(\psi(y) + q(t,y,x)), \tag{71}$$

where

$$\lim_{t\to\infty} \sup_{|y| \le \varepsilon^{-1},\ \varepsilon\sqrt{t} \le |x| \le \varepsilon^{-1}\sqrt{t}} |q(t,y,x| = 0.$$

Proof. As in Lemma 9.1, formula (71) follows from (70). Lemma 5.7 implies

$$(I + \beta_{cr}A(\lambda))^{-1} = \frac{\beta_{cr}}{\beta(\lambda) - \beta_{cr}} B + O(1), \quad \lambda \to 0,\ \lambda \in \mathbb{C}',$$

where B is the one dimensional operator with the kernel

$$B(x,y) = \frac{v(x)\psi(x)\psi(y)}{\int_{\mathbb{R}^3} v(x)\psi^2(x)dx}.$$

From here, (33) and (38) we get

$$(I + \beta_{cr}A(\lambda))^{-1} = \frac{1}{\beta_{cr}\gamma\sqrt{\lambda}} B + O(1), \quad \lambda \to 0,\ \lambda \in \mathbb{C}',$$

where γ is defined in (39), (40). Hence, for any $f \in C_{\exp}(\mathbb{R}^3)$ and $\lambda \to 0$, $\lambda \in \mathbb{C}'$,

$$h(\lambda, x) := (I + \beta_{cr} A(\lambda))^{-1} f = \frac{\widetilde{\alpha}(f)}{\sqrt{\lambda}} v(x)\psi(x) + g_1(\lambda), \quad \widetilde{\alpha}(f) = \frac{\sqrt{2}\pi \int_{\mathbb{R}^3} \psi(x) f(x) dx}{\beta_{cr}(\int_{\mathbb{R}^3} v(x)\psi(x)dx)^2}, \tag{72}$$

where $g_1(\lambda) \le c||f||_{C_{\exp}(\mathbb{R}^3)}$ for some constant c. Now, similarly to (60), we have

$$u_\beta(t,x) = \frac{-1}{2\pi i}\int_{\Gamma(0)} e^{\lambda t}(R_\beta(\lambda) f)(x) d\lambda = \frac{1}{2\pi i}\int_{\Gamma(0)}\int_{\mathbb{R}^3} e^{\lambda t} \frac{e^{-\sqrt{2\lambda}|x-y|}}{2\pi|x-y|} h(\lambda, y) dy d\lambda.$$

The integral with $g_1(\lambda)$ instead of h can be estimated similarly to the estimate on $u_\beta^{(1)}$ in the case of $\beta < \beta_{cr}$. This leads to following analogue of (63)

$$u_\beta(t,x) = \frac{\widetilde{\alpha}(f)}{2\pi i}\int_{\mathbb{R}^3}\int_{\Gamma(0)} e^{\lambda t}\frac{e^{-\sqrt{2\lambda}|x-y|}}{2\pi\sqrt{\lambda}|x-y|} v(y)\psi(y) d\lambda dy + r_1(t,x),$$

where the remainder $r_1(t,x)$ satisfies

$$\sup_{\varepsilon\sqrt{t} \le |x| \le \varepsilon^{-1}\sqrt{t}} |r_1(t,x)| = ||f||_{C_{\exp}(\mathbb{R}^3)} O(t^{-3/2}) \quad \text{as} \quad t \to \infty. \tag{73}$$

We evaluate the integral over $\Gamma(0)$:

$$\frac{1}{2\pi i}\int_{\Gamma(0)} \frac{e^{\lambda t - \sqrt{2\lambda}|x-y|}}{\sqrt{2\lambda}} d\lambda = \frac{1}{\sqrt{2\pi t}} e^{-\frac{|x-y|^2}{2t}}. \tag{74}$$

This equality simply means that the inverse Laplace transform of the Green function of the one dimensional Helmholtz equation coincides with the fundamental solution of the corresponding heat equation. Thus,

$$u_\beta(t,x) = \frac{\widetilde{\alpha}(f)}{2\pi^{3/2}\sqrt{t}}\int_{\mathbb{R}^3} \frac{1}{|x-y|} e^{-\frac{|x-y|^2}{2t}} v(y)\psi(y) dy + r_1(t,x).$$

This implies (70) since v has a compact support. □

The next theorem concerns the fundamental solution when both y and x are at a distance of order $\sqrt{t}$ away from the origin. Note that now there are two terms in the asymptotic expansion for the fundamental solution which are of the same order in t. The main terms have the order $t^{-3/2}$ when $t \to \infty$, compared with t^{-1} in the case considered in Theorem 10.1 (where y was bounded).

