Smoothness of Wave Functions in Thermal Equilibrium

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Abstract

We consider the thermal equilibrium distribution at inverse temperature β, or canonical ensemble, of the wave function Ψ of a quantum system. Since L^2 spaces contain more nondifferentiable than differentiable functions, and since the thermal equilibrium distribution is very spread-out, one might expect that Ψ has probability zero to be differentiable. However, we show that for relevant Hamiltonians the contrary is the case: with probability one, Ψ is infinitely often differentiable and even analytic. We also show that with probability one, Ψ lies in the domain of the Hamiltonian.

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1 Introduction

We address the question whether the wave function Ψ of a typical system from the canonical ensemble of thermodynamics with inverse temperature β is differentiable. As pointed out in [7], the thermal equilibrium distribution of the wave function, corresponding to the canonical ensemble, is the "Gaussian adjusted projected measure" $GAP(\rho)$, a probability measure on the unit sphere in Hilbert space whose definition we recall in Section 2, for $\rho = \rho_\beta$, the density matrix of the canonical ensemble, given by (see, e.g., [8, 10])

$$\rho_\beta = \frac{1}{Z(\beta, H)} \mathrm{e}^{-\beta H} \quad \text{with } Z(\beta, H) = \mathrm{tr}\, \mathrm{e}^{-\beta H}. \tag{1}$$

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Thus, we take Ψ to be a random unit vector with distribution $GAP(\rho_\beta)$. The surprising result is that in many relevant cases Ψ has probability one to be infinitely often differentiable and even analytic, i.e., $GAP(\rho_\beta)(C^\infty) = GAP(\rho_\beta)(C^\omega) = 1$.

We explore four kinds of arguments concerning the smoothness of Ψ, each requiring somewhat different assumptions on the Hamiltonian H and leading to somewhat different conclusions. Some of the arguments do not depend on the special measure $GAP(\rho_\beta)$ but show that, for suitable Hamiltonians H, every distribution whose density matrix is ρ_β will be concentrated on the smooth (resp. analytic) functions; other arguments use the way the measure $GAP(\rho)$ is constructed from a Gaussian measure. The measure $GAP(\rho)$ is discussed in detail in [7]. It has density matrix ρ and is stationary if ρ is.

The first argument aims at showing that the Fourier coefficients of Ψ go to zero so fast that they are still square-summable after multiplication by any power of the wave number k. This can be easily applied to cases in which the eigenfunctions of H are plane waves, such as for the free Schrödinger equation in a box. The second argument is based on the assumption that the eigenfunctions of H are smooth, and the theorem asserting that, for a series of functions, summation and differentiation commute if the series of the derivatives converges uniformly. We formulate a condition on H that entails this kind of convergence almost surely (a.s.) for the expansion of Ψ in eigenfunctions of H. The third argument, which supposes that Ψ is a function on an interval $I \subseteq \mathbb{R}$, aims at showing that the increments are not too large, $|\Psi(q+\Delta q) - \Psi(q)| \lesssim \Delta q$, which suggests differentiability; however, the rigorous version of this argument provides only a very weak result. The fourth argument, the simplest and most elegant one, is of a more abstract nature: it concerns not the question $\Psi \in C^\infty$ but instead the related question $\Psi \in \mathrm{domain}(H^\ell)$ for $\ell \in \mathbb{N}$; indeed, we obtain without further assumptions on H that a.s. $\Psi \in C^\infty(H) := \bigcap_{\ell=1}^\infty \mathrm{domain}(H^\ell)$ for almost all β for which thermal equilibrium exists at all. We also provide a variant of this argument concerning the space of analytic vectors of H.

The paper is organized as follows. In Section 2, we recall from [7] the definition of the measure $GAP(\rho_\beta)$ representing the canonical ensemble. In Section 3, we study as an example of H the Laplacian on the circle. We conclude smoothness and analyticity of Ψ from an analysis of the decay behavior of the Fourier coefficients of Ψ. In Section 4, we apply the same argument to the (relativistic or nonrelativistic) ideal gas in a box. In Section 5, we take into account the symmetrization of the wave function for describing bosons or fermions. In Section 6, we give the second kind of argument, providing a general criterion on the Hamiltonian that is sufficient for concluding that Ψ is a.s. smooth. The criterion concerns bounds on the derivatives of the eigenfunctions of H. In Section 7, we discuss the third argument, which concerns the direct estimation of the difference quotients of Ψ. In Section 8, we describe the fourth argument, which allows to conclude that Ψ lies in the domain of H and all its powers. In Section 9, we conclude, as an application of our results, that Ψ a.s. possesses a Bohmian velocity field.

2 The Canonical Ensemble

In this section we give the definition of the measure $GAP(\rho)$ on the unit sphere $\mathscr{S}(\mathscr{H})$ of Hilbert space $\mathscr{H}$, as introduced in [7].

The measure $GAP(\rho)$ is defined for every density matrix ρ (positive operator with $\operatorname{tr}\rho = 1$) on $\mathscr{H}$. We obtain the thermal equilibrium measure $GAP(\rho_\beta)$ by using the canonical density matrix (1) for a self-adjoint operator H (the Hamiltonian) and a number $\beta > 0$ (the inverse temperature) such that

$$Z(\beta, H) = \operatorname{tr} \mathrm{e}^{-\beta H} < \infty \,. \tag{2}$$

The measure $GAP(\rho)$ is defined as the distribution of the random vector

$$\Psi^{GAP} = \Psi^{GA} / \|\Psi^{GA}\| \,, \tag{3}$$

where Ψ^{GA} is a random vector with distribution $GA(\rho)$ (the "Gaussian adjusted measure") defined by

$$GA(\rho)(\mathrm{d}\psi) = \|\psi\|^2 \, G(\rho)(\mathrm{d}\psi) \,, \tag{4}$$

where $G(\rho)$ is the Gaussian measure on $\mathscr{H}$ with covariance matrix ρ.

