Semi-classical predictions of cosmological wave-packets from ridge-lines

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ABSTRACT: We introduce a concept of ridge-lines to investigate the semi-classical prediction from wave-packets with arbitrary width in conventional quantum mechanics and the Wheeler–DeWitt quantum cosmology. Two primary approaches are applied to the exact calculation of the ridge-lines, namely the contour and the stream approach. Moreover, aspects of these are discussed and compared to other scenarios and approaches, i.e. the narrow WKB wave-packets and the first-derivative test. As the main result, we show that the semi-classical predictions in toy models have more abundant solutions than in the classical theory, and most interestingly they may deviate from classical solutions due to the quantum corrections.
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### 1 Introduction

As the prevailing theory of gravitation, the general theory of relativity successfully describes classical gravitation, but has yet to be consistently quantised, despite the efforts of generations of physicists in over a hundred years.
One of the first attempts to quantise general relativity directly is the Wheeler—DeWitt approach, see e.g. [1, 2]. It begins with the Hamiltonian formulation of this theory by Arnowitt, Deser and Misner, and applies the quantisation scheme of Dirac, designed for constrained systems, including the Dirac spinors and the Maxwell theory, among others. This approach, also known as quantum geometrodynamics, is successful with the semi-classical methods of Wentzel—Kramers—Brillouin (WKB) [3] and Born—Oppenheimer [4], and has been applied to quantum models of universes and black holes.

Unfortunately, because of the constrained nature of general relativity (from another perspective, its diffeomorphism invariance), its quantised version à la Dirac lacks many properties that are crucial in conventional quantum theory. Particularly, a positive-definite scalar product of quantum states is difficult to define, rendering the non-existence of a Hilbert space, and of the analysis of self-adjoint operators. As a consequence, one cannot use the usual way to make predictions as in conventional quantum mechanics. This includes, on the one hand, interpreting the inner product as a probability amplitude; on the other hand, analysing self-adjoint operators and studying their spectra.

Quantum cosmology is an application of quantum geometrodynamics to the universe as a whole, see e.g. [1, ch. 8], where the Wheeler–DeWitt equation plays the central role. The emergence of classical trajectories can be realised if the forms of wave functions are similar to the “coherent states”, which strongly peak about a single classical trajectory [5]. However, such an analogue of “coherent state” can only be achieved for simple examples.

In contrast, the emergence of classical trajectories from wave-packets is relatively natural, where the wave-packets of universe are constructed by the superposition of wave functions, and follow the classical trajectories in configuration space, when their width becomes narrow [6–8]. This corresponds to the principle of constructive interference. Nevertheless, the correspondence between classical and quantum theories can only be implemented with the narrowness condition. In this work, we try to address these problems by porting conventional tools in physics and mathematics to this context, aiming to derive the classical prediction from wave-packet with arbitrary width.

The outline of topics in each section is as follows. In section 2, we summarise previous results of a two-dimensional minisuperspace model [9], which can be solved exactly and will be used as the basics to investigate the classical prediction from the corresponding wave-packets in this paper. Next, under the WKB approximation, we show that a narrow Gaussian wave-packet has “maxima” on the classical trajectory and can be compared to the one derived by the method of ridge-lines discussed later, that works for wave-packets with arbitrary width. In section 3, we construct a framework of stationary wave-packets, that makes sense for both the minisuperspace Wheeler–DeWitt equation and the stationary Schrödinger equation. The framework is then tested by the model of a two-dimensional hydrogen atom. In section 4, the concept of ridge-lines is introduced, and an intuitive approach, the first-derivative test, is applied to derive the ridge-lines from wave-packets. The deviation from classical theory emerges apparently near the turning point, which is interpreted as a quantum correction. In sections 5 and 6, we discuss two further approaches to find the ridge-lines as classical predictions from wave-packets with arbitrary width, one is the contour approach, the other one is the stream approach. We provide exact mathemat-
ical descriptions of ridge-lines, which were historically developed for Riemannian geometry with a Euclidean metric signature. Then we try to generalise these descriptions to the pseudo-Riemannian geometry with a Lorentzian metric signature, which is the usual case of minisuperspaces. After that, we apply both approaches in various examples, and discuss their advantages as well as deficits. The section 7 includes a discussion of the relation between these two approaches. Finally, we give a summary and conclusion in section 8, as well as proposals of prospective physical applications. The section A collects the WKB approach used in section 2.2.

2 A two-dimensional minisuperspace model

In this section 2, we study a prototype minisuperspace model that traces back to [9–11], which is described by the minisuperspace action

\[ S = \text{Vol}_3 \int dt M(t) \left\{ \frac{s}{2M(t)} \left( -\frac{3}{\kappa} \dot{\gamma}^2 + \frac{1}{2} \dot{\chi}^2 \right) + V e^{\varphi} \right\} \]

\[ = \int dt \left\{ \frac{1}{2M(t)} G_{IJ} q^I q^J - M(t) V(q) \right\}, \]

where \( s^2 = l^2 = v^2 = 1 \) are signs, \( v := \text{sgn} V; g > 0 \) is a coupling factor; \( G_{IJ} \)'s are the components of the inverse minisuperspace DeWitt metric [1], \( V \) the potential, and \( q^I \) denotes collectively the minisuperspace variables \( \{ \gamma, \chi \} \) in configuration space. One sees that \( M \) corresponds to a lapse function and has no dynamics, whereas \( \gamma \) and \( \chi \) are the dynamic variables.

This prototype model contains several homogeneous cosmological models as its special cases, including the closed Friedmann–Lemaître model with a free scalar field [1, sec. 8.1.2], the flat Friedmann–Lemaître model with a Liouville scalar field [9], and the vacuum Kantowski–Sachs model. Moreover, it is exactly solvable at both the classical and the quantum levels, which facilitates the further study of the model.

At the classical level, the trajectory in the minisuperspace spanned by \( (\gamma, \chi) \) has a uniform representation

\[ e^{\varphi \chi} \text{trig} \left( \sqrt{\frac{3}{2\kappa}} g (\gamma - \gamma_0) \right)^2 = \frac{\varphi \gamma_0^2}{12\text{Vol}_3^2 |V|}, \]

where \( \gamma_0 \) is a constant, trig is a trigonometric function which depends on the four possible signs \( (l, sv) \), see table 1.

At the quantum level, the dynamics of cosmology is governed by the Wheeler–DeWitt equation [12]

\[ 0 = H_\perp (\gamma, \chi, \frac{\hbar}{i} \partial_\gamma, \frac{\hbar}{i} \partial_\chi) \psi(\gamma, \chi) \]

\[ = \left[ \frac{\hbar^2}{\text{Vol}_3} \left( \frac{\kappa}{12} \gamma^2 - \frac{1}{2} \chi^2 \right) + \text{Vol}_3 V e^{\varphi \chi} \right] \psi(\gamma, \chi), \]
\[
\begin{array}{|c|c|}
\hline
(l, sv) & \text{trig}\left(\sqrt{\frac{3}{2g}}g(\gamma - \gamma_0)\right)^2 \\
\hline
(-, -) & -\sin\left(\sqrt{\frac{3}{2g}}g(\gamma - \gamma_0)\right)^2 \\
(-, +) & \sin\left(\sqrt{\frac{3}{2g}}g(\gamma - \gamma_0)\right)^2 \\
(+, -) & \sinh\left(\sqrt{\frac{3}{2g}}g(\gamma - \gamma_0)\right)^2 \\
(+, +) & \cosh\left(\sqrt{\frac{3}{2g}}g(\gamma - \gamma_0)\right)^2 \\
\hline
\end{array}
\]

**Table 1:** Four cases of the trigonometrical function in eq. (2.2). The first case \((-,-)\) does not leave a real and physical trajectory for \((\gamma, \chi)\); \((-,+\)) gives infinitely many isolated trajectories due to the periodicity of the sine function, \((+, -)\) gives two, and \((+, +)\) gives one.

\[
\begin{array}{|c|c|}
\hline
(l, sv) & \text{Bessel}_\nu(x) \\
\hline
(-, -) & c_1K_\nu(x) + c_2I_\nu(x) \\
(-, +) & c_1J_\nu(x) + c_2Y_\nu(x) \\
(+, -) & c_1F_{i\nu}(x) + c_2G_{i\nu}(x) \\
(+, +) & c_1K_{i\nu}(x) + c_2I_{i\nu}(x) \\
\hline
\end{array}
\]

**Table 2:** Four cases of the Bessel function in eq. (2.4). Branches that diverge at the infinite boundary are in grey, which are to be dropped. The remaining branches are all real and have no imaginary part.

which provides a naive solution

\[
\psi \propto e^{i\pi p_\gamma} \text{Bessel}_\nu(x), \quad \text{where} \quad \nu := \frac{1}{\hbar g} \sqrt{\frac{2\kappa}{3}} p_\gamma, \quad x := 2\sqrt{2} \sqrt{\text{Vol}_3 \sqrt{|V|}} \frac{e^{\omega /2}}, \tag{2.4}
\]

and \(\text{Bessel}_\nu(x)\) is the Bessel-type function of order \(\nu\), the type of which depends on the signs \((l, sv)\), see table 2, where \(F_{i\nu}(x)\) and \(G_{i\nu}(x)\) are the unmodified Bessel functions adapted to purely imaginary orders, defined in [13].

The \((l, sv) = (-, +)\)- and \((+, -)\)-branches are not essentially self-adjoint, which was discovered in [9]; a family of self-adjoint extensions is characterised by a number \(a \in [0, 2)\). For \((+, -)\), the spectrum is continuous, and the orthonormal eigenfunction corresponding to \(\nu\) is

\[
\Xi^{(a)}_{\nu}(y) = N_{\Xi, \nu}\left(F_{i\nu}(x) \cos \frac{\pi a}{2} + G_{i\nu}(x) \sin \frac{\pi a}{2}\right), \tag{2.6}
\]

where \(N_{\Xi, \nu}\) is the \(\delta\)-normalisation factor [9]. For \((-, +)\), the spectrum is discrete with

\[
\nu = 2n + a, \quad n \in \mathbb{N}, \tag{2.7a}
\]
and the corresponding orthonormal eigenfunctions read

\[ \Phi^{(n)}_n(y) = N_{J,n} J_{2n+a}(x), \quad (2.7b) \]

\[ \left( N_{J,n} \right)^{2} = \frac{1}{k(2n+a)}. \quad (2.7c) \]

These motivate the study of the minisuperspace model due to the potential of integrability.

### 2.1 An exact wave-packet

Like the stationary Schrödinger equation in conventional quantum mechanics, the Wheeler–DeWitt equation is also a linear differential equation. For a family of mode functions \( \{\psi_\nu\} \), which are complete integrals of the Wheeler–DeWitt equation, one could therefore choose an amplitude \( A(\nu) \) and construct a \textit{wave-packet}

\[ \Psi = \int d\nu A(\nu)\psi_\nu, \quad (2.8) \]

which is a general solution of the Wheeler–DeWitt equation, independent of any interpretations. It is scarce that an exact expression of a wave-packet in minisuperspace models can be found. In this section 2.1 we will study such a case.

Making use of [14, eq. (6.795.3)], we have

\[ \int_{-\infty}^{+\infty} d\nu \nu e^{i\nu y} K_{|\nu|}(x) = i\pi x e^{-x\cosh y} \sinh y, \quad (2.9) \]

and are able to construct the exact wave-packet for the \((+,+)\)-case of our prototype model in table 2,

\[ \Psi_{\text{lin}}(\gamma,\chi) \propto e^{\frac{2\pi}{\sqrt{3}}} \sinh \left( \frac{3}{2\pi} g(\gamma - \gamma_0) \right) \cdot \exp \left\{ -\frac{2\sqrt{2} \text{Vol}_3 \sqrt{|V|}}{\hbar g} e^{\frac{2\pi}{\sqrt{3}}} \cosh \left( \frac{3}{2\pi} g(\gamma - \gamma_0) \right) \right\}, \quad (2.10) \]

with an amplitude that “seems to be” \( A_{\text{lin}}(\nu) \propto p_\gamma \propto \nu \) (c.f. eq. (2.5)). This is a typical profile of the norm square \( |\Psi|^2 \) of a wave-packet in Wheeler–DeWitt quantum cosmology, which forms a tube around some classical trajectory in the asymptotic region, see fig. 1a.

