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Cauchy data and Hadamard singularities in time-dependent backgrounds

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We obtain the most general Cauchy data that produce Hadamard singularities in the propagator of a scalar field in the following backgrounds: (a) space-times with general homogeneous plane cosmological metrics; (b) Robertson-Walker space-times with arbitrary spatial curvature. Using this result we discuss the propagator's structure derived from two recently proposed Hamiltonian diagonalizations.

I. INTRODUCTION

The problem of the vacuum definition in quantum field theory in curved space is still unsolved. The requirements usually imposed on a given state to be considered a good candidate fall into two categories: (1) The associated propagator must reproduce, in some sense, the flat-space-time behavior for $x \rightarrow x'$ or, related to this, the energy-momentum tensor ($T_{\mu\nu}$) must be renormalizable (local properties);[1-5] (2) the "energy" must be diagonalized or minimized (global properties).[1-4]

All authors agree with the necessity of imposing requirement (1) in different degrees but the clear requirement of type (2) is not apparent up to now. Waiting for this global property to be established, we have obtained the restrictions which result on the possible vacuum states by applying property (1) in its weakest version, i.e., that the propagator must reproduce only the Hadamard singularities[6] for $x \rightarrow x'$. We remark that we do not ask for the complete Hadamard form nor for the renormalizability of the $T_{\mu\nu}$; our criterion is less restrictive than these.

We will work with some of the metrics (of cosmological interest) which allow the separation of the natural time in the field equation: general homogeneous plane metrics and Robertson-Walker (RW) space-times with an arbitrary scalar curvature (related works in spatially flat RW (Ref. 7) and Bianchi type-I metrics[8] will be commented below).

The organization of the paper is as follows. Hadamard's formalism is briefly reviewed in Sec. II. In Sec. III we show that the WKB vacuum[5] reproduces the Hadamard singularities. In Sec. IV we obtain the relation between the WKB Cauchy data and the most general ones that produce the correct singularity structure in the propagator. The renormalizability of the energy-momentum tensor and the relation of our work to those of Refs. 7 and 8 is also commented there.

It has been recently pointed out[9] that, after performing an appropriate time-dependent canonical transformation, a consistent vacuum definition through Hamiltonian diagonalization can be done in spatially flat RW backgrounds for all values of the coupling constant ξ (see Appendix A for notation). "Consistent" means that the propagator has Hadamard singularities and that the infinite terms in the vacuum expectation value of the Hamiltonian do not depend on the time in which one fixes the vacuum state, allowing a state-independent renormalization. Using the results of Sec. IV we show in Sec. V that this cannot be done if the metric is anisotropic. We also discuss in this section the cases in which the Cauchy data which diagonalize the observer dependent Hamiltonian proposed in Ref. 10 coincide with the ones obtained in Sec. IV.

Finally, we present our conclusions in Sec. VI. Appendixes A and B contain the notation and conventions used as well as some useful formulas.

II. HADAMARD STRUCTURE

Let us consider the propagator

$$G_1(x,x') = \langle 0 \mid \{\phi(x),\phi(x')\} \mid 0\rangle \ . \tag{2.1}$$

The Hadamard solution of the Klein-Gordon equation is given by

$$G_1^H(x,x') = \frac{\Delta^{1/2}(x,x')}{8\pi^2}\left[\frac{2}{\sigma} + v(x,x')\ln\sigma + w(x,x')\right] , \tag{2.2}$$

where $\Delta(x,x') = g^{-1/2}(x)\det(\sigma_{;\mu\nu'})g^{-1/2}(x')$ is the Van-Vleck determinant and $\sigma(x,x')$ is one-half of the square of the geodesic distance between x and x'. The functions $v(x,x')$ and $w(x,x')$ admit the expansions

$$v(x,x') = \sum_{n=0}^{\infty} v_n(x,x')\sigma^n ,$$
$$w(x,x') = \sum_{n=0}^{\infty} w_n(x,x')\sigma^n , \tag{2.3}$$

and the coefficients $v_n(x,x')$ can be recursively calculated inserting (2.2) and (2.3) into the field equation (A2), while the $w_n(x,x')$ are determined once $w_0(x,x')$ is fixed.

As is well known, the Hadamard solution (2.2) is the natural generalization of the flat-space-time kernel

$$\Delta_1(\sigma)=\frac{m^2}{4\pi^2}\,\mathrm{Im}\frac{H_1^{(1)}((2m^2\sigma)^{1/2})}{(2m^2\sigma)^{1/2}} \tag{2.4}$$

(here $H_1^{(1)}$ denotes the first order and type Hankel function and $\sigma=\frac{1}{2}[(\mathbf{x}-\mathbf{x}')^2-(t-t')^2]$). It is easy to see that $\Delta_1(\sigma)$ is of the form (2.2): expanding $H_1^{(1)}((2m^2\sigma)^{1/2})$ one obtains

$$v_n=2\left[\frac{m^2}{2}\right]^{n+1}\Big/ n!(n+1)!\ , \tag{2.5a}$$

$$w_n=2\left[\frac{m^2}{2}\right]^{n+1}\frac{\left[\ln\frac{m^2}{2}-\psi(n+2)-\psi(n+1)\right]}{n!(n+1)!}\ . \tag{2.5b}$$

We will discuss in Sec. IV which are the restrictions that appear on the possible vacuum states by imposing the Hadamard form for the singular part of the propagator in the coincidence limit $x\to x'$. To do this, Eq. (2.2) must be rewritten in terms of some particular coordinates x^a. We can write the square of the geodesic distance $s^2(x,x')$ and the Van-Vleck determinant as

$$s^2(x,x')=2\sigma(x,x')=g_{ab}Y^aY^b\ , \tag{2.6}$$

$$\Delta^{1/2}(x,x')=1+\tfrac{1}{12}R_{ab}Y^aY^b+\cdots\ ,\qquad a,b=0,1,2,3\ , \tag{2.7}$$

where Y^a are the normal coordinates of the point x' with respect to x (Ref. 11) which can be written in terms of the coordinates x^a as

$$Y^a=\Delta x^b+\frac{1}{2!}\Gamma^a_{bc}\Delta x^b\Delta x^c+\frac{1}{3!}(\Gamma^a_{bc,d}+\Gamma^a_{be}\Gamma^e_{cd})\Delta x^b\Delta x^c\Delta x^d\ , \tag{2.8}$$

with $\Delta x^a=x'^a-x^a$.

