

Quantum Maupertuis Principle

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According to the Maupertuis principle, the movement of a classical particle in an external potential $V(x)$ can be understood as the movement in a curved space with the metric $g_{\mu\nu}(x) = 2M[V(x) - E]\delta_{\mu\nu}$. We show that the principle can be extended to the quantum regime, i.e., we show that the wave function of the particle follows a Schrödinger equation in curved space where the kinetic operator is formed with the *Weyl-invariant Laplace-Beltrami* operator. As an application, we use DeWitt's recursive semiclassical expansion of the time-evolution operator in curved space to calculate the semiclassical expansion of the particle density $\rho(x; E) = \langle x | \delta(E - \hat{H}) | x \rangle$.

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The famous principle discovered in 1741 by Pierre Louis Maupertuis and refined by Hamilton and Jacobi laid the foundation to the geometric formulation of Newton's laws, and was an important stimulus for Einstein's general theory of relativity. In this note we want to point out that this geometric view of classical physics remains also valid in the quantum regime, i.e., the quantum mechanics of a particle in a potential $V(x)$ may be described alternatively by a Schrödinger equation in curved space with the Maupertuis metric

$$g_{\mu\nu}(x) \equiv 2M[V(x) - E]\delta_{\mu\nu}. \quad (1)$$

The Hamiltonian of this Schrödinger equation contains the *Weyl-invariant* (conformally-invariant) version

$$\Delta_W = \Delta - \frac{1}{4} \frac{D-2}{D-1} R. \quad (2)$$

of the Laplace-Beltrami operator

$$\Delta = g^{-1/2} \partial_\mu g^{1/2} g^{\mu\nu} \partial_\nu. \quad (3)$$

Our result supplies us with an answer to an old, very fundamental problem left open by Einstein's classical equivalence principle. That principle states that the classical laws of motion of a point particle can be derived from a coordinate transformation in spacetime whose inertial forces simulate the gravitational forces at the position of the particle. Since a quantum particle is always an extended object described by a wave packet, there can be a correction term ξR proportional to the curvature scalar R , whose size ξ is undetermined by the classical equivalence principle. The Quantum Maupertuis Principle fixes the size of the R -term.

1. Consider the *eikonal* of an arbitrary trajectory of a point particle moving in Euclidean space with a potential $V(x)$ which is defined as

$$S(E) \equiv \int \sqrt{g_{\mu\nu}^E(x) dx^\mu dx^\nu}, \quad (4)$$

with the Maupertuis metric (1). The integral (4) is a functional of the trajectory which may be parameterized

with the help of an arbitrary variable λ as $x^\mu(\lambda)$, and rewritten as

$$S(E) \equiv \int d\lambda \sqrt{g_{\mu\nu}(x(\lambda)) \dot{x}^\mu(\lambda) \dot{x}^\nu(\lambda)} \equiv l. \quad (5)$$

The right-hand side coincides with the invariant length of the trajectory.

According to Maupertuis, the eikonal $S(E)$ is extremal for the classical trajectory, i.e., the classical orbit is *geodesic*. If λ is chosen to coincide with the invariant length l , the extremization produces the geodesic differential equation

$$\frac{d^2 x^\delta}{dl^2} + \Gamma_{\alpha\beta}^\delta \frac{dx^\alpha}{dl} \frac{dx^\beta}{dl} = 0, \quad (6)$$

where $\Gamma_{\mu\nu}^\lambda$ are the Christoffel symbols

$$\Gamma_{\mu\nu}^\lambda = \frac{1}{2} g^{\lambda\sigma} (\partial_\mu g_{\sigma\nu} + \partial_\nu g_{\mu\sigma} - \partial_\sigma g_{\mu\nu}). \quad (7)$$

Inserting the metric (1), we see that Eq. (6) is fulfilled if the trajectory follows the Newton equation $x''^\mu = -\partial^\mu V$.