One may wonder how an amplitude that is proportional to the “wave number” \( \nu \) can lead to a smooth wave-packet that makes physical sense. For example, if one naively takes plane waves \((2\pi)^{-1/2} e^{ikx}\) and uses a linear amplitude, one finds

\[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} dk ke^{ikx} = -i\sqrt{2\pi} \delta'(x) \quad (2.11) \]

which is 0 for \( x \neq 0 \).

The doubts can be dispelled if one considers the \textit{Schrödinger normalisation} of \( |\nu|\)(x), which is given in [15–17], leading to the true amplitude

\[ A_{\text{lin}}(\nu) \propto \frac{\nu}{N_{K,\nu}} \propto \frac{\sqrt{\nu}}{\sinh(\nu)} \text{sgn} \nu, \quad (2.12) \]
where we have used a δ-normalisation factor \( N_{K\nu} = k\nu \sinh(\pi \nu)/\pi^2 \) for \( K_{i\nu}(x) \). In turn, the normalisation condition for the amplitude \( f_{-\infty}^{+\infty} d\nu |A_{\text{lin}}(\nu)| = 1 \) gives

\[
A_{\text{lin}}(\nu) = \sqrt{\frac{2\nu}{\sinh(\nu)}} \sgn \nu .
\] (2.13)

To understand more about \( A_{\text{lin}} \), one can turn to the Gaussian amplitude that is popular in the literature, and compare the former with a modified version of the latter, which is flipped with respect to the \( x \)-axis for \( \nu < 0 \) and has the same second moment \( \langle \nu^2 \rangle \) as \( A_{\text{lin}} \). The second moment for the “linear” amplitude in eq. (2.13) reads

\[
\int_{-\infty}^{+\infty} d\nu \nu^2 |A_{\text{lin}}(\nu)|^2 = \frac{1}{2} .
\] (2.14)

One therefore uses the one-dimensional Gaussian distribution

\[
\text{GD}_1 \left( 0, \frac{1}{2} ; \nu \right) = \pi^{-1/2} e^{-\nu^2}
\] (2.15)

and constructs the amplitude as

\[
A_{\text{hfg}}(\nu) = \sqrt{\text{GD}_1 \left( 0, \frac{1}{2} ; \nu \right) \sgn \nu} = \pi^{-1/4} e^{-\frac{\nu^2}{2}} \sgn \nu .
\] (2.16)
The corresponding wave-packet, which is constructed numerically, is plotted in fig. 1b. One sees that it indeed resembles that with $A_{\text{lin}}$ in fig. 1a.

One may ask about a possible classical correspondence of this wave-packet, which many other wave-packets do have. Generally speaking, the familiar scenario would be that the wave-packet is constructed by superposing mode functions with quantum number $\nu \in \mathbb{R}$ by a normal Gaussian amplitude, that is centred at $\nu_0$. Then the claim is that, this wave-packet corresponds to the classical trajectory with a classical first-integral $\propto \nu$, see also [9, 18]. This approach is not viable here, since the amplitude is by no means a normal Gaussian one. We will focus on the issue of digging a classical trajectory out of a generic wave-packet in section 4, but before that, let us revisit the traditional WKB approach to derive the classical trajectory.

2.2 Narrow WKB Gaussian wave-packet

In this section 2.2, we study a special case, in which the wave-packet is constructed by superposing the WKB mode functions with a narrow Gaussian amplitude. The mathematical result confirms the heuristic idea, that such a wave-packet peaks near the classical trajectory, which shares the same integral constant as the centre of the Gaussian amplitude.

We begin with the two-dimensional case eq. (2.1b), so that the WKB wave function reads (see appendix A)

$$
\psi(q^1, q^2; \alpha) \approx \sqrt{D} \exp \left[ \frac{i}{\hbar} (S(q^1, q^2; \alpha) - \alpha \beta) \right],
$$

(2.17)

where the additional phase $\alpha \beta$ will become clear soon. The Gaussian wave-packet is the result of

$$
\Psi(q^1, q^2; \alpha, \sigma) = \int dA \psi(q^1, q^2; A) \frac{\text{GD}_1(\alpha, \sigma^2; A)^{1/2}}{\sqrt{2\pi\sigma^2}}.
$$

(2.18a)

$$
\text{GD}_1(\alpha, \sigma^2; A) := \exp \left( -\frac{1}{2} \sigma^{-2} (A - \alpha)^2 \right).
$$

(2.18b)

Applying Taylor’s theorem to the exponent of the integrand in eq. (2.18a) with respect to $A$ at $\alpha$ gives

$$
\psi(q^1, q^2; A) \frac{\text{GD}_1(\alpha, \sigma^2; A)^{1/2}}{\sqrt{2\pi\sigma^2}} = \exp \left[ \frac{i}{\hbar} \left( S(q^1, q^2; \alpha) - \alpha \beta \right) - \frac{1}{2} (A - \alpha)^2 d_1^{(2)} \right] g(A),
$$

(2.19)

where

$$
d_1^{(0)} := \frac{1}{\hbar} (S(q^1, q^2; \alpha) - \alpha \beta),
$$

(2.20a)

$$
d_1^{(1)} := \frac{1}{\hbar} (\partial_\alpha S - \beta),
$$

(2.20b)

$$
d_1^{(2)} := \frac{1}{2} \sigma^{-2} - \frac{i}{\hbar} \partial_\alpha^2 S;
$$

(2.20c)

$$
g(A) := \sqrt{D} \exp \left( \hbar(A - \alpha)^2 \right), \quad \hbar(\alpha) = 0.
$$

(2.20d)
Consider the WKB mode function plotted in fig. 2. Gaussian wave-packets of \( d \) near \( G \) are given that the wave-packet is constructed to be dominated in eq. (2.19), i.e. 
\[
\frac{\sigma}{d_1^{(2)}} \approx \exp \left( \frac{-\sigma^2}{d_1^{(2)}} \right)^{1/2} \left[ \partial_S d_1^{(1)} - \frac{d_1^{(1)}}{2d_1^{(2)}} \right]^2,
\]
and the corresponding Schrödinger density reads
\[
\rho = \rho(q^1, q^2; \alpha, \sigma) = |\Psi|^2 = \sqrt{2\pi} \frac{D}{\sigma d_1^{(2)}} \exp \left[ -\frac{\Re d_1^{(2)}}{d_1^{(1)}} \right]^2.
\]

Given that \( D, d_1^{(2)} \) and \( \Re d_1^{(2)} \) vary slowly with respect to \( (q^1, q^2) \), the peak of \( \rho \) dominates near \( d_1^{(1)} = 0 \), i.e. \( \partial_S S = \beta \) (c.f. eq. (A.16b)), which is just the classical trajectory. Narrow Gaussian wave-packets of \((-+, +), (+, -)\) and \((+, +)\) cases are summarized in table 3 and plotted in fig. 2.

The above result in two dimensions can easily be generalised to higher dimensions. Consider the WKB mode function
\[
\psi(q^i; \alpha_k) \approx \sqrt{D} \exp \left[ \frac{i}{\hbar} \left( S(q^1 \ldots q^n; \alpha_1 \ldots \alpha_m) - \sum_{k=1}^m \alpha_k \beta_k \right) \right],
\]
where \( m = n - 1 \) is the number of integral constants.

Choosing a non-degenerate \( m \)-dimensional Gaussian amplitude leads to the Gaussian wave-packet
\[
\Psi(q^i; \alpha_j, \Sigma_{jk}) = \int dA_1 \ldots dA_m \psi(q^i; A_k) GD_m(\alpha_k, \Sigma_{kl}; A_k)^{1/2},
\]
Figure 2: Narrow Gaussian wave-packets of the WKB mode functions with $S_{\pm}$ by eq. (2.22) as dashed contours, the expressions of which are listed in table 3. One sees that for each $S_{\pm}$, the wave-packet peaks around one asymptotic branch of the classical trajectory, which fails to hold near the turning point. Moreover, for the $(+, -)$- and $(+, +)$-cases, where $g\chi \to -\infty$ is a region that the corresponding Bessel functions are sinusoidal, the wave-packets form uniform tubes near the classical trajectory. For the $(-, +)$- and $(+, -)$-cases, where $g\chi \to +\infty$ is a region that the corresponding Bessel functions decay exponentially in amplitude, the wave-packets also decay.
where
\[
\text{GD}_m(\alpha_k, \Sigma_{kl}; A_k) := \frac{\exp\left[ -\frac{1}{2} \sum_{k,l=1}^{m} (\Sigma^{-1})_{kl} (A - \alpha)_k (A - \alpha)_l \right]}{\sqrt{(2\pi)^m \det \Sigma}}
\] (2.24b)
is the probability density function of the multivariate Gaussian distribution [19, ch. 5], 
\(m = n - 1\), and \(\Sigma\) is the non-degenerate, positive definite covariance matrix. The integral in eq. (2.24a) can also be estimated by the stationary phase method as
\[
\Psi(q^i; \alpha_k, \Sigma_{kl}) \approx \left( \frac{(2\pi)^m}{\det \Sigma} \right)^{1/4} \left( \frac{D}{\det d_m^{(2)}} \right)^{1/2} \cdot \exp \left[ id_m^{(0)} - \frac{1}{2} \sum_{k,l} \left( d_m^{(2)} \right)_{kl} \left( d_m^{(1)} \right)_k \left( d_m^{(1)} \right)_l \right],
\] (2.25)
where
\[
d_m^{(0)} := \frac{1}{\hbar} \left( S(q^i; \alpha^k) - \sum_{k=1}^{m} \alpha_k \beta_k \right),
\] (2.26a)
\[
\left( d_m^{(1)} \right)_k := \frac{1}{\hbar} \left( \partial_{\alpha_k} S - \beta_k \right),
\] (2.26b)
\[
\left( d_m^{(2)} \right)_{kl} := \left( \frac{1}{2} \Sigma^{-1} - \frac{i}{\hbar} \text{Hess}_{\alpha} S \right)_{kl};
\] (2.26c)
\[
(\text{Hess}_{\alpha} S)_{kl} := \partial_{\alpha_k} \partial_{\alpha_l} S.
\] (2.26d)
The Schrödinger density of the wave-packet reads
\[
\rho = \rho(q^i, \alpha_k, \Sigma_{kl}) = |\Psi|^2
\]
\[
= \sqrt{\frac{(2\pi)^m}{\det \Sigma} \frac{D}{\det d_m^{(2)}}} \exp \left[ -\text{Re} \left( \sum_{k,l} \left( d_m^{(2)} \right)_{kl} \left( d_m^{(1)} \right)_k \left( d_m^{(1)} \right)_l \right) \right].
\] (2.27)
The corresponding classical trajectory is \(\left( d_m^{(1)} \right)_k = 0\), or \(\beta_k = \partial_{\alpha_k} S\), which is identical to eq. (A.16a).

Therefore, we can be confident that a classical universe is likely to emerge from a quantum wave-packet constructed by a narrow Gaussian amplitude, and in regions where the WKB approximation is good. The amplitudes near the peak also seem to be constant. Departure from classical theory is expected where these conditions are violated, for example when the wave-packet spreads (and becomes wider), is damped (and the amplitude becomes smaller), or near the classical turning point (and the WKB approximation fails).

The idea of the “peak” of a wave-packet, that was used in eqs. (2.22) and (2.27), is heuristic. If a wave-packet does not have a form as in eqs. (2.22) and (2.27), the heuristic idea does not easily apply, which has already happened in eq. (2.10). One needs a mathematical description for this idea, which will be studied in section 4. One will see that in the contour approach of ridge-lines, as well as in the simple first-derivative test, the classical trajectories in eqs. (2.22) and (2.27) can be confirmed.
3 Stationary wave-packets

In quantum cosmology, the usual way of constructing a wave-packet is linearly superposing
the complete integrals \( \psi_\nu \), containing constants \( \nu \), of the Wheeler–DeWitt equation which
is comparable to the stationary Schrödinger equation in quantum mechanics,

\[
H\psi_\nu = E\psi_\nu ,
\]

the solution \( \psi_\nu \) to which is called the wave function of a stationary state, where \( \nu \) is another
quantum number that marks different states in a degenerate level. If one writes \( H_\perp = H - E \)
and fixes the energy level \( E \), eq. (3.1) becomes \( H_\perp \psi_\nu = 0 \), which looks identical to eq.
(2.3a). In this resemblance, constructing a wave-packet corresponds to the superposition of
degenerate stationary states in the same energy level, the result of which is also an energy
eigenstate of the same level.

