THE HOHENBERG-KOHN THEOREM FOR MARKOV SEMIGROUPS

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ABSTRACT. At the basis of much of computational chemistry is density functional theory, as initiated by the Hohenberg-Kohn theorem. The theorem states that, when nuclei are fixed, electronic systems are determined by 1-electron densities. We recast and derive this result within the context of Markov semigroups.

1. Introduction

In quantum mechanics, the probability distribution of the ground state of an N-electron system[1] is a permutation-symmetric probability measure μ on $\mathbf{R}^{3N}$, and its 1-electron marginal is the probability measure ρ on $\mathbf{R}^3$ given by

$$\int_{\mathbf{R}^3} f\, d\rho = \int_{\mathbf{R}^{3N}} f(x_1)\, d\mu(x_1, \dots, x_N).$$

The potential acting on the electrons is a sum $V_0 + V$ of potentials, where V_0 is the repulsive Coulomb potential between electrons, and V is the attractive nuclear or external potential[2]

$$V(x_1, \dots, x_N) = \frac{v(x_1) + \cdots + v(x_N)}{N}, \tag{1}$$

for some function v on $\mathbf{R}^3$. The system is specified by the external potential v, as V_0 is the same for all N-electron systems.

Then the electronic ground state energy is given by

$$E(V_0 + V) = \inf_{\psi} \int_{\mathbf{R}^{3N}} \left(|\operatorname{grad} \psi|^2 + V_0\psi^2 + V\psi^2\right) dx_1 \dots dx_N, \tag{2}$$

where the infimum is over all real ψ satisfying $\int \psi^2 dx_1 \dots dx_N = 1$, and the distribution corresponding to the ground state ψ is $d\mu = \psi^2\, dx_1 \dots dx_N$.

The Hohenberg-Kohn theorem [8] states that the external potential v — and thus the electronic system — is determined by the marginal ρ: If μ_1, μ_2 are distributions of ground states ψ_1, ψ_2 corresponding to external potentials v_1, v_2, and their marginals agree, $\rho_1 = \rho_2$, then $v_1 - v_2$ is a constant. The thrust of the theorem is to reduce the study of electronic systems from $3N$ variables down to 3 variables.

Date: January 15, 2018.

1991 *Mathematics Subject Classification.* 46N50, 47N30, 60J25, 60J35 .

Key words and phrases. Hohenberg-Kohn theorem, Markov semigroup, principal eigenvalue , density functional theory.

[1]An atom, molecule, or solid where nuclei are fixed.

[2]The $1/N$ normalization is not standard.

In this paper we generalize this result from the above electronic setting to the general (non-self-adjoint) Markov semigroup setting. To help simplify matters, instead of $\mathbf{R}^3$, we take a compact metric space X as our position space.

Let X be a compact metric space and let P_t, $t \geq 0$, be a Markov semigroup on $C(X)$ with generator L defined on its dense domain $\mathcal{D} \subset C(X)$. Examples of semigroups which satisfy all our assumptions below are

- X is a compact manifold and L is a nondegenerate elliptic second order differential operator with smooth coefficients, given by
$$Lf(x) = \sum a_{ij}(x) \frac{\partial^2 f}{\partial x_i \partial x_j} + \sum b_i(x) \frac{\partial f}{\partial x_i}$$
in local coordinates.
- $X = \{1, \dots, d\}$ and L is a $d \times d$ matrix with nonnegative off-diagonal entries whose row-sums vanish and whose adjacency graph is connected.

Given V in $C(X)$, let P_t^V, $t \geq 0$, denote the Schrodinger semigroup on $C(X)$ generated by $L + V$. Then the principal eigenvalue

$$\lambda_V \equiv \lim_{t \uparrow \infty} \frac{1}{t} \log \|P_t^V\|$$

exists and is given by the Donsker-Varadhan formula [4]

$$\lambda_V = \sup_{\mu} \left(\int_X V \, d\mu - I(\mu) \right) \tag{3}$$

where the supremum is over all probability measures μ on X and

$$I(\mu) = - \inf_{u \in \mathcal{D}^+} \int_X \frac{Lu}{u} \, d\mu.$$

Here the infimum is over all positive u in $\mathcal{D}$. In the electronic case, (3) reduces to (2) and $\lambda_V = -E(-V)$.

Given $f \in C(X)$ and a probability measure μ on X, let $\mu(f)$ denote the integral of f against μ. Let $M(X)$ denote the space of probability measures on X, and let V be in $C(X)$.

An *equilibrium measure for* V is a $\mu \in M(X)$ achieving[3] the supremum in (3), $\lambda_V = \mu(V) - I(\mu)$.

A *ground measure for* V is a $\pi \in M(X)$ satisfying

$$\int_X e^{-\lambda_V t} P_t^V f \, d\pi = \int_X f \, d\pi, \qquad t \geq 0, f \in C(X). \tag{4}$$

By positivity,

$$P_t^V f(x) = \int_X p^V(t, x, dy) f(y) \tag{5}$$

for some family $(t, x) \mapsto p^V(t, x, \cdot)$ of bounded positive measures on X. Thus $0 \leq P_t^V f(x) \leq +\infty$ is well-defined for f nonnegative Borel on X. Let μ be in $M(X)$.

[3] The supremum is always achieved as I is lower semicontinuous (Lemma 1).

A *ground state for V relative to μ* is a nonnegative Borel function ψ on X satisfying $\psi > 0$ a.e. μ and

$$e^{-\lambda_V t} P_t^V \psi = \psi, \qquad a.e.\mu, t \geq 0.$$

Thus a ground state ψ plays the role of a right eigenvector for $L+V$, and a ground measure π plays the role of a left eigenvector for $L+V$, both with eigenvalue λ_V.

When $N = 1$, the Hohenberg-Kohn theorem states that if μ is the distribution of a ground state ψ corresponding to V_1 and to V_2, then $V_1 - V_2$ is a constant. In the electronic case, $d\mu = \psi^2\, dx$ and this is an immediate consequence of the Schrodinger equations $L\psi + V_i\psi = \lambda_{V_i}\psi$, $i = 1, 2$. In the general case, however, establishing this turns out to be the heart of the matter, as the correspondence between equilibrium measures μ and ground states ψ is not as direct. The following sheds light on the relation between μ, ψ, and π.

Theorem 1. *Let $\mu, \pi \in M(X)$ and let $V \in C(X)$. Suppose $\mu << \pi$ and suppose $\psi = d\mu/d\pi$ satisfies $\log\psi \in L^1(\mu)$. Then the following hold.*

1. *If ψ is a ground state for V relative to μ and π is a ground measure for V, then μ is an equilibrium measure for V.*
2. *If π is a ground measure for V and μ is an equilibrium measure for V, then ψ is a ground state for V relative to μ.*
3. *If μ is an equilibrium measure for V and ψ is a ground state for V relative to μ, then π is a ground measure for V.*

In the electronic case, L is self-adjoint relative to $dx_1 \dots dx_N$, so heuristically a right eigenvector is a left eigenvector, so by Theorem 1, a ground state ψ leads to a ground measure $d\pi = \psi\, dx_1 \dots dx_N$ and to an equilibrium measure $d\mu = \psi\, d\pi = \psi^2\, dx_1 \dots dx_N$.