On the other hand, the coincidence limits of the first two functions $v_n(x,x')$ are[12]

$$\lim_{x\to x'} v_0(x,x')=m^2+(\xi-\tfrac{1}{6})R\equiv v_0(x)\ , \tag{2.9a}$$

$$\lim_{x\to x'} v_1(x,x')=\frac{m^4}{4}+\frac{m^2}{2}(\xi-\tfrac{1}{6})R+\tfrac{1}{4}(\xi-\tfrac{1}{6})^2R^2-\tfrac{1}{12}(\xi-\tfrac{1}{5})\Box R+\tfrac{1}{360}(R_{abcd}R^{abcd}-R_{ab}R^{ab})\equiv v_1(x)\ . \tag{2.9b}$$

In the following section we will obtain explicit expressions for $G_1^H(x,x')$ in the limit $x\to x'$ using Eqs. (2.6)–(2.9) and the geometric identities of Appendix A.

III. WKB VACUUM AND SINGULARITIES

As we said in Sec. I we will restrict ourselves to cases in which we can separate variables in the field equation. We shall consider two types of metrics:

$$(\mathrm{A})\quad ds^2=-dt^2+g_{ij}(t)dx^idx^j\ , \tag{3.1a}$$

$$(\mathrm{B})\quad ds^2=-dt^2+a^2(t)[d\chi^2+f^2(\chi)(d\theta^2+\sin^2\theta\, d\varphi^2)]\ ,$$

with

$$f(\chi)=r=\begin{cases}\sin\chi, & \chi\in[0,2\pi)\ ,\\ \sinh\chi, & \chi\in[0,+\infty)\end{cases} \tag{3.1b}$$

(these are RW metrics with $K=\pm1$, respectively).

The action for the scalar field is

$$S=-\tfrac{1}{2}\int d^4x(-g)^{1/2}[g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi+(m^2+\xi R)\phi^2]\ ,$$

where $g_{\mu\nu}$ is the metric tensor, g is the determinant of $g_{\mu\nu}$, and R is the Ricci scalar. The field equation is then

$$(\Box-m^2-\xi R)\phi=0\ .$$

Setting

$$\phi(x)=\int d\mu(\mathbf{k})[a_\mathbf{k}u_\mathbf{k}(x)+\mathrm{H.c.}] \tag{3.2}$$

and $u_\mathbf{k}(x)=E_\mathbf{k}(\mathbf{x})T_\mathbf{k}(t)_a{}^{-3/2}$, the temporal and spatial equations which result are

$$\ddot T_\mathbf{k}+T_\mathbf{k}[\omega_\mathbf{k}{}^2+\xi(R-{}^{(3)}R)-\tfrac{9}{4}H^2-\tfrac{3}{2}\dot H]=0\ ,$$

$$\Delta^{(3)}E_\mathbf{k}(\mathbf{x})=-(k^2-K)E_\mathbf{k}(\mathbf{x})\ ,$$

where $\omega_\mathbf{k}{}^2=m^2+g_{ij}k^ik^j$, ${}^{(3)}R=K=0$ for type (A) and $\omega_\mathbf{k}{}^2=m^2+k^2a^{-2}+(\xi-\frac{1}{6})^{(3)}R$, ${}^{(3)}R=6K/a^2$, $K=\pm1$ for type (B) metrics; a always denotes $(-g)^{1/6}$ and $H=\dot a/a$. The separation constant is $\mathbf{k}$ and the measure $d\mu(\mathbf{k})$ in (3.2) is

$$\int d\mu(\mathbf{k})=\begin{cases}\int d^3k, & \text{type(A)}\ ,\\ \sum_{k=0}^{\infty}\sum_{j=0}^{k-1}\sum_{m=-J}^{J}\ , & K=+1\ ,\\ \int_0^\infty dk\sum_{J=0}^{\infty}\sum_{m=-J}^{J}\ , & K=-1\ .\end{cases}$$

Using the normalization condition

$$\dot T_\mathbf{k}^*T_\mathbf{k}-T_\mathbf{k}^*\dot T_\mathbf{k}=i\ ,$$

the pure temporal part of the normal modes can be written as

$$T_{\mathbf{k}}(t)=\frac{\exp\left[-i\int^{t}V_{\mathbf{k}}(t')dt'\right]}{[2V_{\mathbf{k}}(t)]^{1/2}}\ , \tag{3.3}$$

where $V_{\mathbf{k}}(t)$ is a real function. Replacing (3.3) in the temporal equation one obtains

$$V_{\mathbf{k}}{}^{2}=\omega_{\mathbf{k}}{}^{2}+\mathcal{F}_{\mathbf{k}}(\ddot{V}_{\mathbf{k}},\dot{V}_{\mathbf{k}},V_{\mathbf{k}})\ , \tag{3.4}$$

where the function $\mathcal{F}_{\mathbf{k}}(\ddot{V}_{\mathbf{k}},\dot{V}_{\mathbf{k}},V_{\mathbf{k}})$ will be given below for each case considered.

The WKB solution can be computed replacing the asymptotic expansion

$$\Omega_{\mathbf{k}}\sim\sum_{n\geq 0}\frac{An}{\omega_{\mathbf{k}}{}^{2n-1}}\ , \tag{3.5}$$

into (3.4); the adiabatic solution of order m can be obtained retaining those terms in (3.5) which contain less than m derivatives of the metric.

Using Eqs. (2.1), (3.2), and (3.3) the WKB propagator can be written as

$$G_{1}^{\mathrm{WKB}}(x,x')=\int d\mu(\mathbf{k})\frac{E_{\mathbf{k}}(\mathbf{x})E_{\mathbf{k}}^{*}(\mathbf{x})\cos\int_{t}^{t'}\Omega_{\mathbf{k}}(z)dz}{[\Omega_{\mathbf{k}}(t)\Omega_{\mathbf{k}}(t')a^{3}(t)a^{3}(t')]^{1/2}}\ , \tag{3.6}$$

where $\Omega_{\mathbf{k}}$ is given by (3.5).