More explicitly, for a random vector Ψ^G to be $G(\rho)$-distributed means that for any $\phi_1, \phi_2 \in \mathscr{H}$ the components $Z_1 = \langle \phi_1 | \Psi^G \rangle$ and $Z_2 = \langle \phi_2 | \Psi^G \rangle$ of Ψ^G are complex Gaussian random variables with mean zero and covariance

$$\mathbb{E} Z_1 Z_2^* = \mathbb{E} \langle \phi_1 | \Psi^G \rangle \langle \Psi^G | \phi_2 \rangle = \langle \phi_1 | \rho | \phi_2 \rangle, \tag{5}$$

where $\mathbb{E}$ denotes expectation. In particular, if $\{|\varphi_n\rangle\}$ is an orthonormal basis of $\mathscr{H}$ consisting of eigenvectors of ρ with eigenvalues p_n, then the coefficients $\langle \varphi_n | \Psi^G \rangle$ of Ψ^G are independent complex Gaussian random variables with mean zero and variances

$$\mathbb{E} \big| \langle \varphi_n | \Psi^G \rangle \big|^2 = p_n \,. \tag{6}$$

If ρ is of the form (1) then the φ_n are also eigenvectors of H.

Although we are interested only in those ρ of the form (1) for physically relevant Hamiltonians, we will sometimes, when this makes the mathematics clearer and more elegant, formulate facts or conditions in terms of an arbitrary density matrix ρ.

For any probability measure μ on $\mathscr{S}(\mathscr{H})$, its density matrix is given by

$$\rho_\mu = \int\limits_{\mathscr{S}(\mathscr{H})} \mu(\mathrm{d}\psi) \, |\psi\rangle\langle\psi| \,, \tag{7}$$

or $\rho_\mu = \mathbb{E}_\mu |\psi\rangle\langle\psi|$, where $\mathbb{E}_\mu$ denotes the expectation with respect to μ. In particular, $\mathbb{E}_\mu \big| \langle \varphi | \psi \rangle \big|^2 = \langle \varphi | \rho_\mu | \varphi \rangle$ for every fixed $\varphi \in \mathscr{H}$. (If a probability measure μ on $\mathscr{H}$ is not concentrated on $\mathscr{S}(\mathscr{H})$, the notion of density matrix of μ does not make sense any more; however, (7), or $\mathbb{E}_\mu |\psi\rangle\langle\psi|$, is still the *covariance matrix* of μ.) As mathematically expressed by $\mathbb{E}_\mu\langle\psi|P|\psi\rangle = \mathrm{tr}(\rho_\mu P)$ for every projection P, ρ_μ provides the distribution of outcomes of any quantum experiment on a system with μ-distributed random wave function. The density matrix of $GAP(\rho)$ is indeed ρ. This and other fundamental properties of the measure $GAP(\rho)$ are discussed in [7].

The following simple fact will sometimes be useful as it reduces the task of showing smoothness of $\Psi = \Psi^{GAP}$ to showing smoothness of the Gaussian random vector Ψ^G with distribution $G(\rho)$. For any subspace W of $\mathscr{H}$, we have that

$$\text{if } G(\rho)(W) = 1 \text{ then } GAP(\rho)(W) = 1\,. \tag{8}$$

To see this, note that $GA(\rho)$ has the same null sets as $G(\rho)$ (as it is absolutely continuous with respect to $G(\rho)$ with a density that vanishes only at one point), so that, if $G(\rho)(W) = 1$, $0 = G(\rho)(\mathscr{H}\setminus W) = GA(\rho)(\mathscr{H}\setminus W)$ and thus $GA(\rho)(W) = 1$; but, by definition (3), if $\Psi^{GA} \in W$ then also $\Psi^{GAP} \in W$.

3 A Case Study: The Laplacian on the Circle

In this section we consider a single particle moving on a circle S^1 with the free Schrödinger Hamiltonian,

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2}, \tag{9}$$

where m denotes the mass of the particle, q the angular coordinate on the circle, and wave functions are written as periodic functions of q. The result we derive is that relative to any measure μ on $\mathscr{S}(\mathscr{H})$ with density matrix ρ_β with $\beta > 0$ (or, in fact, any measure μ on $\mathscr{H}$ with covariance matrix ρ_β), almost every wave function ψ is smooth, $\psi \in C^\infty(\mathbb{R})$; we then go on to show that μ-almost every wave function is analytic, $\psi \in C^\omega(\mathbb{R})$.

We begin with considering, instead of differentiability, a closely related property: existence (in L^2) of the distributional derivative. In other words, we consider the property of a wave function ψ that $|k|\,\widehat{\psi}(k)$ is still square integrable where $\widehat{\psi}$ is the Fourier transform of ψ. Since the functions we are considering are 2π-periodic in q, the appropriate property is that the Fourier coefficients c_k, defined by

$$\psi(q) = \sum_{k\in\mathbb{Z}} c_k\, \mathrm{e}^{\mathrm{i}kq}, \tag{10}$$

are still square-summable after multiplication with $|k|$. Let W^ℓ denote the ℓ-th Sobolev space, i.e., the subspace of $L^2([0, 2\pi])$ containing those functions whose Fourier coefficients c_k satisfy

$$|k|^\ell\, c_k \text{ is square-summable, i.e., } \sum_{k\in\mathbb{Z}} |k|^{2\ell}\,|c_k|^2 < \infty. \tag{11}$$

We ask whether $\psi \in W^\ell$ for a random wave function ψ with distribution μ. Since the eigenfunctions of H are the plane waves,

$$\varphi_n(q) = \frac{1}{\sqrt{2\pi}}\, \mathrm{e}^{inq}\,, \quad n \in \mathbb{Z}, \tag{12}$$

the energy coefficients of a wave function are just the Fourier coefficients. The eigenvalues are

$$E_n = \frac{\hbar^2}{2m} n^2, \quad n \in \mathbb{Z}. \tag{13}$$

Thus, our question about ψ amounts to asking for which $\ell \in \mathbb{N}$ we have

$$\sum_{n\in\mathbb{Z}} n^{2\ell} \big|\langle \varphi_n|\psi\rangle\big|^2 < \infty. \tag{14}$$