Given ψ nonnegative, let

$$P_t^{V,\psi} f = \frac{e^{-\lambda_V t} P_t^V (f\psi)}{\psi}. \tag{6}$$

Then $P_t^{V,\psi} f(x)$ is defined at a point x if $P_t^V(|f|\psi)(x) < \infty$ and $\psi(x) > 0$.

Theorem 2. *Fix $V \in C(X)$ and suppose*

$$C \equiv \sup_{t \geq 0} \left(e^{-\lambda_V t} \| P_t^V \| \right) < \infty, \tag{7}$$

and let μ be an equilibrium measure for V. Then there is a ground state ψ for V relative to μ and a ground measure π for V such that

- $\log\psi \in L^1(\mu)$,
- $\mu << \pi$ *and* $d\mu/d\pi = \psi$, *and*
- $P_t^{V,\psi}$, $t \geq 0$, *is a Markov semigroup on* $L^1(\mu)$, *and* μ *is* $P_t^{V,\psi}$, $t \geq 0$, *invariant*

$$\int_X P_t^{V,\psi} f \, d\mu = \int_X f \, d\mu, \qquad f \in L^1(\mu), t \geq 0.$$

Note this existence result is not just a Perron-Frobenius result, as ψ and π are determined subordinate to the given equilibrium measure μ.

Now we list our assumptions on the Markov semigroup P_t, $t \geq 0$.

We assume a strong uniformity condition

(A) There is a $T > 0$ and an $\epsilon = \epsilon(T) > 0$ such that $P_T|f|(x) \geq \epsilon P_T|f|(y)$ for all $x, y \in X$ and $f \in C(X)$.

As we shall see, (A) implies (7). We also assume

(B) There is a $T > 0$ such that $f \geq 0$ in $C(X)$ implies $P_T f > 0$ everywhere in X.

A core for P_t, $t \geq 0$, is a subspace $\mathcal{D}^\infty \subset \mathcal{D}$ whose closure in the graph norm $\|f\| + \|Lf\|$ equals $\mathcal{D}$. We assume

(C) There is a core $\mathcal{D}^\infty$ that is closed under multiplication and division: If $f, g \in \mathcal{D}^\infty$ then $fg \in \mathcal{D}^\infty$, and if moreover $g > 0$, then $f/g \in \mathcal{D}^\infty$.

Let $[A, B] = AB - BA$ denote the bracket of operators A, B. Given $g \in C(X)$, let g also denote the corresponding multiplication operator on $C(X)$. Then (Lemma 2) the double bracket $[[L, g], g]$ is a positive operator

$$f, fg, fg^2 \in \mathcal{D} \text{ and } f \geq 0 \text{ implies } [[L, g], g]f \geq 0.$$

The square-field operator is

$$\Gamma(g) \equiv [[L, g], g]1 = L(g^2) - 2gLg \qquad g \in \mathcal{D}^\infty.$$

By the positivity of the double bracket, $\Gamma(g) \geq 0$. We assume the nondegeneracy condition

(D) If $g \in \mathcal{D}^\infty$ and $\Gamma(g) \equiv 0$, then g is a constant.

Let $B(X)$ denote the bounded Borel functions on X. We say a potential V is *smooth* if P_t^V maps $B(X)$ into $\mathcal{D}^\infty$ for $t > 0$. This depends on both L and V.

For the examples above, (A) and (B) are valid, and (C) and (D) are valid if we take $\mathcal{D}^\infty = C^\infty(X)$, and V is smooth in the above sense if V is in $C^\infty(X)$ (for the second example, $C^\infty(X) = C(X) = B(X)$ equals all functions on X).

Theorem 3. *Assume (A), (B), (C), (D) and let V_1, V_2 be smooth potentials. If μ is an equilibrium measure for V_1 and for V_2, then $V_1 - V_2$ is a constant.*

This result should hold more broadly, in which case one should obtain $V_1 - V_2$ is a constant on the support of μ. This restriction is natural because one cannot expect to determine the potential in regions outside the electron cloud. The more general result is easily verified when $L \equiv 0$ for any $V_1, V_2 \in C(X)$, so nondegeneracy should not play a role in a broader formulation. A discrete time version of Theorem 3 in the case $X = \{1, \ldots, d\}$ is in [6].

Note that μ is an equilibrium measure for V iff V is a subdifferential of I at μ, i.e. iff

$$I(\nu) \geq I(\mu) + \nu(V) - \mu(V), \qquad \nu \in M(X).$$

Subdifferentials at a given μ need not exist. When subdifferentials do exist, Theorem 3 provides conditions under which uniqueness holds at the given μ, up to a constant.

Next we look at Markov semigroups on $C(X^N)$.

Let $N \geq 1$ and X^N be the N-fold product of X. Let P_t, $t \geq 0$, be a Markov semigroup on $C(X^N)$, representing the motion of N particles, and let L be its generator. Let P_t^i, $t \geq 0$, $1 \leq i \leq N$, be Markov semigroups on $C(X)$. When P_t, $t \geq 0$, is the product of P_t^i, $t \geq 0$, $1 \leq i \leq N$, with the i-th semigroup acting on the i-th component in $C(X^N)$,

$$(P_t^i f)(x_1, \ldots, x_N) = P_t^i(f(x_1, \ldots, x_{i-1}, \cdot, x_{i+1}, \ldots, x_N))(x_i), \qquad 1 \leq i \leq N,$$

we have non-interacting particles. When the semigroups P^i_t, $t \geq 0$, $1 \leq i \leq N$, are the same, we have identical non-interacting particles. If $V(x_1, \dots, x_N)$ is a potential in $C(X^N)$, particle interactivity is then modelled by the Schrodinger semigroup P^V_t, $t \geq 0$, on $C(X^N)$.

If (A) holds for single particle Markov semigroups P^i_t, $t \geq 0$, $1 \leq i \leq N$, on $C(X)$, then (A) holds (with ϵ replaced by ϵ^N) for the product Markov semigroup P_t, $t \geq 0$, on $C(X^N)$, corresponding to non-interacting particles. Similarly for (B). If (C) and (D) hold for P^i_t, $t \geq 0$, $1 \leq i \leq N$, on $C(X)$, then (C) and (D) hold for the product Markov semigroup P_t, $t \geq 0$, on $C(X^N)$, assuming $\mathcal{D}^\infty(X^N)$ can be chosen to be a tensor product of $\mathcal{D}^\infty(X)$ in a suitable sense. This is the case for the examples above when $\mathcal{D}^\infty(X^N) = C^\infty(X^N)$ and $\mathcal{D}^\infty(X) = C^\infty(X)$.

