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Cosmological particle creation as above-barrier reflection: approximation method and applications

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Abstract. For the example of conformally-coupled massive Klein–Gordon particles in a Robertson–Walker universe the analogy between the Fock-space formulation of pair creation caused by the contraction and expansion of the universe on one hand and the pair creation in time-dependent electric fields as well as the reflection above a barrier in one-dimensional Schrödinger quantum mechanics on the other hand is described. This analogy is taken as the basis for the transcription of exact results and for the transcription of a WKB approximation method which allows an easy calculation of the relative probability of cosmological pair creation. For time-symmetric contraction–expansion behaviour the latter can be reduced to a real quadrature. Apart from the mathematical conditions for the application of the approximation procedure, the coherent calculation demands as an additional physical condition that the Cauchy hypersurfaces taken as the in- and out-regions admit free WKB particles. This implies conditions for the metric which are discussed in detail. Generalisations to other cosmologies and other particle equations are indicated. Several applications of the exact transcription procedure and of the approximation formulae are given, mainly with regard to the question of whether the spectrum of created particles is a thermal one.

1. Introduction

During the last five years there has been an ever increasing interest in the study of the creation of elementary particles by strong gravitational fields in the vicinity of black holes and during the early stages of the universe. For motivations, difficulties and a survey of the results see the review articles by DeWitt (1975), Parker (1977), Davies (1978) and Gibbons (1978). In order to better 'understand' a physical process like cosmological particle creation one needs—apart from the study of its underlying principles and main calculation schemes—an acquaintance with the results of as many particular examples as possible. Restricting the intended results to the number of the created particles and their spectrum, the corresponding rigorous calculations are often based on the explicit behaviour of exact solutions of the respective particle field equations and are therefore obtained only for appropriate special space–times in a laborious manner. Usually nothing is known about the stability of the characteristic traits of the primary situation. Therefore, to survey quickly the results of particle creation for a wide class of expansion laws one requires an approximation formula which is generally applicable and which can be handled easily. The purpose of this paper is (i) to draw attention to the analogies between cosmological pair creation, electric pair creation and above-barrier reflection which permit an understanding of

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one process in terms of another, (ii) to describe a quasi-classical (WKB) approximation method for the calculation of the probability of pair production caused by the time dependence of cosmological metric fields and (iii) to indicate the usefulness of these considerations in applying them to several examples. The procedure has been sketched briefly by Audretsch (1978).

To describe the essentials of the method we specialise to conformally-coupled massive Klein–Gordon particles in a three-flat Robertson–Walker universe with given (i.e. otherwise determined) contraction–expansion law $R(t)$. The metric remains unquantised and the back reaction of the created matter on the expansion is neglected. Particle creation is thereby represented by the fact that an in-vacuum contains out-states. The process of cosmological pair creation we are dealing with is described by a pure state (coherent superposition) and not by a mixture (density matrix) as it is if an horizon is present.

The starting point of our considerations is the analogy between the Fock-space formulation of the cosmological creation process with the respective formulation of relativistic pair creation in time-dependent electric fields on one hand, and the analogy with the Hilbert-space formulation of the reflection above a barrier in the framework of non-relativistic one-dimensional Schrödinger quantum mechanics on the other hand. This analogy is described briefly in § 2. If the cosmological contraction–expansion law does not approach a constant value asymptotically (statistically bounded behaviour), the problem of the appropriate definition of 'positive' frequency solutions, i.e. the problem of the definition of free particle states, and, correspondingly, the definition of the vacuum arises. It is shown in § 3 how different particle definitions answer differently the directly related additional question of whether or not a space–time admits Cauchy surfaces where the particles become free according to these definitions, i.e. where the interaction has finished (in- and out-regions). Based on the analogies described in § 2, we discuss in § 4 a method which allows the approximate calculation of the relative probability of pair creation in a given mode. In the case of a time-symmetric expansion–contraction behaviour of the metric of the cosmological space–time, the evaluation can be reduced to a real quadrature.

The whole scheme can be generalised to field equations describing other sorts of particles and different types of couplings as shown in § 5. The underlying space–time can be generalised to other types of Robertson–Walker universes and to anisotropically contracting–expanding universes. In § 6 we give several applications of the transcription procedure and of the approximation formulae mainly in relation to the question of whether the spectrum of created particles is a thermal one.

2. Cosmological particle creation, electromagnetic particle creation and non-relativistic above-barrier reflection

We restrict our description to a cosmological background described by the Robertson–Walker metric with flat spatial sections†

$$ds^2 = dt^2 - R^2(t)(dx^2 + dy^2 + dz^2) \qquad (2.1a)$$

$$ds^2 = R^2(\eta)(d\eta^2 - dx^2 - dy^2 - dz^2) \qquad (2.1b)$$

† $\hbar = 1$, $c = 1$. Signature of the metric tensor $g_{\alpha\beta}$: $(---+)$. ∇_α and $\|\alpha$ denote the covariant and ∂_α and $|\alpha$ the partial derivative.

and contraction–expansion law $R(\eta)$. For other metrics see § 5. Physical statements refer to cosmic observers with world-lines $x=\text{constant}$, $y=\text{constant}$, $z=\text{constant}$.