This indeed holds μ-a.s. for all $\ell \in \mathbb{N}$; to see this, note that[1]

$$\mathbb{E}_\mu \sum_{n\in\mathbb{Z}} n^{2\ell} \big|\langle \varphi_n|\psi\rangle\big|^2 = \sum_{n\in\mathbb{Z}} n^{2\ell} \mathbb{E}_\mu \big|\langle \varphi_n|\psi\rangle\big|^2 = \tag{15a}$$

$$\overset{(6)}{=} \sum_{n\in\mathbb{Z}} n^{2\ell} \frac{\mathrm{e}^{-\beta E_n}}{Z(\beta,H)} \overset{(13)}{=} \frac{1}{Z(\beta,H)} \sum_{n\in\mathbb{Z}} n^{2\ell} \mathrm{e}^{-(\beta\hbar^2/2m)n^2} < \infty \tag{15b}$$

because for any constant $\gamma > 0$ and for sufficiently large $|n|$,

$$(2\ell+2)\log|n| < \gamma|n|^2 \quad \text{and thus} \quad |n|^{2\ell}\, \mathrm{e}^{-\gamma|n|^2} < \frac{1}{|n|^2}. \tag{16}$$

If the expectation (15) of a $[0,\infty]$-valued random variable is finite, the variable is a.s. finite. Thus,

$$\mu\Big(\sum_{n\in\mathbb{Z}} n^{2\ell} \big|\langle \varphi_n|\psi\rangle\big|^2 = \infty\Big) = 0 \text{ or } \mu(W^\ell) = 1 \tag{17}$$

for all $\ell \in \mathbb{N}$.

We now make the connection between W^ℓ and C^ℓ, i.e., with classical differentiability: by the Sobolev lemma [9, p. 52], every function in W^ℓ is equal Lebesgue-almost-everywhere to a function in $C^{\ell-1}$. Hence, every function in $\bigcap_{\ell=1}^\infty W^\ell$ is equal Lebesgue-almost-everywhere to a function in C^∞. In particular, μ-a.s. there is a $\phi \in C^\infty$ such that $\psi(q) = \phi(q)$ Lebesgue-almost-everywhere.

We now turn to analyticity. By a similar argument as given in (15) and (16), one can see that

$$\mu\Big(\sum_{n\in\mathbb{Z}} \mathrm{e}^{2\alpha|n|} \big|\langle \varphi_n|\psi\rangle\big|^2 = \infty\Big) = 0 \tag{18}$$

for every $\alpha > 0$, so that

$$\mathrm{e}^{\alpha|k|}\, c_k \text{ is a.s. square-summable.} \tag{19}$$

[1] Numbers on top of equality signs indicate which equation is being applied.

Regarding the variable q in (10) as complex, we observe that the right hand side of (10) converges, as a consequence of (19), uniformly in every strip $-\alpha+\varepsilon < \operatorname{Im} q < \alpha-\varepsilon$ with $0<\varepsilon<\alpha$. (To see this, we use that square-summable sequences are bounded, $\mathrm{e}^{\alpha|k|}\,|c_k| \leq C$, so that for q in the strip, $|c_k\,\mathrm{e}^{\mathrm{i}kq}| = |c_k|\,\mathrm{e}^{-k\operatorname{Im} q} < |c_k|\,\mathrm{e}^{|k|(\alpha-\varepsilon)} \leq C\,\mathrm{e}^{-|k|\varepsilon}$, which is summable over $k\in\mathbb{Z}$.) Since the uniform limit of analytic functions on an open set in the complex plane is analytic (by virtue of the Cauchy integral formula), ψ is analytic in the strip $-\alpha < \operatorname{Im} q < \alpha$; since α was arbitrary, ψ is entire (i.e., analytic on the whole complex plane). More precisely, μ-a.s. there is an entire function ϕ such that $\psi(q)=\phi(q)$ Lebesgue-almost-everywhere in $\mathbb{R}$.

4 The Ideal Gas in a Box

In a similar way, we can treat any Hamiltonian whose eigenfunctions are plane waves. A particularly relevant case is that of the ideal gas: N noninteracting particles in a d-dimensional box $[0,\pi]^d$ with Hamiltonian

$$H = -\sum_{i=1}^{N} \frac{\hbar^2}{2m}\Delta_i \tag{20}$$

with Dirichlet boundary conditions, where Δ_i is the Laplacian acting on the coordinates of the i-th particle. Our conclusion will again be that $\mu(C^\infty)=\mu(C^\omega)=1$ for every measure μ on $\mathscr{H}$ whose covariance matrix is ρ_β, and in particular for $\mu = GAP(\rho_\beta)$. For the moment, we ignore the symmetrization postulate; we will treat bosons and fermions in Section 5.

The Hamiltonian H on $\mathscr{H}=L^2([0,\pi]^{Nd})$ has eigenfunctions [3, p. 78]

$$\varphi_n(q) = \Bigl(\frac{2}{\pi}\Bigr)^{Nd/2} \prod_{i=1}^{N}\prod_{a=1}^{d} \sin(n_{i,a}q_{i,a}) \tag{21}$$

where $n=(n_{1,1},\dots,n_{N,d})\in\mathbb{N}^{Nd}$ and $q=(q_{1,1},\dots,q_{N,d})\in[0,\pi]^{Nd}$, and eigenvalues

$$E_n = \sum_{i=1}^{N}\sum_{a=1}^{d} \frac{\hbar^2}{2m} n_{i,a}^2 = \frac{\hbar^2}{2m}\|n\|^2. \tag{22}$$

The right hand side of (21) extends in an obvious way to a function on $\mathbb{R}^{Nd}$ that is 2π-periodic in every variable, which we also call φ_n; using the coefficients $\langle\varphi_n|\psi\rangle$ of the energy expansion we have a natural extension of any $\psi\in\mathscr{H}$ to a function ϕ on $\mathbb{R}^{Nd}$ that is 2π-periodic in every variable, $\phi=\sum_n\langle\varphi_n|\psi\rangle\,\varphi_n$. Its Fourier coefficients are

$$c_k = (-i)^{Nd}\Bigl(\prod_{i=1}^{N}\prod_{a=1}^{d}\operatorname{sign}(k_{i,a})\Bigr)\Bigl\langle \varphi_{|k_{1,1}|,\dots,|k_{N,d}|}\Bigm|\psi\Bigr\rangle \tag{23}$$

where $k = (k_{1,1}, \ldots, k_{N,d}) \in \mathbb{Z}^{Nd}$ and we set $\operatorname{sign}(0) = 0$.

