An alternate Hamiltonian formulation of fourth–order theories and its application to cosmology

Hans-Jürgen Schmidt

Universität Potsdam, Institut für Mathematik, Projektgruppe Kosmologie
D-14415 POTSDAM, PF 601553, Am Neuen Palais 10, Germany
e-mail hjschmi@rz.uni-potsdam.de

Abstract

An alternate Hamiltonian $H$ different from Ostrogradski’s one is found for the Lagrangian $L = L(q, \dot{q}, \ddot{q})$, where $\partial^2 L/\partial(\ddot{q})^2 \neq 0$. We add a suitable divergence to $L$ and insert $a = q$ and $b = \ddot{q}$. Contrary to other approaches no constraint is needed because $\ddot{a} = b$ is one of the canonical equations. Another canonical equation becomes equivalent to the fourth–order Euler–Lagrange equation of $L$. Usually, $H$ becomes quadratic in the momenta, whereas the Ostrogradski approach has Hamiltonians always linear in the momenta.

For non–linear $L = F(R)$, $G = dF/dR \neq 0$ the Lagrangians $L$ and $\tilde{L} = \tilde{F}(\tilde{R})$ with $\tilde{F} = 2R/G^3 - 3L/G^4$, $\tilde{g}_{ij} = G^2 g_{ij}$ and $\tilde{R} = 3R/G^2 - 4L/G^3$ give conformally equivalent fourth–order field equations being dual to each other. This generalizes Buchdahl’s result for $L = R^2$.

The exact fourth–order gravity cosmological solutions found by Accioly and Chimento are interpreted from the viewpoint of the instability of fourth–order theories and how they transform under this duality.

Finally, the alternate Hamiltonian is applied to deduce the Wheeler–De Witt equation for fourth–order gravity models more systematically than before.
1 Introduction

Higher-order theories, especially fourth-order gravity theories, are subject to conflicting facts: On the one hand, they appear quite naturally from generally accepted principles; on the other hand, they are unstable and so, they should be considered unphysical.

Here, we want to attack this conflict from two directions. First: The Ostrogradski approach [1] to find a Hamiltonian formulation for a higher-order theory is the most famous (see e.g. refs. [1 - 9]) but possibly not the best method. To check this hypothesis, we present an alternate Hamiltonian formalism for fourth-order theories in sect. 2. It systematizes what has been sporadically done in the literature for special examples.

Sect. 3 deals with fourth-order gravity following from a non-linear Lagrangian $L(R)$. The conformal equivalence of these theories to theories of other types is widely known, but the conformal equivalence of these theories to theories of the same type but essentially different Lagrangian is much less known. We fill this gap by proving a duality theorem between pairs of such fourth-order theories in subsection 3.1. The instability of these theories from the point of view of the Cauchy problem is subject of subsection 3.2.

Sect. 2 applies to arbitrary theories, sect. 3 to gravity, and both are applied to fourth-order cosmology in sect. 4. We re-interpret known exact solutions (Friedmann models in subsection 4.1 and Kantowski–Sachs models in 4.2) under the stability criteria mentioned before.

In the final sect. 5 we discuss quantum effects and give hints (which shall be outlined in a future paper with S. Reuter) how to apply the alternate
Hamiltonian formalism of sct. 2 to the Wheeler–De Witt equation for a cosmological minisuperspace model within fourth–order gravity.

The rest of this introduction shortly reviews papers on higher–order theories. Eliezer and Woodard [1] and Jaen, Llosa and Molina [2] represent standard papers for the generalization of the Ostrogradski approach to non–local systems (see also [3]) and to systems with constraints (see also [4 - 6]) applying Dirac’s approach.

Let the Lagrangian \( L \) be a function of the vector \( q_\alpha \) and its first \( n \) temporal derivatives \( \dot{q}_\alpha, \ddot{q}_\alpha, \ldots, q^{(n)}_\alpha \). The Hessian is

\[
H_{\alpha\beta} = \frac{\partial^2 L}{\partial q^{(n)}_\alpha \partial q^{(n)}_\beta} \tag{1.1}
\]

and the non–vanishing of its determinant defines the regularity of \( L \). In the following we do not write the subscript \( \alpha \); one can think of \( q \) as being a point particle in a (one– or higher–dimensional) space. In the Ostrogradski approach, \( Q = \dot{q} \) is taken as additional position variable. This leads to an ambivalence of the procedure, because it is not trivial to see at which places \( \dot{q} \) has to be replaced with \( Q \), cf. [7]. We prevent this ambivalence in our alternate Hamiltonian, cf. sct. 2, by putting \( Q = \ddot{q} \).

Ref. [8] discusses higher–order field theories. The problem is the lack of an energy bound, typically two kinds of oscillators with different signs of energy exist. Usually, one restricts the space of initial conditions to prevent negative energy solutions. The authors of ref. [8] redefine the energy analogous to the Timoshenko model, so one gets a positive mechanical energy inspite of an indefinite Ostrogradski Hamiltonian, they write: "An appealing aspect of this approach is the absence of any constraint.” So it has this property in common with our approach sct. 2, but it is otherwise a different one.