To demonstrate an analogy and also for later use we write out some well known separations of different particle field equations. The conformally-coupled massive Klein–Gordon equation

$$(\nabla_\mu \nabla^\mu + m^2 + \tfrac{1}{6}\hat{R})\Psi = 0 \qquad \hat{R} = 6R^{-3}\,\partial^2 R/\partial\eta^2 \tag{2.2}$$

leads after separation of the variables according to

$$\Psi = \frac{1}{R(\eta)}\Phi = \frac{1}{(2\pi)^{3/2}}\frac{1}{R(\eta)} f(\eta)\exp(\pm i\boldsymbol{k}\boldsymbol{x}) \qquad \boldsymbol{k} = \text{constant} \tag{2.3}$$

to the generalised oscillator equation with time-dependent frequency

$$f'' + \omega^2(\eta) f = 0 \qquad \omega = (R^2(\eta)m^2 + k^2)^{1/2} \tag{2.4}$$

with $(\partial' = \partial/\partial\eta)$ and $f(\eta)$ complex. The measured momentum is $\boldsymbol{p}(\eta) = \boldsymbol{k}/R(\eta)$. The Klein–Gordon scalar product

$$\mathrm{i}\int_\Sigma \Psi_1^* \overleftrightarrow{f^\mu} \Psi_2 \,\mathrm{d}\Sigma_\mu \qquad \overleftrightarrow{f^\mu} = \sqrt{-g}\, g^{\mu\nu}\, \overrightarrow{\partial_\nu} - \overleftarrow{\partial_\nu}\, g^{\mu\nu}\sqrt{-g} \tag{2.5}$$

taken with regard to the Cauchy hypersurface Σ given by $\eta = \text{constant}$ reduces to

$$(f_1, f_2) = \mathrm{i}(f_1^* f_2' - f_1^{*\prime} f_2). \tag{2.6}$$

It is independent of the hypersurface Σ for Klein–Gordon solutions f of (2.4). The Φ solutions are thereby normalised to δ functions.

On the other hand, the solution Φ of the Klein–Gordon equation for a particle of mass m and charge e

$$[(\partial_\mu + \mathrm{i}eA_\mu)(\partial^\mu + \mathrm{i}eA^\mu) + m^2]\Phi = 0 \tag{2.7}$$

in an external linearly-polarised time-dependent electric field $\boldsymbol{E}(\eta) = E(\eta)\boldsymbol{e}_z$ in Minkowski space–time (η is taken as the usual time coordinate) is, after the separation

$$\Phi = \frac{1}{(2\pi)^{3/2}} f(\eta)\exp[\pm\mathrm{i}(\hat{p}_x x + \hat{p}_y y + \hat{p}_z z)], \tag{2.8}$$

$(\hat{p}_x, \hat{p}_y, \hat{p}_z = \text{constant})$ also determined by an oscillator equation with time-dependent frequency

$$f'' + \omega^2(\eta) f = 0 \tag{2.9a}$$

$$\omega^2 = (\hat{p}_z - eA(\eta))^2 + \mu^2 \qquad \mu^2 = \hat{p}_x^2 + \hat{p}_y^2 + m^2. \tag{2.9b}$$

We have chosen $A^\mu = (0, 0, A(\eta), 0)$; accordingly we have $E(\eta) = -A'(\eta)$ and $p_z(\eta) = -eA(\eta) + \text{constant}$. The scalar product

$$\int_\Sigma \Phi_1^*(\mathrm{i}\,\partial^\mu - 2eA^\mu)\Phi_2\,\mathrm{d}\Sigma_\mu \tag{2.10}$$

reduces with (2.8) for the Σ hypersurface $\eta = \text{constant}$ to

$$(f_1, f_2) = \mathrm{i}(f_1^* f_2' - f_1^{*\prime} f_2), \tag{2.11}$$

which agrees with the form of (2.6). It is independent of the hypersurface for Klein–Gordon solutions f of (2.9).

Finally the one-dimensional one-particle Schrödinger equation for stationary solutions $u(x)$ in a potential $V(x)$ is of the form

$$u''(x)+\omega^2(x)u(x)=0 \qquad \omega(x)=[2m(E-V(x))]^{1/2} \tag{2.12}$$

with $(\ )'=\partial/\partial x$. Taking η instead of x, equation (2.12) has the same structure as (2.4) and (2.9a). The product which agrees with (2.6) and (2.12) is the Wronskian

$$(u_1, u_2)=\mathrm{i}(u_1^* u_2' - u_1^{*\prime} u_2). \tag{2.13}$$

It is conserved for two Schrödinger solutions of (2.12). For $u_1=u_2$ it represents a current.

All three physical systems therefore agree with regard to field equations and scalar product if apart from $\eta \leftrightarrow x$ one identifies the respective external fields according to

$$R^2(\eta)m^2 \leftrightarrow (\hat{p}_z - eA(\eta))^2 \leftrightarrow -2mV(x) \tag{2.14}$$

and the remaining parameters according to

$$k^2 \leftrightarrow \hat{p}_x^2+\hat{p}_y^2+m^2 \leftrightarrow 2mE, \tag{2.15}$$

which implies $V\leqslant 0$, $E\geqslant 0$ for the Schrödinger problem.

With regard to the process of particle creation the quantised Klein–Gordon field is expanded according to

$$\Phi=\frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^3k[a_k^{\mathrm{in}}\ {}_{+}f_k(\eta)\exp(\mathrm{i}\boldsymbol{kx})+(b_k^{\mathrm{in}})^{\dagger}\ {}_{-}f_k \exp(-\mathrm{i}\boldsymbol{kx})] \tag{2.16a}$$

$$\Phi=\frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^3k[a_k^{\mathrm{out}}\ {}^{+}f_k(\eta)\exp(\mathrm{i}\boldsymbol{kx})+(b_k^{\mathrm{out}})^{\dagger}\ {}^{-}f_k \exp(-\mathrm{i}\boldsymbol{kx})] \tag{2.16b}$$