Theorem 10.2. *Let $d = 3$, $\beta = \beta_{cr}$, $\varepsilon > 0$. We have the following asymptotics for the fundamental solution of the parabolic equation:*

$$p_\beta(t,y,x) = p_0(t,y,x) + \frac{1}{(2\pi)^{3/2}|y||x|\sqrt{t}} e^{-(|y|+|x|)^2/2t}(1 + \overline{q}(t,y,x)), \tag{75}$$

where

$$\lim_{t\to\infty} \sup_{\varepsilon\sqrt{t} \le |y|, |x| \le \varepsilon^{-1}\sqrt{t}} |\overline{q}(t,y,x| = 0. \tag{76}$$

Proof. Let $p_\beta(t,y,x)=p_0(t,y,x)+u$. Then $u_t=H_\beta u+\beta v p_0,\quad u|_{t=0}=0$, and therefore by the Duhamel formula

$$u(t,y,x)=\int_0^t\int_{\mathbb{R}^3}p_\beta(t-s,z,x)\beta v(z)p_0(s,y,z)dzds.$$

Using (71), we get

$$u(t,y,x)=\int_0^t\int_{\mathbb{R}^3}\frac{\varkappa}{|x|\sqrt{t-s}}\exp(-|x|^2/2(t-s))(\psi(z)\beta v(z)p_0(s,y,0)dzds+h_1+h_2 \quad (77)$$

with

$$h_1=\int_0^t\int_{\mathbb{R}^3}\frac{\varkappa}{|x|\sqrt{t-s}}\exp(-|x|^2/2(t-s))(\psi(z)\beta v(z)(p_0(s,y,z)-p_0(s,y,0))dzds,$$

$$h_2=\int_0^t\int_{\mathbb{R}^3}\frac{\varkappa}{|x|\sqrt{t-s}}\exp(-|x|^2/2(t-s))(q(t-s,z,x)\beta v(z)p_0(s,y,z)dzds,$$

where q is the same as in (71). The integral in the right hand side of (77) (let us denote it by w) is a convolution of two functions and can be evaluated using the Laplace transform (see (74)). It gives the second term in the right hand side of (75). The contribution from the other two terms can be shown to satisfy (76). Let us prove the statement about w. In fact,

$$w=\varkappa_1(w_1*p_0(t,y,0)),\quad \varkappa_1=\frac{\varkappa\sqrt{2\pi}}{|x|}\int_{\mathbb{R}^3}\beta v(z)\psi(z)dz=\frac{1}{|x|},\quad w_1=\frac{1}{\sqrt{2\pi t}}\exp(-|x|^2/2t)).$$

The Laplace transform $\widehat{w}_1(\lambda)$ of the function w_1 is equal to $e^{-\sqrt{2\lambda}|x|}/\sqrt{2\lambda}$ (see (74)), and the Laplace transform of $p_0(t,y,0)$ is equal to $e^{-\sqrt{2\lambda}|y|}/2\pi|y|$. Thus

$$\widehat{w}(\lambda)=\frac{1}{2\pi|x||y|}\frac{e^{-\sqrt{2\lambda}(|x|+|y|)}}{\sqrt{2\lambda}}.$$

It remains to apply (74) one more time. □

As in Section 9, we shall study the limit, as $T\to\infty$, of the family of processes $y^T(t)=x(tT)/\sqrt{T}$, $0\le t\le 1$. For $0\le s<t\le 1$, $y,x\in\mathbb{R}^3$, define

$$p_\beta^T(s,t,y,x)=p_\beta(T(t-s),y\sqrt{T},x\sqrt{T}),$$

$$\overline{p}_\beta(s,t,0,x)=\lim_{T\to\infty}(Tp_\beta^T(s,t,0,x))=\lim_{T\to\infty}(Tp_\beta(T(t-s),0,x\sqrt{T})),\ \ x\neq 0,$$

$$\overline{p}_\beta(s,t,y,x)=\lim_{T\to\infty}(T^{3/2}p_\beta^T(s,t,y,x))=\lim_{T\to\infty}(T^{3/2}p_\beta(T(t-s),y\sqrt{T},x\sqrt{T})),\quad y,x\neq 0.$$