The Maupertuis metric (1) differs from the flat Euclidean metric $\bar{g}_{\mu\nu} \equiv \delta_{\mu\nu}$ only by a conformal factor

$$\Omega^2(x) \equiv 2M[V(x) - E], \quad (8)$$

it is therefore called *conformally flat*. The geometric properties of this space can be calculated directly as functions of $\Omega(x)$. We observe that under the *Weyl transformation* $\bar{g}_{\mu\nu}(x) \rightarrow g_{\mu\nu} = \Omega^2(x) \bar{g}_{\mu\nu}(x)$, the symbols (7) change like

$$\Gamma_{\mu\nu}^\lambda = \bar{\Gamma}_{\mu\nu}^\lambda + \Omega^{-1} (\delta_\nu^\lambda \partial_\mu \Omega + \delta_\mu^\lambda \partial_\nu \Omega - \bar{g}^{\sigma\lambda} \bar{g}_{\mu\nu} \partial_\sigma \Omega). \quad (9)$$

Because of this, the Riemann tensor defined by the covariant curl [1]

$$R_{\mu\nu\lambda}^\sigma = \partial_\mu \Gamma_{\nu\lambda}^\sigma - \partial_\nu \Gamma_{\mu\lambda}^\sigma - \Gamma_{\mu\lambda}^\tau \Gamma_{\nu\tau}^\sigma + \Gamma_{\nu\lambda}^\tau \Gamma_{\mu\tau}^\sigma \quad (10)$$

is related to $\bar{R}_{\mu\nu\lambda}^\sigma$ by

$$\begin{aligned} R_{\mu\nu\lambda}^\sigma &= \bar{R}_{\mu\nu\lambda}^\sigma \\ &+ \left(2\bar{g}_{\lambda[\nu} \delta_{\mu]\beta} \bar{g}^{\sigma\alpha} - 2\delta_{[\nu}^\sigma \delta_{\mu]\alpha} \delta_{\lambda\beta} + \delta_{[\nu}^\sigma \bar{g}_{\mu]\lambda} \bar{g}^{\alpha\beta} \right) \frac{(\partial_\alpha \Omega)(\partial_\beta \Omega)}{\Omega^2} \\ &+ \left(\delta_{[\nu}^\sigma \delta_{\mu]\alpha} \delta_{\lambda\beta} + \bar{g}^{\sigma\alpha} \bar{g}_{\lambda[\mu} \delta_{\nu]\beta} \right) \frac{\bar{\nabla}_\alpha \bar{\nabla}_\beta \Omega}{\Omega}, \end{aligned} \quad (11)$$

where $\bar{\nabla}_\mu v_\nu \equiv \partial_\mu v_\nu - \bar{\Gamma}_{\mu\nu}^\lambda v_\lambda$ stands for the covariant derivative, and $\bar{g}_{\lambda[\nu}\delta_{\mu]\beta}\bar{g}^{\sigma\alpha}$ is defined as the antisymmetrized expression $\bar{g}_{\lambda[\nu}\delta_{\mu]\beta}\bar{g}^{\sigma\alpha} \equiv \bar{g}_{\lambda\nu}\delta_{\mu\beta}g^{\sigma\alpha} - \bar{g}_{\lambda\mu}\delta_{\nu\beta}g^{\sigma\alpha}$. The Ricci scalar $R \equiv g^{\nu\lambda}R_{\mu\nu\lambda}^\mu$ is obtained from (10) as

$$R = \frac{\bar{R}}{\Omega^2} - 2(D-1)\bar{g}^{\alpha\beta}\frac{\bar{\nabla}_\alpha\bar{\nabla}_\beta\Omega}{\Omega^3} - (D-1)(D-4)\bar{g}^{\alpha\beta}\frac{(\partial_\alpha\Omega)(\partial_\beta\Omega)}{\Omega^4}. \quad (12)$$

Inserting $\Omega(x)$ from (8), this becomes

$$R = \frac{1-D}{4} \left[\frac{2\partial^\mu\partial_\mu V}{M(E-V)^2} + \frac{(D-6)\partial^\mu V\partial_\mu V}{2M(E-V)^3} \right]. \quad (13)$$

2. Consider now the quantum mechanics of the point particle of energy E in the potential $V(x)$. It is described by the Schrödinger equation

$$(\hat{H} - E)\psi(x) \equiv \left(\frac{\hat{\mathbf{p}}^2}{2M} + V(x) - E \right) \psi(x) = 0, \quad (14)$$

where $\hat{\mathbf{p}} \equiv -i\hbar\nabla$. Using the metric (1), this can be rewritten as $[\Omega^{-2}(x)\hat{\mathbf{p}}^2 + 1]\psi(x) = 0$, or as

$$[\hbar^2\Delta_W - 1]\psi(x) = 0, \quad (15)$$

where $\Delta_W \equiv \Omega^{-2}(x)\sum_\mu\partial_{x^\mu}^2$. It is easy to verify that this is equal to the Weyl-invariant combination (2) of the Laplace-Beltrami operator (3) and R .

Equation (15) is a simple but very fundamental result. The Maupertuis metric (1) governs not only the classical motion, but also the quantum mechanics, provided that the Laplace-Beltrami operator is extended to the Weyl-invariant form (2).