where the $f_k(\eta)$ are solutions of the oscillator equations (2.4) or (2.9a). We assume that asymptotically for $\eta\to-\infty$ and $\eta\to+\infty$ an in-region Σ^{in} and an out-region Σ^{out} exist which allow the existence of free particles. According to the definition of free particles, which will be specified in the next section, the solutions ${}_{\pm}f_k(\eta)$ and ${}^{\pm}f_k(\eta)$ are additionally specified by demanding that asymptotically for $\eta\leftrightarrow-\infty$ and $\eta\to+\infty$ respectively they fulfil particular conditions. They represent different Fock bases and define particles (plus sign) or antiparticles (minus sign) in the corresponding region. Because our definition of free particles will be based on an asymptotical WKB behaviour of $f(\eta)$ (see next section) we have asymptotically ${}_{-}f_k={}_{+}f_k^*$. The relative probability ρ_k for the creation of a pair with opposite momentum (momentum parameter $\boldsymbol{k}$) is then given by

$$\rho_k=|\beta_k|^2/|\alpha_k|^2=|({}^{+}f_k, {}_{-}f_k)|^2/|({}^{+}f_k, {}_{+}f_k)|^2=|({}^{+}f_k, {}_{+}f_k^*)|^2/|({}^{+}f_k, {}_{+}f_k)|^2. \tag{2.17}$$

Because the Bogolubov coefficients α_k and β_k are connected by $|\alpha_k|^2-|\beta_k|^2=1$, the mean total number of pairs created per coordinate volume in the channel $\boldsymbol{k}$ is

$$\langle N_k\rangle=|\beta_k|^2=\rho_k/(1-\rho_k). \tag{2.18}$$

The analogous process described by the Schrödinger equation (2.12) is the above-barrier reflection with potential $V(x)\leqslant 0$ where a stream of particles with energy $E\geqslant 0$, which is assumed to be incident from the right (i.e. $x=+\infty$), is partly reflected back to $x=+\infty$ and partly transmitted to $x=-\infty$. Let ${}^{+}f$ be a solution of (2.12) normalised by means of (2.13) which shows for $x\to-\infty$ the same asymptotic behaviour as demanded in (2.16) above and let ${}_{+}f$ be a solution with this property for $x\to+\infty$ and let both be propagating in the negative x direction. Above-barrier reflection can then be described by the following solution u which is also normalised by means of (2.13):

$$u(x) = {}^{+}f(x) = A_{+}f(x) + B_{+}f^{*}(x). \tag{2.19}$$

This normalisation implies $|A|^2 - |B|^2 = 1$. For the reflection coefficient ρ we obtain

$$\rho = |B|^2/|A|^2 = |({}^{+}f, {}_{+}f^{*})|^2/|({}^{+}f, {}_{+}f)|^2, \tag{2.20}$$

which formally agrees with (2.17).

Comparing (2.20) and (2.17) we therefore obtain the following *result.* If one identifies apart from $\eta \leftrightarrow x$ according to (2.14) and (2.15) and if one demands the same asymptotical behaviour of the solutions $f(\eta)$ and $u(x)$ in the in- and out-regions (thus defining the particle states and the vacua), the relative probability of pair creation in the cosmological and the electric field case on one hand and the reflection coefficient for above-barrier reflection on the other hand agree:

$$\rho(\text{cosmological}) = \rho(\text{electric}) = \rho(\text{above-barrier reflection}). \tag{2.21}$$

The same applies for $\langle N \rangle$.

This implies several advantages for the discussion of cosmological pair creation. (i) Rigorous results for pair creation in time-dependent electric fields and of above-barrier reflection already obtained for various potentials can easily be transcribed. (ii) Approximation methods elaborated in either of the two fields can simply be rearranged for the calculation of the probability of cosmological pair creation. (iii) Especially when looking at the equivalent situation of the more familiar above-barrier reflection one easily obtains a deeper intuitive insight into what is to be expected for cosmological pair creation caused by a particular contraction–expansion behaviour of a universe.

3. Different concepts of free particles

A central question of quantum field theory in curved space–time is 'what are particles?', i.e. what are the 'positive frequency' solutions in the space–time regions in question? For a survey of different approaches and references see Parker (1977) and Gibbons (1978). Since we are concerned with an in–out calculation based on Fock representations we are interested only in the definition of *free particles*, by which we mean particles in a region in which the particle producing interactions have not yet started or are already finished.

To define the vacuum we take a *generally covariant WKB particle approach* and demand that the wavefunctions in order to define free particles should be on the Cauchy hypersurfaces Σ^{in} and Σ^{out} respectively: (i) exact Klein–Gordon solutions (KG solutions) and (ii) exact solutions of the WKB equations (WKB solutions) also, thus restricting the Cauchy data for the Klein–Gordon field equations. A consequence justifying this definition physically is that in terms of the creation and annihilation operators corresponding to these free particles the Hamiltonian taken with regard to the preferred time coordinate becomes diagonal (Mamaev *et al* 1976) and the solutions describing free particles lie future- or past-pointing on the mass shell (see below). This corresponds to a process of state preparation or observation which is based on an energy measurement whereby the energy–momentum condition fulfilled guarantees that the particles are not produced by the detector. For a less restrixtive WKB approach see, e.g., Woodhouse (1976). For an extended WKB approach see below (Parker and Fulling 1974). Often it is only demanded that the states 'look like' WKB states.