By Theorems 10.1 and 10.2,

$$\overline{p}_\beta(s,t,0,x) = \frac{\varkappa\psi(0)}{|x|\sqrt{t-s}}\exp(-|x|^2/2(t-s)), \quad x \neq 0,$$

$$\overline{p}_\beta(s,t,y,x) = p_0(t-s,y,x) + \frac{1}{(2\pi)^{3/2}|y||x|\sqrt{t-s}}\exp(-(|y|+|x|)^2/2(t-s)) \quad ,y,x \neq 0. \tag{78}$$

For $0 < t_1 < ... < t_n \leq 1$, let the density of the random vector $(y^T(t_1),...,y^T(t_n))$ with respect to the Lebesgue measure on $\mathbb{R}^{dn}$ be denoted by $\rho^T(x_1,...,x_n)$.

For $0 \leq s < t \leq 1$ and $y, x \in \mathbb{R}^3$, define

$$Q^T(s,t,y,x) = p^T_\beta(s,t,y,x)\int_{\mathbb{R}^3} p^T_\beta(t,1,x,z)dz(\int_{\mathbb{R}^3} p^T_\beta(s,1,y,z)dz)^{-1}, \quad t<1,$$

$$Q^T(s,1,y,x) = p^T_\beta(s,1,y,x)(\int_{\mathbb{R}^3} p^T_\beta(s,1,y,z)dz)^{-1}.$$

Thus

$$\rho^T(x_1,...,x_n) = Q^T(0,t_1,0,x_1)Q^T(t_1,t_2,x_1,x_2)...Q^T(t_{n-1},t_n,x_{n-1},x_n).$$

In order to find the limit of the finite dimensional distributions of y^T, we need to identify the limit of Q^T as $T\to\infty$. For $0 \leq s < t \leq 1$, $y \in \mathbb{R}^3$ and $x \in \mathbb{R}^3 \setminus \{0\}$, define

$$Q(s,t,y,x) = \lim_{T\to\infty} Q^T(s,t,y,x). \tag{79}$$

By Theorems 10.1 and 10.2,

$$Q(s,t,y,x) = \overline{p}_\beta(s,t,y,x)\int_{\mathbb{R}^3} \overline{p}_\beta(t,1,x,z)dz(\int_{\mathbb{R}^3} \overline{p}_\beta(s,1,y,z)dz)^{-1}, \quad t<1, \tag{80}$$

$$Q(s,1,y,x) = \overline{p}_\beta(s,1,y,x)(\int_{\mathbb{R}^3} \overline{p}_\beta(s,1,y,z)dz)^{-1}. \tag{81}$$

We additionally define $Q(s,t,y,0) = 0$.

Using (79), (80) and (81), we can identify the limit of the densities $\rho^T(x_1,...,x_n)$ for $x_2,...,x_n \neq 0$. In order to identify the weak limit of the finite dimensional distributions of the processes y^T, we are going to show that the limit of the densities is the density of a probability distribution, i.e. the mass does not escape to the origin or infinity. This is done in Lemma 10.4, where we show that Q serves as the transition density for a Markov process. First, however, we show that Q satisfies a Fokker-Plank type equation on $\mathbb{R}^3 \setminus \{0\}$.