We will call such a quantum wave-packet a stationary wave-packet, that encompasses
both conventional quantum mechanics and the Wheeler–DeWitt quantum cosmology. Relat-
ing a tentative theory of quantum gravitation to quantum mechanics can lead to analogue
models, which has been realised in the study of black holes [20–23] and quantum field theory
in curved space-time [24, 25]. For a review of analogue gravitation, see [26].

On the other hand, we noticed that the Rydberg or highly-excited atom, has indeed
a description of such a superposition as a wave-packet [27–29]. Independent of this exper-
imental aspect, in section 3.1 we introduce the two-dimensional hydrogen atom as a toy
model, and then construct stationary wave-packets in section 3.2. Meanwhile, we discuss
the choice of superposition amplitudes, arguing in favour of Gaussian, binomial and Pois-
son amplitudes, etc., which maximises the entropy. In the end, we turn to the study of the
classical limit, and verify the correspondence principles in section 3.3.

3.1 Two-dimensional hydrogen atom

Consider a spinless non-relativistic two-dimensional hydrogen atom, described by the action

\[
S = \int dt \left[ \frac{m}{2} \left( \dot{\varrho}^2 + \varrho^2 \dot{\varphi}^2 \right) + \frac{\alpha}{\varrho} \right] , \quad \alpha > 0
\]

in polar coordinates \((\varrho, \varphi)\). The classical trajectory can be solved in terms of the conserved
energy and angular momentum \((E, L)\) as

\[
\varrho = \frac{L^2}{m\alpha + \sqrt{m(2EL^2 + m\alpha^2)} \cos(\varphi - \varphi_0)} .
\]

For \( E < 0 \), the system is bounded, and the trajectory is an ellipse. Fixing \( \varphi_0 = 0 \), the
trajectory passing through \((\varrho, \varphi) = (\varrho_0, 0)\) and \((\varrho, \pi)\) can be worked out in terms of

\[
E = - \frac{\alpha}{\varrho_0 + \varrho_\pi} < 0 , \quad L = \pm \sqrt{\frac{2m\alpha}{\varrho_0^{-1} + \varrho_\pi}} .
\]
Upon canonical quantisation, the stationary Schrödinger equation reads

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 - \alpha / \varrho \right) \psi(\varrho, \varphi) = E \psi(\varrho, \varphi),
\]

(3.5)

where the Laplace–Beltrami operator

\[
\nabla^2 := \partial_{\varrho}^2 + \varrho^{-1} \partial_\varrho - \frac{1}{\hbar^2 \varrho^2} L^2, \quad L := -i \hbar \partial_\varphi
\]

(3.6)

is chosen. The stationary wave functions, with definite main and angular quantum numbers, are

\[
\psi_{nl}(\xi, \varphi) = P_{nl}(\xi) \Phi_l(\varphi),
\]

(3.7a)

\[
P_{nl}(\xi) = N_{nl} \xi^{\left|l\right|} e^{-\xi/2} G_{nl}(\xi),
\]

(3.7b)

\[
N_{nl} = \frac{1}{(2\left|l\right|)!} \left( \frac{(n + \left|l\right|)!}{(2n + 1)(n - \left|l\right|)!} \right)^{1/2},
\]

(3.7c)

\[
\Phi_l(\varphi) = (2\pi)^{-1/2} e^{i l \varphi}, \quad l = 0, \pm 1, \pm 2, \ldots ,
\]

(3.7d)

where

\[
\xi := \beta_n \varrho, \quad \beta_n := \frac{2m\alpha}{\hbar^2} \left( n + \frac{1}{2} \right)^{-1}
\]

(3.7e)

are the dimensionless radial coordinate, and \( G_{nl} \) can be given in terms of a Kummer’s [30] confluent hypergeometric function [31, sec. 13.2], Sonin’s [32, sec. 40] associated Laguerre polynomial [31, eq. (18.11.2)], or a Whittaker function [31, eq. (13.14.4)] as

\[
G(\xi) = _1F_1(\left|l\right| - n, 2\left|l\right| + 1, \xi) N_{nl}
\]

(3.8a)

\[
= L_{\mu}^{(a)}(\xi) \frac{a!}{(\mu + 1)_{2\left|l\right|}} N_{nl} \quad a = 2\left|l\right|, \quad \mu = n - \left|l\right|;
\]

(3.8b)

\[
= M_{\nu,\left|l\right|}(\xi) \xi^{-\left|l\right|/2} \xi / 2 N_{nl} \quad \nu = n + \frac{1}{2},
\]

(3.8c)

where \((a)_n := a(a - 1) \ldots (a - n + 1)\) is the Pochhammer’s [33] symbol [31, sec. 5.2(ii)]. Note that eq. (3.7c) is chosen such that eq. (3.7a) is normalised with respect to \( \xi \), rather than \( \varrho \). The energy levels for the bounded states are

\[
E_n := -\frac{m\alpha^2}{2\hbar^2} \left( n + \frac{1}{2} \right)^{-2}.
\]

(3.9)

The normalisation condition for scattering states \( E \geq 0 \) does not lead to a closed-form expression for the normalisation factor, see e.g. [34, eq. (2.28)]. For simplicity, we focus on the case \( E < 0 \) in the following.
3.2 Stationary wave-packets for the hydrogen atom

For bounded states of the two-dimensional hydrogen atom in eq. (3.2), one fixes $E$ or $n$ and chooses a probability amplitude for different $l$’s to construct a stationary wave-packet,

$$\Psi_{nq} := \sum_{k=-n}^{n} A_{nk;q} \psi_{nk}.$$  \hspace{1cm} (3.10)

We would like to find a choice for the $A_{nk;q}$’s, such that the expectation value of angular momentum

$$\langle \Psi_{nq}, L \Psi_{nq} \rangle = q \hbar,$$  \hspace{1cm} (3.11)

where $q \in [-n, n]$, $q \in \mathbb{R}$. Since $k \in [-n, n] \cap \mathbb{Z}$, a “natural” choice for the probability masses seems to be the binomial distribution, where the probability mass function is

$$BD(k; u, s) := \binom{u}{k} s^k (1-s)^{u-k},$$  \hspace{1cm} (3.12a)

$$\binom{u}{k} := \frac{u!}{k!(u-k)!},$$  \hspace{1cm} (3.12b)

$$k = 0, 1, \ldots, u, \quad s \in [0, 1].$$  \hspace{1cm} (3.12c)

In our case, the amplitude satisfies

$$|A_{nk;q}|^2 = BD\left(n + k, 2n, \frac{n + q}{2n}\right)$$

$$= (2n)^{-2n} (n-q)^{-k} (n+q)^{n+k} \binom{2n}{n+k}.$$  \hspace{1cm} (3.13a)

The most naive choice

$$A_{nk;q} = \sqrt{BD\left(n + k, 2n, \frac{n + q}{2n}\right)}.$$  \hspace{1cm} (3.13b)

leads to stationary wave-packets that “peak around” a classical trajectory for $|q| \lesssim n$, see fig. 3.

3.3 Ridge-line of a wave-packet and the correspondence principles

In quantum cosmology, people argue that the ridge-line of a wave-packet peaks along a classical trajectory [5]. This would be more convincing if the statement also holds for the stationary wave-packets in conventional quantum mechanics.

For the binomial wave-packets here, defined by eqs. (3.7a), (3.7d), (3.10) and (3.13b), we approximate the ridge by finding the two highest peaks of the wave-packet, and find the elliptic classical trajectory passing them, see fig. 3. The approximate ridge-line is described by the integral constants $(E_{ar}, L_{ar})$ given by eq. (3.4).

One sees that this approximation is good as $n$ increases, which fits Bohr’s correspondence principle [35], stating that the quantum system reproduces its classical behaviour in
Figure 3: Stationary wave-packets $|\Psi_{nq}(\xi, \phi)|^2$ of the two-dimensional hydrogen atom. The green lines denote a classical trajectory in eq. (3.3) with $\phi_0 = 0$, $E = E_n$ and $L = q\hbar$. The orange lines are the classical trajectories passing through the two highest peaks of the wave-packet, with the integral constants $(E, L)$ given by eq. (3.4). Apparently, the green line in fig. 3b fits the orange line better than in fig. 3a, but worse than in fig. 3c. In fig. 3d we show the normal projection of fig. 3c on the $\sin \phi = 0$ line (in logarithm scale). One sees that there are multiple maxima; the highest two were chosen for plotting fig. 3c.

the limit of large main quantum number $n$. This can be seen in fig. 4a, where one fixes $q/n$ and observes the relative difference between $(E_{ar}, L_{ar})$ and $(E_n, L)$ vanishes polynomially as $n \to +\infty$.

In our application, on the other hand, we are more concerned with fixed $n$ or $E_n$, and varying $q$. In this case, the ridge-line gets closer to the classical trajectory as the effective angular quantum number $q \to n^-$, in the sense that the relative differences between $(E_{ar}, L_{ar})$ and $(E_n, q\hbar)$ become smaller in the aforementioned limit, see fig. 4b. The differences, however, will not vanish. This correspondence phenomenon is relevant in quantum cosmology, where the “main quantum number” is to be fixed, and only the other quantum numbers in the degenerate “energy eigenspace” can change.
Figure 4: Correspondence principles shown in terms of the difference between $(E_{ar}, L_{ar})$ and $(E_n, q\hbar)$, where the former with subscript $ar$ denotes the integral constants that give a trajectory passing through the two highest peaks of the binomial wave-packet (fig. 3). In fig. 4a, the difference vanishes as $n \to +\infty$, which is accordance with Bohr. The solid line is the best fit with the generalised linear model \[ y = g^{-1}(\beta_0 + \beta_1 \ln n) \] with $g(y) = \ln y$. In fig. 4b, the difference becomes smaller as $q \to n^{-}$, but will not vanish; this correspondence phenomenon is relevant in quantum cosmology.

4 Ridge-lines of wave-packets

4.1 The conception of ridge-lines

In the remaining sections of this paper, we try to quantify the qualitative arguments in the literature, that a classical trajectory can be read off from wave-packets in specific forms. Intuitively, one may imagine the profile of a wave-packet as a terrain in its configuration space, where the hills and valleys are the most and least probable places to “find” the system. In physical geography, chains of mountains or hills stretch a distance, where the “highest points” form the ridge-lines; conversely, one can define the valleys or the dale-lines by the “lowest points”.

The ridge- and dale-lines are in some sense the generalisation of local maxima and minima, which are isolated points. The latter are also easier to be solved in terms of local extrema as $\nabla \rho = 0$ as necessary but not sufficient conditions, and distinguishing them is more involved. One may give a sufficient condition when the Hessian is non-singular, but when it is, more works need to be done. For simplicity and clearance, we will study the ridge- and dale-lines on the equal foot.

The ridge- and dale-lines have been studied by the computer scientists working on imaging and vision [37–39], where the ridge- and dale-lines have rich applications, especially in two-dimensional Euclidean geometry. In physical configuration spaces having a higher-dimensional (pseudo-)Riemannian geometry, the ridge- and dale-lines have not been much used, to our knowledge. In addition, the Euclidean experience from computer science also
needs to be thought twice.

From now on, we will not use the analogy with terrain any further, which we argue as follows. For terrain, the altitude has the dimension of length, which is comparable to the dimension of the geographic coordinates. For a wave-packet, in contrast, the dimension of its profile is not comparable to the dimensions of the configuration space coordinates; the former might be the inverse of the configuration volume if one has the Schrödinger normalisation condition in mind,

$$\int \text{dVol} |\Psi|^2 = 1,$$

which is dependent on the configuration space coordinates. Based on these considerations, we shall find an intrinsic description of the ridge-lines of a wave-packet, where the wave-packet is not to be plotted in an additional dimension.

4.2 First-derivative test and Hessian matrix

Heuristically, one can simply use the first partial derivative to find the ridge- and dale-lines. In two dimensions with Cartesian coordinates \((x, y)\), it reads

$$\rho_x = 0 \quad \text{or} \quad \rho_y = 0,$$

which is weaker than the extremum condition \(\rho_x = 0 \quad \text{and} \quad \rho_y = 0\).

Geometrically, eq. (4.2) can be interpreted as a directional extremum test, namely to find the extremum with respect to only the \(x\)- or \(y\)-direction.