In order to show that $G_{1}^{\mathrm{WKB}}(\mathbf{x},\mathbf{x}',t,t')$ has Hadamard singularities we will compute $G_{1}^{\mathrm{WKB}}(\mathbf{x},\mathbf{x}',t,t)\ \forall\ t$ and compare it with $G_{1}^{H}(\mathbf{x},\mathbf{x}',t,t)$, both up to the second adiabatic order [obviously this assures that $\partial_{t}G_{1}^{\mathrm{WKB}}(\mathbf{x},\mathbf{x}',t,t)$ also has the Hadamard behavior].

(a) Metrics of type (A). In this case one has

$$E_{\mathbf{k}}(\mathbf{x})=\frac{1}{(2\pi)^{3/2}}e^{ig_{ij}k^{i}x^{j}}=\frac{1}{(2\pi)^{3/2}}e^{ik_{j}x^{j}} \tag{3.7}$$

and

$$\mathcal{F}_{\mathbf{k}}=\xi R-\tfrac{9}{4}H^{2}-\tfrac{3}{2}\dot{H}+\frac{1}{4}\left[\frac{\dot{V}_{\mathbf{k}}}{V_{\mathbf{k}}}\right]^{2}-\frac{1}{2}\left[\frac{\dot{V}_{\mathbf{k}}}{V_{\mathbf{k}}}\right]^{\cdot}\ ,$$

so

$$\Omega_{\mathbf{k}}\sim\omega_{\mathbf{k}}\left\{1+\frac{1}{2\omega_{\mathbf{k}}{}^{2}}\left[(\xi-\tfrac{1}{6})R+\frac{1}{4}\left[\frac{\dot{b}}{b}\right]^{2}-\frac{1}{2}\left[\frac{\dot{b}}{b}\right]^{\cdot}-\tfrac{9}{4}H^{2}-\tfrac{3}{2}\dot{H}+\tfrac{1}{6}R\right]+\cdots\right\}$$
$$\simeq\omega_{\mathbf{k}}\left[1+\frac{A_{1}}{\omega_{\mathbf{k}}{}^{2}}+\cdots\right]\ , \tag{3.8}$$

where $b\equiv(g_{ij}k^{i}k^{j})^{1/2}$ and $\omega_{\mathbf{k}}{}^{2}=b^{2}+m^{2}$.

The WKB propagator is thus

$$G_{1}^{\mathrm{WKB}}(\mathbf{x},\mathbf{x},'t,t)=\int\frac{d^{3}k}{(2\pi a)^{3}}\frac{e^{ik_{j}x^{j}}}{\omega_{\mathbf{k}}}\left[1-\frac{A_{1}}{2\omega_{\mathbf{k}}{}^{2}}+\cdots\right]\ . \tag{3.9}$$

The successive terms in (3.9) can be evaluated using the following well-known formulas:

$$\omega_{\mathbf{k}}{}^{-2n-1}=\frac{2^{n}}{(2n-1)!!}\left[-\frac{\partial}{\partial m^{2}}\right]^{n}\omega_{\mathbf{k}}{}^{-1}\ , \tag{3.10}$$

$$\Delta_{1}(\tfrac{1}{2}r^{2})=\frac{1}{(2\pi)^{3}}\int d^{3}k\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(k^{2}+m^{2})^{1/2}}\ , \tag{3.11}$$

and performing the change of variables $\mathbf{k}'=B^{-1}\mathbf{k}$ such that $g_{ij}k^{i}k^{j}=k'^{2}$. After a tedious, but straightforward calculation (sketched in Appendix B) we obtain

$$G_{1}^{\mathrm{WKB}}(\mathbf{x},\mathbf{x}',t,t)=\frac{1}{8\pi^{2}}\left[\frac{2}{x}+[m^{2}+(\xi-\tfrac{1}{6})R]\ln x-\frac{h_{ij}h_{kl}}{48x^{2}}r^{i}r^{j}r^{k}r^{l}+\tfrac{1}{12}(\dot{h}^{ij}+3hh^{ij}+h^{li}h_{l}^{j})\times\frac{r_{i}r_{j}}{x}+O(x\ln x)\right]\ , \tag{3.12}$$

where

$$x=\tfrac{1}{2}g_{lk}r^{l}r^{k},\quad r^{k}=x'^{k}-x^{k},\quad\text{and}\quad h_{ij}=\dot{g}_{ij}\ .$$

It is interesting to note that only the term $(\xi-\frac{1}{6})R$ in A_{1} [cf. (3.8)] contributes to the logarithmic divergence since $A_{1}-(\xi-\frac{1}{6})R$ produces a finite term (which has no well-defined limit for $\mathbf{x}\to\mathbf{x}'$).

The Hadamard propagator can be evaluated using the expressions (2.6) up to the second adiabatic order,

$$Y^{0}(t=t')=\tfrac{1}{4}h_{ij}r^{i}r^{j}\ , \tag{3.13a}$$

$$Y^{i}(t=t')=r^{i}+\tfrac{1}{24}h_{k}^{i}h_{jp}r^{k}r^{j}r^{p}\ , \tag{3.13b}$$

$$2\sigma(t=t')\equiv 2\bar{\sigma}=g_{ij}r^{i}r^{j}+\tfrac{1}{48}h_{kl}h_{ij}r^{k}r^{l}r^{i}r^{j}\ , \tag{3.13c}$$

$$\Delta^{1/2}(t=t')=1+\frac{r^{i}r^{j}}{12}[\tfrac{1}{2}\dot{h}_{ij}+\tfrac{1}{4}(6hh_{ij}-2h_{i}^{l}h_{jl})]\ . \tag{3.13d}$$

Replacing Eqs. (3.13) and (2.9a) into (2.2) one can verify that $G_{1}^{H}(\mathbf{x},\mathbf{x}',t,t)$ coincides with the one given in (3.12) so the WKB solution has an associated propagator with Hadamard singularities.