We begin with the existence in L^2 of the ℓ-fold distributional derivative. We assert that μ-a.s. for all $\ell \in \mathbb{N}$

$$\sum_{k\in\mathbb{Z}^{Nd}} \|k\|^{2\ell}\, |c_k|^2 < \infty. \tag{24}$$

This follows from

$$\mathbb{E}_\mu \sum_{k\in\mathbb{Z}^{Nd}} \|k\|^{2\ell}\, |c_k|^2 = 2^{Nd} \sum_{n\in\mathbb{N}^{Nd}} \|n\|^{2\ell}\, \mathbb{E}_\mu \big|\langle\varphi_n|\psi\rangle\big|^2 = \tag{25a}$$

$$\overset{(6)}{=} \frac{2^{Nd}}{Z(\beta,H)} \sum_{n\in\mathbb{N}^{Nd}} \|n\|^{2\ell}\, \mathrm{e}^{-\beta E_n} \overset{(22)}{=} \frac{2^{Nd}}{Z(\beta,H)} \sum_{n\in\mathbb{N}^{Nd}} \|n\|^{2\ell}\, \mathrm{e}^{-(\beta\hbar^2/2m)\|n\|^2} \leq \tag{25b}$$

$$\overset{(26)}{\leq} \frac{2^{Nd}}{Z(\beta,H)} \sum_{n\in\mathbb{N}^{Nd}} (1+n_{1,1})^{2\ell} \cdots (1+n_{N,d})^{2\ell}\, \mathrm{e}^{-(\beta\hbar^2/2m)\|n\|^2} = \tag{25c}$$

$$= \frac{1}{Z(\beta,H)} \Big(2 \sum_{\nu\in\mathbb{N}} (1+\nu)^{2\ell}\, \mathrm{e}^{-(\beta\hbar^2/2m)\nu^2}\Big)^{Nd} \overset{(16)}{<} \infty, \tag{25d}$$

where we used

$$\|n\|^2 = \sum_{i,a} n_{i,a}^2 \leq \prod_{i,a} (1 + 2n_{i,a} + n_{i,a}^2) = \prod_{i,a} (1+n_{i,a})^2. \tag{26}$$

Inequality (24) means that ϕ lies in the Sobolev space W^ℓ, and by the Sobolev lemma [9, p. 52] also in C^m for all $m < \ell - Nd/2$. Since ℓ was arbitrary, ϕ is μ-a.s. smooth, and thus so is ψ, its restriction to $[0,\pi]^{Nd}$.

The same argument can be applied to the relativistic case, in which the Hamiltonian is the free Dirac operator

$$H = -\sum_{i=1}^{N} \Big(\mathrm{i}c\hbar\alpha_i \cdot \nabla_i + mc^2\beta_i\Big) \tag{27}$$

with c the speed of light, m the mass, and α_i and β_i the Dirac alpha and beta matrices acting on the i-th spin index of the wave function. Again, one obtains that $\mu(C^\infty) = 1$ for all μ with covariance matrix ρ_β.

We turn to analyticity and to this end assert that μ-a.s. for all $\alpha > 0$

$$\sum_{k\in\mathbb{Z}^{Nd}} \mathrm{e}^{2\alpha\|k\|}\, |c_k|^2 < \infty. \tag{28}$$

This follows from the fact that, by the same reasoning as in (25),

$$\mathbb{E}_\mu \sum_{k\in\mathbb{Z}^{Nd}} \mathrm{e}^{2\alpha\|k\|}\, |c_k|^2 = \frac{2^{Nd}}{Z(\beta,H)} \sum_{n\in\mathbb{N}^{Nd}} \mathrm{e}^{2\alpha\|n\|}\, \mathrm{e}^{-(\beta\hbar^2/2m)\|n\|^2} < \infty$$

because for any constant $\gamma > 0$ and for all but finitely many $n \in \mathbb{N}^{Nd}$, $2\alpha\|n\| - \gamma\|n\|^2 < -(\gamma/2)\|n\|^2$, while $\mathrm{e}^{-(\gamma/2)\|n\|^2}$ is summable over $\mathbb{N}^{Nd}$ by (16). By the same argument as in the last paragraph of Section 3, one can conclude from (28) that ϕ is analytic in the cylinder $\{q \in \mathbb{C}^{Nd} : \|\mathrm{Im}\, q\| < \alpha\}$. Since α was arbitrary, ϕ is entire. Thus, μ-a.s. there is an entire function ϕ such that $\psi(q) = \phi(q)$ Lebesgue-almost-everywhere in $[0,\pi]^{Nd}$. (For the Dirac equation, since the energy eigenvalues grow like $c\hbar\|k\|$, ψ a.s. possesses an analytic continuation to the cylinder $\|\mathrm{Im}\, q\| < \beta c\hbar/2$.)

5 Bosons and Fermions

In the previous section, we ignored the symmetrization of the wave function for systems of bosons or fermions. If one takes the symmetrization into account, one reaches the same conclusion: smoothness is almost sure. But instead of going through the calculation of the previous section again, we provide a simple argument why $GAP(\rho_\beta)$ must be concentrated on C^∞ for indistinguishable particles (with symmetrized wave functions) if it is concentrated on C^∞ for distinguishable particles (with unsymmetrized wave functions).

The symmetric (respectively anti-symmetric) state vectors form a subspace of $\mathscr{H} = L^2([0,\pi]^{Nd})$; let P denote the projection to that subspace; the subspace can be written $P\mathscr{H}$. Since the Hamiltonian (20) is invariant under permutations, we have that $HP = PH = PHP$. Thus, the canonical density matrix for indistinguishable particles is

$$\rho_\beta(PH, P\mathscr{H}) = c\, P\rho_\beta(H, \mathscr{H})P \tag{29}$$

where we have made explicit the dependence of ρ_β on the given Hamiltonian and Hilbert space, and $c = Z(\beta, H)/Z(\beta, PHP)$.

Now observe that for a Gaussian measure with covariance ρ, we have that $G(P\rho P) = G(\rho) \circ P^{-1}$, where P^{-1} is understood as mapping subsets of $P\mathscr{H}$ to their pre-images in $\mathscr{H}$, in other words $\Psi^{G(P\rho P)} = P\Psi^{G(\rho)}$ in distribution.

In our case, P is the symmetrization (respectively anti-symmetrization) operator, which maps smooth functions to smooth functions. Since Ψ^G is a.s. smooth (by the result of the previous section), so is $P\Psi^G$; with (8) we conclude that $GAP(\rho_\beta(PH, P\mathscr{H}))(C^\infty) = 1$. The same argument works with analyticity.