A potential V in $C(X^N)$ is separable if it is of the form (1) for some v in $C(X)$. We are interested in Schrodinger semigroups on $C(X^N)$ with generators of the form $L + V_0 + V$ with V_0, V in $C(X^N)$ and V separable.

Given $f \in C(X^N)$ and a permutation σ of $(1, \dots, N)$, let

$$f^\sigma(x_1, \dots, x_N) = f(x_{\sigma 1}, \dots, x_{\sigma N}).$$

Given a measure μ on X^N, let μ^σ be the measure with action $\mu^\sigma(f) = \mu(f^\sigma)$. A potential V on X^N is symmetric if $V^\sigma = V$ and a measure μ on X^N is symmetric if $\mu^\sigma = \mu$, both for all permutations σ.

Let P_t, $t \geq 0$, be a Markov semigroup on $C(X^N)$ with generator L. We say the semigroup P_t, $t \geq 0$, is symmetric if $(P_t f)^\sigma = P_t f^\sigma$, $t \geq 0$, for all permutations σ. When the semigroup is symmetric and V is symmetric, we can restrict the supremum in (3) (with X replaced by X^N) to symmetric measures. As before, if μ is a symmetric probability measure on X^N, its 1-particle marginal is the probability measure ρ on X satisfying

$$\int_X f \, d\rho = \int_{X^N} f(x_1) \, d\mu(x_1, \dots, x_N), \qquad f \in C(X).$$

Note for μ symmetric with marginal ρ and V separable, we have $\mu(V) = \rho(v)$.

Here is the Hohenberg-Kohn theorem in this setting.

Theorem 4. *Let P_t, $t \geq 0$ be a Markov semigroup on $C(X^N)$ satisfying (A), (B), (C), (D) and let V_0 be a potential and V_1, V_2 separable potentials, all in $C(X^N)$, with V_1, V_2, arising from v_1, v_2 in $C(X)$. Assume $V_0 + V_1$ and $V_0 + V_2$ are smooth. Let μ_1, μ_2 be symmetric equilibrium measures for $V_0 + V_1$, $V_0 + V_2$ and let ρ_1, ρ_2 denote their 1-particle marginals. Then $\rho_1 = \rho_2$ implies $v_1 - v_2$ is constant.*

For example this applies if V_0 is symmetric and P_t, $t \geq 0$, corresponds to non-interacting identical particles.

The proof of this is so short we present it right away.

Proof of Theorem 4. If μ_1 is an equilibrium measure for $V_0 + V_2$, then by Theorem 3, $V_1 - V_2 = (V_0 + V_1) - (V_0 + V_2)$ is constant on X^N, but $V_1 - V_2$ is separable, hence $v_1 - v_2$ is constant on X. Otherwise, we have

$$\mu_1(V_0 + V_2) - I(\mu_1) < \lambda_{V_0+V_2} = \lambda_{V_0+V_2} - \lambda_{V_0+V_1} + \mu_1(V_0 + V_1) - I(\mu_1)$$

which implies

$$\rho_1(v_2 - v_1) = \mu_1(V_2 - V_1) < \lambda_{V_0+V_2} - \lambda_{V_0+V_1}$$

hence

$$\rho_1(v_2 - v_1) < \lambda_{V_0+V_2} - \lambda_{V_0+V_1}.$$

Reversing the roles of V_1, V_2,

$$\rho_2(v_1 - v_2) < \lambda_{V_0+V_1} - \lambda_{V_0+V_2}.$$

Since $\rho_1 = \rho_2$, this is a contradiction. $\square$

Let $I(\mu)$ correspond to a symmetric Markov semigroup on $C(X^N)$, and let V_0, V be in $C(X^N)$ with V_0 symmetric and V separable. Let

$$I_{HK}(\rho) \equiv \inf_{\mu \to \rho} \left(I(\mu) - \int_{X^N} V_0 \, d\mu \right),$$

where the infimum is over all symmetric μ in $M(X^N)$ with marginal ρ in $M(X)$. Then (3) written over $M(X^N)$ reduces to

$$\lambda_{V_0+V} = \sup_{\mu} \left(\int_{X^N} (V_0 + V) \, d\mu - I(\mu) \right) = \sup_{\rho} \left(\int_X v \, d\rho - I_{HK}(\rho) \right).$$

Thus the computation of the principal eigenvalue is reduced to computing the $M(X^N)$ universal object I_{HK} followed by an optimization over $M(X)$. In the electronic case, density functional theory is the study of approximations of I_{HK} [9], [10].

The following sections contain the proofs of Theorems 1, 2, 3 and supporting Lemmas. Many of the Lemmas are basic and go back to the early papers [4], [5] and the book [3].

2. The Schrodinger semigroup

Let X be a compact metric space, let $C(X)$ denote the space of real continuous functions with the sup norm $\|\cdot\|$, and let $M(X)$ denote the space of Borel probability measures with the topology of weak convergence. Then $M(X)$ is a compact metric space. Throughout $\mu(f)$ denotes the integral of f against μ.

A strongly continuous positive semigroup on $C(X)$ is a semigroup P_t, $t \geq 0$, of bounded operators on $C(X)$ preserving positivity $P_t f \geq 0$, for $f \geq 0$, $t \geq 0$, and satisfying $\|P_t f - f\| \to 0$ as $t \to 0+$. Then the $C(X)$-valued map $t \mapsto P_t f$ is continuous on $[0, \infty)$ for $f \in C(X)$. A Markov semigroup on $C(X)$ is a strongly continuous positive semigroup on $C(X)$ satisfying $P_t 1 = 1$, $t \geq 0$.

Let $C^+(X)$ the strictly positive functions in $C(X)$. Then $P_t f \in C^+(X)$ when $f \in C^+(X)$.

The subspace $\mathcal{D} \subset C(X)$ of functions $f \in C(X)$ for which the limit

$$\lim_{t \to 0+} \frac{1}{t} (P_t f - f) \tag{8}$$

exists in $C(X)$ is dense. If Lf is defined to be this limit, then $P_t(\mathcal{D}) \subset \mathcal{D}$, $t \geq 0$, the $C(X)$-valued map $t \mapsto P_t f$ is differentiable on $(0, \infty)$ for $f \in \mathcal{D}$, and $(d/dt)P_t f = L(P_t f) = P_t(Lf)$, for $f \in \mathcal{D}$ and $t > 0$.