3. The advantage of the curved-space reformulation (15) of the Schrödinger equation (14) is that, in curved space, the particle is without a potential. It is a *free particle* moving through the Maupertuis metric (1). For such movements, there exist well-developed methods of calculating quantum properties pioneered by Bryce DeWitt [2, 3]. In particular, DeWitt has given a semiclassical expansion of the matrix elements of the resolvent operator

$$\langle x|\hat{\mathcal{R}}|x'\rangle \equiv \langle x|\frac{i\hbar}{\mathcal{E} - \hat{\mathcal{H}}}|x'\rangle, \quad (16)$$

where $\hat{\mathcal{H}}$ is a curved-space translation operator in some *pseudotime* parameter τ , and \mathcal{E} is the associated pseudoenergy. The pseudotime τ is commonly called *Schwinger time* or *fifth time*. The Green function $G(x, x') = \langle x|\hat{R}|x'\rangle$ can be written as an integral

$$G(x, x') = \int_0^\infty d\tau \langle x, \tau | x', 0 \rangle \quad (17)$$

over the pseudotime displacement amplitude

$$\langle x, \tau | x', 0 \rangle = \langle x | e^{-i(\hat{\mathcal{H}} - \mathcal{E})\tau/\hbar} | x' \rangle. \quad (18)$$

This amplitude satisfies the Schrödinger equation

$$i\hbar\partial_\tau \langle x, \tau | x', 0 \rangle = \hat{\mathcal{H}} \langle x, \tau | x', 0 \rangle \quad (19)$$

with the boundary condition in D dimensions

$$\langle x, 0 | x', 0 \rangle = \delta^{(D)}(x - x'). \quad (20)$$

The Lagrangian treated by DeWitt is

$$\mathcal{L} = \frac{1}{2}g_{\mu\nu}(x)\dot{x}^\mu\dot{x}^\nu. \quad (21)$$

This has the pseudotime Hamiltonian $\mathcal{H} = \frac{1}{2}g^{\mu\nu}(x)p_\mu p_\nu \equiv \frac{1}{2}p^\mu p_\mu$, where $g^{\mu\nu}(x)$ is the inverse of the metric $g_{\mu\nu}(x)$, and the action

$$\mathcal{A}(x, x'; \tau - \tau') = \int_{x, \tau}^{x', \tau'} d\tau \mathcal{L} = \frac{\sigma(x, x')}{\tau - \tau'}. \quad (22)$$

where $\sigma(x, x') \approx \frac{1}{2}g_{\mu\nu}(x)(x - x')^\mu(x - x')^\nu + \dots$ is the geodetic interval. The action depends on the pseudotime only via this ratio. This is a consequence of the “free motion” in the metric $g_{\mu\nu}(x)$.

From the Hamilton-Jacobi equations it follows that

$$\frac{\partial \mathcal{A}}{\partial x^\mu} = p_\mu = \frac{\sigma_\mu}{(\tau - \tau')}, \quad (23)$$

$$-\frac{\partial \mathcal{A}}{\partial \tau} = \frac{\sigma(x, x')}{(\tau - \tau')^2} = \mathcal{H} = \frac{1}{2}p_\mu p^\mu. \quad (24)$$

DeWitt gave the solution of the Schrödinger equation (19) as a power series in τ for the Hamiltonian

$$\hat{\mathcal{H}} = \frac{1}{2}(-\Delta + \xi R + m^2), \quad (25)$$

with an arbitrary parameter ξ . For small τ and x close to x' , the solution is simply

$$\langle x, \tau | x', \tau' \rangle \approx \frac{D_{\text{MV}}^{1/2}(x, x')}{(2\pi i \hbar s)^{D/2}} e^{i\sigma(x, x')/s\hbar}, \quad (26)$$

where $s \equiv \tau - \tau'$ and $D_{\text{MV}} \equiv \det[-\partial_\mu \partial'_\nu \sigma(x, x')]$ is the Morette-van Vleck determinant [4, 6]. For arbitrary s , the result is (26)

$$\langle x, \tau | x', \tau' \rangle = \frac{D_{\text{MV}}^{1/2}(x, x')}{(2\pi i \hbar s)^{D/2}} e^{i\sigma(x, x')/s\hbar} \sum_{n=0}^{\infty} a_n (is/2\hbar)^n, \quad (27)$$

