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Born's Postulate and Reconstruction of the ψ-Function in Nonrelativistic Quantum Mechanics

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A continuous family of self-adjoint operators is constructed such that their measurement data are insufficient to reproduce uniquely via Born's postulate the underlying quantum state. Moreover, no pair of operators has a common invariant subspace. This rejects a conjecture given by Moroz. On the other hand, strengthening results obtained by Kreinovitch, it is shown that already one special potential and the related localization measurement data at different moments of time can guarantee the uniqueness of reconstruction.

1. It is a basic problem in the foundations of quantum mechanics to describe how one can reconstruct the state vector of an ensemble of particles from the experimental data obtained in the course of observation. According to Born (1953, p. 100]:

> Physical significance is confined to the quantity $|\psi|^2$ (the square of the amplitude), and other similarly constructed quadratic expressions (matrix elements) which only partially define ψ, it follows, that even when the physically determinable quantities are completely known at time $t=0$, the initial value of ψ-function is necessarily not completely definable.

To be more precise, one may ask whether the data

$$|\psi_A(\lambda)|, \qquad A\in\mathscr{A}$$

determine the state vector ψ up to a constant phase factor. Here $\mathscr{A}$ is a given set of self-adjoint operators in a complex Hilbert space X and $|\psi_A(\lambda)|^2$ is the spectral density of the operator A w.r.t. the state vector ψ, so that

$$\langle\psi|f(A)\psi\rangle=\int |\psi_A(\lambda)|^2 f(\lambda)\,d\sigma(\lambda) \tag{1}$$

for $A\in\mathscr{A}$, $\psi\in X$ (cf. Section 2). In particular, let $X=L^2(\mathbb{R}^3, d\lambda)$ be the Hilbert space of complex-valued L^2 functions on $\mathbb{R}^3$; one may ask to what extent the absolute values $|\psi(x)|$ and $|\hat{\psi}(p)|$ determine the function, that is,

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how to describe the set of solutions of the system of equations

$$|\psi(x)| = f(x), \qquad |\hat{\psi}(p)| = g(p), \qquad \psi \in L^2(\mathbb{R}^3) \tag{2}$$

for two given functions f and g; here $\hat{\psi}$ denotes the Fourier transform of ψ and one should assume, of course, that $f(x) \geq 0$, $g(p) \geq 0$ for λ-a.e. $x \in \mathbb{R}^3$, $p \in \mathbb{R}^3$. Even in this special case, corresponding to the position and momentum measurements for an ensemble of spinless, nonrelativistic particles, this problem remains unsolved. It has been shown (Moroz, 1974), however, that given a solution of (2), one can construct another solution; thus, position and momentum measurements are in general not sufficient to reproduce the state vector of a spinless particle (in accordance with the remark of Born's cited above). Developing this idea further, we construct here an infinite system $\{A(\alpha)|\alpha \in \mathbb{R}\}$ of self-adjoint operators, such that although the operators $A(\alpha)$ and $A(\beta)$ have no common invariant subspace when $\alpha \neq \beta$, there are two vectors ψ^+ and ψ^- such that $\psi^+ \neq c\psi^-$ with $c \in \mathbb{C}$, but $|\psi^+_{A(\alpha)}(\lambda)| = |\psi^-_{A(\alpha)}(\lambda)|$ for $a \in \mathbb{R}$. Thereby we give a counterexample to a conjecture of Moroz's (1983, p. 333). The general problem of describing the set of solutions $\{\psi|\psi \in X\}$ to the system of equations (1) when A varies over a given set $\mathscr{A}$ of self-adjoint operators remains unsolved. One may ask, for example, whether equations (2) have only a finite number of solutions or, more generally, what conditions one should impose on $\mathscr{A}$ to guarantee uniqueness (up to a constant factor) of the solution to the system of equations (1). Already in 1933 E. Feenberg suggested another approach to the discussed reconstruction problem and gave a heuristic argument suggesting that one could uniquely reproduce the ψ-function from position measurements during a short interval of time (cf. Kemble, 1937, p. 71). His argument however, is false: Consider two spinless particles moving freely on the n-dimensional torus with period L and having the state functions $\psi_1(X) = 1$ and $\psi_2(X) = \exp[(2\pi i/L) \sum_{j=1}^{n} x_j]$ at the moment of time $t = 0$; a brief consideration shows that position measurements cannot distinguish between ψ_1 and ψ_2. On the other hand, we show that position measurements carried out at different moments of time on an ensemble of particles placed in a suitable potential can provide data sufficient to reproduce the initial state of the ensemble. This results strengthens the results of Kreinovitch (1977). To conclude this introduction, we refer to Band and Park (1979) for some other results in one space dimension, which seem to be relevant in this context.