A second standard procedure [2, 8, 9] for dealing with higher–order Lagrangians is to consider them as a sequence in a parameter \( \epsilon \), so one can break the Euler–Lagrange–equation into a sequence of second order ones. In [9] this is called "reduction of higher–order Lagrangians by a formal power series in an ordering parameter.” [9] deals also with the Lie–Königs theorem: a local Hamiltonian is always possible, and they consider some global questions.
Let us repeat the famous counter-example [10] Douglas (1941): it is an example of a second order system not following from a Lagrangian:

\[ \ddot{x} + \dot{y} = 0 \quad \ddot{y} + y + \epsilon \dot{x} = 0 \]

It follows from the Lagrangian

\[ L = \frac{1}{2}[\dot{y}^2 - y^2 + \epsilon(x\dot{y} - \dot{x}y - \dot{\dot{x}})] \]

for \( \epsilon \neq 0 \) and has no Lagrangian otherwise. We mention this example to show that the following recipe need to to work always. Recipe for higher-order theories: "Write down the Euler–Lagrange equations, break them into a sequence of second order ones by introducing further coordinates. Find Lagrangians for these second order equations."

A powerful method for dealing with a classical Lagrangian

\[ L = \frac{1}{2} g_{ij} \dot{q}^i \dot{q}^j - V(q) \]

is given in [11] and shall be applied in cosmological minisuperspace models like in sect. 5. The Euler–Lagrange equation to Lagrangian (1.2) reads

\[ \ddot{q}^i + \Gamma^i_{jk} \dot{q}^j \dot{q}^k = -g^{ik} V_k \]

and is fulfilled for geodesics in the Jacobi–metric

\[ \hat{g}_{ij} = (E - V) g_{ij} \]

Remark: For constant potentials \( V \) this is trivial, for non-constant potentials the constant \( E \) must be correctly chosen to get the result, for \( E = V \) it breaks down, of course.

Stelle [12] cites Ostrogradski [1] but uses other methods to extract different spin modes for fourth-order gravity. In [13], a regular reduction of fourth-order gravity similar to the method with an ordering parameter mentioned above has been proposed as follows: In the Newtonian limit one has

\[ \Delta \Phi + \beta \Delta \Delta \Phi = 4\pi G \rho, \]
then one restricts to solutions which can be expanded into powers of the coupling parameter $\beta$. Argument: If $\beta$ is a parameter, this is well justified, if it is a universal constant, then this restriction is less satisfying. Comment: This restriction excludes the usual Yukawa–like potential $\frac{1}{r} \exp(-r/\sqrt{\beta})$, so one may doubt whether this method gives the right solutions. Let us further mention ref. [14] for non–local gravitational Lagrangians like $L = R\Box^{-1}R + \Lambda$ in two dimensions and refs. [15, 16] for the linearized $R^2$–theory.

To facilitate the reading of sect. 2, we pick up the example eq. (5) of [5]:

$$\tilde{L} = \left[q^2 + 4\dot{q}\ddot{q}^2 + 4\dot{q}^4\right]e^{3q}$$  \hspace{1cm} (1.3)

The equation of motion is [5, eq. (6)]

$$2q^{(4)} + 12\dot{q}q^{(3)} + 9(\ddot{q})^2 + 18\dot{q}^2\ddot{q} = 0$$  \hspace{1cm} (1.4)

A good check of the validity of the formalism is the following: For a constant $c > 0$ and $\dot{q} > 0$, each solution of

$$\ddot{q} = -2\dot{q}^2 + c\sqrt{\dot{q}}$$

is also a solution of eq. (1.4).

By adding a divergence to eq. (1.3) one gets $L = (\dot{q})^2 e^{3q}$. The alternate formalism requires to use $q^1 = q$ and $q^2 = \ddot{q}$ as new coordinates. So we get

$$L = (q^2)^2 \exp(3q^1)$$  \hspace{1cm} (1.5)

Eq. (1.5) represents the ultralocal Lagrangian mentioned in [5]. It is correctly stated in [5], that the alternate formalism does not work for this version eq. (1.5) of the system. This clarifies that the addition of a divergence to a higher–order Lagrangian sometimes influences the applicability of the alternate Hamiltonian formalism. So one should add a ”suitable” total derivative to the Lagrangian. ”Suitable” means, that the space of solutions is the same at both sides, and that the relation between the various coordinates is ensured without imposing any constraints. It turns out, that the Lagrangian $\hat{L}$ differing from $\tilde{L}$, eq. (1.3) by a divergence only

$$\hat{L} = -[\dddot{q}^2 + 6\dot{q}\ddot{q}^2 + 2\dot{q}q^{(3)}]e^{3q}$$  \hspace{1cm} (1.6)
does the job. Of course, the variations of $L$, $\tilde{L}$, and \( \hat{L} \) with respect to $q$ all give the same equation of motion (1.4). But only in version (1.6) the alternate formalism (insertion of the equation $Q = \ddot{q}$ and then apply the usual formulas of classical mechanics - to avoid ambiguities with the square–sign we have replaced $q^1$ by $q$ and $q^2$ by $Q$) leads correctly to the Hamiltonian [5, eq. (7)]:

$$H = -\frac{1}{2}(pP - 3P^2Q)e^{-3q} + Q^2e^{3q}$$ \hspace{1cm} (1.7)