Take the “linear” wave-packet in eq. (2.10) as an example. With \(\rho_{\text{lin}} = |\Psi_{\text{lin}}|^2\), the condition \(\partial_\chi \rho_{\text{lin}} = 0\) gives

$$e^{g\chi} \cosh \left[ \sqrt{\frac{3}{2\pi}} g(\gamma - \gamma_0) \right]^2 = \frac{g^2 h^2}{8\text{Vol}_2^2 |V|}.$$

Compared with eq. (2.2) and table 1, eq. (4.3) has exactly the form of a classical trajectory, with

$$p_\gamma^2 = \frac{3g^2 h^2}{2\pi}.$$

On the other hand, the condition \(\partial_\gamma \rho_{\text{lin}} = 0\) gives

$$e^{g\chi} \cosh \left[ \sqrt{\frac{3}{2\pi}} g(\gamma - \gamma_0) \right]^2 = \frac{g^2 h^2}{8\text{Vol}_2^2 |V|} \coth \left[ \sqrt{\frac{3}{2\pi}} g(\gamma - \gamma_0) \right]^4.$$

Since \(\coth \left[ \sqrt{\frac{3}{2\pi}} g(\gamma - \gamma_0) \right] \to 1\) as \(\sqrt{\frac{3}{2\pi}} g(\gamma - \gamma_0) \to \pm \infty\), eq. (4.5) also coincides asymptotically with a classical trajectory, with the same \(p_\gamma\) as in eq. (4.4). In contrast to eq. (4.3), one has two distinct trajectories, which approach the same classical trajectory in the above-mentioned asymptotic region, while they depart from the trajectory near the classical turning point. The result is plotted in fig. 5.

Now consider a classical trajectory that is implicitly given by an equation \(f(x, y) = 0\). This works only in two dimensions; for \(d\)-dimensions, \(d > 2\), one needs \(d - 1 > 1\) equations
to specify an implicit curve. One can intuitively imagine a wave-packet that “peaks around” this trajectory, the density of which is given by [5, eq. (6.3)]

$$\rho = e^{-f^2}, \quad (4.6)$$

so that the density $\rho$ peaks to 1 at $f = 0$, and is less than 1 for $f \neq 0$.

Using the first-derivative test with an arbitrary variable $x$, one has

$$0 = \partial_x \rho = -2f \partial_x f, \quad (4.7)$$

and therefore

$$f = 0, \quad \text{or} \quad \partial_x f = 0. \quad (4.8)$$

Hence the trajectory $f = 0$ is included in the result of the first-derivative test.

The first-derivative test is intuitive and easy to implement. However, it is not covariant under coordinate transformation; moreover, one can construct examples where the test does not give sensible results, see fig. 14b. One may imagine using the eigenvector field of the Hessian $\partial_i \partial_j \rho$ as the “principle directions” and perform a directional derivative test with respect to them. This is the approach in [39].

Unfortunately, the directional derivative test is not practical in higher dimensions, where no generic expression for roots of the algebraic eigenvalue equation exists. In addition, the smoothness of the eigenvector field is difficult to establish. Moreover, upon moving to (pseudo-)Riemannian geometry, one needs to deal with the $(1,1)$-Hessian tensor, which is not symmetric as a matrix, and the analysis is lost in challenging calculations. We now move forward to the other two approaches of ridge-lines.

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**Figure 5**: The first-derivative approach shown with the “linear” wave-packet in eq. (2.10). The orange and purple lines are the results from eq. (4.5), whereas the pink line is from eq. (4.3).
5 Classical predictions as contour ridge-lines

In subsection 5.1 we first describe the ridge-lines in terms of a certain character of the contour lines. One can imagine finding the \textit{locally most curved neighbourhoods} on the contour lines, the trajectory of which forms a ridge- or dale-line. The defining equation of this approach was first written down by Barré de Saint-Venant in 1852 \[40\] without derivation. We refer to \[39\] for a comprehensive explanation.

We will begin with the two-dimensional Euclidean case, where there are two equivalent definitions of the contour ridge-lines, both of which can be generalised to higher dimensions, as well as to (pseudo-)Riemannian geometry. For the “linear” wave-packet in eq. (2.10), the contour approach can directly be applied.

In this subsection 5.2 we establish a scenario with an exponential wave-packet, in which the contour approach gives intuitive results. We then generalise this scenario with a slowly varying amplitude and show that an intuitive result is still contained in the result. We show how the redundant results can be identified with a toy example.

5.1 The contour ridge-lines

First definition In topography, contour lines give the altitude intrinsically. One can formulate the ridge- and dale-lines in terms of the contour lines as follows \[41, \text{sec. 4.1}\]:

When representing ridges, contour lines are elongated towards ridge stretch and they are convex as they are turned towards the fall of the ridge or the ground...

Mathematically, one considers a $C^2$ real function $\rho(x,y)$, the contour lines $\gamma_c$ of which are given by the implicit equation $\rho \equiv c$.

Having the idea of “locally most curved neighbourhoods” in the introduction in mind, now let $\kappa(x,y)$ be a \textit{characteristic function}, such that the crossing of a ridge and the contour $\gamma_c$ is an extremum of $\kappa$ on $\gamma_c$. This gives the first definition of a contour ridge-line, namely the \textit{ridge-line is regarded as the locus of extrema of $\kappa$ under the constraint $\rho = c$}.

The statement can be formulated by the method of Lagrange multipliers,

\begin{align}
\text{d}\rho &= \lambda_c \text{d}\kappa, \\
\rho &= c,
\end{align}

where $\lambda_c$ is the Lagrange multiplier. Equation (5.1a) can be separated into a system of equations in the bases $\text{d}x$ and $\text{d}y$. Then eliminating $\lambda_c$ gives

\begin{equation}
0 = \rho_x \kappa_y - \rho_y \kappa_x,
\end{equation}

where “,” denotes partial derivative \[42, \text{eq. (2.25)}\].

In practice, one can use the squared norm of $\text{d}\rho$ as the characteristic function

\begin{equation}
\kappa = \kappa_{\text{sq}}(x,y) = \rho_x^2 + \rho_y^2.
\end{equation}

Substituting eq. (5.3) in eq. (5.2) results in the \textit{de Saint-Venant equation for ridges (dSVr)} \[37, 40\]

\begin{equation}
0 = \rho_{x} \rho_{y}(\rho_{x,x} - \rho_{y,y}) - (\rho_{x,x}^2 - \rho_{y,y}^2) \rho_{x,y}.
\end{equation}
Second definition  To see the mathematical structure more clearly, we use the generalisation of eq. (5.3) in eq. (5.7). Substituting the latter in eq. (5.1a) gives the tensorial equation
\[ \rho_{;i} = 2\lambda c \rho_{;j} \rho_{;j} \cdot \]
In other words, \( \rho^{ij} \) is an eigenvector of its Hessian \( \rho^{ij,j} \). This gives the second characteristic of a contour ridge-line: it is the locus of points where the gradient is an eigenvector of the Hessian.

Generalisations  The results above in two dimensions can easily be generalised to higher dimensional (pseudo-)Riemannian spaces. From eq. (5.1a) one can derive
\[ 0 = d\rho \wedge d\kappa, \]
which takes the place of eq. (5.2). For eq. (5.3), the generic version reads
\[ \kappa^{\text{sq}} = \ast^{-1}(d\rho \wedge \ast d\rho) = d\rho^\flat \ast d\rho = g^{ij} \rho_{;i} \rho_{;j}, \]
where \( \ast \) is the Hodge star operator [43, sec. 28], \( \ast \) is a musical isomorphism, \( \ast \) is the interior product or contraction [43, sec. 23], \( g^{ij} \) is the inverse metric, and the symbol \( \ast \) denotes the covariant derivative with respect to an affine connection [44, sec. 85].

Inserting eq. (5.7) in eq. (5.6) gives the covariant dSVr equation
\[ 0 = d\rho \wedge d\left(d\rho^\flat \ast d\rho\right). \]
This equation is to be understood as imposing all its components to be zero, and therefore defining an implicit curve.

Application to the “linear” wave-packet  The contour approach can immediately be applied to the “linear” wave-packet in eq. (2.10). Using the DeWitt metric in eq. (2.1b), the de Saint-Venant equations for ridges (5.8) can be factorised such that
\[ 0 = y, \quad \text{or} \quad 0 = x^3 \sinh(y)^4 - x^2 \cosh(y) \sinh(y)^2 - x \cosh(y)^2 + \cosh(y), \]
where \( x > 0 \) is given in eq. (2.5), \( y = \sqrt{\frac{3}{2\kappa}} g(\gamma - \gamma_0) \). One can solve \( x \) from eq. (5.9b) in terms of \( y \),
\[ 3x_k = 1 + 4 \cos \frac{2k\pi + \arctan\left[19 - 8\cosh(2y), 3\sqrt{48\cosh(2y) - 33}\right]}{3}, \]
\[ k = 0, 1, 2, \]
where \( \arctan(x, y) \) gives \( \varphi \in [0, 2\pi) \) such that \( \cos \varphi = \frac{x}{\sqrt{x^2 + y^2}}, \ \sin \varphi = \frac{y}{\sqrt{x^2 + y^2}}. \)

In eq. (5.10), since
\[ \lim_{y \to \infty} \arctan\left[19 - 8\cosh(2y), 3\sqrt{48\cosh(2y) - 33}\right] = \pi, \]

\[ -19 - \]
one obtains
\[
\lim_{y \to \infty} x_k = (-)^{k+1} \chi.
\] (5.12)

Therefore, the cases \( k = 0 \) and \( 2 \) give positive \( x \) and real \( \chi \) as \( \chi \to \infty \), whereas \( k = 1 \) does not. Exact calculation shows that \( x_2 < 0 \) for all \( y \in \mathbb{R} \), and is to be excluded.

These results are plotted in fig. 6. One sees a redundant line \( y = 0 \) that is a dale, a pink line that resembles a classical trajectory, and two further solid lines that converge to the same classical trajectory as \( \gamma \to \pm \infty \). Nevertheless, the deviation from classical trajectory is apparent. More precisely, the classical prediction from the ridge-lines by the contour approach does not match the classical trajectory around the turning point, which can be regarded as quantum correction to the classical theory.

**Curvature as the characteristic function**  In two dimensions, it is tempting and intuitive to use the curvature of the contours as the characteristic function. We argue that this choice will not fit our purpose. Upon generalising to higher dimensions, the curvature of an \((n-1)\)-dimensional contour becomes the scalar-valued second fundamental form, which is a symmetric tensor. One may want to further analyse this tensor, and study its orthonormal eigenvectors [39].

Unfortunately, for the cases where the (DeWitt) metric is indefinite (e.g. Lorentzian), the second fundamental form is defined differently for the time- and space-like patches [45, sec. 1.2.4], which discontinues at the null edge, where the second fundamental form is again defined differently [46]. The reason is that, for time- and space-like hypersurfaces, the second fundamental form depends on the choice of a unit normal vector, which of course discontinues going from a time-like patch to a space-like patch. Moreover, the eigenvectors of the second fundamental form may also not exist ([45, sec. 2.5.(2)]).
The contour ridge-line is based on first- and second-derivatives of \( \rho \) and always give equations for an algebraic curve. However, aside from sensible ridge-lines, this approach also gives counter-intuitive curves.

5.2 Aspects of the contour approach

**Invariance under regular transformation and applications** For a transformation \( \rho \to F \circ \rho \), the dSVr equation (5.8) transforms to
\[
0 = \left( \frac{dF}{d\rho} \right)^3 \frac{\delta \rho}{\delta \rho} \wedge d\left( \frac{\delta^2 \rho}{\delta \rho} \right). \tag{5.13}
\]
If \( F \) is strictly monotonic, i.e. \( \frac{dF}{d\rho} \neq 0 \), the extra factor is non-zero, and eq. (5.13) gives the same ridge-line as eq. (5.8).

Now we move back to the two-dimensional wave-packet eq. (4.6). Since \( e^x \) increases monotonically with respect to \( x \), applying the above-mentioned property gives the ridge-line
\[
0 = d(f^2) \wedge d\left( \frac{d(f^2)^2}{df} \right)
= 8f^3 df \wedge \left( \frac{df^2}{df} \right), \tag{5.14}
\]
which means
\[
0 = f \quad \text{or} \quad 0 = df \wedge \left( \frac{df^2}{df} \right). \tag{5.15a/b}
\]
Equation (5.15a) gives what we wanted to set up, whereas eq. (5.15b) gives the ridge- (or dale-)line of \( f \) itself.