Given V and f in $C(X)$, the Schrodinger semigroup may be constructed as the unique $C(X)$-valued continuous map $t \mapsto u(t) = P_t^V f$, $t \geq 0$, satisfying

$$u(t) = P_t f + \int_0^t P_{t-s} V u(s) \, ds, \qquad t \geq 0. \tag{9}$$

For $f \geq 0$, this implies

$$e^{t \min V} P_t f \leq P_t^V f \leq e^{t \max V} P_t f, \qquad t \geq 0, \tag{10}$$

which implies

$$\min V \le \lambda_V \le \max V.$$

Then P_t^V, $t \ge 0$, is a strongly continuous positive semigroup on $C(X)$, and the limit

$$\lim_{t\to 0+} \frac{1}{t}\left(P_t^V f - f\right) \tag{11}$$

exists in $C(X)$ if and only if $f \in \mathcal{D}$, in which case it equals $(L+V)f$. Moreover $P_t^V(\mathcal{D}) \subset \mathcal{D}$, $t \ge 0$, the $C(X)$-valued map $t \mapsto P_t^V f$ is differentiable on $(0,\infty)$ for $f \in \mathcal{D}$, and $(d/dt)P_t^V f = (L+V)(P_t^V f) = P_t^V(Lf + Vf)$, for $f \in \mathcal{D}$ and $t > 0$.

Let $\mathcal{D}^+$ be the strictly positive functions in $\mathcal{D}$. For μ in $M(X)$, let

$$I^V(\mu) \equiv I(\mu) - \int_X V\,d\mu + \lambda_V = -\inf_{u\in\mathcal{D}^+} \int_X \frac{(L+V-\lambda_V)u}{u}\,d\mu$$

Then $I^0(\mu) = I(\mu)$ and $I^V(\mu) = 0$ iff μ is an equilibrium measure for V.

Lemma 1. *For V in $C(X)$, I^V is lower semicontinuous, convex, and $0 \le I^V \le +\infty$. In particular, I is lower semicontinuous, convex, and $0 \le I \le +\infty$.*

Proof. Lower semicontinuity and convexity follow from the fact that I^V is the supremum of continuous affine functions. The Donsker-Varadhan formula implies I^V is nonnegative. □

Lemma 2. *If $f, gf, g^2 f$ are in $\mathcal{D}$ and $f \ge 0$, then $[[L,g],g]f \ge 0$.*

Proof. Expanding

$$\int_X p(t,x,dy) f(y) \left(g(y) - g(x)\right)^2$$

yields

$$P_t(fg^2) - 2gP_t(fg) + g^2 P_t f \ge 0$$

hence

$$(P_t(fg^2) - fg^2) - 2g(P_t(fg) - fg) + g^2(P_t f - f) \ge 0.$$

Dividing by t and sending $t \to 0+$ yields

$$[[L,g],g]f = L(fg^2) - 2gL(fg) + g^2 Lf \ge 0. \quad \square$$

Note when P_t, $t \ge 0$, is a diffusion, e.g. our first example above, one has $[[L,g],g]f = f \cdot \Gamma(g)$ is multiplication by the symbol of L, a standard characterization of second-order differential operators.

For $t > 0$ and u in $C^+(X)$, (10) implies

$$\log\left(\frac{e^{-\lambda_V t} P_t^V u}{u}\right)$$

is in $C(X)$.

Lemma 3. *For V in $C(X)$, $\mu \in M(X)$, and u in $C^+(X)$,*

$$\int_X \log\left(\frac{e^{-\lambda_V t} P_t^V u}{u}\right) d\mu \ge -tI^V(\mu), \qquad t \ge 0. \tag{12}$$

The proof follows that of Lemma 3.1 in [5].

Proof. By definition of $I^V(\mu)$,

$$\int_X \frac{(L+V-\lambda_V)u}{u}\,d\mu \geq -I^V(\mu), \qquad u \in \mathcal{D}^+. \tag{13}$$

When $I^V(\mu) = +\infty$, the result is valid, hence we may assume $I^V(\mu) < \infty$. For $t = 0$, (12) is an equality. Moreover for $t > 0$ and $u \in \mathcal{D}^+$, by (10) we have $e^{-\lambda_V t} P_t^V u \in \mathcal{D}^+$ and

$$\frac{d}{dt}\int_X \log\left(\frac{e^{-\lambda_V t}P_t^V u}{u}\right) d\mu = \int_X \frac{(L+V-\lambda_V)(e^{-\lambda_V t}P_t^V u)}{e^{-\lambda_V t}P_t^V u}\,d\mu \geq -I^V(\mu).$$

This establishes (12) for $u \in \mathcal{D}^+$. Since $\mathcal{D}^+$ is dense in $C^+(X)$, (12) is valid for u in $C^+(X)$. □

3. Equilibrium Measures

Let $L^1(\mu)$ denote the μ-integrable Borel functions on X with

$$\|f\|_{L^1(\mu)} = \int_X |f|\,d\mu = \mu(|f|).$$

The following strengthening of Lemma 3 is necessary in the next section. Let $B(X)$ denote the bounded Borel functions on X. Recall (5) $0 \leq P_t^V u(x) \leq +\infty$ is well-defined for $u \geq 0$ Borel, for all $x \in X$.

Lemma 4. *Fix $V \in C(X)$ and $\mu \in M(X)$. Let $u > 0$ Borel satisfy $\log u \in L^1(\mu)$. Then for $t \geq 0$,*

$$tI^V(\mu) + \int_X \log^+\left(\frac{e^{-\lambda_V t}P_t^V u}{u}\right) d\mu \geq \int_X \log^-\left(\frac{e^{-\lambda_V t}P_t^V u}{u}\right) d\mu. \tag{14}$$

Here the integrals may be infinite.

Proof. We may assume $I^V(\mu) < \infty$, otherwise (14) is true.

Let $u > 0$ be Borel with $\log u \in L^1(\mu)$. We establish (14) in three stages, first for $\log u \in B(X)$, then for $\log u$ bounded below, then in general. Let $Q_t = e^{-\lambda_V t}P_t^V$, $t \geq 0$.

Suppose $|\log u| \leq M$ and suppose $u_n > 0$, $n \geq 1$, satisfy $|\log u_n| \leq M$, $n \geq 1$. If $u_n \to u$ pointwise on X, it follows that $Q_t u_n \to Q_t u$ pointwise on X. Assume (12) is valid for u_n, $n \geq 1$. Since by (10)

$$t(\min V - \lambda_V) - 2M \leq \log\left(\frac{Q_t u_n}{u_n}\right) \leq t(\max V - \lambda_V) + 2M, \qquad n \geq 1,$$

it follows that (12) is valid for u. Thus the set of Borel f in $B(X)$ with $u = e^f$ satisfying (12) is closed under bounded pointwise convergence. Since (12) is valid when $f = \log u \in C(X)$, it follows that (12) hence (14) is valid for all Borel u satisfying $\log u \in B(X)$. Here both sides of (14) are finite.