First, in order to compare in a covariant manner the KG and WKB solutions, we decompose Ψ of (2.2) according to

$$\Psi = a(\boldsymbol{x}, \eta)\exp(\pm \mathrm{i} W(\boldsymbol{x}, \eta)) \tag{3.1}$$

with real functions $a(\boldsymbol{x}, \eta)$ and $W(\boldsymbol{x}, \eta)$. Then the Klein–Gordon equation (2.2) decomposes according to

$$a^{|\alpha}{}_{\|\alpha} + \tfrac{1}{6}\hat{R} - a(W^{|\alpha}W_{|\alpha} - m^2) = 0 \tag{3.2a}$$

$$\frac{1}{a}(a^2 W^{|\alpha})_{\|\alpha} = 0. \tag{3.2b}$$

The generally covariant *WKB equations* for Klein–Gordon particles, which after reintroducing $\hbar$ are formally obtained by letting $\hbar \to 0$, are:

$$W^{|\alpha}W_{|\alpha} - m^2 = 0 \tag{3.3a}$$

$$(a^2 W^{|\alpha})_{\|\alpha} = 0. \tag{3.3b}$$

Explicitly, for the line element (2.1) we obtain from (3.3a) after separating according to (2.3), i.e. restricting to WKB solutions which are momentum eigenfunctions,

$$W_{|\eta} = -(R^2(\eta)m^2 + k^2)^{1/2} = -\omega \tag{3.4a}$$

$$W_{|\boldsymbol{x}} = \boldsymbol{k}, \tag{3.4b}$$

and correspondingly from (3.3b)

$$a = \text{constant} \times \frac{1}{R(R^2m^2 + k^2)^{1/4}} = \text{constant}\,\frac{1}{R\sqrt{\omega}}, \tag{3.5}$$

which implies

$$a^{|\alpha}{}_{\|\alpha} + \tfrac{1}{6}\hat{R}a = R^{-3}(Ra)'' = R^{-3}[(R^2m^2 + k^2)^{-1/4}]'' \tag{3.6}$$

with $(\ )' = \partial/\partial\eta$.

The current $j_\alpha = \mp(a^2/m)W_{|\alpha}$, where the two signs correspond to the signs in (3.1), is because (3.3b) is divergence free and tangent to a geodesic congruence. The Hamiltonian–Jacobi equation (3.3a) guarantees that the four-momentum fulfils the energy–momentum relation, i.e. that the solution lies on the mass shell. The different signs $+/-$ in (3.1) correspond to future/past pointing j^α and p^α and accordingly represent positive/negative frequency solutions. The corresponding solutions ${}_+f, {}^+f/{}_-f, {}^-f$ are in the region $(*)$, where they represent free particles/antiparticles given by

$${}_+f, {}^+f/{}_-f, {}^-f \overset{*}{=} \frac{1}{(2m\omega(\eta))^{1/2}}\exp\left(-/+\mathrm{i}\int \omega(\eta)\,\mathrm{d}\eta\right). \tag{3.7}$$

Note for the following that for the particular asymptotic hypersurfaces Σ characterised by $R^2 \to 0$ or $R^2 \to \infty$ we have $|a| \to \infty$ or $|a| \to 0$. Note additionally that in order to represent the energy–momentum relation (Hamilton–Jacobi equation) for any particular time, we have to use as the WKB equation the equation (3.3a) without any multiplication by a function of a. Therefore, with regard to the definition of free particles, the demand that the wavefunctions in the decomposition (2.16) are KG solutions at all Cauchy hypersurfaces and additionally fulfil exactly the WKB equations at the Cauchy hypersurfaces Σ^{in} and Σ^{out} implies (compare (3.2a) and (3.3a)) that $a^{-1}(a^{|\alpha}{}_{\|\alpha}+\frac{1}{6}\hat{R})=0$ at Σ^{in} and Σ^{out}. This covariant condition results independently of a possible multiplication of the Klein–Gordon equation (3.2) by a factor.

We assume that the other conditions necessary for describing particles (for example, being an orthonormal basis) are fulfilled at Σ^{in} and Σ^{out}. We then have the following definition of free particles together with the related condition a space–time region has to fulfil in order that the particle-producing interaction is absent, and accordingly the concept of free particles makes sense at all.

Definition: *(KG → WKB) particles.* A Klein–Gordon solution of (3.2) goes over into an exact WKB solution (i.e. fulfils (3.3)) at Σ^{in} and Σ^{out}. The corresponding necessary condition for the space–time is

$$0=\frac{1}{a}(a^{|\alpha}{}_{\|\alpha}+\tfrac{1}{6}\hat{R})\Big|_{\Sigma^{\text{in}}/\Sigma^{\text{out}}} \stackrel{*}{=} \frac{1}{R^2}(R^2m^2+k^2)^{1/4}[(R^2m^2+k^2)^{-1/4}]''\Big|_{\eta^{\text{in}}/\eta^{\text{out}}}. \tag{3.8}$$

(Here $\stackrel{*}{=}$ refers to the space–time (2.1) with $\Sigma^{\text{in}}/\Sigma^{\text{out}}$ being Cauchy hypersurfaces described by $\eta^{\text{in}}/\eta^{\text{out}}=$ constant including $\eta^{\text{in}}/\eta^{\text{out}}\to -/+\infty$.)

The approximation procedure of the next section is based on a Liouville transformation of the oscillator equations (2.4), (2.9a) and (2.12):

$$(\mathrm{d}^2f/\mathrm{d}\eta^2)+\omega^2(\eta)f=0. \tag{3.9}$$

This transformation has also been used as starting point for a particle definition. The transformation (Liouville 1837)

$$f\to f_2=\sqrt{\omega}\,f \qquad \eta\to\eta_2=\int\omega\,\mathrm{d}\eta \tag{3.10}$$

leads to an equivalent new oscillator equation†

$$(\mathrm{d}^2f_2/\mathrm{d}\eta_2^2)+[1+\epsilon_2(\eta_2)]f_2=0 \tag{3.11}$$

with

$$\epsilon^2=\frac{1}{\omega^{3/2}}\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}\left(\frac{1}{\sqrt{\omega}}\right)=\frac{3}{4}\frac{\omega^{12}}{\omega^4}-\frac{1}{2}\frac{\omega''}{\omega^3}. \tag{3.12}$$