(b) Metrics of type (B). In this case $G_{1}^{\mathrm{WKB}}(\mathbf{x},\mathbf{x}',t,t)$ can be evaluated using similar arguments. Setting $\omega_{\mathbf{k}}{}^{2}=k^{2}/a^{2}+m^{2}(\xi-\frac{1}{6})\,{}^{(3)}R$ one has

$$\mathcal{F}_{\mathbf{k}}=\xi(R-{}^{(3)}R)-\tfrac{9}{4}H^{2}-\tfrac{3}{2}\dot{H}+\frac{1}{4}\left[\frac{\dot{V}_{\mathbf{k}}}{V_{\mathbf{k}}}\right]^{2}-\frac{1}{2}\left[\frac{\dot{V}_{\mathbf{k}}}{V_{\mathbf{k}}}\right]^{\cdot}\ ,$$

and in consequence, the WKB expansion gives

$$\Omega_{\mathbf{k}}\sim\omega_{\mathbf{k}}\left[1+(\xi-\tfrac{1}{6})\frac{R-{}^{(3)}R}{2\omega_{\mathbf{k}}{}^{2}}+\cdots\right]\ . \tag{3.14}$$

The WKB propagator is thus

$$G_1^{\rm WKB}(\mathbf{x},\mathbf{x}',t,t)=\int \frac{d\mu(\mathbf{k})}{a^3(t)}\frac{E_{\mathbf{k}}(\mathbf{x})E_{\mathbf{k}}^*(\mathbf{x}')}{\omega_{\mathbf{k}}}\times\left[1-\frac{(\xi-\frac{1}{6})(R-{}^{(3)}R)}{2\omega_{\mathbf{k}}^2}+\cdots\right]. \tag{3.15}$$

This expression can be evaluated using the fact that for the static case, the propagator $G_1(\mathbf{x},\mathbf{x}',t,t)$ is of Hadamard form.[5] Without losing generality, we can consider $\Delta\theta=\Delta\varphi=0$ so

$$\int \frac{d\mu(\mathbf{k})}{a^3(t)}\frac{E_{\mathbf{k}}(\mathbf{x})E_{\mathbf{k}}^*(\mathbf{x}')}{\omega_{\mathbf{k}}}=\frac{1}{8\pi^2}\left[\frac{2}{x}+[m^2+(\xi-\tfrac{1}{6})^{(3)}R]\times\ln x+O(x\ln x)\right], \tag{3.16}$$

where $x=\frac{1}{2}a^2(\mathcal{X}-\mathcal{X}')^2$. In consequence, using (3.10),

$$G_1^{\rm WKB}(\mathbf{x},\mathbf{x}',t,t)=\frac{1}{8\pi^2}\left[\frac{2}{x}+[m^2+(\xi-\tfrac{1}{6}R)]\ln x+O(x\ln x)\right]. \tag{3.17}$$

The Hadamard propagator can be easily calculated. Because of the isotropy there are no terms without a well-defined limit for $\mathbf{x}\to\mathbf{x}'$ and then only the first term in (2.6)–(2.8) must be retained so

$$Y^{\mathcal{X}}(t=t')\simeq\mathcal{X}'-\mathcal{X},\quad Y^0(t=t')=Y^{\varphi}(t=t')=Y^{t}(t=t')\simeq 0\ , \tag{3.18a}$$

$$\Delta^{1/2}(t=t')\simeq 1\ , \tag{3.18b}$$

$$\bar\sigma\simeq\tfrac{1}{2}(\mathcal{X}-\mathcal{X}')^2\ . \tag{3.18c}$$

Replacing in (2.2) we see again the coincidence between the divergences of $G_1^H(\mathbf{x},\mathbf{x}',t,t)$ and $G_1^{\rm WKB}(\mathbf{x},\mathbf{x}',t,t)$.

IV. ARBITRARY CAUCHY DATA AND SINGULARITIES

Let us consider an arbitrary basis $\{T_{\mathbf{k}}(t),T_{\mathbf{k}}^*(t)\}$ of the space of solutions to Eq. (A8a). One can always write

$$T_{\mathbf{k}}(t)=\alpha_{\mathbf{k}}T_{\mathbf{k}}^{\rm WKB}(t)+\beta_{\mathbf{k}}T_{\mathbf{k}}^{\rm WKB*}(t)\ , \tag{4.1}$$

where $\{T_{\mathbf{k}}^{\rm WKB},T_{\mathbf{k}}^{\rm WKB*}\}$ is the WKB basis. Since $T_{\mathbf{k}}$ and $T_{\mathbf{k}}^{\rm WKB}$ are normalized, the coefficients $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ satisfy

$$|\alpha_{\mathbf{k}}|^2=1+|\beta_{\mathbf{k}}|^2\ . \tag{4.2}$$

Using Eqs. (4.1) and (4.2) $G_1(x,x')$ can be rewritten as

$$G_1(x,x')=\frac{2\,\mathrm{Re}}{[a(t)a(t')]^{3/2}}\int d\mu(\mathbf{k})E_{\mathbf{k}}(\mathbf{x})E_{\mathbf{k}}^*(\mathbf{x}')\{T_{\mathbf{k}}^{\rm WKB}(t)T_{\mathbf{k}}^{\rm WKB*}(t')+2|\beta_{\mathbf{k}}|^2T_{\mathbf{k}}^{\rm WKB}(t)T_{\mathbf{k}}^{\rm WKB*}(t')+2\alpha_{\mathbf{k}}\beta_{\mathbf{k}}^*T_{\mathbf{k}}^{\rm WKB}(t)T_{\mathbf{k}}^{\rm WKB}(t')\}\ . \tag{4.3}$$

Let us suppose that the basis $\{T_{\mathbf{k}},T_{\mathbf{k}}^*\}$ is fixed by the Cauchy data at $t=t_0$, i.e.,

$$T_{\mathbf{k}}(t_0)=\frac{1}{[2V_{\mathbf{k}}(t_0)]^{1/2}}\ , \tag{4.4a}$$

$$T_{\mathbf{k}}(t_0)=-\left[\frac{1}{2}\frac{\dot V_{\mathbf{k}}(t_0)}{V_{\mathbf{k}}(t_0)}+iV_{\mathbf{k}}(t_0)\right]T_{\mathbf{k}}(t_0)\ ; \tag{4.4b}$$

then one has

$$\beta_{\mathbf{k}}=\alpha_{\mathbf{k}}\frac{T_{\mathbf{k}}^{\rm WKB}(t_0)}{T_{\mathbf{k}}^{\rm WKB*}(t_0)}\frac{\frac{1}{2}\left[\frac{\dot V_{\mathbf{k}}(t_0)}{V_{\mathbf{k}}(t_0)}-\frac{\dot\Omega_{\mathbf{k}}(t_0)}{\Omega_{\mathbf{k}}(t_0)}\right]+i[\Omega_{\mathbf{k}}(t_0)-V_{\mathbf{k}}(t_0)]}{\frac{1}{2}\left[\frac{\dot V_{\mathbf{k}}(t_0)}{V_{\mathbf{k}}(t_0)}-\frac{\dot\Omega_{\mathbf{k}}(t_0)}{\Omega_{\mathbf{k}}(t_0)}\right]-i[\Omega_{\mathbf{k}}(t_0)+V_{\mathbf{k}}(t_0)]}\ . \tag{4.5}$$

The first term in (4.3) gives the Hadamard singularities so, as we shall demonstrate below, $\beta_{\mathbf{k}}$ must be $O(k^{-3})$ in order to ensure that the second and third terms do not introduce new divergences. We will again separately treat the metrics of types (A) and (B).