6 A General Sufficient Condition for Smoothness

We now present a second kind of argument, different from the one used in the previous sections; it applies to the measure $GAP(\rho)$ but not to all measures with density matrix ρ. The argument provides us with a condition, see (30) below, on any given density matrix ρ (and thus, for $\rho = \rho_\beta$, on the Hamiltonian) ensuring that $GAP(\rho)(C^\infty) = 1$.

Theorem 1 *Let $\mathcal{Q}$ be an open subset of $\mathbb{R}^d$. Suppose that the density matrix ρ on $\mathscr{H} = L^2(\mathcal{Q}, \mathbb{C}^m)$ has C^∞ eigenfunctions $\varphi_n(q)$ with $\|\varphi_n\| = 1$ and eigenvalues p_n, such that for all n and all $\ell = 0, 1, 2, 3, \ldots$, the ℓ-th derivative of φ_n is bounded,*

$$\|\nabla^\ell \varphi_n\|_\infty = \sup_{q \in \mathcal{Q}} |\nabla^\ell \varphi_n(q)| < \infty,$$

where by absolute values we mean

$$|\nabla^\ell \psi(q)|^2 = \sum_{i_1,\ldots,i_\ell=1}^{d} \sum_{s=1}^{m} \Big| \frac{\partial^\ell \psi_s}{\partial q_{i_1} \cdots \partial q_{i_\ell}}(q) \Big|^2.$$

If for all $\ell = 0, 1, 2, 3, \ldots$,

$$\sum_n \|\nabla^\ell \varphi_n\|_\infty \sqrt{p_n} < \infty \tag{30}$$

then $GAP(\rho)\big(C^\infty(\mathcal{Q}, \mathbb{C}^m)\big) = 1$.

Proof. To begin with, for a complex Gaussian random variable Z with $\mathbb{E}Z = 0$ and $\mathbb{E}|Z|^2 = \sigma^2$ one can determine that

$$\mathbb{E}|Z| = \int_{\mathbb{R}^2} dx\, dy\, \frac{\sqrt{x^2+y^2}}{\pi\sigma^2} \exp\Big(-\frac{x^2+y^2}{\sigma^2}\Big) = \frac{\sqrt{\pi}}{2}\sigma. \tag{31}$$

Setting $Z = \langle \varphi_n | \Psi^G \rangle$, we obtain that

$$\mathbb{E} \sum_n \Big\| \nabla^\ell \varphi_n \, \langle \varphi_n | \Psi^G \rangle \Big\|_\infty = \mathbb{E} \sum_n \big| \langle \varphi_n | \Psi^G \rangle \big| \, \|\nabla^\ell \varphi_n\|_\infty =$$
$$= \sum_n \mathbb{E} \big| \langle \varphi_n | \Psi^G \rangle \big| \, \|\nabla^\ell \varphi_n\|_\infty \stackrel{(31)}{=} \sum_n \frac{\sqrt{\pi}}{2} \sqrt{p_n} \, \|\nabla^\ell \varphi_n\|_\infty \stackrel{(30)}{<} \infty,$$

and therefore

$$\mathrm{Prob}\Big(\sum_n \Big\| \nabla^\ell \varphi_n \, \langle \varphi_n | \Psi^G \rangle \Big\|_\infty < \infty \Big) = 1.$$

Since this is true of every ℓ, we have that in the expansion

$$\Psi^G(q) = \sum_n \varphi_n(q) \, \langle \varphi_n | \Psi^G \rangle \tag{32}$$

(having C^∞ partial sums), a.s. the ℓ-th derivatives of the partial sums converge uniformly; and in particular, (32) itself converges uniformly. It is a standard theorem (see, e.g., [4, p. 118]) that if a sequence f_n of functions converges pointwise and the derivatives ∇f_n uniformly, then the limit function f is differentiable and has derivative $\nabla f = \lim \nabla f_n$. Therefore, a.s. $\Psi^G \in C^\infty(\mathcal{Q})$, and the derivatives are

$$\nabla^\ell \Psi^G(q) = \sum_n \nabla^\ell \varphi_n(q) \, \langle \varphi_n | \Psi^G \rangle. \tag{33}$$

By (8), a.s. $\Psi \in C^\infty(\mathcal{Q})$, which completes the proof. $\square$

By applying this proof to local coordinates, we can generalize the result to Riemannian manifolds and vector bundles as follows. *Let $\mathcal{Q}$ be a Riemannian C^∞ manifold, E a C^∞ complex vector bundle over $\mathcal{Q}$ with positive-definite C^∞ Hermitian inner products on the fiber spaces, and let ∇ be the covariant derivative operator corresponding to a C^∞ connection on E. Let $\mathscr{H} = L^2(E)$ be the Hilbert space of square-integrable (with respect to the Riemannian volume) measurable cross-sections of E, and $C^\infty(E)$ the space of smooth cross-sections. Suppose that the density matrix ρ on $\mathscr{H}$ has C^∞ eigen-cross-sections $\varphi_n(q)$ with $\|\varphi_n\| = 1$ and eigenvalues p_n, such that for all n and all $\ell = 0, 1, 2, 3, \ldots$, the ℓ-th covariant derivative of φ_n is bounded,*

$$\|\nabla^\ell \varphi_n\|_\infty = \sup_{q\in\mathcal{Q}} |\nabla^\ell \varphi_n(q)| < \infty, \tag{34}$$

where the absolute values are taken with respect to the Riemannian inner product on tangent spaces and the Hermitian inner product on fiber spaces. If for all $\ell = 0, 1, 2, 3, \ldots$,

$$\sum_n \|\nabla^\ell \varphi_n\|_\infty \sqrt{p_n} < \infty \tag{35}$$

then $GAP(\rho)\big(C^\infty(E)\big) = 1$.