This transformation can correspondingly be repeated, always leading to oscillator equations of type (3.11) with a frequency of the form $\omega_n^2=1+\epsilon_n$. Thereby n is usually counted in steps $\Delta n=2$ (Chakraborty 1973). Putting the respective ϵ_n equal to zero one obtains different levels of a WKB-type approximation for (3.9). Comparing (2.3), (3.1), (3.4) and (3.5) with the solution f_2 or f of (3.11) or (3.10) for $\epsilon_2=0$ one verifies that this f agrees with the WKB solution in the sense used above. The conditions $\epsilon_n=0$ again imply conditions for the space–time. For $n=2$ we have with (2.4) and (3.13),

$$\epsilon_2=\frac{1}{\omega^{3/2}}\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}\left(\frac{1}{\sqrt{\omega}}\right)=\frac{3}{4}\frac{\omega^{12}}{\omega^4}-\frac{1}{2}\frac{\omega''}{\omega^3}. \tag{3.13}$$

† For a more general transformation which preserves the form of the oscillator equation see Fröman and Fröman (1965).

In the framework of adiabatic regularisation (Parker and Fulling 1974, Fulling *et al* 1974) the *definitions of particles* are based on functions which fulfil the oscillator equation with $\epsilon_n = 0$ for a certain n. With regard to the question of whether a Cauchy hypersurface admits free particles, the main objection against these definitions, apart from being non-covariantly formulated, is that they are based on an equation for $f(\eta)$ instead of the physical function Ψ as in the definition above. In fact, for $\epsilon_2 = 0$ only equation (3.11) with the left side multiplied by a time-dependent factor is equivalent to the WKB equation. Because of this there is for $R^2 \to 0$ even for $n = 2$ a difference between $\epsilon_2 = 0$ on one hand and (3.8) on the other. The condition (3.8) is stronger. The difference between the two conditions is illustrated physically by the example in § 6.6 where, demanding $\epsilon_2 = 0$ only, the big bang would represent an in-region with no particle production. For $R^2 \to \infty$ the conditions (3.8) and $\epsilon_2 = 0$ both agree.

That the wavefunctions of free particles should solve the Klein–Gordon as well as the WKB equations has been stated by Audretsch and Schäfer (1978b), while the (KG→WKB) particle definition has been used implicitly by Schäfer (1978), who showed that, according to this definition, in the DeSitter space no free particles are possible time-asymptotically, i.e. that the particle-producing interaction continues. In the framework of this paper the condition $\epsilon_2 = 0$ is essential for the following approximation method.

4. Approximation method to calculate the pair creation probability

The approximation method to calculate ρ of (2.27) is a quasiclassical approach which is based on the comparison of WKB-type solutions of the oscillator equation (3.9) in an in- and an out-region. The discussion of the definitions of the preceeding chapter is necessary because, before applying the resulting approximation formula, it has to be proved whether or not the WKB particle concept can sensibly be applied asymptotically according to one of the definitions. The latter presupposes (3.8), in contrast to the approximation formula below for which $\epsilon_2 = 0$ will have to be fulfilled. Following the analogies of § 2, we transcribe for cosmological pair creation by identifying according to (2.14) and (2.15) a result which has been derived and discussed widely in the framework of above-barrier reflection and of particle creation by time-dependent electric fields.

The solution of (3.9) has the general form

$$A(\eta)\frac{1}{\sqrt{\omega(\eta)}}\exp\left(-\mathrm{i}\int \omega \, \mathrm{d}\eta\right) + B(\eta)\frac{1}{\sqrt{\omega(\eta)}}\exp\left(+\mathrm{i}\int \omega \, \mathrm{d}\eta\right). \tag{4.1}$$

If at $\eta \to \pm\infty$ free particles exist according to § 3, the situation of pair creation (above-barrier reflection, $\eta = x$) is described by $A = 1$, $B = 0$ at $\eta \to -\infty$ and $\rho = |B/A|^2$ at $\eta \to +\infty$. In the framework of the WKB approximation one cannot determine ρ by moving along the real axis. To connect the asymptotic solutions one therefore moves in the complex η plane. Thereby the behaviour of the differential equation at the zeros of η, which are called transition points (turning points, reflections points), needs special consideration because of the singular behaviour of ϵ_2. In contrast to barrier transmission we have in our case complex transition points representing the fact that the reflection is classically impossible. Without repeating its proof, we state the following theorem which allows the approximate determination† of ρ.

† For a different method to treat particle creation or reflection above a barrier see Migdal (1977).

Theorem: *Approximation formula.* We assume (i) that the criterion for the applicability of the WKB approximation to the oscillator equation (3.9) with $\omega^2 = R^2(\eta)m^2 + k^2$ is everywhere fulfilled on the real axis (take, e.g. $\epsilon_2 \ll 1$), (ii) that the solutions of (3.10) become exact WKB solutions for $\eta \to \pm\infty$, i.e. $\epsilon_2 \to 0$, (iii) that $R^2(\eta)$ is an analytic function in the complex η plane and (iv) that the complex transition point η_0 (where $\omega^2(\eta_0) = 0$) nearest to the real axis is a simple root of ω^2, i.e. $\omega \to C(\eta - \eta_0)^{1/2}$, $C \neq 0$ for $\eta \to \eta_0$ and that all other zeros and singularities of ω^2 lie far away from the real axis.

Then ρ is given approximately by

$$\rho = \exp(-4 \operatorname{Im} I) \tag{4.2a}$$

with

$$I = \int_{\eta_1}^{\eta_0} \omega(\eta)\, d\eta \tag{4.2b}$$

where $\operatorname{Im} \eta_0 \geqslant 0$ and η_1 is a point on the real axis with $\eta_1 \leqslant \operatorname{Re} \eta_0$. Because of (i), the approximation is valid for $\operatorname{Im} I \gg 1$ or, equivalently, $\rho \ll 1$.