Next, assume $\log u$ in $L^1(\mu)$ and $u \geq \delta > 0$ and let $u_n = u \wedge n$, $n \geq 1$. Then

$$\log\left(\frac{Q_t u}{u}\right) \geq \log\left(\frac{Q_t u_n}{u}\right) = \log\left(\frac{Q_t u_n}{u_n}\right) + \log\left(\frac{u_n}{u}\right)$$

so

$$\log^+\left(\frac{Q_t u}{u}\right) \geq \log^-\left(\frac{Q_t u}{u}\right) + \log\left(\frac{Q_t u_n}{u_n}\right) + \log\left(\frac{u_n}{u}\right).$$

Hence

$$\int_X \log^+\left(\frac{Q_t u}{u}\right) d\mu \geq \int_X \log^-\left(\frac{Q_t u}{u}\right) d\mu - tI^V(\mu) + \int_{u>n} (\log n - \log u)\, d\mu.$$

Discarding the $\log n$ term and passing to the limit $n \to \infty$ yields (14). Note $u \geq \delta$ and (10) imply

$$\log^-\left(\frac{Q_t u}{u}\right) = \log^+\left(\frac{u}{Q_t u}\right) \leq |\log u| + (\lambda_V - \min V)t + \log\frac{1}{\delta}$$

so the right side of (14) is finite in this case and in fact (12) is valid.

Now assume $\log u$ in $L^1(\mu)$ and let $u_\delta = u \vee \delta$. Then

$$\log^+\left(\frac{Q_t u_\delta}{u}\right) = \log^-\left(\frac{Q_t u_\delta}{u}\right) + \log\left(\frac{Q_t u_\delta}{u_\delta}\right) + \log\left(\frac{u_\delta}{u}\right)$$

so

$$\int_X \log^+\left(\frac{Q_t u_\delta}{u}\right) d\mu \geq \int_X \log^-\left(\frac{Q_t u_\delta}{u}\right) d\mu - tI^V(\mu) + \int_{u<\delta} \log\left(\frac{\delta}{u}\right) d\mu$$

hence

$$tI^V(\mu) + \int_X \log^+\left(\frac{Q_t u_\delta}{u}\right) d\mu \geq \int_X \log^-\left(\frac{Q_t u_\delta}{u}\right) d\mu, \tag{15}$$

where we discarded the right-most integral as its integrand is nonnegative. To establish (14), we pass to the limit $\delta \downarrow 0$ in (15). We may assume

$$\int_X \log^+\left(\frac{Q_t u}{u}\right) d\mu < \infty,$$

otherwise (14) is true. This implies $\log^+(Q_t u/u)(x) < \infty$ for μ-a.a x which implies $Q_t u(x) < \infty$ for μ-a.a. x. Since $u_\delta \leq u + 1$ for $\delta < 1$, it follows by the dominated convergence theorem that $Q_t u_\delta \to Q_t u$ a.e. μ as $\delta \downarrow 0$.

Since

$$\log^-\left(\frac{Q_t u_\delta}{u}\right), \qquad \delta > 0,$$

increases as $\delta \downarrow 0$, the right side of (15) converges to the right side of (14). Using $2\log^+(a+b) \leq 2\log 2 + \log^+ a + \log^+ b$, (10), and $u_\delta \leq u + 1$ for $\delta < 1$, we have

$$2\log^+\left(\frac{Q_t u_\delta}{u}\right) \leq 2\log 2 + \log^+\left(\frac{Q_t u}{u}\right) + |\log u| + t(\max V - \lambda_V),$$

hence the dominated convergence theorem shows the left side of (15) converges to the left side of (14). □

Let $P_t^{V,\psi}$ be as in (6).

Corollary 1. *Fix $V \in C(X)$, $\mu \in M(X)$, let $\log\psi \in L^1(\mu)$, and let $u > 0$ Borel satisfy $\log u \in L^1(\mu)$. Then for $t \geq 0$,*

$$tI^V(\mu) + \int_X \log^+\left(\frac{P_t^{V,\psi} u}{u}\right) d\mu \geq \int_X \log^-\left(\frac{P_t^{V,\psi} u}{u}\right) d\mu. \tag{16}$$

Here the integrals may be infinite.

Proof. Since $\log\psi$ is in $L^1(\mu)$, $\log(u\psi)$ is in $L^1(\mu)$ iff $\log u$ is in $L^1(\mu)$. Now apply Lemma 4. □

Corollary 2. *Let* $V \in C(X)$ *and* $\log \psi \in L^1(\mu)$*. Then* $\mu \in M(X)$ *is an equilibrium measure for* V *iff*

$$\int_X \log^+ \left(\frac{P_t^{V,\psi} u}{u} \right) d\mu \geq \int_X \log^- \left(\frac{P_t^{V,\psi} u}{u} \right) d\mu$$

for $t \geq 0$ *and* $u > 0$ *satisfying* $\log u \in L^1(\mu)$*.*

Proof. If μ is an equilibrium measure, $I^V(\mu) = 0$ so the result follows from Corollary 1. Conversely, assume the inequality holds for all $u > 0$ satisfying $\log u \in L^1(\mu)$. For $u \in C^+(X)$, the function u/ψ satisfies $\log(u/\psi) \in L^1(\mu)$. Inserting u/ψ in the inequality yields

$$\int_X \log^+ \left(\frac{e^{-\lambda_V t} P_t^V u}{u} \right) d\mu \geq \int_X \log^- \left(\frac{e^{-\lambda_V t} P_t^V u}{u} \right) d\mu.$$

For u in $C^+(X)$, the integrals are finite hence

$$\int_X \log \left(\frac{e^{-\lambda_V t} P_t^V u}{u} \right) d\mu \geq 0.$$

For $u \in \mathcal{D}^+$, with $Q_t = e^{-\lambda_V t} P_t^V$, $t \geq 0$, we have $Q_t u \in \mathcal{D}^+$ so

$$Q_t u = u + t(L + V - \lambda_V)u + o(t), \qquad t \to 0,$$

$$\frac{Q_t u}{u} = 1 + t\frac{(L + V - \lambda_V)u}{u} + o(t), \qquad t \to 0,$$

$$\log \left(\frac{Q_t u}{u} \right) = t\frac{(L + V - \lambda_V)u}{u} + o(t), \qquad t \to 0,$$

all uniformly on X. Hence dividing by t and sending $t \to 0$ yields

$$\int_X \frac{(L + V - \lambda_V)u}{u} d\mu \geq 0.$$

This implies $I^V(\mu) \leq 0$, hence $I^V(\mu) = 0$. □

A strongly continuous positive semigroup on $L^1(\mu)$ is a semigroup P_t, $t \geq 0$, of bounded operators on $L^1(\mu)$ preserving positivity $P_t f \geq 0$ a.e. μ, for $f \geq 0$ a.e. μ, $t \geq 0$, and satisfying $\|P_t f - f\|_{L^1(\mu)} \to 0$ as $t \to 0+$. A Markov semigroup on $L^1(\mu)$ is a strongly continuous positive semigroup on $L^1(\mu)$ satisfying $P_t 1 = 1$ a.e. μ, $t \geq 0$.