Let

$$g(t,x) = \ln(\int_{\mathbb{R}^3} \overline{p}_\beta(t,1,x,z)dz), \quad 0 \leq t < 1, \quad |x| > 0, \tag{82}$$

Let L be the differential operator acting on $C^2(\mathbb{R}^3 \setminus \{0\})$ according to the formula

$$(Lf)(t,x) = \frac{1}{2}\Delta_x f(t,x) + (\frac{\partial g(t,x)}{\partial r})\frac{\partial f}{\partial r}(t,x), \quad |x| > 0,$$

and let L^* be the formal adjoint of L, i.e.

$$L^* v = \frac{1}{2}\Delta_x v - \frac{1}{r^2}\frac{\partial[(\partial g/\partial r)v]}{\partial r}.$$

Lemma 10.3. *For $0 \le s < 1$ and $y \in \mathbb{R}^3$, the function $Q(s,t,y,x)$ satisfies the equation*

$$\frac{\partial Q(s,t,y,x)}{\partial t} = L^* Q(s,t,y,x), \quad |x| > 0, \quad s < t < 1. \tag{83}$$

Proof. Let us consider the case when $y \neq 0$ (the other case is similar). Let

$$v_1(s,t,y,x) = \frac{1}{(2\pi)^{3/2}|y||x|\sqrt{t-s}} \exp(-(|y|+|x|)^2/2(t-s)),$$

$$v_2(t,x) = \int_{\mathbb{R}^3} \frac{1}{(2\pi)^{3/2}|x||z|\sqrt{1-t}} \exp(-(|x|+|z|)^2/2(1-t))dz.$$

Observe that

$$(\frac{\partial}{\partial t} - \frac{1}{2}\Delta_x)v_1 = 0, \quad (\frac{\partial}{\partial t} + \frac{1}{2}\Delta_x)v_2 = 0. \tag{84}$$

For fixed s and y, the function $Q(s,t,y,x)$ is proportional to

$$u(t,x) = (p_0(t-s,y,x) + v_1(s,t,y,x))[1 + v_2(t,x)].$$

By (84),

$$(\frac{\partial}{\partial t} - \frac{1}{2}\Delta_x)u = -(\frac{\partial p_0}{\partial r} + \frac{\partial v_1}{\partial r})\frac{\partial v_2}{\partial r} + 2(p_0 + v_1)\frac{\partial v_2}{\partial t}. \tag{85}$$

For any two functions A and B we have

$$(A\frac{\partial}{\partial r} + B)u = A(\frac{\partial p_0}{\partial r} + \frac{\partial v_1}{\partial r})(1+v_2) + A(p_0+v_1)\frac{\partial v_2}{\partial r} + B(p_0+v_1)(1+v_2). \tag{86}$$

Thus

$$(\frac{\partial}{\partial t} - \frac{1}{2}\Delta_x + A\frac{\partial}{\partial r} + B)u =$$

$$(\frac{\partial p_0}{\partial r} + \frac{\partial v_1}{\partial r})(-\frac{\partial v_2}{\partial r} + A(1+v_2)) + 2(p_0+v_1)(\frac{\partial v_2}{\partial t} + A\frac{\partial v_2}{\partial r} + B(1+v_2)) = 0$$

if

$$A = \frac{\partial v_2}{\partial r}(1+v_2)^{-1}, \quad B = -(2\frac{\partial v_2}{\partial t} + A\frac{\partial v_2}{\partial r})(1+v_2)^{-1}.$$

Since $g(t,x) = \ln(1+v_2)$ and $2\partial v_2/\partial t = -\partial^2 v_2/\partial r^2 - 2\partial v_2/\partial r$ (see (84)), it is easy to check that the operator in the left hand side of the equation for u is $\frac{\partial}{\partial t} - L^*$, and this justifies (83). □

Lemma 10.4. *The function $Q(s,t,y,x)$, $0 \le s < t \le 1$, $y,x \in \mathbb{R}^3$, is the transition density for a Markov process on $\mathbb{R}^3$.*

Proof. To show the existence of a Markov process, we need to verify that

$$\int_{\mathbb{R}^3} Q(t_1,t_2,x_1,x_2)dx_2 = 1, \quad t_1 < t_2 \tag{87}$$

and

$$\int_{\mathbb{R}^3} Q(t_1,t_2,x_1,x_2)Q(t_2,t_3,x_2,x_3)dx_2 = Q(t_1,t_3,x_1,x_3), \quad t_1 < t_2 < t_3. \tag{88}$$