If the metric is of type (A) then it is trivial to prove that $\beta_{\mathbf{k}}=O(k^{-3})$ is a sufficient condition, since the spatial functions $E_{\mathbf{k}}(\mathbf{x})$ are simply exponentials. In the case of RW with $K=\pm 1$ [type (B) metrics] these functions are more complicated but, since $\alpha_{\mathbf{k}}$ and $\beta_{\mathbf{k}}$ do not depend on $\hat{\mathbf{k}}$ (this fact is due to isotropy), the integration or summation over angular variables can be performed (see Appendix A). The results are, for $K=+1$,

$$G_1(x,x')=\frac{4\,\mathrm{Re}}{[a(t)a(t')]^{3/2}}\frac{1}{\pi}\sum_{k=1}^{\infty}k\frac{\sin k(\mathcal{X}-\mathcal{X}')}{\sin(\mathcal{X}-\mathcal{X}')}\{T_k^{\rm WKB}(t)T_k^{\rm WKB*}(t')+2|\beta_k|^2T_k^{\rm WKB}(t)T_k^{\rm WKB*}(t')+2\alpha_k\beta_k^*T_k^{\rm WKB}(t)T_k^{\rm WKB}(t')\}\ ; \tag{4.6a}$$

and for $K=-1$,

$$G_1(x,x')=\frac{4\,\mathrm{Re}}{\pi[a(t)a(t')]^{3/2}}\int_0^\infty dk\,k\frac{\sin k(\chi-\chi')}{\sinh(\chi-\chi')}\{T_k^{\mathrm{WKB}}(t)T_k^{\mathrm{WKB}*}(t')+2\,|\beta_k|^2T_k^{\mathrm{WKB}}(t)T_k^{\mathrm{WKB}*}(t')+2\alpha_k\beta_k^*T_k^{\mathrm{WKB}}(t)T_k^{\mathrm{WKB}}(t')\}\ . \tag{4.6b}$$

From these equations it is now trivial to see that, if $\beta_k=O(k^{-3})$, then no new singularity appears.

In terms of $\Omega_{\mathbf{k}}$ and $V_{\mathbf{k}}$ the condition $\beta_{\mathbf{k}}=O(k^{-3})$ can be rewritten as

$$\Omega_{\mathbf{k}}{}^2(t_0)-V_{\mathbf{k}}{}^2(t_0)=O(k^{-2})\ , \tag{4.7a}$$

$$\frac{\dot\Omega_{\mathbf{k}}}{\Omega_{\mathbf{k}}}(t_0)-\frac{\dot V_{\mathbf{k}}}{V_{\mathbf{k}}}(t_0)=O(k^{-2})\ , \tag{4.7b}$$

so we conclude that the most general Cauchy data compatible with Hadamard singularities in the propagator are the ones which coincide with that of the WKB solution up to k^{-2}.

It is interesting to note that Eqs. (4.7) are necessary and sufficient conditions in RW metrics but only sufficient conditions in the anisotropic case. For instance, if

$$\Omega_{\mathbf{k}}{}^2(t_0)-V_{\mathbf{k}}{}^2(t_0)=A(\hat{\mathbf{k}})=O(k^0)\ , \tag{4.8a}$$

$$\frac{\dot\Omega_{\mathbf{k}}}{\Omega_{\mathbf{k}}}(t_0)-\frac{\dot V_{\mathbf{k}}}{V_{\mathbf{k}}}(t_0)=O(k^{-2})\ , \tag{4.8b}$$

with $\int A(\hat{\mathbf{k}})d\Omega=0$ then $\beta_{\mathbf{k}}=O(k^{-1})$, but one can show that the singularities for $x\to x'$ are not modified. An example of this type is

$$V_{\mathbf{k}}{}^2=\omega_{\mathbf{k}}{}^2+(\xi-\tfrac{1}{6})R\ , \tag{4.9}$$

since $A_1-(\xi-\frac{1}{6})R$ produces a finite term [see the comment below Eq. (3.12b)]. Nevertheless, these Cauchy data (4.8) are not suitable because nonlocal singularities (i.e., for $x-x'\neq 0$) can appear.

In Refs. 7 and 8 similar results to our Eqs. (4.7) have been derived in spatially flat RW and Bianchi type-I metrics. We have generalized these results to metrics of types (A) and (B) using a little different approach which allows us to deduce that if the singular part of $G_1\ (\mathbf{x},\mathbf{x}',t_0,t_0+\epsilon)$ is of the form (2.2), then the singular part of $G_1(\mathbf{x},\mathbf{x}',t,t+\epsilon)$ is also of this form for all values of t (Ref. 13).

A related theorem has been shown in Ref. 14: if $G_1(x,x')$ has the complete Hadamard form in the neighborhood of a Cauchy hypersurface, then it will maintain this form on the whole manifold.

On the other hand we have tacitly supposed that there are not infrared divergences in the second and third term of (4.3). If this is not the case then nonlocal singularities can appear, as has been discussed in Ref. 7.

Finally, we want to mention that the conditions which we have found are necessary for the renormalizability of the energy-momentum tensor but, in general, they are not sufficient. This is because the vacuum expectation value (VEV) of $T_{\mu\nu}$ is constructed through

$$\langle T_{\mu\nu}(x)\rangle=\lim_{x\to x'}\mathcal{L}_{\mu\nu}G_1(x,x')\ , \tag{4.10}$$

where $\mathcal{L}_{\mu\nu}$ is a second-order differential operator and in consequence the term $\sigma\ln\sigma$ also contributes to the infinite part of $\langle T_{\mu\nu}\rangle$. Only if $\xi=\frac{1}{6}$ it can be shown that this term does not contribute to the divergences and this is the reason why the "weak vacuum" of Ref. 2 produces a renormalizable $T_{\mu\nu}$.