Another easy generalization of Theorem 1 concerns analyticity: *Let $\mathcal{Q}_\mathbb{C}$ be an open subset of $\mathbb{C}^d$ and $\mathcal{Q} := \{(q_1, \ldots, q_d) \in \mathcal{Q}_\mathbb{C} : q_1, \ldots, q_d \in \mathbb{R}\} \subseteq \mathbb{R}^d$. Suppose that the density matrix ρ on $\mathscr{H} = L^2(\mathcal{Q}, \mathbb{C}^m)$ has eigenvalues p_n with normalized eigenvectors $\varphi_n \in C^\omega(\mathcal{Q}_\mathbb{C})$, with $C^\omega(\mathcal{Q}_\mathbb{C})$ the space of L^2 functions on $\mathcal{Q}$ that possess analytic continuations to $\mathcal{Q}_\mathbb{C}$. If for every compact set $K \subseteq \mathcal{Q}_\mathbb{C}$,*

$$\sum_n \big\|\varphi_n|_K\big\|_\infty \sqrt{p_n} < \infty\,, \tag{36}$$

(writing also φ_n for the analytic continuation and $\varphi_n|_K$ for its restriction to K), then $GAP(\rho)\big(C^\omega(\mathcal{Q}_\mathbb{C})\big) = 1$.

Proof. By (36) and (31),

$$\mathbb{E}\sum_n \big\|\varphi_n|_K\big\|_\infty \big|\langle\varphi_n|\Psi^G\rangle\big| = \sum_n \big\|\varphi_n|_K\big\|_\infty \frac{\sqrt{\pi}}{2}\sqrt{p_n} < \infty\,,$$

and thus a.s. $\sum_n \big\|\varphi_n|_K\big\|_\infty \big|\langle\varphi_n|\Psi^G\rangle\big| < \infty$. As a consequence, the expansion

$$\Psi^G(q) = \sum_n \varphi_n(q)\,\langle\varphi_n|\Psi^G\rangle \tag{37}$$

converges not only for $q \in \mathcal{Q}$ but also for $q \in \mathcal{Q}_\mathbb{C}$, in fact uniformly on every compact set $K \subseteq \mathcal{Q}_\mathbb{C}$. Since uniform limits of analytic functions are analytic, Ψ^G and thus also Ψ^{GAP} are a.s. analytic. $\square$

In order to demonstrate that the conditions (30), (35) and (36) are not unreasonably strong, we show that they are satisfied for the Laplacian on the circle. Here the eigenfunctions are given by (12), and their derivatives, respectively analytic continuations to disks $K = \{q \in \mathcal{Q}_{\mathbb{C}} = \mathbb{C} : |q| \leq \alpha\}$, have bounds

$$\|\nabla^\ell \varphi_n\|_\infty = \frac{|n|^\ell}{\sqrt{2\pi}}, \quad \big\|\varphi_n|_K\big\|_\infty = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{\alpha|n|} .$$

In this case, (30) respectively (35) is satisfied since

$$\sum_{n\in\mathbb{Z}} \|\nabla^\ell \varphi_n\|_\infty \, \mathrm{e}^{-\frac{1}{2}\beta E_n} = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} |n|^\ell \, \mathrm{e}^{-(\beta\hbar^2/4m)n^2} < \infty$$

by (16), and similarly (36) since

$$\sum_{n\in\mathbb{Z}} \big\|\varphi_n|_K\big\|_\infty \, \mathrm{e}^{-\frac{1}{2}\beta E_n} = \frac{1}{\sqrt{2\pi}} \sum_{n\in\mathbb{Z}} \mathrm{e}^{\alpha|n|} \, \mathrm{e}^{-(\beta\hbar^2/4m)n^2} < \infty .$$

7 Estimating Difference Quotients

In this section, we follow another line of reasoning for studying regularity properties of Ψ, based on a standard theorem on the regularity of sample paths of a Gaussian process. However, the result is much weaker than what we obtained in the previous section.

Assume for simplicity that the configuration space is an open interval $I \subseteq \mathbb{R}$, and that $\mathscr{H} = L^2(I, \mathbb{C})$. The idea in this section is to consider the increments $\Psi^G(q+\Delta q) - \Psi^G(q)$ of the Gaussian process Ψ^G and to argue that for reasonable Hamiltonians they are of the order of magnitude of $\Delta q > 0$,

$$\big|\Psi^G(q + \Delta q) - \Psi^G(q)\big| \lesssim \Delta q, \tag{38}$$

which suggests that difference quotients converge to differential quotients as $\Delta q \to 0$, i.e., that Ψ^G be differentiable. However, what can rigorously be concluded from a statement about the variance of the increment analogous to (38) is less than differentiability, namely Hölder continuity with exponent $1 - \varepsilon$.

We now describe the argument in detail. We pretend that Ψ^G is everywhere defined in I (although, strictly speaking, vectors in Hilbert space are equivalence classes of functions coinciding Lebesgue-almost-everywhere) in such a way that it is a Gaussian process in the sense that, for any choice of $q_1, \ldots, q_n \in I$, the joint distribution of $\Psi^G(q_1), \ldots, \Psi^G(q_n)$ in $\mathbb{C}^n$ is Gaussian. It follows that for any $\Delta q > 0$, the increment $\Psi^G(q + \Delta q) - \Psi^G(q)$ is a Gaussian variable, and we can compute its variance,

$$\mathbb{E}\big|\Psi^G(q + \Delta q) - \Psi^G(q)\big|^2 = \rho(q + \Delta q, q + \Delta q) - 2\mathrm{Re}\, \rho(q, q + \Delta q) + \rho(q, q), \tag{39}$$

where $\rho(q, q') = \langle q|\rho|q'\rangle$ are the "matrix elements" in the position representation of the density matrix $\rho = \rho_\beta$. Assuming that

$$\rho(q, q') \text{ is a smooth function,} \tag{40}$$

which would appear to be a reasonable assumption on the Hamiltonian, we can employ a Taylor expansion of ρ to the second order around (q,q) and obtain from (39) that

$$\mathbb{E}\big|\Psi^G(q+\Delta q)-\Psi^G(q)\big|^2 = \frac{\partial^2\rho}{\partial q\,\partial q'}\bigg|_{q'=q}\Delta q^2 + O(\Delta q^3). \tag{41}$$

It is a standard result [6, Thm. 8 of Chap. III] that for a Gaussian process Ψ^G with the following bound on the variances of the increments:

$$\mathbb{E}\big|\Psi^G(q+\Delta q)-\Psi^G(q)\big|^2 \le K\,\Delta q^p, \tag{42}$$

where $K>0$ and $p>0$ are constants, the realization a.s. satisfies

$$\big|\Psi^G(q+\Delta q)-\Psi^G(q)\big| \le K'\,\Delta q^{p/2}\,\big|\log\Delta q\big|^{1+\delta} \tag{43}$$

for arbitrary $\delta>0$ and a suitable constant $K'=K'(\delta)>0$. Inserting (41) into (42), we obtain from (43), in case $\partial^2\rho/\partial q\,\partial q'\neq 0$, that a.s.

$$\big|\Psi^G(q+\Delta q)-\Psi^G(q)\big| \le K''\,\Delta q^{1-\varepsilon} \tag{44}$$

for arbitrary $\varepsilon>0$, i.e., Hölder continuity of degree $1-\varepsilon$.