In the next section we describe our counterexample to the Moroz conjecture; in Section 3 we construct a system of potentials that ensures uniqueness of reconstruction of the initial state of an ensemble of particles.

2. Let A be a self-adjoint (s.a.) operator in a rigged Hilbert space $\phi \subset X \subset \phi'$ with spectral decomposition $A = \int \lambda \, dE_\lambda$ (cf. Gelfand and

Vilenkin, 1964, Chapter 1.4). The operator A has a complete system of generalized eigenvectors

$$\{e_\lambda | \lambda \in \operatorname{spec} A\} \subset \phi'$$

so that each $\psi \in \phi$ can be uniquely decomposed as follows:

$$\psi = \int \psi_A(\lambda) e_\lambda \, d\sigma(\lambda)$$

where σ is the Borel measure on spec A determined by A and ψ_A is the σ-measurable function on spec A determined by ψ and A satisfying the following condition:

$$\langle \psi | f(A) \psi \rangle = \int |\psi_A(\lambda)|^2 f(\lambda) \, d\sigma(\lambda)$$

for every Borel-measurable function f. According to Born's postulate, the probability distribution of the results of the measurements of the observable A upon an ensemble of particles prepared in the state $\psi \in \phi$ is given by the following function:

$$B \to \langle \psi | \chi_B(A) \psi \rangle / \langle \psi | \psi \rangle$$

where B ranges over Borel subsets of $\mathbb{R}$ and χ_B denotes the characteristic function of B. This probability distribution is uniquely determined by the spectral density ψ_A, So that the probability of finding the value of A in B is equal to

$$\frac{1}{\langle \psi | \psi \rangle} \int |\psi_A(\lambda)|^2 \chi_B(\lambda) \, d\sigma(\lambda)$$

Thus, two states $\psi^{(1)}$ and $\psi^{(2)}$ with the same A-spectral density, that is, for which

$$|\psi_A^{(1)}(\lambda)| = |\psi_A^{(2)}(\lambda)|, \qquad \sigma = \text{a.e.}$$

cannot be distinguished by the measurements of A. Let $A_1, \ldots, A_n$ be s.a. operators on $\phi \subset X \subset \phi'$ such that no pair A_i, A_j with $i \neq j$ has a common invariant subspace. Moroz (1983, p. 333; 1984) conjectured that if $n \geq 3$ (or at least sufficiently large), then it follows from the equations

$$|\psi_{A_i}(\lambda)| = |\varphi_{A_i}(\lambda)|, \qquad \sigma_{A_i}\text{-a.e.}, \quad 1 \leq i \leq n$$

that $\psi = c\psi$, $c \in \mathbb{C}$, $\psi \in \phi$, $\varphi \in \phi$.

We need the Baker-Campbell-Hausdorff formula, as stated, e.g., in (Frölich, 1977, p. 135). Let A, B, N be the symmetric operators on ϕ satisfying the following conditions:

(i) N is essentially s.a. on ϕ and $N \geq 1$.
(ii) There is a K_1 in $\mathbb{R}$ such that

$$\pm A \leq K_1 N, \quad \pm i[N, A] \leq K_1 N, \quad \pm B \leq K_1 N, \quad \pm[N, [N, B]] \leq K_1 N$$

in the sense of quadratic forms on $\phi \times \phi$.
(iii) Let $c_0 = A$, $c_n := i[B, c_{n-1}]$ for $n \geq 1$; then there is K_2 in $\mathbb{R}$ such that

$$C_n \leq (K_2)^n n!\, N, \qquad \pm i[N, C_n] \leq (K_2)^n n!\, N$$

By Nelson's commutator theorem (Reed and Simon, 1975, p. 193) it follows from (ii) that the operators H and B are essentially self-adjoint on ϕ.