This is easier to see with the toy example
\[
f(x,y) = y - x^2, \tag{5.16}
\]
so that \( f = 0 \) gives the parabola \( y = x^2 \). There is an additional solution to the dSVr equation, \( x = 0 \), satisfying eq. (5.15b). See fig. 7.

The parabola \( y = x^2 \) is what we wanted. However, we also get \( x = 0 \), which is a dale-line for the density function \( f = y - x^2 \); as for \( \rho = e^{-f^2} \), it is a ridge-line for \( y < 0 \), and a dale line for \( y > 0 \). This line is a concrete mathematical result, although it does not fit our expectation.

**Modulation and redundant lines** The results for the wave-packet in eq. (4.6) can be generalised to the narrow wave-packet with varying amplitude
\[
\rho(x,y) = g(x,y)e^{-\frac{(x,y)^2}{2\sigma^2}}, \tag{5.17}
\]
where \( \sigma \) is a constant, \( \sigma \ll |\nabla g| \) characterising the narrowness, and \( g \) is a modulation. Substituting eq. (5.17) into eq. (5.4) gives
\[
0 = g^3 f^3 (p_{rs} q_{rs}(r_{rs} - t_{rs}) - (p_{rs}^2 - q_{rs}^2) s_{rs}) + O(\sigma^2), \tag{5.18}
\]
Figure 7: Density function $\rho = e^{-(y-x^2)^2}$ and the contour ridge-lines, which are $x = 0$ (green, ridge-line for $y < 0$ and dale-line for $y > 0$) and $y = x^2$ (orange). Incidentally, these lines are also given by the first-derivative test $\rho_x = 0$, $\rho_y = 0$.

where $(p_f, \ldots, t_f)$ are the symbols with respect to $f$.

As $\sigma \to 0^+$, the wave-packet becomes sharper and sharper; except for an additional factor $g^3$, the leading-order dSVr equation recovers the case without modulation. At the limit $\sigma = 0^+$, the wave-packet becomes a wall with zero width, and extends along the classical trajectory $f = 0$. Equation (5.18) shows that a slow modulation does not drastically change the ridge-lines.

The narrow WKB Gaussian wave-packets in section 2.2 is an instance of this model. The heuristic arguments we used in that section can now be replaced with the derivation in eq. (5.18).

Exact calculation reveals that the approximation we used to derive eq. (5.18) loses details. To see this, we also modulate eq. (5.16) by

$$g = e^{-2\epsilon y}, \quad \epsilon = \frac{1}{2}, \frac{1}{10}.$$  \hspace{1cm} (5.19)

The dSVr equation for $\rho = g e^{-(y-x^2)^2}$ with $g$ given in eq. (5.19) reads

$$0 = 16x[-2y^3 + 2y^2 (3x^2 - \epsilon) + y(-6x^4 + 8\epsilon x^2 + \epsilon)] + 2x^6 - 6\epsilon x^4 - \epsilon x^2 + \epsilon^2,$$  \hspace{1cm} (5.20)

which has been factorised into $x = 0$, and a term cubic in $y$. One can solve $y$ in terms of $x$ from the factor in a square bracket, where the three roots $y = y(x)$ are all real. See fig. 8.

Only one of the three roots approaches $y = x^2$ as $x \to \infty$. This can be seen by expanding $y(x) - x^2$ at $\epsilon = 0^+$, which yields

$$y_{1,2}(x) - x^2 = \pm \sqrt{\frac{1 + 4x^2}{2}} e^{1/2} + \left(-1 + \frac{1}{1 + 4x^2}\right) \frac{\epsilon}{2} + O(\epsilon^{3/2}),$$  \hspace{1cm} (5.21a)

$$y_3(x) - x^2 = -\epsilon \frac{1}{1 + 4x^2} + O(\epsilon^2).$$  \hspace{1cm} (5.21b)
\( (a) \rho = e^{-(y-x^2)^2-y/2} \)

\( (b) \rho = e^{-(y-x^2)^2-y/10} \)

**Figure 8**: Density function \( \rho = g e^{-(y-x^2)^2} \) and the contour ridge-lines for \( g = e^{-y/2} \) and \( g = e^{-y/10} \) with a Euclidean metric. The green line \( x = 0 \) and the orange line are (qualitatively) the same as in fig. 7; however, the dSVr equation (5.8) also gives the purple and the pink lines, which are apparently neither ridge- nor dale-lines.

As \( x \to \pm \infty \), \( y_3 - x^2 \) converges to 0, whereas \( y_{1,2} - x^2 \) diverge, and can be interpreted as the locus of the "locally flattest places on the contour", resembling \( x = 0 \) for \( y = x^3 \).

The extra curves in eq. (5.21a) seem to be a common feature of the dSVr equation. Here we have managed to remove them by asymptotic analysis at infinity, recovering the intuitive result \( y_3 \). The extra line \( x = 0 \) has been discussed at the end of the last part.

**Two-dimensional hydrogen atom revisited**  The binomial stationary wave-packets of two-dimensional hydrogen atom, described in section 3, can also be studied by the contour approach. For \( n = 1 \), the dSVr equation is a sextic equation with respect to the dimensionless radial coordinate \( \xi \), which has a quadratic and a quartic factor

\[
0 = -x^2(\sqrt{\ldots \cos \varphi - 1})^2 \\
+ x\left(\sqrt{\ldots \cos(2\varphi) + 3\sqrt{\ldots ^2} - 6\sqrt{\ldots \cos \varphi + 2}\right) \\
+ \sqrt{\ldots (2\cos \varphi - 3\sqrt{\ldots )}, \quad \text{or}
\]

\[
0 = +4x^4(\sqrt{\ldots \cos \varphi - 1})^3 \\
+ x^3\left[-4\sqrt{\ldots ^3 \cos(3\varphi) + 30\sqrt{\ldots ^2 \cos(2\varphi) - 4(5\sqrt{\ldots ^2} + 16)\sqrt{\ldots \cos \varphi + 38\sqrt{\ldots ^2} + 20} \right] \\
+ x^2\left[6\sqrt{\ldots ^2} + 2(3\sqrt{\ldots ^2} + 8) \cos \varphi \\
- 5\sqrt{\ldots \cos(2\varphi) \right] - 74\sqrt{\ldots ^2} - 28} \right]
\]

\[
+ 4x \left[-2(3\sqrt{\ldots ^2} + 4) \sqrt{\ldots \cos \varphi + 13\sqrt{\ldots ^2} + 2} \right. \\
- 12\sqrt{\ldots ^2},
\]

(5.22b)
Figure 9: Stationary wave-packet $\Psi_1,23(\xi,\varphi)^2$ of the two-dimensional hydrogen atom with $n = 1$, $q = \frac{23}{24}$. See section 3 for details. The thick lines with colour are solutions of the dSVr equation, whereas the dash-dotted line is the “best-fit trajectory” that crosses the maxima, adapted from the orange line in fig. 3b. The discontinuities within the same color are a numerical artefact.

where $\sqrt{\cdots} := \sqrt{1 - q^2}$. We are therefore able to obtain solutions in terms of roots. Aside from $\sin \varphi = 0$, there are six solution $\xi = \xi(\varphi)$, three in which are real and positive near $\varphi = 0$ and $\varphi = \pi$; one is from the quadratic factor and has a simple form, while the other two are very complicated. We managed to plot them in fig. 9.

One sees that the orange ridge given by the dSVr equation is very close to the “best-fit trajectory” that passes through the maxima of the wave-packet. Like in the case $\rho = g e^{-f^2}$, there are two additional lines, which might be the locally flattest points of the contours.

**Lorentzian signature** In quantum cosmology, the minisuperspace DeWitt metric usually has a Lorentzian signature. For the Lorentzian metric

$$ds^2 = -dt^2 + dx^2,$$

(5.23)

the Lorentzian dSVr, according to eq. (5.8), reads

$$0 = -\rho_x\rho_t(\rho_{xx} + \rho_{tt}) + (\rho^2_x + \rho^2_t)\rho_{xt}. \quad (5.24)$$

In fig. 6, we have already shown a sensible result with contour ridge-lines in a Lorentzian signature.

For the $\rho = g e^{-f^2}$ model, we can also mimic the scenario by replacing $y \to t$ in eqs. (5.16) and (5.19), and using the metric in eq. (5.23). The result can still be factorised to $x = 0$ and a cubic algebraic equation with respect to $t$, see fig. 10.

Intriguingly, none of the three curves given by the latter factor lies on the intuitive ridge globally; instead, for the turning and asymptotic regions, there is one branch for each case that fits well with intuition.
Figure 10: Density function $\rho = e^{-(t-x^2)^2-t/2}$ and the contour ridge-lines for $g = e^{-t/2}$ and $g = e^{-t/10}$ with an Lorentzian metric (5.23). The green line $x = 0$ is the same as in figs. 7 and 8. The orange line fits intuition better near $x = 0$, whereas the other two lines both have a sharp turning point, and one of the branches fits the intuitive ridge in the asymptotic region.

6 Classical predictions as stream ridge-lines

Now we consider the ridges in terms of singular stream-lines of the gradient vector field, which dates back to Rudolf Rothe in 1915 [47]. Heuristically, one imagines that water slowly flows from the top of a hill along the stream-lines of the gradient vector field. The water stream diverges from a ridge and converges to a dale. This is the intuitive notion of the singularity of the stream-lines along ridge- and dale-lines.

The stream approach is also adapted by modern computer scientists in image processing and computer vision [37, 38]. The mathematics behind this approach is the inverse integral factor and inverse Jacobi multiplier, which work for two- and higher-dimensional cases, respectively [48, 49]. We will focus on the two-dimensional case.

After a general discussion in section 6.1, we examine two families of density function, for which the stream ridge-lines can be exactly solved in section 6.2. We then show that the toy model $\rho = e^{-(y-x^2)^2}$ introduced in section 5.2 belongs to one of the families. In the end we investigate the cases with a Lorentzian metric signature.

6.1 The stream ridge-lines

Inverse integral factor In $\mathbb{R}^2$ with Cartesian coordinates $(x, y)$, the contours of $\rho$ are defined by $d\rho = 0$, or $\rho = c$; dual to them are the stream-lines, characterised by $dw = 0$ or $w = c$, where

$$\theta \, dw = \star d\rho = -\rho_y \, dx + \rho_x \, dy,$$

(6.1)
in which \( \theta \) compensates the non-integrability of the right-hand side and is therefore called an inverse integral factor. One also has

\[
0 = \rho_{,x} w_{,x} + \rho_{,y} w_{,y} = \star^{-1}(d\rho \wedge \star dw).
\]

(6.2)

\((\theta, w)\) is unique up to

\[
\theta \rightarrow \theta/F(w) , \quad w \rightarrow F(w) ,
\]

(6.3)

where \( F(w) \) is an arbitrary function. One may worry that this arbitrariness renders the stream approach not giving definite results, which fortunately does not seem to be the case, see section 7.

One sees that if \( \theta = 0 \) and \( \rho_{,x} \neq 0 \neq \rho_{,y} \) at \((x_0, y_0)\), \( w \) cannot be expanded by the Taylor theorem at \((x_0, y_0)\), since the linear term blows up by eq. (6.1) \[47, \text{sec. 7}\]. \((x_0, y_0)\) is said to be on a singular stream-line.

One can imagine that if the ridge- and dale-lines are required also to be stream-lines themselves, then the neighbouring stream-lines converge to the former, and diverge from the latter along the direction of the gradient vector field. In other words, stream ridge- and dale-lines are singular stream-lines. It has been shown that along these stream-lines, one has \[48\]

\[
\theta(x, y) = 0 .
\]

(6.4a)

The integrability condition \( d \wedge dw = 0 \), or \( \theta_{,xy} = \theta_{,yx} \), gives the differential equation for \( \theta \),

\[
\rho_{,x} \theta_{,x} + \rho_{,y} \theta_{,y} = (\rho_{,xx} + \rho_{,yy}) \theta .
\]

(6.4b)

Equations (6.4a) and (6.4b) define the stream ridge- and dale-lines.