It essentially differs from the Ostrogradski approach because terms only linear in the momenta do not appear; so one of the criteria for unboundedness of energy fails to be fulfilled. The integrability condition $Q = \ddot{q}$ and the equation of motion (1.4) both follow from the canonical equations of eq. (1.7); no constraint is necessary to get this.

## 2  The alternate Hamiltonian formalism

Let us consider the Lagrangian

$$L = L(q, \dot{q}, \ddot{q})$$ \hspace{1cm} (2.1)

for a point particle $q(t)$, a dot denoting $\frac{d}{dt}$ and

$$q^{(n)} = \frac{d^n q}{dt^n}$$

The corresponding Euler–Lagrange equation reads

$$0 = \frac{\partial L}{\partial q} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}} + \frac{d^2}{dt^2} \frac{\partial L}{\partial \ddot{q}}$$ \hspace{1cm} (2.2)

We suppose this Lagrangian to be non-degenerated, i.e., $L$ is non-linear in $\ddot{q}$. The highest-order term of eq. (2.2) is

$$q^{(4)} \frac{\partial^2 L}{\partial(\ddot{q})^2}$$

therefore, non-degeneracy (= regularity, cf. eq. (1.1)) is equivalent to require that eq. (2.2) is of fourth order, i.e.

$$\frac{\partial^2 L}{\partial(\ddot{q})^2} \neq 0$$
(If \(q\) is a vector consisting of \(m\) real components then this condition is to be written as Hessian determinant.)

If we add the divergence \(\frac{d}{dt}G(q, \dot{q})\) to \(L\), we do not alter the Euler–Lagrange equation (2.2). Furthermore, the expression \(\frac{d}{dt}G\) is linear in \(\dot{q}\), and so its addition to \(L\) does not influence the condition of non-degeneracy. The addition of such a divergence can therefore simply absorbed by a suitable redefinition of \(L\).

In the next two subsections we add a special and a more general divergence to get a Hamiltonian formulation different from Ostrogradski’s one. In the preprint by Kasper [4] a similar consideration has been made at the Lagrangian’s level. Subsection 2.1 represents only a special case of subsection 2.2, but we write it down, because it has the advantage that the formulas can be given explicitly, and so the formalism becomes more transparent.

### 2.1 A special divergence

The addition of the following divergence is no more done by a redefinition of \(L\)

\[
L_{\text{div}} = \frac{d}{dt}[f(q) \dot{q} \ddot{q}], \quad f(q) \neq 0
\]  

(2.3)

and we consider \(\hat{L} = L + L_{\text{div}}\). The Euler–Lagrange equation is again eq. (2.2). Using

\[
f'(q) \equiv \frac{df}{dq}
\]

we get

\[
\hat{L} = L + f'(q)q^2 \ddot{q} + f(q)[(\ddot{q})^2 + \dot{q}q^{(3)}]
\]  

(2.4)

which contains third derivatives of \(q\).

We introduce new coordinates

\[
a = q, \quad b = \ddot{q}
\]  

(2.5)

(In the Ostrogradski approach, the second coordinate is \(\dot{q}\), instead.) It is obvious that there is exactly this one compatibility condition:

\[
\ddot{a} = b
\]  

(2.6)
Let us insert eq. (2.5) into eq. (2.4). This insertion becomes unique by the additional requirement that \( \hat{L} \) does not depend on second and higher derivatives of \( a \) and \( b \), i.e.,

\[
\hat{L} = \hat{L}(\dot{a}, \dot{b}, \ddot{b})
\]

giving

\[
\hat{L} = L(a, \dot{a}, b, \dot{b}) + f'(a)\dddot{\dot{a}}b + f(a)[\dddot{\dot{b}} + \dddot{\dot{a}}]
\] (2.7)

(In the Ostrogradski approach, there remains an ambivalence which of the \( \dot{q} \) in the original Lagrangian is to be interpreted as second coordinate and which as time derivative of the first one.)