Let us suppose that $\mathcal{L}_{\mu\nu}$ applied to the first term of (4.3) gives the Hadamard form (including the term $\sigma\ln\sigma$) up to the fourth adiabatic order. In this case, the sufficient condition to have a renormalizable $T_{\mu\nu}$ can be written as

$$\partial_\mu\partial_\nu\int d\mu(\mathbf{k})\alpha_{\mathbf{k}}\beta_{\mathbf{k}}^*T_{\mathbf{k}}^{\mathrm{WKB}}(t)T_{\mathbf{k}}^{\mathrm{WKB}}(t')<\infty\ , \tag{4.11}$$

so $\beta_{\mathbf{k}}$ must be $O(k^{-5})$ and the Cauchy data must coincide with the WKB ones up to terms of order k^{-4}.

V. HAMILTONIAN DIAGONALIZATION

The most natural global property to require for vacuum fixing is that of the Hamiltonian diagonalization (or VEV minimization). Nevertheless, it is well known that in general, the associated propagator does not have Hadamard singularities.[1-3] For example, if one works with the metric Hamiltonian (constructed with T_{00}), the Cauchy data which minimize the energy VEV coincide with the WKB ones in the sense of (4.7) only for $\xi=\frac{1}{6}$ in the isotropic case.[2]

But, on the other hand, using the ambiguity in the election of the canonical Hamiltonian,[15] it has been shown in Ref. 9 that one can construct (in spatially flat RW universes) a canonical Hamiltonian such that its ground state produces the Hadamard singularities in the propagator for all values of ξ. Is this fact true for more general backgrounds? We will answer this question in this section.

The canonical transformation proposed in Ref. 9 is of the form

$$\phi(\mathbf{x},t)=h^{-1}(t)\chi(\mathbf{x},t)\ , \tag{5.1}$$

where $h(t)$ is an unknown function which will be fixed at the end of the calculation. The Hamiltonian is

$$H=\tfrac{1}{2}\int\frac{d^3x}{h^2}\,|g|^{1/2}\{(\partial_0\chi)^2-g^{ij}\partial_i\chi\partial_j\chi+[m^2+\xi R-f(h)]\chi^2\}\ , \tag{5.2}$$

where

$$f(h)=\left[\frac{\dot h}{h}\right]^2+\frac{h^2}{a^2}\left[a^3\frac{\dot h}{h^3}\right]^{\cdot} .$$

The Cauchy data which minimize this Hamiltonian VEV can be evaluated using standard manipulations.[1-3,9] The results are, for type (A),

$$V_{\mathbf{k}}^{\mathrm{ME}}=[g_{ij}k^ik^j+m^2+\xi R-f(h)]^{1/2} , \quad (5.3a)$$

$$\frac{\dot V_{\mathbf{k}}^{\mathrm{ME}}}{V_{\mathbf{k}}^{\mathrm{ME}}}=2\dot h/h-3\dot a/a \quad (5.3b)$$

and, for type (B),

$$V_{\mathbf{k}}^{\mathrm{ME}}=\frac{(k^2-K)}{a}+m^2+\xi R-f(h) , \quad (5.3c)$$

$$\frac{\dot V_{\mathbf{k}}^{\mathrm{ME}}}{V_{\mathbf{k}}^{\mathrm{ME}}}=2\dot h/h-3\dot a/a . \quad (5.3d)$$

Comparing Eqs. (5.3) with Eqs. (4.7) we conclude the following.

(1) In the isotropic case, the data (5.3) are correct if $h=a$, since $f(a)=(R-{}^{(3)}R)/6$ and $\dot V_{\mathbf{k}}^{\mathrm{ME}}/V_{\mathbf{k}}^{\mathrm{ME}}=-H$. This is Weiss's result[9] for $K=0$, which we have generalized for $K=\pm1$. The canonical transformation is such that $V_{\mathbf{k}}^{\mathrm{ME}}$ coincides with $\Omega_{\mathbf{k}}$.

(2) If the metric is not isotropic then the canonical transformation does not give good results because (4.7b) is $\hat{\mathbf{k}}$ dependent and (5.3b) is not. The use of a more general type of canonical transformation [for example, $\phi_{\mathbf{k}}(t)=h_{\mathbf{k}}{}^{-1}(t)\chi_{\mathbf{k}}(t)$ or $\phi(\mathbf{x},t)=h^{-1}(\mathbf{x},t)\chi(\mathbf{x},t)$] is not appealing because the new Hamiltonian density becomes nonlocal or nonuniform in terms of the new field.

To conclude this section we shall mention the properties of the vacuum associated to the observer-dependent Hamiltonian of Ref. 10. The Cauchy data which minimize $\langle H\rangle$ for a geodesic observer in type (A) metrics are[2,10]

$$V_{\mathbf{k}}^{\mathrm{ME}}=[\omega_{\mathbf{k}}{}^2+6\xi H(1-6\xi)]^{1/2} , \quad (5.4a)$$

$$\frac{\dot V_{\mathbf{k}}^{\mathrm{ME}}}{V_{\mathbf{k}}^{\mathrm{ME}}}=-3H(1-4\xi) , \quad (5.4b)$$

so the propagator has Hadamard singularities only in some particular cases: RW with $\xi=\frac16$ for all t; at $t=t_0$ if $h_{ij}(t_0)=0$, etc., (see Ref. 2).

For type (B) metrics one has[10] that the Cauchy data which minimize $\langle H\rangle$ are

$$V_{\mathbf{k}}^{\mathrm{ME}}=m^2+\frac{k^2-K}{a^2}+\xi^{(3)}R+6\xi(1-6\xi)H^2 , \quad (5.5a)$$

$$\frac{\dot V_{\mathbf{k}}^{\mathrm{ME}}}{V_{\mathbf{k}}^{\mathrm{ME}}}=-3H(1-4\xi) . \quad (5.5b)$$

The WKB data are given by (3.14) and $\dot\Omega_{\mathbf{k}}/\Omega_{\mathbf{k}}=-H$. The situation is then similar to the $K=0$ case since for $\xi=\frac16$ or $H=0$ the singularities of $G_1^{\mathrm{ME}}(x,x')$ are the correct ones.