This theorem has been derived by Pokrovskii and Khalatnikov (1961). For a more heuristic illustration see Landau and Lifshitz (1965). Using a different approach, the result has also been obtained by Fröman and Fröman (1965). Applications to electric pair creation are discussed by Popov (1972) and Marinov and Popov (1977). Since ω^2 is real on the real axis we have $\omega^2(\eta_0^*) = [\omega^2(\eta_0)]^*$ so that there are two complex conjugate zeros: η_0 with $\operatorname{Im} \eta_0 \geqslant 0$ and η_0^*. The formula (4.2) takes into account only the contribution from the nearest transition point and its complex conjugate. If there are more transition points their contributions to ρ are additive. For further details see Pokrovskii and Khalatnikov (1961). An essential statement of the theorem is the term 1 before the exponential in (4.2*a*). The condition (iv) is most likely fulfilled for cosmological pair creation. If $\omega \to C(\eta - \eta_0)^{\alpha-1}$, $C \neq 0$, $\alpha > 0$ for $\eta \to \eta_0$, the right-hand side of (4.2*a*) is to be multiplied by $4\cos^2(\pi/2\alpha)$.

Because ω of (2.4), (2.9) and (2.12) is a real square root on the real axis we find after cutting the complex plane from η_0^* to η_0 that

$$4 \operatorname{Im} I = 2 \operatorname{Im} \int_{\eta_0^*}^{\eta_0} \omega\, d\eta = \operatorname{Im} \oint_C \omega\, d\eta \tag{4.3}$$

where in the first integral the path of integration lies on the left-hand side of the cut and the path C surrounds the cut clockwise on the upper sheet. In favourable cases the second integral may be evaluated using the residue theorem.

For special cosmological cases the calculation of ρ can be further simplified. Restricting our considerations to a cosmological evolution with a *time-symmetric contraction–expansion law*, it is useful to describe this in the form (symmetry axis: $\eta = 0$)

$$R^2(\eta) = \tilde{R}^2(\eta) + R_0^2 \qquad R_0^2 = R^2(\eta = 0) \tag{4.4}$$

by means of a time-antisymmetric function $\tilde{R}(\eta)$:

$$\tilde{R}(\eta) = -\tilde{R}(-\eta) \tag{4.5a}$$

$$\partial\tilde{R}/\partial\eta > 0, \tag{4.5b}$$

where for (4.5*b*) we have additionally assumed $\partial\tilde{R}/\partial\eta \neq 0$. For $R_0^2 = 0$ a singularity appears at $\eta = 0$. Without difficulty we can enclose $R_0^2 = 0$ as a limiting case in our considerations by describing the corresponding 'passage through the singularity' of the Klein–Gordon test field by means of a conformal method as has been done by Audretsch and Schäfer (1978a), though from the physical point of view it is doubtful if the approximation of unquantised geometry can be maintained if the curvature radius becomes very much smaller than the Planck radius.

Because of the structure (2.4) of ω we can combine k^2 and R_0^2 by

$$\tilde{k}^2 = k^2 + R_0^2 m^2 \qquad \omega^2 = \tilde{R}^2 m^2 + \tilde{k}^2. \tag{4.6}$$

In the contour integral of (4.3) we now transform the complex variable according to $\eta \to u = (m/\tilde{k})\tilde{R}(\eta)$, $\tilde{k} > 0$, which implies transition points at $u = \pm \mathrm{i}$. As a consequence of (4.5), the functions $\tilde{R}^2$ and $\tilde{R}'$ are real on the imaginary axis also. Therefore after rotating the imaginary axis by the transformation $u \to v = -\mathrm{i}u$ on the real axis, we find that the contour integral reduces to a *real quadrature*

$$4 \operatorname{Im} I = \frac{2\tilde{k}^2}{m} \int_{-1}^{+1} \frac{(1-v^2)^{1/2}}{\tilde{R}'(v)} \, \mathrm{d}v \tag{4.7}$$

where the real function $\tilde{R}'(v)$ is obtained from $\tilde{R}'(\eta)$ by substituting the inverse of the function $v = -\mathrm{i}(m/\tilde{k})\tilde{R}(\eta)$. It may be easier after substituting $\eta = \mathrm{i}\xi$ to invert $v = v(\xi)$, thus obtaining $\xi = \xi(v)$. One then has

$$\frac{1}{\tilde{R}'(v)} = \frac{m}{\tilde{k}} \frac{\mathrm{d}\xi}{\mathrm{d}v}. \tag{4.8}$$

5. Generalisations

For a wide class of space–times separable coordinate systems can be found with regard to which the time dependence of the minimally- or the conformally-coupled Klein–Gordon equation reduces to an oscillator equation with variable frequency (Dietz 1976), so that the approximation formulae of the preceeding section can be applied if in- and out-regions with free particles exist. Before applying the scheme above one has to see if the whole space–time is covered by the respective coordinate system and if, for example by the existence of horizons, pure states may be changed into superpositions so that our coherent calculation does not apply.