Generalisations The results above in two dimensions can readily be generalised to \( n \)-dimensional curved spaces. Consider local coordinates \((x^1, \ldots, x^n)\), \( n \geq 2 \). The gradient vector field \( v \) of \( \rho \) is given by

\[
v^i \partial_i \equiv v = d\rho^i := g^{ij} f_j \partial_i .
\]

(6.5)

One has \((n - 1)\) linearly independent \(w\)’s for the stream-lines, satisfying

\[
0 = v^i \partial_i w = v(w) ,
\]

(6.6)

which is the generalisation of eq. (6.2). They are nothing else but the \((n - 1)\) first integrals \[50\], that require \((n - 1)\) inverse integral factors \( \theta \).

Similar to eq. (6.1), one has for instance

\[
\theta \, dw = v^1 \, dx^j - v^j \, dx^1 , \quad 2 \leq j \leq n ,
\]

(6.7)

given \( v^i \neq 0, 1 \leq i \leq n \). All of the \( \theta \)’s satisfying the linear, first-order partial differential equation

\[
v^i \theta_{,i} = \theta v_i , \quad \text{or} \quad v_{,i} \, d\theta = \theta \, d^i v^i ,
\]

(6.8)
where \(d^1\) is the codifferential or the adjoint [43, sec. 29]. The solutions to eq. (6.8) are called inverse Jacobi multipliers [49], first appeared in [51].

For Riemannian geometry, the stream approach seems to always give sensible results, in contrast with the contour approach and the simple first-derivative test. However, the approach involves giving the general integral [52, sec. 3.1.2] of the partial differential equation (6.6) or (6.8), which is only possible in very limited cases. Moreover, Lorentzian geometry gives rise to counter-intuitive configurations of gradient vector fields, where the time-like component of the gradient one-form fields is flipped. This leaves us problems that are yet to be solved. See sections 7 and 6.2.

6.2 Aspects of the stream approach

Stream ridge-lines of two function families

For density functions of the following two forms

\[
\rho(u, v) = f(f^u(u) + f^v(v)), \tag{6.9a}
\]

\[
\rho(u, v) = f(f^u(u)f^v(v)) \tag{6.9b}
\]

with the metric

\[
ds^2 = h(u, v)^2(g \, du^2 + dv^2), \tag{6.10}
\]

the stream-lines of the gradient vector field can be exactly solved. Note that for the Euclidean signature \(g = +\), eq. (6.10) includes the bipolar, Cartesian, elliptic and planar parabolic coordinates for the flat geometry, and the stereographic coordinates for the spherical geometry, so that it is quite comprehensive. The Hodge-stars of the coordinate differentials read

\[
\star du = g \, dv, \quad \star dv = -du; \tag{6.11}
\]

one therefore gets

\[
\theta dw = \star dp = -\rho_u du + g \rho_u dv. \tag{6.12}
\]

By using eqs. (6.2), (6.10) and (6.11), one obtains for eq. (6.9a)

\[
w = F \left( -g \int^u \frac{d\mu}{f^{\mu}(\mu)} + \int^v \frac{d\nu}{f^{\nu}(\nu)} \right), \tag{6.13a}
\]

\[
\theta = -\frac{1}{F} f' f^{uu}(u) f^{v}(v), \tag{6.13b}
\]

and for eq. (6.9b)

\[
w = F \left( -g \int^u \frac{d\mu}{(\ln f^{\mu}(\mu))^7} + \int^v \frac{d\nu}{(\ln f^{\nu}(\nu))^7} \right), \tag{6.14a}
\]

\[
\theta = -\frac{1}{F} f' f^{uu}(u) f^{v}(v), \tag{6.14b}
\]

Curiously, both eqs. (6.13b) and (6.14b) includes the result from the first-derivative test, \(\rho_u = 0\) or \(\rho_v = 0\).
Figure 11: Density function $\rho = e^{-(y-x^2)^2}$, the stream-lines of the gradient vector field in both Euclidean and Lorentzian geometry, and the stream ridge-lines which are $x = 0$ (green) and $y = x^2$ (orange). The Lorentzian results are to be understood with $y$ having the negative signature in the Minkowski metric.

Application to the toy model The toy model $\rho = e^{-(y-x^2)^2}$ in section 5.2 has the form of eq. (6.9a). One can adapt the results in eqs. (6.13a) and (6.13b) and get

$$w = F\left(g y + \frac{1}{2} \ln x\right),$$  \hspace{1cm} (6.15a)

$$\theta = 4g e^{-(y-x^2)^2} \frac{x(y-x^2)}{F'(gy + \frac{1}{2} \ln x)}.$$  \hspace{1cm} (6.15b)

See fig. 11. The Lorentzian results are to be understood with $y$ having the negative signature in the Minkowski metric. Equation (6.15b) gives the same ridge-lines as in the contour approach, as well as in the first-derivative test, $y = x^2$ and $x = 0$.

Now we move to the modulated toy model $\rho = g(x,y) e^{-(y-x^2)^2}$. Using $g_\epsilon = e^{-2\epsilon y}$, eq. (7.7) becomes

$$g(-x^2 + y + \epsilon) w_{,y} + 2x(x^2 - y) w_{,x} = 0.$$  \hspace{1cm} (6.16)

For $\epsilon \ll 1$, one uses the series test solution

$$w = \sum_{n=0}^{\infty} w_n \epsilon^n \quad \text{with} \quad w_0 = F\left(g y + \frac{1}{2} \ln x\right),$$  \hspace{1cm} (6.17)

and for $n \geq 0$,

$$(y - x^2)(2gx \partial_x w_{n+1} - \partial_y w_{n+1}) = \partial_y w_n.$$  \hspace{1cm} (6.18)

On the other hand,

$$\theta = g \frac{\rho_x}{w_{,y}} = -\frac{\rho_y}{w_{,x}}.$$  \hspace{1cm} (6.19)
where \( \rho \) can also be expanded with respect to \( \epsilon \), i.e.

\[
\rho = \rho_0 \left( 1 + \sum_{n=0}^{+\infty} \frac{\epsilon^n}{n!} \left. \frac{\partial^n e^{-2\epsilon y}}{\partial \epsilon^n} \right|_{\epsilon=0} \right), \quad \rho_0 = e^{-(y-x^2)^2}.
\]

This implies that \( \theta \propto \partial_x \rho_0 \propto x(y-x^2) \).

We failed to obtain a general integral \( w \) for the modulated toy model \( \rho = g e^{-(y-x^2)^2} \). Numerically integrated stream-lines of the gradient vector field are plotted in fig. 12. One sees that for the Euclidean signature, the stream-lines indicate the fastest up-hill direction, in which the singular stream-lines are ridge- or dale-lines that fit the intuition. Moreover, the dash-dotted orange line \( y = x^2 \) is a good approximation of the actual ridge-line for small \( \epsilon \) (fig. 12b), but fails for larger \( \epsilon \) (fig. 12a); in other words, there are non-perturbative effects that cannot be revealed by the perturbative analysis above.

With the Lorentzian signature shown in figs. 12c and 12d, things become more complicated. The above-mentioned property, that the gradient vector field points to the up-hill direction, is lost. Furthermore, the apparent ridge in the plot is no longer accompanied by a possible singular stream-line; instead, on the plot one sees a series of turning points that could play the role of indicating a ridge-line that also fits human cognition.

**Numerical applications to other models** As mentioned before, the stream approach is difficult to obtain analytic results. For the two-dimensional hydrogen atom and the “linear” wave-packet that were studied before, we make numeric plots of the stream-lines of the gradient vector fields, see fig. 13.

One sees again the good quality in the case with a Euclidean signature in fig. 13a, that no counter-intuitive lines are present. There seems to be a singular stream-line that is very close to the “best-fit” classical trajectory. For the Lorentzian geometry, the “best-fit” classical trajectory lies again near the “turning points” of the stream-lines, instead of being near a singular stream-line.

## 7 Relations of the contour and stream approaches

In this section 7 we compare the contour and stream approaches, as well as argue against the first-derivative test. Much of the material is adapted from [37, 47].

The contour and stream ridge-lines can be derived on the same footing. In \( \mathbb{R}^2 \), from \( d\rho = \rho_x \, dx + \rho_y \, dy \), eqs. (5.3) and (6.1), one deduces that [47, sec. 5]

\[
\frac{1}{2} d\kappa_{\text{sqr}} = R \, d\rho + \theta S \, dw, \tag{7.1}
\]

where

\[
R := \frac{\rho_x^2 \rho_x,xx + 2 \rho_x \rho_y \rho_x,xy + \rho_y^2 \rho_y,yy}{\kappa_{\text{sqr}}^2}, \tag{7.2a}
\]

\[
S := \frac{\rho_x \rho_y (\rho_x,xx - \rho_y,yy) - (\rho_y^2 - \rho_x^2) \rho_x,yy}{\kappa_{\text{sqr}}^2}. \tag{7.2b}
\]
Figure 12: Density function $\rho = g e^{-(y-x^2)^2-y^2/2}$ and the contour ridge-lines for $g = e^{-y^2/2}$ and $g = e^{-y^2/10}$ with the Euclidean and Lorentzian metrics. The green solid line $x = 0$ remains a ridge-dale-line, whereas the orange dash-dotted line is merely an approximation in the Euclidean case; the actual singular stream-lines seem to be under the orange lines. The stream ridge-line in the Lorentzian signature is apparently more intriguing.

Imposing $\kappa_{sq}$ to be stationary in the direction of $w$ gives

$$0 = \frac{1}{2} \frac{\partial \kappa_{sq}}{\partial w} = \theta S,$$

which gives either $\theta = 0$ or $S = 0$; they corresponds to the contour and stream ridge-lines defined in eqs. (5.4) and (6.4a), respectively.

The contour and stream ridge-lines are distinct, except for two special cases. Breton de Champ (see [47, sec. 2]) has shown that, stream-lines satisfying $S = 0$ are necessarily straight lines; otherwise, contour ridge-lines should not be stream-lines, and they are therefore no stream ridge-line. However, it seems to us that points satisfying $\rho_x = \rho_y = 0$ also lie on
both the contour and stream ridge-lines, see sections 5.2 and 6.2 for an example.

The differences, of the contour and stream ridge-lines, as well as the simple first-derivative test, can be shown with a so-called two-dimensional helicoidal gutter [37, sec. 6]; in polar coordinates \((\rho, \varphi)\) the metric and the gutter are

\[
ds^2 = g_{ij} \, dx^i \, dx^j = d\rho^2 + \rho^2 \, d\varphi^2,
\]

\[
\rho > 0, \quad 0 \leq \varphi < 2\pi;
\]

\[
\rho(\rho, \varphi) = \varphi + \frac{1}{2} \left( \frac{\rho}{\rho_0} - 1 \right)^2,
\]

see fig. 14.

The contour ridge-lines of eq. (7.4b) are given by the dSVr equation, or \(S = 0\) in eq. (7.2b). From the covariant expression in eq. (5.8), one derives

\[
0 = \left( \frac{\rho}{\rho_0} \right)^4 - \left( \frac{\rho}{\rho_0} \right)^3 - 1.
\]

The only positive root reads

\[
\frac{\rho}{\rho_0} \approx 1.38028.
\]

See fig. 14a. Roughly speaking, it crosses the contours where the latter are curved more.

As for the stream ridge-lines, using eq. (6.6) yields the equation for \(w\)

\[
d\rho^\sharp \, dw = 0, \quad \text{or} \quad 0 = \rho_i g^{ij} w_{,j} = \left( \frac{\rho}{\rho_0} - 1 \right) \frac{w,\rho}{\rho_0} + \frac{w,\varphi}{\rho^2}.
\]
(a) Contour and stream ridge-lines  

(b) First-derivative lines

(c) Section at $\varphi = \frac{2\pi}{3}$

**Figure 14:** The so-called helicoidal gutter in eq. (7.4b), its contours (dashed lines) and gradient vector field (represented by the grey stream-lines with arrows), and its ridge-lines. In fig. 14a, the green line is the stream ridge-line given by $\theta = 0$, and the orange line is the contour ridge-line predicted by the dSVr equation. In fig. 14b, the pink and the purple lines are $\rho_{,x} = 0$ and $\rho_{,y} = 0$, respectively. In fig. 14c, the section at $\varphi = 2\pi/3$ is plotted, where the round, square and diamond points are the stream and contour ridge-lines, as well as the first-derivative line. One sees that it is the *stream ridge-line* that picks the highest point in the sense of constant $\varphi$-section.