The momenta are defined as in classical mechanics by

\[
p_a = \frac{\partial \hat{L}}{\partial \dot{a}}, \quad p_b = \frac{\partial \hat{L}}{\partial \dot{b}}
\] (2.8)

(In the Ostrogradski approach, an additional term is necessary.) Inserting eq. (2.7) into eqs. (2.8) we get

\[
p_a = \frac{\partial L}{\partial \dot{a}} + 2f'(a)\dddot{\dot{a}}b + f(a)\dddot{\dot{b}}
\] (2.9)

and

\[
p_b = f(a)\dddot{\dot{a}}
\] (2.10)

Because of \( f(a) \neq 0 \), cf. eq. (2.3), we can invert eq. (2.10) to

\[
\dddot{\dot{a}} = \frac{p_b}{f(a)}
\] (2.11)

Inserting eq. (2.11) into eq. (2.9) and dividing by \( f(a) \) we get

\[
\dddot{\dot{b}} = \frac{1}{f(a)}[p_a - \frac{\partial L}{\partial \dot{a}} - 2f'(a)b\frac{p_b}{f(a)}]
\] (2.12)

It is instructive to make a more general consideration: The question, whether eqs. (2.9, 10) can be inverted to \( \dddot{\dot{a}}, \dddot{\dot{b}} \), can be answered by calculating the Jacobian

\[
J = \frac{\partial(p_a, p_b)}{\partial(\dddot{\dot{a}}, \dddot{\dot{b}})} = \frac{\partial p_a}{\partial \dddot{\dot{a}}} \frac{\partial p_b}{\partial \dddot{\dot{b}}} - \frac{\partial p_a}{\partial \dddot{\dot{b}}} \frac{\partial p_b}{\partial \dddot{\dot{a}}}
\] (2.13)

We insert eqs. (2.9, 10) into eq. (2.13) and get

\[
J = - [f(a)]^2
\] (2.14)
Because of $f \neq 0$ one has also $J \neq 0$ and the inversion is possible. This more general consideration gave the additional information that the Jacobian is always negative; this may be the hint to some kind of instability.

We define the Hamiltonian $H$ as usual by

$$H = \dot{p}_a + \dot{b}p_b - \dot{L}$$

i.e., with eq. (2.7) we get

$$H = \dot{a}p_a + \dot{b}p_b - L - f'(a)a^2b - f(a)[b^2 + \dot{a}b]$$

(2.15)

Here we insert $\dot{a}$ according to eq. (2.11) and get the Hamiltonian $H = H(a, p_a, b, p_b)$. The factor of $\dot{b}$ in $H$ automatically vanishes, so we do not need eq. (2.12). The canonical equations read

$$\frac{\partial H}{\partial p_a} = \dot{a}$$

(2.16)

further

$$\frac{\partial H}{\partial p_b} = \dot{b}$$

(2.17)

and

$$\frac{\partial H}{\partial a} = -\dot{p}_a$$

(2.18)

and

$$\frac{\partial H}{\partial b} = -\dot{p}_b$$

(2.19)

The whole procedure is intended to give the following results: The Hamiltonian $H$ shall be considered to be a usual Hamiltonian for two interacting point particles $a(t)$ and $b(t)$. One of the canonical equations shall be equivalent to the compatibility condition eq. (2.6) and another one shall be equivalent to the original Euler–Lagrange equation (2.2), whereas the two remaining canonical equations are used to eliminate the momenta $p_a$ and $p_b$ from the system. The next step is to find those Lagrangians $L$ which make this procedure work. From eqs. (2.15) and (2.11) we get

$$H = \frac{p_a p_b}{f'(a)} - L(a, \frac{p_b}{f'(a)}, b) - \frac{p_b^2 f'(a)}{f(a)^2} - f(a)b^2$$

(2.20)
In this form, eq. (2.16) coincides with eq. (2.11) and (2.17) with (2.12). So we may use eqs. (2.9, 10) in the following, because they are equivalent to eqs. (2.11, 12).

Now, we use eqs. (2.19), cancel $p_b$ by use of eq. (2.10) and get

$$0 = \frac{\partial L}{\partial b} + 2bf(a) - \ddot{a}f(a)$$

(2.21)

In order that the compatibility relation eq. (2.6) follows automatically from eq. (2.21), one has to ensure that $f(a) \neq 0$ (which is already assumed) and that

$$0 = \frac{\partial L}{\partial b} + bf(a)$$

identically takes place. The condition of non-degeneracy,

$$\frac{\partial^2 L}{\partial b^2} \neq 0$$

is then also automatically fulfilled. One has the following possible Lagrangian

$$L = -\frac{1}{2}f(a)b^2 + K(a, \dot{a})$$

(2.22)

where $K$ is an arbitrary function, but, for simplicity, we put $K = 0$.