In order to obtain a stronger estimate than (44), one might hope that

$$\frac{\partial^2\rho}{\partial q\,\partial q'}\bigg|_{q'=q} = 0 \quad \text{for all } q\in I. \tag{45}$$

This would allow us to replace the exponent in (44) by $3/2-\varepsilon$, which would give us in particular local Lipschitz continuity, so that Ψ^G would be differentiable Lebesgue-almost-everywhere. But any exponent greater than 1 is too good to be true. Indeed, as we shall show presently, (45) holds only for one particular density matrix ρ_0, the projection to the 1-dimensional subspace of constant functions. For $\rho=\rho_0$, $\Psi(q)$ is constant with modulus determined by normalization and random phase.

To see $\rho=\rho_0$, write ρ in terms of its eigenfunctions $\varphi_n(q)$ and eigenvalues p_n, $\rho(q,q')=\sum_n p_n\,\varphi_n(q)\,\varphi_n^*(q')$, and observe that

$$\frac{\partial^2\rho}{\partial q\,\partial q'}\bigg|_{q'=q} = \sum_n p_n\,\varphi_n'(q)\,\varphi_n'^*(q')\bigg|_{q'=q} = \sum_n p_n\,|\varphi_n'(q)|^2\,,$$

where φ_n' denotes the derivative of φ_n. The only way how this quantity can vanish for all q is that all φ_n have identically vanishing derivative and thus are constant, which implies $\rho=\rho_0$.

8 Concentration on the Domain of H

In this section we utilize a fourth kind of argument, different from those of the previous sections. It is our most elegant argument, particularly simple and direct, as it deals only with the eigenvalues and eigenvectors, but also more abstract. This argument applies not only to $GAP(\rho_\beta)$ but to every probability measure μ on $\mathscr{S}(\mathscr{H})$ with density matrix ρ_β.

The question we address is whether $\mu(\text{domain}(H)) = 1$. The answer is yes. Even more, we show that, for any self-adjoint H and almost all β for which $Z(\beta, H) < \infty$, any μ with density matrix ρ_β is supported by the domain of H^ℓ for every $\ell \in \mathbb{N}$. (Whether $\psi \in \text{domain}(H)$ implies differentiability depends of course on H.) After that, we show further that $GAP(\rho_\beta)$ for sufficiently large β is concentrated on the *subspace of analytic vectors* [1] of H.

Theorem 2 *Let ρ be a density matrix on the Hilbert space $\mathscr{H}$, μ a probability measure on $\mathscr{S}(\mathscr{H})$ with density matrix ρ, and $f : [0,\infty) \to \mathbb{R}$ a measurable function. If*

$$\mathrm{tr}\big(\rho\, f(\rho)^2\big) < \infty \tag{46}$$

then $\mu\big(\text{domain}\big(f(\rho)\big)\big) = 1$, where the domain of $f(\rho)$ can be defined, in terms of an orthonormal basis $\{|\varphi_n\rangle\}$ of eigenvectors of ρ with eigenvalues p_n, by

$$\text{domain}\big(f(\rho)\big) = \Big\{\psi \in \mathscr{H} : \sum_n \big|f(p_n)\langle\varphi_n|\psi\rangle\big|^2 < \infty\Big\}. \tag{47}$$

Proof. From (46) it follows that

$$\mathbb{E}_\mu \sum_n \big|f(p_n)\langle\varphi_n|\psi\rangle\big|^2 = \sum_n f(p_n)^2\, \mathbb{E}_\mu \big|\langle\varphi_n|\psi\rangle\big|^2 = \sum_n f(p_n)^2\, p_n < \infty.$$

Therefore, μ-a.s. $\sum_n \big|f(p_n)\langle\varphi_n|\psi\rangle\big|^2 < \infty$, or $\mu\big(\text{domain}(f(\rho))\big) = 1$. □

Corollary 1 *Let H be a self-adjoint operator on the Hilbert space $\mathscr{H}$. Suppose $Z(\beta_0, H) < \infty$ for some $\beta_0 > 0$, which implies $Z(\beta, H) < \infty$ for every $\beta > \beta_0$. Then for every $\beta > \beta_0$ and every probability measure μ on $\mathscr{S}(\mathscr{H})$ with density matrix ρ_β, $\mu(C^\infty(H)) = 1$, where $C^\infty(H) = \bigcap_{\ell=1}^\infty \text{domain}(H^\ell)$.*

Proof. For ρ given by (1), we have that $H = -\frac{1}{\beta}\log\rho + E_0\,\mathrm{id}$ for some constant E_0. Define $f(x) = (-\frac{1}{\beta}\log x + E_0)^\ell$ for $x > 0$ and $f(x) = 0$ for $x = 0$. Since $f(\rho) = H^\ell$, Theorem 2 yields the claim if we can confirm the condition (46), which we do now.