Theorem 0 (cf. Fröhlich, 1977). The following identity holds:

$$\exp(itB)\exp(isA)\exp(-itB) = \exp\left(is \sum_{n=0}^{\infty} C_n \frac{t^n}{n!}\right)$$

for $|t| < (K_2)^{-1}$, $s \in \mathbb{R}$. Moreover, the operator $\sum_{n=0}^{\infty} (C_n t^n / n!)$ is essentially s.a. on $D(N)$ and $D(N) \supset \phi$.

Let $\phi = \gamma$ be the Schwartz space of rapidly decreasing functions on $\mathbb{R}^n$ and let $X = L^2(\mathbb{R}^n, d\lambda)$ be the Hilbert space of L^2-complex-valued functions on $\mathbb{R}^n$ w.r.t. the Lebesgue measure $d\lambda$; we denote by x_j and p_j the operators $f \mapsto x_j f$ and $f \mapsto i(\partial/\partial x_j)f$, respectively, for $f \in \phi$. Let

$$N = p^2 + x^2 + 1 = 1 + \sum_{j=1}^{n} (p_j^2 + x_j^2)$$

Then p_j, x_j, N are essentially s.a. on ϕ and $N \geq 1$, and it can be easily shown that one may apply Theorem 0 to any real polynomial in x_j, p_j of degree ≤ 2; moreover, the constant K_2 can be chosen to be arbitrarily small by a proper rescaling of N. To construct a system of operators $\{A(\alpha) | \alpha \in \mathbb{R}\}$ violating Moroz's conjecture, we shall work in one space dimension and let $n = 1$. Although the following result is well known, we give a short proof of it to make our exposition self-contained.

Lemma 1. The operators p and x have no common nontrivial subspace.

Proof. Write

$$\{[\exp(-p^2]\psi\}(x) = \tfrac{1}{2} \int_{-\infty}^{\infty} \exp(-\tfrac{1}{4}|x-y|^2)\psi(y)\, dy$$

so that if $\psi \geq 0$, $\varphi \geq 0$ almost everywhere, and $\langle \varphi | [\exp(-p^2)] \psi \rangle = 0$, then $\psi = 0$ a.e. or $\varphi = 0$ a.e. Let U be a common invariant subspace for x and p and let $\psi \in U$, $\varphi \in U^{\perp}$; let

$$\eta_{\psi}(x) := \chi_B(x) \overline{\psi(x)} / |\psi(x)|; \qquad B := \psi^{-1}(\mathbb{C} \backslash \{0\})$$

and let

$$\eta_{\varphi}(x) := \chi_{B'}(x) \overline{\varphi(x)} / |\varphi(x)|; \qquad B' := \varphi^{-1}(\mathbb{C} \backslash \{0\})$$

Then $\eta_{\psi}(x)\psi(x) \geq 0$ and $\eta_{\varphi}(x)\varphi(x) \geq 0$ for x a.e., and

$$\bar{\eta}_{\varphi}[\exp(-p^2)] \eta_{\psi} \psi \in U$$

so that

$$\langle \varphi | \bar{\eta}_{\varphi} [\exp(-p^2)] \eta_{\psi} \psi \rangle = 0$$

or $\langle \eta_{\varphi} \varphi | [\exp(-p^2)] \eta_{\psi} \psi \rangle = 0$. Therefore, it follows that $\varphi = 0$ or $\psi = 0$. ■

Remark 1. Nonvanishing of the commutator of two s.a. operators on every nontrivial subspace of a Hilbert space does not imply that these operators have no common nontrivial invariant subspace: let $-\Delta_{\partial \Lambda}$ be the Laplacian on $L^2(\mathbb{R}, d\lambda)$ with Dirichlet boundary conditions on $\partial \Lambda$; then $L^2(\Lambda, d\lambda)$ is a common invariant subspace of $L^2(\mathbb{R}, d\lambda)$ for x and $-\Delta_{\partial \Lambda}$.

Theorem 1. Let $A(\alpha) := \alpha p + x^2$, $\alpha \in \mathbb{R}$. The operator $A(\alpha)$ is essentially s.a. on the Schwartz space ϕ and the two operators $A(\alpha)$ and $A(\beta)$ have no common nontrivial invariant subspace when $\alpha \neq \beta$.