The general integral to eq. (7.7) reads

$$w = F\left(-\frac{\varrho_0}{u} + \varphi - \ln\left(1 - \frac{\varrho_0}{\varrho}\right)\right),$$

where $F$ is an arbitrary function, see eq. (6.3). In order to obtain $\theta$, one applies eq. (6.1)

$$\theta \, dw = \ast d\varrho = -\frac{\rho_{,\varphi}}{\varrho} \, d\varphi + \varrho \rho_{,\varphi} \, d\varphi.$$
The result is
\[
\theta = \frac{\varrho}{\varrho_0} \left( \frac{\varrho}{\varrho_0} - 1 \right) \left\{ F' \left( -\frac{\varrho_0}{\varrho} + \varphi - \ln \left( 1 - \frac{\varrho_0}{\varrho} \right) \right) \right\}^{-1}.
\] (7.10)

The stream ridge-lines are then given by \( \theta = 0 \), or
\[
\varrho = \varrho_0.
\] (7.11)

See fig. 14a. One sees that the arbitrariness of \( w \) encoded in \( F \) does not affect the effectiveness of the stream approach. Furthermore, the stream ridge-line really marks the highest point for a constant \( \varphi \)-section. As a stream-line by itself, the stream ridge-line is also a limit cycle [50, sec. 1.6.3] of the gradient vector field, and is also a watershed for two distinct families of stream-lines, one spirals inwards and another outwards. The contour ridge-line, on the other hand, is close to the highest point, see fig. 14b.

Finally, the curves given by the first-derivative test with respect to \((x, y)\) can also be easily worked out, see fig. 14b. They do not respect the rotational symmetry of \( \rho \) and is therefore not very sensible. One may argue for an alternative test with respect to \((\varrho, \varphi)\), but the choice itself cannot be arbitrary and needs a mathematical description, which renders the method losing its simpleness.

8 Summary and outlook

In current work, we have discussed the classical prediction from the ridge lines of stationary wave-packet in quantum theory. Our results show that the predictions from ridge lines are more abundant than the solutions solved from the classical theories; moreover, there may exist distinct deviation in the predictions from the classical solutions in certain range of minisuperspace, which arises from the quantum behaviour. This implies that the real classical trajectory should be corrected in this range.

First of all, the stationary wave-packets are realised in quantum mechanics with the superposition of degenerate energy eigenstates. Such cases are illustrated by the toy model of a two-dimensional hydrogen atom. In reality, the Rydberg atom can also be described by such a superposition, providing a chance to verify the theoretical statements. Wave-packets constructed by superposing solutions of the Wheeler–DeWitt are also formally stationary. It is imaginable to make use of this fact and use quantum systems in laboratory to simulate a quantum universe or a quantum black hole. However, one crucial difference between common quantum mechanical systems and quantum cosmology is that, the latter usually has a Lorentzian “kinetic energy term” in the Hamiltonian constraint, whereas the former mostly have a Euclidean kinetic energy term. One needs to be very creative to set up a simulated quantum cosmology system in laboratory.

Secondly, the contour approach to ridge-lines, which dates back to Barré de Saint-Venant in 1852, gives us an implicit equation (5.8) that can readily be plotted. It may not give results that are directionally minimal, but the difference can be small, see fig. 14c. The curves given by the dSVr equations are typically higher-order algebraic equations, which can at least be numerically solved. For the “linear” wave-packet, as well as for narrow
Gaussian WKB wave-packets, this approach gives sensible results, as discussed in section 5 and earlier in this section. With a Euclidean signature, redundant curves can appear, as we have seen in this section with the modulated toy model $\rho = g e^{-f^2}$, as well as with the two-dimensional hydrogen atom, that may arise from the fact that the dSVr equations collect not only the most convex and concave neighbourhoods, but also the flattest points. For the toy model, the redundant lines can be removed by careful asymptotic analysis, leaving results that also fit intuition. As for the Lorentzian signature, however, it can happen that no result fully agrees with intuition, as we have seen in the modulated toy model. We have to decide whether to believe in mathematics and abandon our intuition, or stick to the intuition and find a better mathematical description. Finally, an algorithm is needed to find the contour ridge-lines for numerically constructed wave-packets. This is to be investigated in the future.

Lastly, the stream approach to ridge-lines, which dates back to Rudolf Rothe in 1915, tells us to solve for a generic first integral $w$ of the gradient vector field from eq. (6.2), so that an inverse integral factor $\theta$ can be calculated, and $\theta = 0$ gives the singular stream-lines, that define the stream ridge-lines. As has been shown with fig. 14c, it can give results that are also directionally minimal. With the Euclidean signature, directions of the gradient vector field give the fastest ascent. The stream approach here gives results that agree with intuitive expectations, and no redundant lines appear except for those given by symmetries. We have shown this with the helicoidal gutter, as well as the toy model $\rho = e^{-f^2}$ analytically; numerically, the modulated toy model $\rho = g e^{-f^2}$ as well as the two-dimensional hydrogen atom also seem to perform pretty well under this approach. As for the Lorentzian signature, the singular stream-lines of the gradient vector field do not seem to agree with the intuitive ridge-lines, as we have seen in the numeric results of the “linear” wave-packet in fig. 13b. The reason is that, for Lorentzian geometry, the directions of the gradient vector field differ from those of the gradient one-form field, and the former field no longer points to the direction of the fastest ascent. One can either discard intuition and embrace what mathematical generalisation gives, or invent a novel notion of ridge-lines, keeping in mind that this new notion is also to work with the Euclidean case. Finally, an algorithm is needed to find the singular ridge-lines for an analytically given gradient vector field, since the generic first integral is difficult to solve. Moreover, for the cases where wave-packets are already constructed numerically, another algorithm is needed to find the singular ridge-lines from the numerically given gradient vector field.

The systematics of ridge-lines enables us to calculate the classical trajectories that emerge from a quantum wave-packet with arbitrary width. In fig. 5, for example, one sees three trajectories, one of which coincides or is close to a classical trajectory; with the profile of the wave-packet considered, one may understand it as predicting a tunnelling between two branches of the wave-packet, in that the wave-packet describes a semi-classical universe evolving from one classical trajectory in the asymptotic region to another classical trajectory, tunnelling near the origin of the plot. In contrast, the other two trajectories depart from classical trajectories near the classical turning point, giving a semi-classical behaviour that essentially differs from the classical one. The tunnelling picture can be useful for the singularity avoidance, which also tells a semi-classical fate.
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A Semi-classical approach of WKB

The WKB approach, named after Wentzel, Kramers and Brillouin [53–55], is an important approximation in conventional quantum mechanics that separates the rapidly varying phase from the slowly varying amplitude [56, ch. 7; 1, sec. 5.3.2]. It is also one of the standard ways to connect quantum geometrodynamics with classical general relativity.

In contrast, the connection between the quantum and classical gravitational theories in the scenario of wave-packets, is not very clear, and mostly ad hoc case by case, shown with plots [8, 9, 18]. In [57], the author observed that a superposition of WKB states can be chosen to have support only in a thin “tube” around a classical trajectory. Moreover, in [58], it was suggested that in the WKB approximation, an integral across a narrow section near a classical trajectory is related to the lapse function. Furthermore, in [59], the author interpreted WKB wave-packets as containing higher-order WKB effects. And finally in [60], it was suggested that the wave function of the universe forms a narrow wave-packet in the classical region.

It is common to construct a wave-packet by superposing mode functions with an amplitude that refers to a quantum number, e.g. superposing plane waves with a Gaussian amplitude that refers to the momenta of the plane waves. At the classical level, the quantum numbers correspond to first integrals, and using the former implies the existence of the latter. Therefore, this practice implicitly assumes that the system is Liouville integrable [61, sec. 49], containing a number of first integrals. Systems that do not have sufficient first integrals belong to the regime of classical and quantum chaos [62], and will not be studied here. For a criterion of integrable systems that can be separated in the Hamilton–Jacobi formulation, see [63].

In this section A, we will first describe the general WKB theory in mathematics and minisuperspace models, and explain the relation between the WKB mode functions and the classical trajectories in section A.1. Then we will derive the WKB approximation for our prototype minisuperspace model, both by analysing the obtained exact solution in section A.2, and by working the WKB mode functions out from scratch in section A.3. Observing that these mode functions all contain a quantum number, we will show in section A.4 that these quantum numbers have their correspondence at the classical level as first integrals of the system, and the phase of the WKB mode functions is just the Hamilton’s principal function. Finally, we will apply the theory established in section A.4 to wave-packets in section 2.2. We will show that these wave-packets, if constructed by superposing the WKB mode
functions with a narrow Gaussian amplitude, necessarily peak near a classical trajectory, which has the first integrals corresponding to the centre of the Gaussian amplitude.

A.1 General theory

This section A.1 briefly introduces the WKB approximation in mathematics and the Wheeler–DeWitt approach.

Mathematically, the WKB approximation belongs to the class of \textit{global} approximations to the solution of a linear differential equation, in which the highest derivative is controlled by a small parameter \( \delta \) \cite[ch. 10]{64}, with respect to which the solution \( y = y(x) \) is expanded as a formal power series on the exponent:

\[
\phi(x) \sim \exp \left( \frac{1}{\delta} \sum_{n=0}^{+\infty} \delta^n S_n(x) \right), \quad \delta \to 0.
\]  \hspace{1cm} (A.1)

In conventional quantum mechanics as well as in the Wheeler–DeWitt approach of quantum gravitation, the highest derivatives are controlled by the reduced Planck constant \( \hbar \). The meaning of a power expansion with respect to such a \textit{dimensionful} quantity is questioned at the end of this subsection.

At the next-to-leading order, the WKB wave function is often taken as the test solution \cite{18}

\[
\psi \approx \sqrt{D} e^{i S},
\]  \hspace{1cm} (A.2)

where \( S \) is the leading order term, \( D = e^{i S_1} \) corresponds to the real part of the next-to-leading order term, which is called \textit{Van Vleck factor}, named after its eponymous founder \cite{65}.\footnote{See \cite[ch. 7]{66} for a viable introduction of the Van Vleck factor; for historical remarks, see \cite{67, 68}.} In the minisuperspace models, inserting eq. (A.2) into the Wheeler-DeWitt equation, the resulting equations read \cite{18}

\[
0 = H_\perp \left( \chi, \gamma; \frac{\partial S_0}{\partial \chi}, \frac{\partial S_0}{\partial \gamma} \right) = \frac{1}{2} G^{IJ} \frac{\partial S}{\partial q^I} \frac{\partial S}{\partial q^J} + \mathcal{V}(q), \quad \hspace{1cm} (A.3a)
\]

\[
G^{IJ} \frac{\partial S}{\partial q^I} \frac{\partial D}{\partial q^J} = -(\Box S) D. \quad \hspace{1cm} (A.3b)
\]

Equation (A.3a) is just the \textit{Hamilton–Jacobi equation} for our singular system. Results for the next orders can be found in e.g. \cite[sec. 5.4.1]{1}, which are not needed here.

A.2 Asymptotic expansion as a WKB approximation

In our prototype model, the exact solution of the minisuperspace Wheeler–DeWitt equation (2.3b) is known. The WKB approach can therefore be realised in two ways. One can start with the generic WKB result, which means the Hamilton–Jacobi equation in (A.3a), and then solve \( S_0 \) for it. This approach will be illustrated later in section A.3. Alternatively, one can also begin with the mode functions in eq. (2.4) which are exact solutions, and find an approximation for the Bessel functions that have the form of eq. (A.1). We will follow this approach in this section A.2.
Since \( \nu, x \propto h^{-1} \) (c.f. eq. (2.5))\), an approximation at small \( h \) means asymptotic expansion of the Bessel functions at large \( \nu \) and \( x \). Note that

\[
\left( \frac{\nu}{x} \right)^2 = \frac{\kappa^2}{12 \text{Vol}_3^2 |V| e^{2\gamma}} \tag{A.4a}
\]

\[= \text{trig} \left( \sqrt{\frac{3}{2\pi}} g(\gamma - \gamma_0) \right)^2 \text{ by substituting eq. (2.2)}. \tag{A.4b}
\]

Equation (A.4b) makes sense if we want to study the behaviour of the mode functions near a classical trajectory.