In view of these results, one sees that properties (1) and (2) are still in general, incompatible. It is interesting to note that the naive attempt to compatibilize them, i.e., to minimize the energy within the subset (M) of Cauchy data which produce Hadamard singularities, does not work. This can be seen as follows. ${}_{(t_0)}\langle 0|H|0\rangle_{(t_0)}$ is a functional of the arbitrary functions of $\mathbf{k}$ $W_{\mathbf{k}}^{\mathrm{ME}}(t_0)$ and $\dot W_{\mathbf{k}}^{\mathrm{ME}}(t_0)$, but it does not depend on their $\mathbf{k}$ derivatives. As a consequence, given $\epsilon>0$ one can always find, in M, functions $W_{\mathbf{k}}^{\epsilon}(t_0)$ and $\dot W_{\mathbf{k}}^{\epsilon}(t_0)$ such that

$$|E(W_{\mathbf{k}}^{\epsilon},\dot W_{\mathbf{k}}^{\epsilon},t_0)-E(W_{\mathbf{k}}^{\mathrm{ME}},\dot W_{\mathbf{k}}^{\mathrm{ME}},t_0)|<\epsilon , \quad (5.6)$$

so, in general, there is no minimum in M. This is so because the Cauchy data $W_{\mathbf{k}}^{\epsilon}$ and $\dot W_{\mathbf{k}}^{\epsilon}$ produce a value of $E(W_{\mathbf{k}}^{\epsilon},\dot W_{\mathbf{k}}^{\epsilon},t_0)$ that, although greater than $E(W_{\mathbf{k}}^{\mathrm{ME}},\dot W_{\mathbf{k}}^{\mathrm{ME}},t_0)$, is arbitrarily close to it.

VI. CONCLUSIONS

We have found the most general Cauchy data which reproduce the Hadamard singularities up to the second adiabatic order. The utility of this result is that it can be used to test if a given state is a good candidate to be the vacuum state, since it is the weakest restriction of type (1) which can be imposed.

As an application, we have shown that the canonical transformation proposed in Ref. 9 can be generalized to type (B) metrics, but it fails in the anisotropic case of type (A). On the other hand, the observer-dependent Hamiltonian of Ref. 10 gives the correct structure only in particular cases, and a minimization within the subset of "good" Cauchy data cannot be performed.

APPENDIX A: NOTATION AND CONVENTIONS

The Lagrangian density for the scalar field is

$$\mathcal{L}=-\tfrac12(-g)^{1/2}[g^{\mu\nu}\partial_\mu\phi\partial_\nu\phi+(m^2+\xi R)\phi^2] , \quad (A1)$$

where $g_{\mu\nu}$ is the metric tensor, g is the determinant of $g_{\mu\nu}$, R is the Ricci scalar, and ξ the coupling constant. The Klein-Gordon equation is then

$$(\Box-m^2-\xi R)\phi=0 ,\qquad \Box\phi\equiv\frac{1}{(-g)^{1/2}}\partial_\mu[(-g)^{1/2}\partial^\mu\phi] . \quad (A2)$$

In this paper we use two types of metrics. The line element is given in each case by the expressions (3.1a) and (3.1b). Throughout the paper we use the notation $a=(-g)^{1/6}$ for type (A) metrics. Some relevant geometric identities for these metrics are the following. Type (A):

$$\Gamma^0_{ij}=\tfrac12\dot g_{ij},\quad \Gamma^i_{j0}=\tfrac12 g^{il}\dot g_{lj} \quad (A3)$$

(other Christoffel symbols vanish). Defining

$$h_{ij}=\dot g_{ij},\quad h^{ij}=-\dot g^{ij},\quad H=\tfrac16 h_i{}^i=\tfrac16\frac{\dot g}{g} , \quad (A4)$$

the Ricci tensor is given by

$$R_{00}=-3\dot H-\tfrac14 h_{ij}h^{ij} , \quad (A5a)$$

$$R_{ij}=\tfrac{1}{2}\dot{h}_{ij}+\tfrac{1}{4}(6h_{ij}h-2h_i^l h_{lj}),\quad R_{0i}=0\ , \tag{A5b}$$

and the scalar curvature is

$$R=6\dot{h}+\tfrac{1}{4}(36h^2+h_{ij}h^{ij})\ . \tag{A5c}$$

Type (B): we will only need in this case the scalar curvature. It is given by

$$R=6\left[\dot{H}+2H^2+\frac{K}{a^2}\right]=6(\dot{H}+2H^2)+{}^{(3)}R\ , \tag{A6}$$

where $\dot{H}=\dot{a}/a$ and $K=\pm 1$ for closed and hyperbolic RW metrics, respectively. Both types of metrics admit variable separation in the Klein-Gordon equation. Setting, as usual,

$$\phi(x)=\int d\mu(\mathbf{k})[a_{\mathbf{k}}u_{\mathbf{k}}(x)+\text{H.c.}] \tag{A7}$$

and $u_{\mathbf{k}}(x)=E_{\mathbf{k}}(\mathbf{x})T_{\mathbf{k}}(t)a^{-3/2}$, the temporal and spatial equations result:

$$\ddot{T}_{\mathbf{k}}+T_{\mathbf{k}}[\omega_{\mathbf{k}}^2+\xi(R-{}^{(3)}R)-\tfrac{9}{4}H^2-\tfrac{3}{2}\dot{H}]=0\ , \tag{A8a}$$

$$\Delta^{(3)}E_{\mathbf{k}}(\mathbf{x})=-(k^2-K)E_{\mathbf{k}}(\mathbf{x})\ . \tag{A8b}$$

Equations (A7) and (A8) are valid for both types of metrics: ${}^{(3)}R=K=0$, $\omega_{\mathbf{k}}^2=m^2+g_{ij}k^ik^j$ for type (A) and $K=\pm 1$, $\omega_{\mathbf{k}}^2=m^2+k^2a^{-2}+(\xi-\frac{1}{6})^{(3)}R$ for type (B). The separation constant is $\mathbf{k}$ and the measure $d\mu(\mathbf{k})$ is given by

$$\int d\mu(\mathbf{k})=\begin{cases}\int d^3k, & K=0\ ,\\ \sum_{k=0}^{\infty}\sum_{J=0}^{k-1}\sum_{m=-J}^{J}\ , & K=+1\ ,\\ \int_0^\infty dk\sum_{J=0}^{\infty}\sum_{m=-J}^{J}\ , & K=-1\ .\end{cases} \tag{A9}$$