where $D_{\text{MV}}^{1/2}(x, x') \equiv g^{1/4}(x)\Delta_{\text{MV}}^{1/2}(x, x')g^{1/4}(x')$ and $\Delta_{\text{MV}}(x, x')$ has the endpoint expansion (i.e., the derivatives are evaluated at the endpoint x)

$$\Delta_{\text{MV}}^{1/2} = 1 + \frac{1}{12}R_{\mu\nu}\sigma^\mu\sigma^\nu - \frac{1}{24}R_{\mu\nu;\rho}\sigma^\mu\sigma^\nu\sigma^\rho + \left(\frac{1}{288}R_{\mu\nu}R_{\rho\tau} + \frac{1}{360}R_{\mu\nu}^{\alpha\beta}R_{\alpha\rho\beta\tau} + \frac{1}{80}R_{\mu\nu;\rho\tau} \right) \sigma^\mu\sigma^\nu\sigma^\rho\sigma^\tau + \dots \quad (28)$$

DeWitt allowed for the presence of an extra term ξR in addition to the Laplace-Beltrami operator Δ on the right-hand side of (19). Then he derived a recursion relation for the expansion coefficients [2]

$$\sigma_\mu(a_0);^\mu = 0 \quad (29)$$

$$(n+1)a_{n+1} + \sigma_\mu(a_{n+1});^\mu = \Delta_{\text{MV}}^{-1/2} \left(\Delta_{\text{MV}}^{1/2} a_n \right);^\mu - \xi R a_n, \quad (30)$$

whose lowest terms are

$$a_1 = \left(\frac{1}{6} - \xi \right) R \quad (31)$$

$$a_2 = \frac{1}{6} \left(\frac{1}{5} - \xi \right) R;^\mu_\mu + \frac{1}{2} \left(\frac{1}{6} - \xi \right)^2 R^2 - \frac{1}{180} R_{\mu\nu} R^{\mu\nu} + \frac{1}{180} R_{\mu\nu\rho\sigma} R^{\mu\nu\rho\sigma}. \quad (32)$$

4. We now come to the announced application of the quantum Maupertuis principle by calculating the particle density of the Schrödinger equation (14)

$$\rho(x; E) \equiv \langle x | \delta(E - \hat{H}) | x \rangle = \frac{1}{2\pi\hbar} \text{disc} \left(\frac{i\hbar}{E - E_n} \right). \quad (33)$$

A simple algebra shows that

$$\langle x | \hat{R} | x' \rangle = \frac{1}{2} \langle x | \hat{R} | x' \rangle [V(x') - E]^{-1}. \quad (34)$$

Now we insert the DeWitt expansion (27) which reduces for $x = x'$ to

$$\langle x | \hat{R} | x \rangle = \frac{g^{1/2}(x)}{(2\pi i \hbar)^{D/2}} \sum_{n=0}^{\infty} a_n (-\partial_{m^2})^n \int_0^\infty \frac{ds e^{-im^2 s/2\hbar}}{s^{D/2}}, \quad (35)$$

where the integral is simply $\Gamma(1 - D/2)(m^2)^{D/2-1}$, so that the sum on the right-hand side becomes

$$\sum_{n=0}^{\infty} a_n \Gamma(n+1 - D/2) (m^2)^{D/2-(n+1)}. \quad (36)$$

To be used in in Eq. (34) we must take Eq. (35) for $\xi = (D-2)/4(D-1)$ and $m^2 = 1$ and evaluate a_n with curvature terms of the Maupertuis metric (1), where

$$\begin{aligned} \langle x | \hat{R} | x \rangle &= \left(\frac{M}{2\pi\hbar^2} \right)^{D/2} \left\{ \Gamma(1 - D/2) (V - E)^{D/2} \right. \\ &\quad - \frac{\hbar^2}{12M} \Gamma(3 - D/2) \partial_\mu \partial^\mu V (V - E)^{D/2-2} \\ &\quad \left. + \frac{\hbar^2}{24M} \Gamma(4 - D/2) \partial_\mu V \partial^\mu V (V - E)^{D/2-3} + \dots \right\}. \quad (37) \end{aligned}$$