Proof. We assume without loss of generality that $\beta \neq 0$. Then

$$\begin{aligned} &\exp[itA(\alpha)] \exp[isA(\beta)] \exp[-itA(\alpha)] \\ &\quad = \exp\{is[A(\beta) + 2t(\alpha - \beta)x + t^2 \alpha(\alpha - \beta)]\} \end{aligned}$$

Let U be a common invariant subspace for $A(\alpha)$ and $A(\beta)$ then it is also $[A(\beta) + \eta x]$-invariant, $\eta := 2t(\alpha - \beta)$. Let us define two unitary operators B_1 and B_2:

$$(B_1 \psi)(x) := \exp(i\beta^{-1} x^3/3)\, \psi(x) \qquad \text{for } x \text{ a.e.}$$

$$(B_2 \psi)(x) := \exp(ix^2 \eta/2)\, \psi(x) \qquad \text{for } x \text{ a.e.}$$

Let $\mathcal{F}$ be the Fourier transform, and let $\tilde{B} = B_1 \mathcal{F} B_2$. The operator $\tilde{B}$ is unitary and, moreover,

$$\tilde{B} A(\beta) \tilde{B}^{-1} = x, \qquad \tilde{B}[A(\beta) + \eta x] \tilde{B}^{-1} = p$$

By Lemma 1, we have $U = \{0\}$ or $U = X$. This proves the theorem. ■

This theorem can be used to construct a counterexample to the conjecture of Moroz (1983, p. 333). Indeed, by the theorem, no pair of these operators have a common nontrivial invariant subspace; therefore, the system $\{A(\alpha)|\alpha \in \mathbb{R}\}$ satisfies the conditions of the conjecture. The operator $A(\alpha)$ is unitary equivalent to a Hamiltonian of a spinless particle in a linear potential. We use the unitary operator B_1 and the generalized eigenvectors of p to recover the system of the generalized eigenvectors of $A(\alpha)$:

$$e_\lambda^\alpha(x) := \exp[i(X\lambda/\alpha + X^3/3\alpha)]$$

$$A(\alpha)e_\lambda^\alpha = \lambda e_\lambda^\alpha$$

for $\alpha \neq 0$. Let now φ, η be two real-valued even functions in ϕ, and let

$$\psi^+(x) := \varphi(x)e^{i\eta(x)}, \qquad \psi^-(x) := \varphi(x)e^{-i\eta(x)}$$

Obviously, for nonconstant η, we have $\psi^+ \neq c\psi^-$ with $c \in \mathbb{C}$. On the other hand, let

$$\psi_\alpha^\pm(\lambda) := \int \psi^\pm(x)e_\lambda^\alpha(x)\,dx$$

Then

$$|\psi_\alpha^+(\lambda)|^2 = \int \varphi(x)\varphi(y)\exp\{i[\eta(x)-\eta(y)]\} \times \exp\{i[\lambda(x-y)/\alpha] + i(x^3-y^3)/3\alpha\}\,dx\,dy$$

and

$$|\psi_\alpha^-(\lambda)|^2 = \int \varphi(x)\varphi(y)\exp\{i[\eta(y)-\eta(x)]\} \times \exp\{i[\lambda(x-y)/\alpha] + i(x^3-y^3)/3\alpha\}\,dx\,dy$$

The substitution $x \mapsto -x$ and $y \mapsto -y$ transforms the first integral into the second one, since $\varphi(-x) = \varphi(x)$ and $\eta(-x) = \eta(x)$ and we conclude that

$$|\psi_\alpha^+(\lambda)|^2 = |\psi_\alpha^-(\lambda)|^2$$

Thus, the $A(\alpha)$ measurements, $\alpha \in \mathbb{R}$, cannot distinguish between the ensemble of particles prepared in the state ψ^+ and the ensemble of particles prepared in the state ψ^-, contrary to the assertion of the conjecture.

Remark 2. It can be easily seen that one also cannot distinguish between ψ^+ and ψ^- by position measurements or by momentum measurements.