The solutions of the spatial equations are

$$\text{Type (A):}\quad E_{\mathbf{k}}(\mathbf{x})=(2\pi)^{-3/2}e^{ik_jx^j}\ , \tag{A10}$$

$$\text{Type (B):}\quad K=+1, E_{\mathbf{k}}(\mathbf{x})=Y_{JM}(\theta,\varphi)\Pi_{kJ}^+(\chi)\ , \tag{A11a}$$

$$K=-1,\ E_{\mathbf{k}}(\mathbf{x})=Y_{JM}(\theta,\varphi)\Pi_{kJ}^-(\chi)\ , \tag{A11b}$$

where $\Pi_{kJ}^+(\chi)$ are proportional to the Gegenbauer polynomials[16] and $\Pi_{kJ}^-(\chi)$ can be obtained substituting $\chi\to i\chi$ and $k\to ik$ in $\Pi_{kJ}^+(\chi)$, (they are proportional to the Gegenbauer functions). The solutions (A11) satisfy the following identities (sum rules):[16,17] For $K=+1$,

$$\sum_{J=0}^{k-1}\sum_{m=-J}^{J}Y_{JM}(\theta,\varphi)Y_{JM}^*(\theta,\varphi)\Pi_{kJ}^+(\chi)\Pi_{kJ}^{+*}(\chi')=\frac{2k}{\pi}\frac{\sin k(\chi-\chi')}{\sin(\chi-\chi')}\ ; \tag{A12a}$$

for $K=-1$,

$$\sum_{J=0}^{\infty}\sum_{m=-J}^{J}Y_{JM}(\theta,\varphi)Y_{JM}^*(\theta,\varphi)\Pi_{kJ}^-(\chi)\Pi_{kJ}^{-*}(\chi')=\frac{2k}{\pi}\frac{\sin k(\chi-\chi')}{\sinh(\chi-\chi')}\ . \tag{A12b}$$

APPENDIX B: CALCULATION OF $G_1^{\text{WKB}}(\mathbf{x},\mathbf{x}',t,t)$

We will sketch here the calculation from (3.9) to (3.12). The propagator is given by

$$G_1^{\text{WKB}}(\mathbf{x},\mathbf{x}',t,t)=\frac{\text{Re}}{(2\pi a)^3}\int d^3k\frac{e^{ik_jr^j}}{\omega_{\mathbf{k}}}\left[1-\frac{A_1}{2\omega_{\mathbf{k}}^2}+\cdots\right]\ , \tag{B1}$$

where

$$\begin{aligned}A_1&=(\xi-\tfrac{1}{6})R+\left[\frac{R}{6}-\tfrac{9}{4}H^2-\tfrac{3}{2}\dot{H}\right]-\frac{1}{4}\ddot{g}^{ij}\frac{k_ik_j}{\omega_{\mathbf{k}^2}}+\frac{5}{16}\frac{(\dot{g}^{ij}k_ik_j)^2}{\omega_{\mathbf{k}}^4}\\&\equiv(\xi-\tfrac{1}{6})R+F+\frac{F^{ij}k_ik_j}{\omega_{\mathbf{k}^2}}+\frac{(G^{ij}k_ik_j)^2}{\omega_{\mathbf{k}}^4}\ .\end{aligned} \tag{B2}$$

Using Eqs. (3.10) and denoting

$$F_1(r)=\text{Re}\int\frac{d^3k}{(2\pi a)^3}\frac{e^{ik_jr^j}}{\omega_{\mathbf{k}}}\ , \tag{B3}$$

Eq. (B1) can be written as

$$\begin{aligned}G_1^{\text{WKB}}(\mathbf{x},\mathbf{x}',t,t)=\Bigg[&1+[(\xi-\tfrac{1}{6})R+F]\frac{\partial}{\partial m^2}+\tfrac{2}{3}F^{ij}\frac{\partial^2}{\partial r_i\partial r_j}\left[\frac{\partial}{\partial m^2}\right]^2\\&+\tfrac{4}{15}G^{ij}G^{lm}\frac{\partial^4}{\partial r^i\partial r^j\partial r^l\partial r^m}\times\left[\frac{\partial}{\partial m^2}\right]^3\Bigg]F_1(r)\ .\end{aligned} \tag{B4}$$

The function $F_1(r)$ can be calculated performing the change of variables $k_i=B_i^jk_j'$ such that $g^{ij}k_ik_j=k_j'k_j'$. The matrix B satisfies

$$B^\dagger gB=\mathbb{1},\quad \det B=(\det g)^{-1/2} \tag{B5}$$

(here, and only here, g denotes the matrix $g_{\mu\nu}$). One finds

$$F_1(r)=\Delta_1(x)\ , \tag{B6}$$

where $x=\frac{1}{2}g_{ij}r^ir^j$. The mass derivatives can be easily evaluated using (2.5). To calculate the r derivatives the following identities are useful:

$$\frac{\partial}{\partial r^i}F(x)=r_iF'(x)\ , \tag{B7a}$$

$$\frac{\partial^2}{\partial r^i \partial r^j} F(x) = r_i r_j F''(x) + g_{ij} F'(x) \,, \tag{B7b}$$

$$\frac{\partial^3 F(x)}{\partial r^l r^j r^k} = r_i r_j r_k F'''(x) + F''(x)(r_k g_{ij} + r_i g_{kj} + r_j g_{ik}) \,, \tag{B7c}$$

$$\frac{\partial F(x)}{\partial r^i r^j r^k r^l} = r_i r_j r_k r_l F''''(x) + F'''(x)(g_{lk} r_i r_j + \text{perm}) + F''(x)(g_{lk} g_{ij} + g_{jl} g_{ik} + g_{kj} g_{il}) \,. \tag{B7d}$$

The final result is then

$$G_1^{\text{WKB}}(\mathbf{x},\mathbf{x}',t,t) = \frac{1}{8\pi^2} \left\{ \frac{2}{x} + [m^2 + (\xi - \tfrac{1}{6})R] \ln x - \tfrac{1}{48} h^{lm} h^{ij} \frac{r_l r_m r_i r_j}{x^2} + \tfrac{1}{12}(\dot{h}^{ij} + 3h h^{ij} + h^{li} h_l^j) \times \frac{r_i r_j}{x} \right\} + \cdots \,. \tag{B8}$$

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