In such a case of fixed \( \nu/x \), the asymptotic representations belong to the “Debye” type [69, sec. 3.14.2]. In the following we give the leading order results. For the \((-+, +)\) case with \( J_\nu(x) \), the Debye expansion reads [31, eq. (10.19.6)]

\[J_\nu(x) = \sqrt{\frac{2}{\pi}} (x^2 - \nu^2)^{-1/4} \cdot \left\{ \sin\left[ \sqrt{x^2 - \nu^2} - \nu \arccos \frac{\nu}{x} + \frac{\pi}{4} \right] + O(x^{-1}) \right\} , \quad x > \nu, \tag{A.5}\]

where \( x > \nu \) holds because \( \text{trig} = \sin \) for \((-+, +)\), and \( x = \nu \) is excluded because it is not contained in the trajectories. The mode function \( e^{i\frac{\pi}{\hbar}(\gamma - \gamma_0)} J_\nu(x) \) contains therefore two WKB branches \( \sim e^{i\frac{\pi}{\hbar}S_\pm} \),

\[S_\pm := \frac{p_\gamma}{\hbar} (\gamma - \gamma_0) \pm \left( \sqrt{x^2 - \nu^2} - \nu \arccos \frac{\nu}{x} + \frac{\pi}{4} \right). \tag{A.6}\]

Note we have introduced an additive constant \( \gamma_0 \) to cancel the extra constant factors and match the classical constant \( \gamma_0 \), which is also related to eqs. (A.16a) and (A.16b). By using eq. (A.16a), one gets

\[0 = \frac{1}{\hbar} \frac{\partial S_\pm}{\partial p_\gamma} = (\gamma - \gamma_0) \mp \sqrt{\frac{2\kappa}{3} \frac{1}{g} \arccos \sqrt{\frac{\kappa^2}{12 \text{Vol}_3^2 |V| e^{2\gamma}}} \hbar} , \tag{A.7}\]

which leads to eq. (2.2) with \( \text{trig} = \sin \).

For the \((+, -)\) case with \( F_{i\nu}(x) \) and \( G_{i\nu}(x) \), the Debye expansions at leading order read [13, eqs. (5.15) and (5.16)]

\[F_{i\nu}(x) = \sqrt{\frac{2}{\pi}} (x^2 + \nu^2)^{-1/4} \cdot \left\{ \sin\left[ \sqrt{x^2 + \nu^2} - \nu \arcsinh \frac{\nu}{x} + \frac{\pi}{4} \right] + O(x^{-1}) \right\} , \tag{A.8a}\]

\[G_{i\nu}(x) = -\sqrt{\frac{2}{\pi}} (x^2 + \nu^2)^{-1/4} \cdot \left\{ \cos\left[ \sqrt{x^2 + \nu^2} - \nu \arcsinh \frac{\nu}{x} + \frac{\pi}{4} \right] + O(x^{-1}) \right\} , \tag{A.8b}\]

\[-37-\]
where \( x, \nu \in \mathbb{R}^+ \) are arbitrary. Both cases contain two WKB branches. Take \( F_\nu(x) \) as an example, one has

\[
S_\pm = \frac{p_\gamma}{\hbar} (\gamma - \gamma_0) \pm \left( \sqrt{\nu^2 + x^2} - \nu \arcsinh \frac{\nu}{x} + \frac{\pi}{4} \right), \quad (A.9)
\]

\[0 = \frac{1}{\hbar} \frac{\partial S_\pm}{\partial p_\gamma} = (\gamma - \gamma_0) \mp \sqrt{\frac{2\nu}{3}} \frac{1}{g} \arcsinh \sqrt{\frac{x p_\gamma^2}{12 \text{Vol}_3^2 \vert V \vert e^{g \chi}}}, \quad (A.10)\]

which also leads to eq. (2.2) with \( \text{trig} = \sinh \). The calculation for \( G_\nu(x) \) is essentially the same, with an extra constant phase shift \( \frac{\pi}{2} \).

Finally, for the \((+,+\rangle\) case, the expansion at leading order reads [69, p. 141–142]

\[
K_{\nu}(x) = \sqrt{\frac{2\pi}{\nu e^{g \chi}}} (\nu^2 - x^2)^{-1/4} \cdot \left\{ \cos \left[ \sqrt{\nu^2 - x^2} - \nu \text{arccosh} \frac{\nu}{x} + \frac{\pi}{4} \right] + O(x^{-1}) \right\} \quad \nu > x, \quad (A.11)
\]

where \( \nu > x \) holds because \( \text{trig} = \cosh \) for \((+,+\rangle\). Equation (A.11) contains, once again, two WKB branches, and one has

\[
S_\pm = \frac{p_\gamma}{\hbar} (\gamma - \gamma_0) \pm \left( \sqrt{\nu^2 - x^2} - \nu \text{arccosh} \frac{\nu}{x} + \frac{\pi}{4} \right), \quad (A.12)
\]

\[0 = \frac{1}{\hbar} \frac{\partial S_\pm}{\partial p_\gamma} = (\gamma - \gamma_0) \mp \sqrt{\frac{2\nu}{3}} \frac{1}{g} \text{arccosh} \sqrt{\frac{x p_\gamma^2}{12 \text{Vol}_3^2 \vert V \vert e^{g \chi}}}, \quad (A.13)\]

which, again, lead to eq. (2.2) with \( \text{trig} = \cosh \).

A.3 WKB approximation by direct calculation

In this section A.3, we obtain the WKB phase \( S \) and the van Vleck factor \( D \) directly from eqs. (A.3a) and (A.3b).

To begin with, one can verify that the \( S_\pm \) given by eqs. (A.6), (A.9) and (A.12) are indeed complete integrals of the Hamilton–Jacobi equation (A.3a), which is a non-linear first-order partial differential equation by itself.

The transport equation (A.3b) in our prototype model reads

\[
\frac{s}{\text{Vol}_3} \left( -\frac{\kappa}{\text{Vol}_3} \frac{\partial S}{\partial \gamma} \frac{\partial D}{\partial \gamma} + \frac{\partial S}{\partial \chi} \frac{\partial D}{\partial \chi} \right) = -\frac{s}{\text{Vol}_3} \left( -\frac{\kappa}{\text{Vol}_3} \frac{\partial^2 S}{\partial \gamma^2} + \frac{\partial^2 S}{\partial \chi^2} \right) D, \quad (A.14)
\]

which is a first-order linear partial differential equation. By using the transformation in eq. (2.5), we are able to derive the general integral, which contains an arbitrary function \( D_0 \), in contrary to the complete integrals for \( S \), where merely arbitrary constants are present. See table 4.

Since \( S_\pm \)'s are complete integrals that result from separation test solutions (see eq. (A.18) below), the full Van Vlack factor should also be in a separated form, which would render \( D_0 \) constant, because it mixes \( \gamma \) with \( \chi \) otherwise. This can be verified if one begins from scratch by inserting the WKB wave function in eq. (A.2) into the Wheeler–DeWitt equation (2.3b), and then adapts a separation test solution. An ordinary differential
Table 4: General integrals of the Van Vleck factor $D_{\pm}$ that are solutions to eq. (A.14) and correspond to $S_{\pm}$. The pre-factors are in accordance with those in eqs. (A.5), (A.8a), (A.8b) and (A.11). The arbitrary function $D_0$ can be argued to be a constant.

| $(l, sv)$ | $D_{\pm}$ |
|-----------|------------|
| $(-, -)$  | no solution |
| $(-, +)$  | $(+x^2 - \nu^2)^{-1/2}D_0\left(\sqrt{\frac{3}{2\kappa}}\ g\gamma \mp \arccos \frac{\nu}{x}\right)$ |
| $(+, -)$  | $(+x^2 + \nu^2)^{-1/2}D_0\left(\sqrt{\frac{3}{2\kappa}}\ g\gamma \mp \arcsinh \frac{\nu}{x}\right)$ |
| $(+, +)$  | $(-x^2 + \nu^2)^{-1/2}D_0\left(\sqrt{\frac{3}{2\kappa}}\ g\gamma \mp \arcosh \frac{\nu}{x}\right)$ |

We conclude that eqs. (A.3b) and (A.14) may not be the best starting point to solve for the Van Vleck factor for systems with multiple degrees of freedom.

A.4 WKB phase as a complete integral

In this section A.4, we study the WKB mode functions and their phases. We will see that the mode functions can be chosen, such that they are labelled with quantum numbers, which are related to classical integrals of motion. Correspondingly, their phases are complete integrals of the classical Hamilton–Jacobi equation, which contain the classical integrals mentions above.

For the Hamilton–Jacobi equation (A.3a), the useful family of solutions is the complete solution or complete integral [70, sec. 47; 52, sec. 3.1; 61, sec. 9.4], that containing integral constants, e.g.

$$S = S(q^i; \alpha_1, \ldots, \alpha_{n-1}) + \alpha_n,$$  \hspace{1cm} (A.15)

where $\alpha_i$ are constants, $i = 1, 2, \ldots, n$. A classical trajectory that corresponds to this WKB solution can then be obtained by the principle of constructive interference [57] as

$$\frac{\partial S}{\partial \alpha_i} = 0.$$  \hspace{1cm} (A.16a)

Meanwhile, in the classical Hamilton–Jacobi formalism, the related equations are

$$\frac{\partial S}{\partial \alpha_i} = \beta_i,$$  \hspace{1cm} (A.16b)

where \{$\alpha_i$\}'s are the constants contained in the complete integral $S$, and \{$\beta_i$\}'s are another set of constants [70, sec. 47].

Now, if $S$ is a complete integral in the form of eq. (A.15), a stationary wave-packet can be constructed by smearing out each constant with an amplitude, see e.g. section 2.2.
In practice, it has been shown in [57] that, in order to be able to derive the Hamilton equations for the canonical momenta in full geometrodynamics, it is sufficient and necessary that \( S \) is a complete integral of the Hamilton–Jacobi equation, containing a number of constants that is equal to the physical degrees of freedom.

In the following we give a construction, in which the phase factor \( S \) in eq. (A.2) is indeed of a form close to the expression in eq. (A.15). Let the system be such that \( m \leq n - 1 \) variables can be iteratively separated [70, sec. 48], so that the following equations can be obtained along a classical trajectory

\[
\phi_1 \left( q^1, \frac{dS_1}{dq^1} \right) =: \alpha_1, \quad \phi_2 \left( q^2, \frac{dS_2}{dq^2}; \alpha_1 \right) =: \alpha_2, \ldots , \quad \phi_m \left( q^m, \frac{dS_m}{dq^m}; \alpha_1, \ldots, \alpha_{m-1} \right) =: \alpha_m ,
\]

(A.17)

and the corresponding complete integral, (A.15), reads

\[
S(q^1, \ldots, q^n; \alpha_1, \ldots, \alpha_m) = S_1(q^1; \alpha_1) + \ldots + S_m(q^m; \alpha_1, \ldots, \alpha_m) + S_{m+1}(q^{m+1} \ldots q^n; \alpha_1, \ldots, \alpha_m) .
\]

(A.18)

From the Hamilton–Jacobi theory, we know that \( \{ \phi_j(q^j, p_j) \} \)’s are in involution [61, sec. 10.1] with \( H_\perp \), i.e. the Poisson brackets vanish,

\[
[\phi_j(q^j, p_j), H_\perp (q^1, \ldots, q^n, p_1, \ldots, p_n)]_P = 0, \quad \forall j = 1, \ldots, m .
\]

(A.19)

Furthermore, we require that \( \{ \phi_j(q^j, p_j) \} \)’s are in mutual involution.

Upon canonical quantisation, the \( H_\perp \) and \( \{ \phi_j \} \)’s are promoted to (if necessary, self-adjoint) operators [1, sec. 5.1], and the condition of mutual involution with respect to \([\cdot, \cdot]_P\) is promoted to commuting \(\frac{i}{\hbar}[\cdot, \cdot]_\perp\). Equation (A.17) are promoted to the simultaneous eigenvalue equations

\[
\phi_1 \left( q^1, \frac{\hbar}{i} \partial_1 \right) \psi = \alpha_1 \psi, \quad \phi_2 \left( q^2, \frac{\hbar}{i} \partial_2; \alpha_1 \right) \psi = \alpha_2 \psi, \quad \ldots , \quad \phi_m \left( q^m, \frac{\hbar}{i} \partial_m; \alpha_1, \ldots, \alpha_{m-1} \right) \psi = \alpha_m \psi ,
\]

(A.20)

so that one can write \( \psi = \psi_{\alpha_1 \ldots \alpha_m} \). Applying a WKB test solution to eq. (A.20) results in the WKB wave function in eq. (A.2) with \( S \) given by eq. (A.18). This finishes our construction.

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