3. In the Heisenberg picture of quantum mechanics the position observable in the jth direction at the moment of time t is represented by the operator

$$e^{itH}x_je^{-itH}, \qquad t \in \mathbb{R}$$

where H denotes the Hamiltonian of the system (assumed to be time-independent). The probability distribution of the experimental data obtained by conducting position measurements at the moment of time t upon an ensemble of particles prepared in the state ψ is given by the function

$$B \mapsto \langle \psi, e^{itH} \chi_B e^{-itH} \psi \rangle / \langle \psi | \psi \rangle$$

where B ranges over the Borel subsets of $\mathbb{R}^n$. The distribution of the results of the position measurements is determined by the mean values

$$\langle \psi | e^{itH} e^{i\lambda x} e^{-itH} \psi \rangle, \qquad \lambda \in \mathbb{R}^n$$

where $\lambda x := \sum_{j=1}^n \lambda_j x_j$. Let now

$$H(\rho) := -\Delta - \sum_{j=1}^{n} \rho_j x_j^2; \qquad \rho_j > 0, \quad 1 \le j \le n$$

It follows that the operator $H(\rho)$ is essentially self-adjoint on ϕ. To make use of Theorem 0, we choose $A = \lambda x$, $B = H(\rho)$, and $N = p^2 + x^2 + 1$. One can prove by induction on n that, in the notations of Theorem 0,

$$C_{2m} = \sum_{j=1}^{n} (-4\rho_j)^m \lambda_j x_j$$

$$C_{2m-1} = -\sum_{j=1}^{n} (-4\rho_j)^m \lambda_j p_j$$

so that

$$e^{itH} e^{i\lambda x} e^{-itH} = e^{iA(\lambda)}$$

with

$$A(\lambda) = \sum_{j=1}^{n} \lambda_j [\cos(2t\rho_j^{1/2})\, x_j - \tfrac{1}{2}\rho_j^{-1/2} \sin(2t\rho_j^{1/2})\, p_j]$$

Proceeding as in Section 2, we can calculate the generalized eigenfunctions

$$\{ e_{\eta_1} \otimes \cdots \otimes e_{\eta_n} | \eta_j \in \mathbb{R} \}$$

of the operator $A(\lambda)$:

$$e_{\eta_j}(x) := \exp(i\mu_j x_j + i\nu_j x_j^2), \qquad 1 \le j \le n$$

where

$$\mu_j = \mu_j(t, \eta, \rho) := 2\eta_j \rho_j^{1/2} [\sin(2t\rho_j^{1/2})]^{-1}$$

$$\nu_j = \nu_j(t, \rho) := \rho_j^{1/2} [\cot\,(2t\rho_j^{1/2})]$$

and

$$A(\lambda)(e_{\eta_1}\otimes\cdots\otimes e_{\eta_n})=\left(\sum_{j=1}^{n}\lambda_j\eta_j\right)(e_{\eta_1}\otimes\cdots\otimes e_{\eta_n})$$

Let

$$\tilde{\psi}(\eta):=\int_{\mathbb{R}^n}\psi(x)(e_{\eta_1}\otimes\cdots\otimes e_{\eta_n})(x)\,dx$$

The distribution of the results of position measurements at the moment of time t is determined by the map

$$\lambda\mapsto\langle\psi|e^{iA(\lambda)}\psi\rangle=\int\tilde{\psi}(\eta)\,e^{i\lambda\eta}\overline{\tilde{\psi}(\eta)}\,d\eta$$

or since the Fourier transformation is unitary, by the map

$$\begin{aligned}\eta\mapsto&|\tilde{\psi}(\eta)|^2\\ &=\int\psi(x)\bar{\psi}(y)\exp\{i[\mu(\eta,t,\rho)(x-y)\\ &\quad+\nu(t,\rho)(x^2-y^2)]\}\,dx\,dy\end{aligned}$$

The substitution $u=x-y$, $v=x^2-y^2$ transforms this integral into the following one:

$$\begin{aligned}&\int\psi\left(\frac{u+vu^{-1}}{2}\right)\overline{\psi\left(\frac{u-vu^{-1}}{2}\right)}\\ &\qquad\exp\{i[\mu(\eta,t,\rho)u+\nu(t,\rho)v]\}\tilde{u}^{-1}\,du\,dy\end{aligned}$$

where we let, for brevity,

$$\tilde{u}^{-1}=\prod_{j=1}^{n}u_j^{-1},\qquad (vu^{-1})_j=v_ju_j^{-1}$$

Thus, the distribution of the results of position measurements at the moment of time t is determined by the map

$$\eta\mapsto\mathcal{F}_\psi(\mu(\eta,t,\rho),\nu(t,\rho))$$

where $\mathcal{F}_\psi$ denotes the Fourier transform of the function

$$(u,v)\mapsto\psi\left(\frac{u+vu^{-1}}{2}\right)\overline{\psi\left(\frac{u-vu^{-1}}{2}\right)}\tilde{u}^{-1}$$