Since $\mathrm{tr}\, \exp(-\beta_0 H) < \infty$, there is a basis $\{|\varphi_n\rangle : n \in \mathbb{N}\}$ of eigenvectors of H with eigenvalues E_n. Furthermore, only finitely many of the eigenvalues lie below zero, so that the set $\mathcal{N} := \{n \in \mathbb{N} : E_n > 0\}$ contains all except finitely many numbers. Observe that for every $\beta > \beta_0$,

$$\infty > \operatorname{tr} \mathrm{e}^{-\beta_0 H} = \sum_{n\in\mathbb{N}} \mathrm{e}^{-\beta_0 E_n} \geq \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta_0 E_n} > \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta E_n},$$

and thus $Z(\beta, H) < \infty$. For $\varepsilon > 0$ with $\varepsilon < \beta - \beta_0$, we find, for any $\ell \in \mathbb{N}$,

$$\infty > \sum_{n\in\mathcal{N}} \mathrm{e}^{-(\beta-\varepsilon)E_n} = \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta E_n}\, \mathrm{e}^{\varepsilon E_n} > \sum_{n\in\mathcal{N}} \mathrm{e}^{-\beta E_n} \sum_{k=0}^{2\ell} \frac{\varepsilon^k E_n^k}{k!} = \sum_{k=0}^{2\ell} \frac{\varepsilon^k}{k!} \sum_{n\in\mathcal{N}} E_n^k\, \mathrm{e}^{-\beta E_n}.$$

In particular,

$$\sum_{n\in\mathcal{N}} E_n^{2\ell}\, \mathrm{e}^{-\beta E_n} < \infty,$$

which implies $\operatorname{tr}\big(\rho_\beta H^{2\ell}\big) < \infty$. □

If $\beta > 2\beta_0$ (with $Z(\beta_0, H) < \infty$), we obtain the stronger result for the measure $GAP(\rho_\beta)$ that it is concentrated on the subspace $C^\omega(H)$ of analytic vectors of H, i.e., those vectors $\psi \in C^\infty(H)$ with

$$\sum_{\ell=0}^{\infty} \frac{\|H^\ell \psi\| \varepsilon^\ell}{\ell!} < \infty \tag{48}$$

for some $\varepsilon > 0$ [1]. It is sufficient for $\psi \in C^\omega(H)$ that

$$\sum_n \mathrm{e}^{\varepsilon |E_n|} \big|\langle n|\psi\rangle\big| < \infty \tag{49}$$

because then

$$\sum_{\ell=0}^{\infty} \frac{\varepsilon^\ell}{\ell!} \|H^\ell \psi\| = \sum_{\ell=0}^{\infty} \frac{\varepsilon^\ell}{\ell!} \Big\| \sum_n E_n^\ell |n\rangle\langle n|\psi\rangle \Big\| \leq$$

$$\leq \sum_n \sum_{\ell=0}^{\infty} \frac{\varepsilon^\ell}{\ell!} |E_n|^\ell \big|\langle n|\psi\rangle\big| = \sum_n \mathrm{e}^{\varepsilon|E_n|} \big|\langle n|\psi\rangle\big| < \infty\,.$$

For $0 < \varepsilon < \beta/2 - \beta_0$, (49) is a.s. true of $\psi = \Psi^G$, and thus also of $\psi = \Psi^{GAP}$, because, assuming without loss of generality that all $E_n > 0$, we have by (31) that

$$\mathbb{E} \sum_n \mathrm{e}^{\varepsilon E_n} \big|\langle n|\Psi^G\rangle\big| = \sum_n \mathrm{e}^{\varepsilon E_n} \frac{\sqrt{\pi}}{2\sqrt{Z(\beta)}} \mathrm{e}^{-\beta E_n/2} \leq \frac{\sqrt{\pi}}{2\sqrt{Z(\beta)}} \sum_n \mathrm{e}^{-\beta_0 E_n} < \infty\,.$$

9 Existence of Bohmian Velocities

As a final remark, we mention an application of smoothness of the wave function: differentiability is needed in Bohmian mechanics [2], a theory ascribing trajectories to the particles of nonrelativistic quantum mechanics. This is because the Bohmian law of motion, which for N particles with masses $m_1, \dots, m_N$ at the configuration $Q(t) = (\boldsymbol{Q}_1(t), \dots, \boldsymbol{Q}_N(t))$ reads

$$\frac{\mathrm{d}\boldsymbol{Q}_i}{\mathrm{d}t} = \boldsymbol{v}_i^{\psi}(Q) = \frac{\hbar}{m_i}\mathrm{Im}\frac{\psi^*\nabla_i\psi}{\psi^*\psi}(Q),$$

involves the derivative of the wave function. Suppose the wave function ψ is chosen at random according to the canonical distribution $GAP(\rho_\beta)$ with inverse temperature β. Then any condition on the Hamiltonian entailing that ψ is a.s. smooth also implies that the Bohmian velocity vector field v^ψ on configuration space $\mathcal{Q} = \mathbb{R}^{3N}$, whose i-th component is $\boldsymbol{v}_i^\psi$, is a.s. well defined everywhere outside the nodes of ψ.

The analogous conclusion holds, as we shall explain presently, for the numerous further variants of Bohmian mechanics that have been considered (such as Bohmian mechanics on curved spaces, on the configuration space of a variable number of particles [5], for wave functions that are cross-sections of a complex vector bundle, and variants suitable for the Dirac equation or for photons). The laws of motion of these variants,

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = v^\psi(Q),$$

are defined by giving the appropriate expression for the velocity vector field v^ψ on the manifold $\mathcal{Q}$, and these definitions of v^ψ can be summarized by the formula [5]

$$v^\psi(q)\cdot\nabla f(q) = \mathrm{Re}\frac{\psi^*(q)\left(\frac{\mathrm{i}}{\hbar}[H,f]\psi\right)(q)}{\psi^*(q)\,\psi(q)} \quad \forall f \in C_0^\infty(\mathcal{Q})\,. \tag{50}$$

Here, $f : \mathcal{Q} \to \mathbb{R}$ is an arbitrary smooth function with compact support playing the role of a coordinate function, and numerator and denominator involve inner products in the value space of ψ (which may be a fiber space of a vector bundle of which ψ is a cross-section). For $\psi \in \mathrm{domain}(H)$ and $f \in C_0^\infty(\mathcal{Q})$, the right hand side of (50) will be well defined since multiplication by f maps the domain of H to itself, since H is the sum of a differential operator (of up to second order) and a multiplication operator. Since the f's from $C_0^\infty(\mathcal{Q})$ suffice for determining v^ψ (up to changes on a null set), one obtains indeed a vector field v^ψ, defined on $\mathcal{Q}\setminus\{q : \psi(q) = 0\}$, for every ψ from the domain of H.

Hence, every wave function ψ from the domain of H is sufficiently regular to define a Bohm-type velocity field. By Corollary 1, the random wave function Ψ with the thermal equilibrium distribution $GAP(\rho_\beta)$ possesses a velocity field v^Ψ with probability one, provided that there is $\beta_0 < \beta$ with $Z(\beta_0, H) < \infty$.

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