Let us assume that (87) has been demonstrated, and prove (88). Observe that

$$\int_{\mathbb{R}^3} T^{2+\alpha} p^T_\beta(t_1,t_2,x_1,x_2)p^T_\beta(t_2,t_3,x_2,x_3)dx_2 = T^{1+\alpha}p^T_\beta(t_1,t_3,x_1,x_3), \quad t_1 < t_2 < t_3,$$

where $\alpha = 1/2$ if $x_1 = 0$ and $\alpha = 0$ otherwise. For $x_3 \neq 0$ we take the limit, as $T \to \infty$, on both sides of this relation. The integrand on the left hand side converges to

$$\overline{p}_\beta(t_1,t_2,x_1,x_2)\overline{p}_\beta(t_2,t_3,x_2,x_3),$$

however, the convergence is not necessarily uniform in x_2, and we can only conclude by the Fatou Lemma that

$$\int_{\mathbb{R}^3\setminus\{0\}} \overline{p}_\beta(t_1,t_2,x_1,x_2)\overline{p}_\beta(t_2,t_3,x_2,x_3)dx_2 \le \overline{p}_\beta(t_1,t_3,x_1,x_3), \quad t_1 < t_2 < t_3, \quad x_3 \neq 0.$$

From (80) and (81) it now follows that

$$\int_{\mathbb{R}^3\setminus\{0\}} Q(t_1,t_2,x_1,x_2)Q(t_2,t_3,x_2,x_3)dx_2 \le Q(t_1,t_3,x_1,x_3), \quad t_1 < t_2 < t_3, \quad x_3 \neq 0.$$

Note that both sides of this inequality are continuous in $x_3 \in \mathbb{R}^3 \setminus \{0\}$. Due to (87), the integrals in x_3 over $\mathbb{R}^3 \setminus \{0\}$ are equal to one for the expressions in both sides of this inequality. Therefore,

$$\int_{\mathbb{R}^3\setminus\{0\}} Q(t_1,t_2,x_1,x_2)Q(t_2,t_3,x_2,x_3)dx_2 = Q(t_1,t_3,x_1,x_3), \quad t_1 < t_2 < t_3, \quad x_3 \neq 0,$$

and thus (87) implies (88).

Now let us verify (87). Put $s = t_1, \tau = t_2, y = x_1$ and $x = x_2$. Again, we shall consider the case $y \neq 0$, the other case being similar. Moreover, we can assume that $\tau < 1$, since the case $\tau = 1$ can be treated by taking the limit $\tau \uparrow 1$. On a formal level, (87) follows from (83) by integrating the both sides of (83) over $\Omega = [s,\tau] \times \mathbb{R}^3 \subset \mathbb{R}^4_{t,x}$:

$$\int_{\mathbb{R}^3} Q(s,\tau,y,x)dx - \lim_{t \downarrow s} \int_{\mathbb{R}^3} Q(s,t,y,x)dx = \langle L^*Q, 1\rangle_{L^2(\Omega)} = \langle Q, L1\rangle_{L^2(\Omega)}. \tag{89}$$

One needs only to note that

$$\lim_{t\downarrow s}\int_{\mathbb{R}^3} Q(s,t,y,x)dx = 1, \tag{90}$$

and that the operator L applied to the identity function gives zero. The latter implies that the left hand side in (89) is zero, and (90) implies that the second term on the left hand side of (89) is one.

In order to make relations (89) rigorous we note that $Q(s,t,y,x)$ is infinitely smooth in (t,x) when $x \neq 0$ and decays exponentially as $|x| \to \infty$. However, it has a singularity at $x = 0$. Thus the integrals over $\mathbb{R}^3$ and Ω in (89) must be understood as limits of the corresponding integrals over the region $|x| > \varepsilon$ as $\varepsilon \to 0$. Let us examine the singularities of Q and of the coefficients of L^* at the origin.

Relation (78) implies that

$$\overline{p}_\beta(s,t,y,x) = \frac{a}{r} + O(r), \quad r = |x| \to 0, \quad a = a(s,t,y). \tag{91}$$