The last of the four canonical equations to be used is eq. (2.18) reading now with eqs. (2.9, 10, 20)

$$0 = \ddot{f}b + 2f' \dot{a} \dot{b} + \frac{3}{2}f'' b^2 + f'' \dot{a}^2 b$$

(2.23)

If we insert here eq. (2.5) we get exactly the same as the Euler–Lagrange equation (2.2) following from the Lagrangian

$$L = -\frac{1}{2}f(q)(\ddot{q})^2$$

(2.24)

Result: For every Lagrangian of type (2.1) which can be brought into type (2.24) with $f \neq 0$ the addition of the divergence (2.3) makes it possible to apply the new coordinates (2.5). Then the system becomes equivalent to a classical Hamiltonian of two particles, and the relation (2.6) between them follows without imposing an additional constraint.
2.2 A general divergence

In this subsection we try to generalize the result of the previous subsection by avoiding to prescribe the special structure (2.3) of the divergence to be added. We substitute eq. (2.3) by

\[ L_{\text{div}} = \frac{d}{dt} h(q, \dot{q}, \ddot{q}) \]  (2.25)

Keeping eqs. (2.5) we get instead of eq. (2.7) now

\[ \hat{L} = L(a, \dot{a}, b) + h_1 \dot{a} + h_2 b + h_3 \dot{b} \]  (2.26)

where \( h_n \) denotes the partial derivative of \( h \) with respect to its \( n \)th argument.

Using eqs. (2.8), (2.10) is now replaced with

\[ p_b = h_3(a, \dot{a}, b) \]  (2.27)

Eq. (2.13) is kept, and (2.14) is replaced with

\[ J = -(h_{23})^2 \]  (2.28)

We have to require that \( h_{23} \neq 0 \), and then the equation \( p_b = h_3 \) is locally invertible as \( \dot{a} = F(p_b, a, b) \). From this definition one immediately gets the identity \( F_1 h_{23} = 1 \). Two further identities to be used later are not so trivial to guess. To derive them, let us for a moment fix \( p_b \) and then calculate the increase of \( h_3 \) with increasing \( a \) and \( b \) resp. The assumed constancy of \( h_3 \) yields the equations

\[ h_{13} + F_2 h_{23} = 0 \]  (2.29)

and

\[ h_{33} + F_3 h_{23} = 0 \]  (2.30)

resp. to be used for deducing the generalization of eq. (2.21). One gets the result: For \( h_{23} \neq 0 \) (which is already presumed), the compatibility relation (2.6) follows automatically from the canonical equation (2.19) if and only if

\[ 0 = L_3 + h_2 \]  (2.31)

is identically fulfilled. One can see: The condition of non–degeneracy of the Lagrangian (2.1) namely

\[ L_{33} \neq 0 \]
is equivalent to the condition $h_{23} \neq 0$. For any given non–degenerate Lagrangian we can find the appropriate divergence by solving eq. (2.31) as follows

$$h(q, \dot{q}, \ddot{q}) = -\int_{0}^{\dot{q}} L_3(q, x, \ddot{q})dx$$

(2.32)

All other things are fully analogous:

$$H = [p_a - h_1(a, F, b)]F - h_2(a, F, b)b - L(a, F, b)$$

(2.33)

where $F = F(p_b, a, b)$. Eq. (2.19) with (2.30) gives the compatibility condition (2.6). Eq. (2.18) with (2.29) is equivalent to the Euler–Lagrange equation (2.2).

Let us summarize this section: For the Lagrangian $L = L(q, \dot{q}, \ddot{q})$ where $\partial^2L/\partial(\ddot{q})^2 \neq 0$ we define $\hat{L} = L + L_{\text{div}}$ where

$$L_{\text{div}} = -\frac{d}{dt} \int \frac{\partial L}{\partial \ddot{q}}(q, x, \ddot{q})dx$$

We insert $a = q$ and $b = \ddot{q}$, define the momenta $p_a = \frac{\partial \hat{L}}{\partial \dot{a}}$ and $p_b = \frac{\partial \hat{L}}{\partial \dot{b}}$ and get the Hamiltonian $H = \dot{a}p_a + \dot{b}p_b - \hat{L}$. One of its canonical equations is $\ddot{a} = b$ and another one is equivalent to the fourth–order Euler–Lagrange equation following from $L$. By these properties, $L_{\text{div}}$ is uniquely determined up to the integration constant. Contrary to other approaches, no constraint is needed.

### 3 Fourth–order gravity

In Rainich (1925, ref. [17]) the electromagnetic field was calculated from the curvature tensor. This was cited in Kuchař (1963, ref. [18]) as example for the geometrization programme; in [18] on meson fields $\psi$ (now called scalar fields), Kuchař gives a kind of geometrization by using a relation between $\psi$ and $R$, then he gets the equation

$$\Box R - \frac{k^2}{2} R = 0$$

which is of fourth order in the metric. It looks like fourth–order gravity as we are dealt with, but he does not deduce it from a curvature squared action.
3.1 Duality theorems

In Bekenstein (1974, ref. [19]) the conformal transformation from Einstein’s theory with a minimally coupled ($\phi$) to a conformally coupled ($\psi$) scalar field is proven where additional conformally invariant matter (radiation) is allowed. For $8\pi G = 1$ one has

$$\psi = \sqrt{6} \tanh(\phi/\sqrt{6})$$

If radiation is absent then it works also with "coth" instead of "tanh". This is reformulated in his theorem 2: If $g_{ij}$ and $\psi$ form an Einstein–conformal scalar solution, then $\hat{g}_{ij} = \frac{1}{6}\psi^2 g_{ij}$ and $\hat{\psi} = 6/\psi$ form a second one. One can see that this is a dual map because by applying the operator $\hat{\ }$ twice, the original solution is re–obtained.