Lemma 5. *Let* $V \in C(X)$ *and suppose* π *and* μ *are measures with* $\mu << \pi$*, and let* $\psi = d\mu/d\pi$*. If* π *is a ground measure for* V*, then* $P_t^{V,\psi}|f|(x) < \infty$ *for* μ*-a.a.* x *and* f *in* $L^1(\mu)$*,* $P_t^{V,\psi}$*,* $t \geq 0$*, is a strongly continuous positive semigroup on* $L^1(\mu)$*, and*

$$\mu(P_t^{V,\psi} f) = \mu(f), \qquad t \geq 0, \tag{17}$$

for f *in* $L^1(\mu)$*. If* ψ *is a ground state for* V *relative to* μ*,* $P_t^{V,\psi}$*,* $t \geq 0$*, is a Markov semigroup on* $L^1(\mu)$*.*

Proof. If π is a ground measure, for f in $C(X)$ we have

$$\begin{aligned}\|e^{-\lambda_V t} P_t^V f\|_{L^1(\pi)} &= \int_X |e^{-\lambda_V t} P_t^V f| \, d\pi \\ &\le \int_X e^{-\lambda_V t} P_t^V |f| \, d\pi = \int_X |f| \, d\pi = \|f\|_{L^1(\pi)}.\end{aligned}$$

Hence $e^{-\lambda_V t} P_t^V$, $t \ge 0$, satisfies

$$\|e^{-\lambda_V t} P_t^V f\|_{L^1(\pi)} \le \|f\|_{L^1(\pi)}, \qquad t \ge 0, \tag{18}$$

for f in $C(X)$. Since the collection of functions f satisfying (18) is closed under bounded pointwise convergence, (18) is valid for $f \in B(X)$. Inserting $f \wedge n$ with f nonnegative Borel and sending $n \to \infty$, (18) is then valid for nonnegative Borel f. It follows that $e^{-\lambda_V t} P_t^V |f|(x) < \infty$, π-a.a. x, for f in $L^1(\pi)$, hence $e^{-\lambda_V t} P_t^V$, $t \ge 0$, are well-defined contractions on $L^1(\pi)$. By (18) and the density of $C(X)$ in $L^1(\pi)$, this implies $\pi(e^{-\lambda_V t} P_t^V f) = \pi(f)$, $t \ge 0$, for f in $L^1(\pi)$ and implies $e^{-\lambda_V t} P_t^V$, $t \ge 0$, is a strongly continuous positive semigroup on $L^1(\pi)$.

Since $\psi \in L^1(\pi)$, (17) follows for $f \in C(X)$. But (18) for f nonnegative Borel implies

$$\|P_t^{V,\psi} f\|_{L^1(\mu)} \le \|f\|_{L^1(\mu)}, \qquad t \ge 0, \tag{19}$$

for f nonnegative Borel, hence $P_t^{V,\psi}|f|(x) < \infty$, μ-a.a. x, for f in $L^1(\mu)$, hence $P_t^{V,\psi}$, $t \ge 0$, are well-defined contractions on $L^1(\mu)$. Moreover

$$\|P_t^{V,\psi} f - f\|_{L^1(\mu)} = \|e^{-\lambda_V t} P_t^V (f\psi) - f\psi\|_{L^1(\pi)} \to 0, \qquad t \to 0+, f \in C(X).$$

By (19) and the density of $C(X)$ in $L^1(\mu)$, we conclude $P_t^{V,\psi}$, $t \ge 0$, is a strongly continuous positive semigroup on $L^1(\mu)$ and (17) holds for $f \in L^1(\mu)$.

If ψ is a ground state relative to μ, $P_t^{V,\psi} 1 = 1$ a.e. μ. Thus in this case $P_t^{V,\psi}$, $t \ge 0$, is a Markov semigroup on $L^1(\mu)$. □

4. Proofs of the Theorems

Proof of Theorem 1. For the first assertion, we have a ground measure π for V and a ground state ψ for V relative to μ satisfying $\log \psi \in L^1(\mu)$. Suppose $\log u \in L^1(\mu)$. Then $P_t^{V,\psi} |\log u|$ is in $L^1(\mu)$ and there is a set N with $\mu(N) = 0$ and $P_t^{V,\psi}(|\log u|)(x) < \infty$ and $P_t^{V,\psi} 1(x) = 1$ for $x \notin N$. Jensen's inequality applied to the integral $f \mapsto (P_t^{V,\psi} f)(x)$ (see (5)) implies

$$\log \left(\frac{P_t^{V,\psi} u}{u} \right)(x) \ge P_t^{V,\psi}(\log u)(x) - (\log u)(x), \qquad x \notin N,$$

hence for $x \notin N$,

$$\log^+ \left(\frac{P_t^{V,\psi} u}{u} \right)(x) \ge \log^- \left(\frac{P_t^{V,\psi} u}{u} \right)(x) + P_t^{V,\psi}(\log u)(x) - (\log u)(x).$$

Integrating over X against μ, the integrals of the right-most two terms cancel by (17) hence by Corollary 2, μ is an equilibrium measure for V, establishing the first assertion.

For the second assertion, assume π is a ground measure for V and μ is an equilibrium measure for V. Note $\int P_t^{V,\psi} 1 \, d\mu < \infty$ so $\int \log^+ \left(P_t^{V,\psi} 1 \right) d\mu < \infty$. By

Corollary 2, it follows that $\int \log^- \left(P_t^{V,\psi}1\right) \, d\mu < \infty$, hence $\log\left(P_t^{V,\psi}1\right)$ is in $L^1(\mu)$. By Jensen's inequality, (17), and Corollary 2,

$$0 = \log(\mu(1)) = \log\left(\int_X P_t^{V,\psi}1 \, d\mu\right) \geq \int_X \log(P_t^{V,\psi}1) \, d\mu \geq 0.$$

Since log is strictly concave, this can only happen if $P_t^{V,\psi}1$ is μ a.e. constant. By (17), the constant is 1. Since $\psi > 0$ a.e. μ is immediate, this establishes the second assertion.