Particular examples leading to an oscillator equation (3.9) are the conformally-coupled Klein–Gordon equation in anisotropic, homogeneous cosmologies (Kasner universes) (Zeldovich and Starobinskii 1972) and the conformally- or minimally-coupled Klein–Gordon equation in Robertson–Walker universes with non-vanishing positive or negative three-curvature (Parker and Fulling 1974, Mamaev *et al* 1976). For later use we note that for the three-flat Robertson–Walker metric (2.1*a*) the minimally-coupled Klein–Gordon equation (i.e. (2.2) with $\hat{R} = 0$) leads after introduction of

$$\tau = \int^t R(t')^{-3} \, \mathrm{d}t' \tag{5.1}$$

for the time-dependent part $g(\tau)$ of the separation $\Psi = g(\tau) Y(\boldsymbol{x})$ to the oscillator equation

$$\frac{\mathrm{d}^2 g}{\mathrm{d}\tau^2} + R^6(\tau)\left(\frac{k^2}{R^2(\tau)} + m^2\right) g = 0. \tag{5.2}$$

The creation of *Dirac particles* by the expansion–contraction of a Robertson–Walker universe is characterised by the fact that there is no interaction with the spin so that one again obtains, after appropriate separation an oscillator equation but with complex frequency (Audretsch and Schäfer 1978a):

$$f'' + (R^2m^2 + k^2 \pm \mathrm{i}mR')f = 0. \tag{5.3}$$

In addition, there is a close similarity with the case of fermions in linear time-dependent electric fields for which the separation leads to

$$f'' + [(\hat{p}_z - eA)^2 + \hat{p}_x^2 + \hat{p}_y^2 + m^2 \mp \mathrm{i}eA']f = 0 \tag{5.4}$$

so that again one may try to transcribe exact results using the identifications (2.14) and (2.15). Because of the complex oscillator frequency (equivalent to a complex barrier) the results of this section cannot be used directly. An approximative treatment of (5.4) has been given by Marinov and Popov (1977).

6. Applications

To indicate the usefulness of the preceeding considerations and to show that there is a wide range of applications for the exact correspondences of § 2 and the approximation formulae of § 4, we discuss several problems which are related mainly to the question of under what condition the spectrum of the created Klein–Gordon particles is a thermal one. We therefore partly reproduce relations published already and partly obtain new results.

6.1. *Conformal coupling, $R^2(\eta) = b^2\eta^2 + R_0^2$ (exact result)*

For the contraction–expansion law

$$R^2(\eta) = b^2\eta^2 + R_0^2 \qquad b = \text{constant} \qquad -\infty < \eta < +\infty, \tag{6.1}$$

which represents a radiation-dominated universe with avoided singularity if $R_0^2 \neq 0$, none of the conditions for free particles is fulfilled for finite η; we also have $\epsilon_2 \neq 0$. Because all conditions are fulfilled for $\eta \to \pm\infty$ we have to take this as the in- and out-region. Then we can transcribe according to § 2 an exact result for particle creation in the uniform electric field E in the z direction $(A^2 = E^2\eta^2)$

$$\langle N \rangle(\text{electric}) = \exp[-\pi(m^2 + \hat{p}_x^2 + \hat{p}_y^2)/eE] \tag{6.2}$$

obtained by means of an asymptotic WKB concept of free particles (Nikiskov (1970). Incorporating R_0^2 according to (4.6) we find with (2.14) and (2.15) for the number of pairs (!) created per unit coordinate volume with mode parameter $\boldsymbol{k}$ out of $[\boldsymbol{k}, \boldsymbol{k} + \mathrm{d}\boldsymbol{k}]$

$$\langle N_k \rangle(\text{cosmological}) = \exp[-\pi(k^2 + R_0^2)/mb]. \tag{6.3}$$

Introducing the physical momentum $\boldsymbol{p} = R^{-1}(\eta)\boldsymbol{k}$ as measured by the cosmological observer and Boltzmann's constant k_{B} we have

$$\langle N_k \rangle(\text{cosmological}) = \exp\left(-\frac{p^2}{2m}\frac{1}{k_{\mathrm{B}}T}\right)\exp(\mu/k_{\mathrm{B}}T) \tag{6.4}$$

which represents a non-relativistic thermal spectrum with temperature T and chemical potential μ as given by

$$T = b/2\pi R^2 k_B \qquad \mu = -b^{-1}\pi m R_0^2 k_B T. \tag{6.5}$$

For this interpretation we have assumed that the created pure state takes part in a thermodynamical process. The expression (6.4) has also been obtained as an exact result by Audretsch and Schäfer (1978b).

6.2. *Conformal coupling, Eckart–Sauter potential (exact result)*

Another transcription of an exact result can be carried out for the Eckart potential (Eckart 1930)

$$V(x) = -\left(\frac{A\xi}{1-\xi} + \frac{B\xi}{(1-\xi)^2}\right) \qquad \xi = -\exp(2\pi x/l) \qquad A, B = \text{constant}. \tag{6.6}$$

We restrict our considerations to the case $B = 0$, which is often attributed to Sauter (1932):

$$V(x) = \frac{A}{1+\exp(-2\pi x/l)} = \tfrac{1}{2}A(1+\tanh(\pi x/l)). \tag{6.7}$$

It represents a step of high A smoothed out between $x = -l$ and $x = +l$. For above-barrier reflection ($E \geqslant 0$, $E \geqslant A$) the reflection coefficient is

$$\rho = \frac{\cosh[2\pi(\alpha-\beta)]-1}{\cosh[2\pi(\alpha+\beta)]-1} = \frac{\sinh^2 \pi(\alpha-\beta)}{\sinh^2 \pi(\alpha+\beta)} \tag{6.8a}$$

where

$$\alpha = l(2mE)^{1/2}/2\pi \qquad \beta = l[2m(E-A)]^{1/2}/2\pi. \tag{6.8b}$$

For the case $B \neq 0$ see Eckart (1930). To obtain the corresponding exact result of particle creation in a universe with a step-like expansion law one has to rewrite (6.8) by means of (2.14) and (2.15). The corresponding result has also been obtained by explicit calculations by Bernhard and Duncan (1977).