Let us comment this theorem 2: For the conformal scalar field one has the effective gravitational constant $G_{eff}$ defined by

$$\frac{1}{8\pi G_{eff}} = 1 - \frac{\psi^2}{6}$$

A positive value $G_{eff}$ implies a negative value $\hat{G}_{eff}$. By changing the overall sign of the Lagrangian one can achieve a positive effective gravitational constant at the price of the scalar field becoming a ghost (wrong sign in front of the kinetic term). So, Bekenstein has given a conformal transformation from Einstein’s theory with a conformally coupled ordinary scalar field to Einstein’s theory with a conformally coupled ghost. From this property one can see that this duality relation is different from the duality theorem to be deduced at the end of this subsection, because there one has effectively ordinary scalar fields at both sides.

Later but independently of [19] the conformal equivalence between minimally and conformally coupled scalar fields with $G_{eff} > 0$ was generalized in [20] by the inclusion of several self–interaction terms. The conformal transformation from fourth–order gravity to Einstein’s theory with a minimally coupled scalar field was deduced in several steps: Bicknell (1974, ref.[21]) found the transformation for $L = R^2$; the conformal
factor is $R$, and after the transformation one gets Einstein’s theory with non-vanishing $\Lambda$-term and a massless minimally coupled scalar field as source. Next steps see e.g. [22]. In [23] besides the conformal transformation it is shown that the trace $\sim R^2$ leads to a term like $R^2 \ln R$ in $L$. Ref. [24] generalizes it

by the inclusion of non-minimally coupled scalar fields. Jakubiec and Kijowski (1988/89, ref. [25]) generalize the conformal transformations to more general transformations of the metric.

Buchdahl (1978, ref. [26]) showed: For $L = R^2$ the conformal factor $R^2$ (if it is $\neq 0$) transforms solutions to solutions and represents a dual map in the set of solutions. (Another conformal factor than in [21]!) [27] generalizes this dual map to other non-linear Lagrangians $L(R)$, the conformal factor being $(\frac{dL}{dR})^2$. (Again, this conformal factor is the square of that conformal factor which is necessary to transform to Einstein’s theory with a minimally coupled scalar field.)

A further type of transformations was presented by Buchdahl in 1959, ref. [28]. For a space-time $V_n$ possessing a non-null hypersurface-orthogonal Killing vector one can produce solutions with a scalar field as follows. Let the Killing vector be $\frac{\partial}{\partial x^1}$, the metric is $g_{kl}$ with $g_{kl,1} = 0$, $g_{11} \neq 0$ and $g_{i\alpha} = 0$ where greek indices take all values except 1. Let $R_{kl} = 0$ and the dimension $n \geq 2$ but $n \neq 3$. We fix two reals $A$ and $B$ and define a new metric $\tilde{g}_{kl}$ by $\tilde{g}_{1\alpha} = 0$,

$$\tilde{g}_{11} = (g_{11})^A \quad \tilde{g}_{\alpha\beta} = (g_{11})^B g_{\alpha\beta}$$

(We consider the case $g_{11} > 0$, the other sign is treated analogously.) This is a conformal transformation for $A = B + 1$. Defining $g_{11} = e^{2\psi}$ one has $R_{11} = 0$ iff (= if and only if) $\Box \psi = 0$. So, $\Box \psi = 0$ is presumed from the beginning.

Further, it holds: $\Box \psi = 0$ is then identically fulfilled iff

$$A = 1 - B(n - 3)$$

(For $n = 4$, this means $A = 1 - B$.)

$B = 0$, $A = 1$ represents the identical transformation. For non-identical transformations the equation is compatible with a conformal transformation.
for \( n = 2 \) only. This is in agreement with the fact that the D’Alembert operator is conformally invariant for \( n = 2 \) only.

Buchdahl’s results are: For \( n = 4 \) and \( A = -1 \), i.e., \( B = 2 \), one gets a vacuum solution which is in general different from the initial one. For \( n = 4 \) and \( |A| \neq 1 \), one gets a solution of Einstein’s theory with a massless minimally coupled scalar field (which is proportional to \( \psi \)) as source. This supplements [21], because here no \( \Lambda \)-term is needed.

In [29, 30] the problem is discussed which of the conformally equivalent metrics in these theorems is the physical metric. Magnano and Sokołowski (1994, ref. [30]) represents a good review to this theme.