The result is valid for $V(x) > E$ where the metric is positive. For $E > V(x)$ se use the property $V - E = e^{\mp i\pi}(E - V)$ to find the discontinuity across the cuts. Remembering the extra factor $(V - E)^{-1}$ in (34) we

obtain from the DeWitt expansion the particle density $\rho_{\text{DW}}(x; E) \equiv \langle x | \delta(E - \hat{H}) | x \rangle$ as

$$\begin{aligned} \rho_{\text{DW}}(x; E) &= \frac{1}{\pi} \left(\frac{M}{2\pi\hbar^2} \right)^{D/2} \sin \left(\frac{\pi D}{2} \right) \\ &\times \left[\Gamma(1 - D/2) (E - V)^{D/2-1} \right. \\ &\quad - \frac{\hbar^2}{12M} \Gamma(3 - D/2) (E - V)^{D/2-3} \partial_\mu \partial^\mu V \\ &\quad \left. - \frac{\hbar^2}{24M} \Gamma(4 - D/2) (E - V)^{D/2-4} \partial_\mu V \partial^\mu V + \dots \right], \quad (38) \end{aligned}$$

Now we employ the reflection formula for Gamma functions $\Gamma(1 - z)\Gamma(z) = \pi/\sin(\pi z)$ to find

$$\begin{aligned} \rho_{\text{DW}}(E; x) &= \left(\frac{M}{2\pi\hbar^2} \right)^{D/2} \left[\frac{1}{\Gamma(D/2)} (E - V)^{D/2-1} \right. \\ &\quad - \frac{\hbar^2}{12M} \frac{1}{\Gamma(D/2 - 2)} (E - V)^{D/2-3} \partial_\mu \partial^\mu V \\ &\quad \left. + \frac{\hbar^2}{24M} \frac{1}{\Gamma(D/2 - 3)} (E - V)^{D/2-4} \partial_\mu V \partial^\mu V + \dots \right]. \quad (39) \end{aligned}$$

This agrees with the result obtained from the original Schrödinger equation (14) $E > V(x)$ [6].

5. By virtue of the bilocal character of the DeWitt techniques in curved space, the expansion of $\langle x | \hat{R} | x \rangle$ exists also for the off-diagonal matrix elements $\langle x | \hat{R} | x' \rangle$ which serves to find also the off-diagonal particle density $\rho(x; E) \equiv \langle x | \delta(E - \hat{H}) | x' \rangle$ beyond the result stated in the literature [7].

6. The extra R -term found above is not universal. This can be seen by comparing the result with the quantum mechanics of another system in curved space: the hydrogen atom in momentum space. It obeys a Schrödinger equation

$$(\mathbf{p}^2 + p_E^2) \Psi(p) = \frac{2}{\hat{r}} \Psi(p). \quad (40)$$

Here \hat{r} is operator of the radial coordinate \mathbf{n} the momentum representation, and $p_E^2 = -2E$ (in natural units with $\hbar = a_H = E_H = 1$, where $a_H \equiv \alpha^2 \hbar / m_e c = \text{Bohr radius}$ and $E_H = \alpha^2 m_e c^2 = \text{Rydberg energy}$). By analogy with the previous approach we rewrite (40) as

$$\{ \frac{1}{4} [\hat{r}(\mathbf{p}^2 + p_E^2)]^2 - 1 \} \Psi(p) = 0. \quad (41)$$

Reordering this we can bring the two operators \hat{r} side by side to express \hat{r}^2 as $\sum_{\mu=1}^D \partial_{p^\mu}^2$, and (41) turns into the differential equation

$$\left(\frac{1}{2} \Delta_p - p_E^2 + 1 \right) \Psi = 0. \quad (42)$$

where Δ_p is now the Laplace-Beltrami operator in momentum space formed from the metric

$$g_{ij} = \frac{2}{(\mathbf{p}^2 + p_E^2)^2} \delta_{ij}, \quad (43)$$

which is again conformally flat. The associated curvature scalar is now $R = 2D(D-1)p_E^2$, so that (44) can be rewritten as

$$\left(\frac{1}{2}\Delta_p - \frac{R}{2D(D-1)} + 1\right)\Psi = 0. \quad (44)$$

Remarkably, the coefficient of the R -term in this momentum space problem does *not* correspond to the Weyl-invariant expression, where the subtracted R -term would have been $(D-2)R/8(D-1) = R/16$ for $D = 3$.

6. The result gives us the possibility of studying the quantum mechanics of an arbitrary potential problem using the well-developed techniques of curved-space quantum mechanics [2]. Conversely, it permits us to understand questions about the quantum mechanics in curved space from the knowledge of Schrödinger theory in flat space.

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- [1] We use the index conventions of the textbooks
H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets*, 5th ed., World Scientific (2009);
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- [5] J.H. Van Vleck, *The Correspondence Principle in the Statistical Interpretation of Quantum Mechanics*, Proceedings of the National Academy of Sciences, **2**, 1928.
- [6] See Eq. (4.262) in the above textbook on path integrals.
- [7] *ibid.* Eq. (4.266).

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