6.3. *Conformal coupling, $R^2(\eta) = b^2\eta^2 + R_0^2$ (approximation)*

To test the results of § 4 we treat the contraction–expansion law (6.1) approximately by means of (4.7). Because of

$$\int_{-1}^{+1} (1-v^2)^{1/2}\, \mathrm{d}v = \tfrac{1}{2}\pi \tag{6.9}$$

we obtain an approximation for $\rho_k \ll 1$:

$$\rho_k \approx \exp[-\pi(k^2 + R_0^2)/bm], \tag{6.10}$$

so that with (2.20) the approximate result for $\langle N_k \rangle$ agrees with the exact result (6.3). This reflects the fact that a WKB approximation method gives exact results for the parabolic potential.

6.4. *Stability of the result*

Because the approximate result for $\langle N_k \rangle$ agrees with the exact one and because the approximation formulae of § 4 are obtained in leaving the real η axis and connecting the in- and out-region in passing along in a curve through the complex η plane, we may infer the following statement concerning the stability of the result. If a contraction–expansion law $R^2(\eta)$ has approximately parabolic shape $\sim\eta^2$ in the region of the complex η plane which contains the transition point and if $R^2(\eta)$ reaches $R^2(\pm\infty)$ smoothly, the result (6.3) for $\langle N_k \rangle \ll 1$ representing a non-relativistic thermal spectrum will be a very good approximation.

On the other hand, to obtain the exact structure of a non-relativistic thermal spectrum it needs a dependence of $\boldsymbol{k}$ of the form

$$\langle N_k \rangle = \exp(-k^2 C^2) \qquad \partial C/\partial k = 0. \tag{6.11}$$

Assuming conformal coupling and a time-symmetric contraction–expansion behaviour we obtain from (4.7) that (6.11) is only fulfilled if

$$\frac{\partial}{\partial k}\int_{-1}^{+1} \frac{(1-v^2)^{1/2}}{\tilde{R}'(v)}\,\mathrm{d}v = 0 \tag{6.12}$$

where, because of (4.8), the function $\tilde{R}'(v)$ is in general dependent on k if $\tilde{R}' \neq$ constant. This verifies the conjecture of Audretsch and Schäfer (1978a) that the radiation-dominated universe with (6.1) is the only one for which the created particles have exactly a non-relativistic thermal spectrum for all values of $\boldsymbol{k}$.

6.5. *Minimal coupling, vanishing mass*

Changing to minimally-coupled particles (equation (5.2)) with vanishing mass $m = 0$, it has been found by Parker (1977; see also Parker 1976) that the expansion law

$$R^4(\tau) = a_1^4 + a_0^4 \exp(\tau/s) \tag{6.13}$$

implies for the created particles a relativistic thermal spectrum

$$\rho_k = \exp(-4\pi s a_1^2 k). \tag{6.14}$$

Parker (1977) conjectured that the relativistic thermal structure

$$\rho_k = \exp(-kC^2) \qquad \partial C/\partial k = 0 \tag{6.15}$$

may hold for rather general expansion laws $R(\tau)$. We can make this precise as follows. Comparing (5.2) with (2.4) we have $\omega^2 = R^4 k^2$ and τ instead of η. Together with (4.2) this implies the approximation

$$\rho_k \approx \exp\left(-k\int_{\tau_1}^{\tau_0} R^2(\tau)\,\mathrm{d}\tau\right) \tag{6.16}$$

and therefore the structure (6.15) whenever the approximation is possible according to the conditions of § 4, i.e. if $\rho_k \ll 0$, for instance because of large k. This result is easily generalised to the case of anisotropic expansion where the different components of $\boldsymbol{k}$ obtain different factors.

On the other hand, it may not be concluded from this that the relativistic thermal structure (6.15) is in general valid for small k as well. To give a counter example we choose

$$R^4(\tau) = A^2\tau^2 + B^2 \qquad A, B = \text{constant}, \tag{6.17}$$

thus reducing the calculation to the case solved exactly with (6.1). Comparing the respective oscillator frequencies ($R_0 = 0$), we obtain from (6.3) as an exact result for the expansion law (6.17)

$$\langle N_k \rangle = \exp[(-\pi B^2/A)k], \tag{6.18}$$

which agrees rigorously with a relativistic thermal spectrum only for large k.

6.6. *Conformal coupling, $R = at$ (approximation)*

Returning to conformal coupling we treat the expansion law

$$R(t) = at \qquad a = \text{constant} \qquad 0 < t < \infty \tag{6.19a}$$

$$R(\eta) = \exp(a\eta) \qquad -\infty < \eta < +\infty. \tag{6.19a}$$

For $t \to 0$ or $\eta \to -\infty$, according to (3.8) no (KG → WKB) particles exist so that there is no asymptotical in-region with free particles. On the other hand, according to (3.13) we have $\epsilon_2 \to 0$ so that at the singularity $t \to 0$, i.e. in the region of strongest gravitational interaction, Liouville ($\epsilon_2 = 0$) particles are possible. Thus justifies again that the definition of free particles should not be based on $\epsilon_2 = 0$ (cf § 3). Nevertheless, because $\epsilon_2 \to 0$ for $\eta \to -\infty$, we can formally (!) apply the approximation formulae of § 4. Evaluating (4.2b) explicitly in the complex plane we obtain by (4.2a)

$$\rho_k \approx \exp(-2\pi/a)k = \exp(-2\pi R(\eta)p(\eta)/a), \tag{6.20}$$

which is valid for large k. This result has also been found by path-integral methods by Chitre and Hartle (1977) and was interpreted by them as a relativistic thermal spectrum. Apart from the fact that there is no interaction-free in-region, an objection against this interpretation is that because $p(\eta) = R^{-1}(\eta)k$ in the out-region with $R \to \infty$, all momenta become non-relativistic.

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