Let us now deduce the duality theorem announced in the introduction which shall close a gap in the set of the aforementioned results.

Let

\[ \hat{g}_{ij} = e^{2U} g_{ij} \]  

(3.1)

and \( \Box_c = \Box - \frac{\hat{R}}{6} \). Then

\[ \Box^c_c = e^{-3U} \Box_c e^U \]  

(3.2)

reflects the conformal invariance of the operator \( \Box_c \) if applied to a scalar. The following consideration is restricted to the case that both \( R \) and \( \hat{R} \) are positive; the other sign can be dealt analogously.

We put \( U = \ln R \) into eq. (3.1) and apply the identity (3.2) to the constant scalar = 1. We multiply by \( (-6R) \) and get the identity

\[ R \hat{R} = 1 - \frac{6}{\hat{R}^2} \Box R \]  

(3.3)

Further, we define the operator \( ^{\wedge} \) given by

\[ \hat{g}_{ij} = R^2 g_{ij} \]  

(3.4)

to be a dual one if it coincides with its inverse operator. Then the following conditions are equivalent:

1. \( ^{\wedge} \) is a dual operator.
2. \( R \hat{R} = 1 \)
3. \( \Box R = 0 \)
4. \( \hat{\Box} R = 0 \)

**Proof.** 1. \( \Leftrightarrow \) 2. is simply the explicit form of the definition of duality. 2. \( \Leftrightarrow \) 3. follows from eq. (3.3). 3. \( \Leftrightarrow \) 4. is a consequence of the duality property.

**Remarks.** 1. The conformal factor \( R^2 \) in eq. (3.4) is crucial for the validity of the duality. Already for spaces with constant curvature scalar one can see: \( \hat{R} = \frac{1}{R} \) requires the conformal factor to be \( R^2 \). 2. This consideration was inspired by Buchdahl’s paper [26] from 1978.

Now we are prepared to show a duality relation between pairs of fourth-order gravity theories. (We formulate it only for dimension 4, other dimensions \( > 2 \) give similar results.) Let \( L = F(R) \) with \( G = \frac{dF}{dR} \neq 0 \), \( H = \frac{dG}{dR} \neq 0 \) and \( \hat{g}_{ij} = G^2 g_{ij} \). If \( g_{ij} \) is a solution of the fourth-order equation following from \( L \) then it holds

\[
\hat{R} = 3R/G^2 - 4F/G^3 \tag{3.5}
\]

One has \( \frac{d\hat{R}}{dR} \neq 0 \) iff (= if and only if)

\[
G^2 \neq 6H(2F - GR) \tag{3.6}
\]

**Remark.** If \( R \) is a constant then \( 2F = GR \) follows from the field equation, (3.6) is automatically fulfilled, and (3.5) reduces to the known relation \( \hat{R} = \frac{R}{G^2} \).

Let (3.6) be fulfilled in the following. Then eq. (3.5) can be inverted locally as \( R = R(\hat{R}) \). We define

\[
\hat{F} = 2R/G^3 - 3F/G^4 \tag{3.7}
\]

where \( R = R(\hat{R}) \) has to be inserted into the r.h.s.

The following theorem holds under the presumptions formulated above.

**Theorem.** \( \hat{L} = \hat{F}(\hat{R}) \) defines a fourth-order theory dual to \( L = F(R) \) and \( \hat{g}_{ij} \) is a solution of its field equation.

Duality means that by applying this procedure twice the original theory with original solution \( g_{ij} \) is obtained.

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Remarks. 1. The most problematic step in formulating this theorem was to find the formulas (3.5) and (3.7); the existence of such a theorem was announced in [27], but these two crucial formulas are presented here for the first time.

2. We call two theories $F, \tilde{F}$ to be similar (i.e., they go into each other by a change of the length unit) if there exist non–vanishing reals $\alpha$ and $\beta$ such that $\tilde{F}(R) = \alpha F(\beta R)$. It holds: Similar theories have similar duals.

Proof of the Theorem. The trace of the field equation following from $L$ reads

$$GR + 3 \Box G = 2F$$

It must be supplemented by the condition that the trace–free part of the tensor $GR_{ij} - G_{ij}$ vanishes. We use identities analogous to eq. (3.3) with $G$ instead of $R$ and the relation holding for the r.h.sides of eqs. (3.5) and (3.7):

$$\frac{d\hat{R}}{dR} = G\frac{d\hat{F}}{dR}$$

This ensures the validity of

$$\hat{G} = \frac{d\hat{F}}{dR} = \frac{1}{G} \neq 0$$

The rest of the proof is lengthy but straightforward.

Examples. 1. Let $L = \frac{R^n}{m}$ with $m \neq 0, 1$. Unequality (3.6) excludes $m = \frac{3}{2}$ and $m = \frac{4}{3}$. For all remaining reals $m$ one gets the dual $\hat{L} = c\hat{R}^{\hat{m}}$ with $\hat{m} = \frac{3m - 4}{2m - 3}$ and a constant $c = c(m)$, cf. [27].