For the third assertion, assume μ is an equilibrium measure for V and ψ is a ground state for V relative to μ. Then $P_t^{V,\psi}1 = 1$ a.e. μ, so for $u \in C^+(X)$,

$$\frac{\min u}{\max u} \leq \frac{P_t^{V,\psi}u}{u} \leq \frac{\max u}{\min u}, \qquad a.e. \mu,$$

hence $\log(P_t^{V,\psi}u/u)$ is in $L^1(\mu)$ for $u \in C^+(X)$. By Corollary 2, for $f \in C(X)$,

$$\beta(\epsilon) \equiv \int_X \log\left(\frac{P_t^{V,\psi}e^{\epsilon f}}{e^{\epsilon f}}\right) d\mu \geq 0, \qquad |\epsilon| < 1,$$

and $\beta(0) = 0$, hence $\dot\beta(0) = 0$. Differentiating at $\epsilon = 0$, we obtain

$$\int_X e^{-\lambda_V t} P_t^V(f\psi) \, d\pi = \int_X f\psi \, d\pi \tag{20}$$

for $f \in C(X)$. Since the collection of functions f satisfying (20) is closed under bounded pointwise convergence, (20) holds for $f \in B(X)$. Now for $f \in C(X)$, $f_\epsilon \equiv f\psi/(\psi+\epsilon) \to f$ boundedly as $\epsilon \downarrow 0$, thus replacing f by $f/(\psi+\epsilon)$ in (20) and letting $\epsilon \downarrow 0$ establishes (4), hence π is a ground measure for V. This establishes the third assertion. □

For μ, π in $M(X)$, the entropy of μ relative to π is

$$H(\mu,\pi) \equiv \sup_V \left(\int_X V \, d\mu - \log \int_X e^V \, d\pi\right)$$

where the supremum is over V in $C(X)$.

Lemma 6. *$H(\mu,\pi) \geq 0$ is finite iff $\mu << \pi$ and $\psi = d\mu/d\pi$ satisfies $\log\psi \in L^1(\mu)$, in which case*

$$H(\mu,\pi) = \int_X \log\psi \, d\mu = \int_X \psi \log\psi \, d\pi.$$

Moreover H is lower-semicontinuous and convex separately in each of μ and π.

This is Lemma 2.1 in [5].

Proof. The lower-semicontinuity and convexity follow from the definition of H as a supremum of convex functions, in each variable π, μ separately. Suppose $H(\mu,\pi) < \infty$. Since the set of V in $B(X)$ satisfying

$$\int_X V \, d\mu - \log \int_X e^V \, d\pi \leq H(\mu,\pi)$$

contains $C(X)$ and is closed under bounded pointwise convergence, it equals $B(X)$. Insert $V = r1_A$ into this inequality, where $\pi(A) = 0$, obtaining

$$r\mu(A) \leq r\mu(A) - \log(\pi(A^c)) \leq H(\mu,\pi).$$

Let $r \to \infty$ to conclude $\mu << \pi$. Since $\psi = d\mu/d\pi \in L^1(\pi)$, let $0 \le f_n \in C(X)$ with $f_n \to \psi$ in $L^1(\pi)$. By passing to a subsequence, assume $f_n \to \psi$ a.e. π. Insert $V = \log(f_n + \epsilon)$ into the definition of H to yield

$$\int_X \log(f_n + \epsilon)\, d\mu - \log \int_X (f_n + \epsilon)\, d\pi \le H(\mu, \pi).$$

Let $n \to \infty$; by Fatou's lemma,

$$\int_X \psi \log(\psi + \epsilon)\, d\pi - \log \int_X (\psi + \epsilon)\, d\pi \le H(\mu, \pi).$$

Since $\pi(\psi + \epsilon) = 1 + \epsilon$, applying Fatou's lemma again as $\epsilon \to 0$, $\int_X \psi \log \psi \, d\pi \le H(\mu, \pi)$.

Conversely, suppose $\psi = d\mu/d\pi$ exists and $\psi \log \psi \in L^1(\pi)$. By Jensen's inequality,

$$\int_X V\, d\mu \le \log \int_X e^V\, d\mu, \qquad V \in B(X).$$

Replace V by $V - \log(\psi \wedge n + \epsilon)$ to get

$$\int_X V\, d\mu - \log \int_X \left(\frac{e^V \psi}{\psi \wedge n + \epsilon} \right) d\pi \le \int_X \psi \log(\psi \wedge n + \epsilon)\, d\pi.$$

Let $\epsilon \to 0$ followed by $n \to \infty$ obtaining

$$\int_X V\, d\mu - \log \int_X e^V\, d\pi \le \int_X \psi \log \psi \, d\pi.$$

Now maximize over V in $C(X)$ to conclude $H(\mu, \pi) \le \int_X \psi \log \psi \, d\pi$. □

Proof of Theorem 2. By (12),

$$\int_X \log\left(\frac{e^{-\lambda_V t} P_t^V u}{u} \right) d\mu \ge -t I^V(\mu), \qquad u \in C^+(X).$$

Thus for $f \in C(X)$,

$$\int_X f\, d\mu - \int_X \log\left(e^{-\lambda_V t} P_t^V e^f \right) d\mu \le t I^V(\mu), \qquad f \in C(X).$$

By Jensen's inequality,

$$\int_X f\, d\mu - \log \int_X \left(e^{-\lambda_V t} P_t^V e^f \right) d\mu \le t I^V(\mu), \qquad f \in C(X).$$

Defining

$$\mu_t(f) = e^{-\lambda_V t} \mu(P_t^V f)$$

and

$$\pi_t(f) = \frac{\mu_t(f)}{\mu_t(1)}$$

yields

$$\int_X f\, d\mu - \log \int_X e^f\, d\pi_t \le t I^V(\mu) + \log \mu_t(1), \qquad f \in C(X).$$

Taking the supremum over all f yields

$$H(\mu, \pi_t) \le t I^V(\mu) + \log \mu_t(1).$$

Note $\mu_t(1) \le C$, $t \ge 0$, hence

$$H(\mu, \pi_t) \le t I^V(\mu) + \log C, \qquad t \ge 0.$$

Now set

$$\bar{\pi}_T = \frac{\int_0^T \mu_t \, dt}{\int_0^T \mu_t(1)\, dt} = \frac{\int_0^T \mu_t(1)\pi_t \, dt}{\int_0^T \mu_t(1)\, dt}, \qquad T > 0.$$

Then π_t is in $M(X)$ for $t > 0$, $\bar{\pi}_T$ is in $M(X)$ for $T > 0$.

Now assume μ is an equilibrium measure for V; then $I^V(\mu) = 0$. By convexity of H.

$$H(\mu, \bar{\pi}_T) \leq \log C, \qquad T > 0.$$

By compactness of $M(X)$, select a sequence $T_n \to \infty$ with $\pi_n = \bar{\pi}_{T_n}$ converging to some π. By lower-semicontinuity of H, we have $H(\mu, \pi) \leq \log C$. Thus $\mu << \pi$ with $\psi = d\mu/d\pi$ satisfying $\psi \log \psi \in L^1(\pi)$. Since

$$\log \mu(e^{-\lambda_V t} P_t^V 1) \geq \mu(\log(e^{-\lambda_V t} P_t^V 1)) \geq 0,$$

we have $\mu_t(1) \geq 1$, $t \geq 0$. This is enough to show

$$\pi_n \left(e^{-\lambda_V T} P_T^V f\right) = \pi_n(f) + o(1), \qquad n \to \infty,$$

for all $T > 0$. Thus π is a ground measure for V. By Theorem 1, ψ is a ground state for V relative to μ. The remaining assertions are in Lemma 5. □

We establish two lemmas used in the proof of Theorem 3.