It is important that (91) does not contain a term of order $O(1)$. From (91), (82) and (80) it follows that

$$\frac{\partial g(t,x)}{r} = -\frac{1}{r} + O(r), \quad Q(s,t,y,x) = \frac{c}{r^2} + O(1), \quad \frac{\partial Q(s,t,y,x)}{\partial r} = -\frac{2c}{r^3} + O(1), \tag{92}$$

where $r \to 0$, $c = c(s,t,y)$. Since Q has a weak singularity at $x = 0$, the integral of the left hand side of (83) over $\Omega_\varepsilon = \Omega \bigcap \{x : |x| > \varepsilon\}$ converges to the left hand side of (89). Hence, in order to prove (87), it remains to show that

$$\int_{\Omega_\varepsilon} L^* Q dt dx \to 0, \quad \varepsilon \to 0.$$

The integral above is equal to

$$\int_s^\tau \int_{|x|=\varepsilon} [-\frac{1}{2}\frac{\partial Q}{\partial r} + \frac{\partial g}{\partial r} Q] d\sigma dt, \tag{93}$$

where $d\sigma$ is the element of the surface area of the sphere $|x| = \varepsilon$. The convergence of (93) to zero follows immediately from (92) □

Lemma 10.5. *The family of processes $y^T(t)$, $T \geq 1$, is tight.*

We shall prove this lemma below. First, however, we formulate the main result of this section.

Theorem 10.6. *The distributions of the processes $y^T(t)$ converge as $T \to \infty$, weakly in the space $C([0,1], \mathbb{R}^3)$, to the distribution of the 3-dimensional Markov process with continuous trajectories. The transition densities for the limiting Markov process are given by (80) and (81).*

Proof. The convergence of the finite dimensional distributions of $y^T(t)$ to those of the Markov process follows from (79) and Lemma 10.4. Since the family $y^T(t)$ is tight, there is a modification of the Markov process which has continuous trajectories. $\square$

Proof of Lemma 10.5. To prove tightness it is enough to demonstrate that for each $\eta, \varepsilon > 0$ there are $0 < \delta < 1$ and $T_0 \geq 1$ such that for all $u \in [0, 1]$ we have

$$\mathrm{P}_{\beta,T}(\sup_{u \leq s \leq \min(t+\delta,1)} |y^T(s) - y^T(u)| > \varepsilon) \leq \delta\eta, \quad T \geq T_0. \tag{94}$$

Let $\eta, \varepsilon > 0$ be fixed. Let $\mathcal{E}_\delta$ be the event that a continuous function $x : [0, T] \to \mathbb{R}^3$ satisfies

$$\sup_{t \leq \delta T,} |x(t) - x(0)|/\sqrt{T} > \varepsilon/8.$$

Using arguments similar to those leading to (69), we can show that (94) follows from

$$\sup_{x \in \mathbb{R}^d, |x| = \varepsilon\sqrt{T}/4} \mathrm{E}^x_{0,T}(\chi_{\mathcal{E}_\delta} \exp(\int_0^T \beta v(x(t))dt)) \leq \delta\eta, \quad T \geq T_0. \tag{95}$$

Let

$$\tau = \min(\delta T, \inf\{t \geq 0 : |x(t) - x(0)| = \varepsilon\sqrt{T}/8\}),$$

The expectation in (95) can be estimated as follows

$$\mathrm{E}^x_{0,T}(\chi_{\mathcal{E}_\delta} \exp(\int_0^T \beta v(x(t))dt)) \leq \mathrm{E}^x_{0,T}(\chi_{\mathcal{E}_\delta} \mathrm{E}^{x(\tau)}_{0,T-\tau} \exp(\int_0^{T-\tau} \beta v(x(t))dt))$$

We claim that

$$\mathrm{E}^{x(\tau)}_{0,T-\tau} \exp(\int_0^{T-\tau} \beta v(x(t))dt) \leq \sup_{x \in \mathbb{R}^d, |x| \geq \varepsilon\sqrt{T}/8} \mathrm{E}^x_{0,T} \exp(\int_0^T \beta v(x(t))dt) \leq c(\varepsilon) \tag{96}$$

for some constant $c(\varepsilon)$ for all sufficiently large T. It then remains to choose δ such that $\mathrm{E}^x_{0,T}(\chi_{\mathcal{E}_\delta}) \leq \delta\eta/c(\varepsilon)$, and the estimate (95) will follow. The second inequality in (96) easily follows from part (2) of Theorem 7.2 and the fact that the probability of reaching the support of v before time T by a Brownian path starting at a distance $\varepsilon\sqrt{T}/8$ away from the origin is of order $O(T^{-1/2})$ if $d = 3$. $\square$

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