If $2t\rho_j^{1/2}\neq 0(\text{mod }\pi)$, $i\leq j\leq n$, we have

$$\{\mu(\eta,t,\rho)|\eta\in\mathbb{R}^n\}=\mathbb{R}^n$$

If, moreover, $\rho_i^{1/2}-\rho_j^{1/2}$ is irrational for $1\le i<j\le n$, then the set

$$\{\nu(t,\rho)|t\in\mathbb{R}\}$$

is a dense subset of $\mathbb{R}^n$. Thus, if this last condition is satisfied, the graph

$$\{[\mu(\eta,t,\rho),\nu(t,\rho)]|\eta\in\mathbb{R}^n,\ t\in\mathbb{R}\}$$

is dense in $\mathbb{R}^{2n}$, and we obtain the following statement:

Theorem 2. Suppose that $\rho_j>0$, $1\le j\le n$, and that $\rho_i^{1/2}-\rho_j^{1/2}$ is irrational for $1\le i<j\le n$ and let

$$H(\rho):=-\Delta-\sum_{j=1}^{n}\rho_j x_j^2$$

Then $H(\rho)$ is essentially self-adjoint on ϕ. Moreover, if ψ_1 and ψ_2 have continuous Fourier transform, $\psi_1\in X$, $\psi_2\in X$, and

$$\langle\psi_1|e^{itH(\rho)}f(x)\,e^{-itH(\rho)}\psi_1\rangle$$
$$=\langle\psi_2|e^{itH(\rho)}f(x)\,e^{-itH(\rho)}\psi_2\rangle$$

for all $f\in\phi$ and all $t\in\mathbb{R}$, so that (by Born's postulate) one can distinguish between the states ψ_1 and ψ_2 by a position measurement at no time, then $\psi_1=e^{ic}\psi_2$ in x for some $c\in\mathbb{R}$.

Proof. By assumption, $\mathscr{F}_{\psi_1}$ and $\mathscr{F}_{\psi_2}$ are two continuous functions on $\mathbb{R}^{2n}$ that, according to the above considerations, coincide on a dense subset. Therefore, $\mathscr{F}_{\psi_1}=\mathscr{F}_{\psi_2}$, so that

$$\psi_1\left(\frac{u+vu^{-1}}{2}\right)\psi_1\left(\frac{u-vu^{-1}}{2}\right)\tilde{u}^{-1}=\psi_2\left(\frac{u+vu^{-1}}{2}\right)\overline{\psi_2\left(\frac{u-vu^{-1}}{2}\right)}\,\tilde{u}^{-1}$$

for u, v a.e., and the assertion follows. ■

Remark 3. The potential $-\rho x^2$ is not physical. However, it can be approximated by a sequence of potentials $V_m\in\mathscr{C}_0^\infty(\mathbb{R}^n)$, $m=0,1,\ldots$, so that

$$V_m f\to(-\rho x^2)f \qquad (L^2\text{-convergence})$$

for each $f\in\phi$. Then (Reed and Simon, 1972), p. 292)

$$-\Delta+V_m\to H(\rho)$$

in the strong resolvent sense, and it follows that the sequence of functions

$$\lambda\mapsto\langle\psi|e^{it(-\Delta+V_m)}\,e^{i\lambda x}\,e^{-it(-\Delta+V_m)}\psi\rangle$$

converges uniformly (in λ) to the function

$$\lambda\mapsto\langle\psi|e^{itH(\rho)}\,e^{i\lambda x}\,e^{-itH(\rho)}\psi\rangle$$

for each ψ in $L^2 \cap L^1$ and each t. Since the Fourier transformation is continuous with respect to this type of convergence, the functions $\mathscr{F}_\psi$ can be arbitrarily good determined by measurements in the potentials V_m and therefore ψ_m may be determined with arbitrarily high precision.

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