Lemma 7. *Let $V \in C(X)$. Under assumption (A), (7) holds.*

This is Lemma 4.3.1 in [3].

Proof. Let $T > 0$ and $\epsilon > 0$ be as in (A). By (10), for $t \geq 0$,

$$\begin{aligned} P_T P_t^V 1 &\leq e^{-T \min V} P_T^V P_t^V 1 = e^{-T \min V} P_t^V P_T^V 1 \\ &\leq e^{T(\max V - \min V)} P_t^V P_T 1 = e^{T(\max V - \min V)} P_t^V 1. \end{aligned}$$

Similarly, one has

$$P_T P_t^V 1 \geq e^{T(\min V - \max V)} P_t^V 1$$

hence

$$e^{T(\max V - \min V)} P_t^V 1 \geq P_T P_t^V 1 \geq e^{T(\min V - \max V)} P_t^V 1.$$

Let $\epsilon' = \epsilon e^{2T(\min V - \max V)}$. By (A) this implies

$$P_t^V 1(x) \geq \epsilon' P_t^V 1(y), \qquad x, y \in X,$$

hence

$$\|P_t^V\| = \sup_x P_t^V 1(x) \geq \phi(t) \equiv \inf_x P_t^V 1(x) \geq \epsilon' \|P_t^V\|, \qquad t \geq 0.$$

But $\phi(t)$ is supermultiplicative so

$$\sup_{t>0} \frac{1}{t} \log \phi(t) = \lim_{t\to\infty} \frac{1}{t} \log \phi(t) \leq \lim_{t\to\infty} \frac{1}{t} \log \|P_t^V\| = \lambda_V.$$

Since $\epsilon' \|P_t^V\| \leq \phi(t)$, this implies (7) with $C \leq 1/\epsilon'$. □

Lemma 8. *Under assumption (A), the ground state ψ in Theorem 2 may be chosen such that $\log \psi$ is in $B(X)$. If moreover (B) holds, $\mathrm{supp}(\mu) = X$. If moreover (C) holds and V is smooth, ψ may be chosen in $\mathcal{D}^\infty$ and strictly positive, and satisfies*

$$L\psi + V\psi = \lambda_V \psi.$$

Proof. With T and ϵ as in (A), let $Q_T = e^{-\lambda_V T} P_T^V$ and $\epsilon' = \epsilon e^{T(\min V - \max V)}$. Then $Q_T\psi = \psi$ a.e. μ. By (A) and (10) we have

$$Q_T|f|(x) \geq \epsilon' Q_T|f|(y), \qquad x, y \in X, \tag{21}$$

for all $f \in C(X)$. Since the collection of functions f satisfying (21) is closed under bounded pointwise convergence, (21) is valid for $f \in B(X)$. Hence

$$Q_T\psi(x) \geq Q_T(\psi \wedge n)(x) \geq \epsilon' Q_T(\psi \wedge n)(y), \qquad x, y \in X.$$

Let $\tilde{\psi} \equiv Q_T\psi$. Sending $n \to \infty$ yields

$$\tilde{\psi}(x) \geq \epsilon' \tilde{\psi}(y), \qquad x, y \in X. \tag{22}$$

Since ψ is a ground state, $\tilde{\psi} = \psi$ a.e. μ. Since $0 < \psi < \infty$ a.e. μ, we have $0 < \tilde{\psi} < \infty$ a.e. μ hence (22) implies $\tilde{\psi}$ is bounded away from zero and away from infinity, i.e. $\log\tilde{\psi}$ is in $B(X)$. Since $d\pi = d\mu/\psi = d\mu/\tilde{\psi}$, Theorem 1 implies $\tilde{\psi}$ is a ground state. Thus we may replace ψ by $\tilde{\psi}$ and assume $\log\psi \in B(X)$.

With $T > 0$ as in (B), $f \in C(X)$ nonnegative implies

$$\mu(f) = \mu(P_T^{V,\psi} f) \geq \frac{\inf\psi}{\sup\psi} e^{T(\min V - \lambda_V)} \mu(P_T f) > 0.$$

Hence $\operatorname{supp}(\mu) = X$.

Now let $\tilde{\psi} \equiv Q_T\psi$ and assume V is smooth. Then $\tilde{\psi} = \psi$ a.e. μ hence as before $\tilde{\psi}$ is a ground state. Since $\tilde{\psi} \in \mathcal{D}^\infty$, we may replace ψ by $\tilde{\psi}$ and assume $\psi \in \mathcal{D}^\infty$.

Since $\operatorname{supp}(\mu) = X$, $e^{-\lambda_V t} P_t^V \psi = \psi$, $t \geq 0$, holds identically on X, hence ψ is strictly positive. Differentiating this yields $L\psi + V\psi = \lambda_V\psi$. □

Proof of Theorem 3. Let $\psi_i \in \mathcal{D}^\infty$ be the strictly positive ground states for V_i relative to μ, $i = 1, 2$, given by Lemma 8. Since μ is $P_t^{V_i,\psi_i}$-invariant, $i = 1, 2$, differentiating (17) yields

$$0 = \int_X \frac{L(\psi_i f)}{\psi_i} + V_i f - \lambda_{V_i} f \, d\mu = \int_X \left(\frac{L(\psi_i f)}{\psi_i} - f\frac{L\psi_i}{\psi_i} \right) d\mu = \int_X \frac{1}{\psi_i} [L, f]\psi_i \, d\mu,$$

for $f \in \mathcal{D}^\infty$, for $i = 1, 2$. Subtract these two equations and insert $f = \psi_1/\psi_2$ to get

$$\int_X \frac{1}{\psi_1} \left[\left[L, \frac{\psi_1}{\psi_2} \right], \frac{\psi_1}{\psi_2} \right] \psi_2 \, d\mu = 0.$$

But $\psi_2 \geq \min\psi_2$ so by Lemma 2 applied with $f = \psi_2 - \min\psi_2$,

$$\frac{1}{\psi_1} \left[\left[L, \frac{\psi_1}{\psi_2} \right], \frac{\psi_1}{\psi_2} \right] \psi_2 \geq \frac{\min\psi_2}{\max\psi_1} \Gamma\left(\frac{\psi_1}{\psi_2} \right) \geq 0$$

so

$$\int_X \Gamma(\psi_1/\psi_2) \, d\mu = 0.$$

Since $\operatorname{supp}(\mu) = X$, $\Gamma(\psi_1/\psi_2) \equiv 0$ which yields by (D) $\psi_1 = c\psi_2 \equiv \psi$. Thus we arrive at $L\psi + V_i\psi = \lambda_{V_i}\psi$ for $i = 1, 2$. Subtracting yields the result. □

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