2. Let $L = R - \alpha R^2$. The inversion of eq. (3.5) is not possible in closed form, but in the vicinity of flat space we may expand into powers of $\hat{R}$ and get up to third order

$$\hat{L} = \hat{R} - \alpha \hat{R}^2 - 4\alpha^2 \hat{R}^3$$

Result: At least a special type of cubic terms in the Lagrangian can be absorbed by a suitable conformal transformation.
3.2 Instability of $R^2$-theories

This subsection deals with the classical instability of fourth-order theories following from a non-linear Lagrangian $L(R)$.

(Quantum instabilities will be commented in sect. 5.)

Teyssandier and Tourrenc (1983, ref. [31]) solved the Cauchy–problem for this theory, let us shortly repeat the main ingredients.

The Cauchy problem is well-posed (a property which is usually required to take place for a physically sensible theory) in each interval of $R$-values where both $dL/dR$ and $d^2L/dR^2$ are different from zero. The constraint equations are similar as in General Relativity: the four 0i-component equations. What is different are the necessary initial data to make the dynamics unique. More exactly: Besides the data of General Relativity one has to prescribe the values of $R$ and $\frac{dR}{dt}$ at the initial hypersurface. This coincides with the general experience: Initial data have to be prescribed till the highest-but-one temporal derivative appearing in the field equation (here: fourth-order field equation, $\frac{dR}{dt}$ contains third-order temporal derivatives of the metric). Under this point of view, classical stability of the field equation means that a small change of the Cauchy data implies also a small change of the solution.

Now we are prepared to classify the stability claims found in refs. [32-36]. To simplify we specialize to the Lagrangian $L = R - \epsilon R^2$ with the non-tachyonic sign $\epsilon > 0$ and restrict to the range $\frac{dL}{dR} > 0$, i.e. $R < \frac{1}{2\epsilon}$.

On the one hand, refs. [32, 33] find a classical instability of the Minkowski space–time for this case. (Mazzitelli and Rodrigues [33] cite Gross, Perry and Yaffe (1982, ref. [34]) with the sentence ”The Minkowski solution in general relativity has been proven to be stable.” which refers to the positive energy theorem of general relativity.)

On the other hand, refs. [35, 36] find out that the Minkowski space–time is here not more unstable than in General Relativity itself. What looks like a contradiction from the first glance is only a notational ambivalence as can be seen now: The main argument in refs. [32, 33] is that an arbitrarily large value $\frac{dR}{dt}$ is compatible with small values of $H^2$ and $R^2$. In refs. [35, 36] however, following the Cauchy–data argument [31], $\left(\frac{dR}{dt}\right)$ being part of
the Cauchy data which are presumed to be small) stability of the Minkowski space–time is obtained in the version: If the Cauchy data are small (meaning: close to the Cauchy data of the Minkowski space–time) then the fourth–order field equation bounds the solution to remain close to the Minkowski space–time.

The argument of ref. [35] is a little bit different: There the conformal transformation to Einstein’s theory with a scalar field $\Phi$ [22] is applied; it is observed that in the $F(R)$-theory there are never ghosts which implies stability. Now, $\Phi$ and $\frac{d\Phi}{dt}$ belong to the Cauchy data which is equivalent to the data $R, \frac{dR}{dt}$ in the conformal picture thus supporting the Cauchy data argument given at the beginning of this subsection.

4 Cosmology

Several papers [37 - 43] apply the conformal transformation theorem [21, 22] to cosmology; so for interpreting the cosmological singularity [37], for dealing with anisotropic models [38], with transformation to Brans–Dicke extended inflation [40]. Ref. [42] mentions that $\Omega_0 < 1$ is possible even if $k = 1$. The other ones apply the theorem mainly as a mathematical device to transform solutions to solutions of the other theory.

In the following two subsections we discuss exact solutions directly found for fourth–order gravity (subsection 4.1: a spatially flat Friedmann model, subsection 4.2: a Kantowski–Sachs model).

4.1 Friedmann models

In 1988, Chimento [44] found an exact solution for fourth–order gravity in a spatially flat Friedmann model. He also found out that in the tachyonic–free case the asymptotic matter-dominated Friedmann solution is stable, and no fine–tuning of initial conditions is necessary to get the final (oscillating) Friedmann stage; particle production of non–conformal fields may backreact to damp the oscillations.
[45] generalizes [44]: here the Dirac equation is considered, the result is that there appear spinor field oscillations and the qualitative behaviour remains essentially the same.

Let us present the exact solution of [44]. For the spatially flat Friedmann model with Hubble parameter $H = \dot{a}/a$ he solves the fourth–order field equation with vacuum polarization term. The zero–zero component equation reads

$$2H\ddot{H} - \dot{H}^2 + 6H^2\dot{H} + \frac{9}{4}H^4 + H^2 = 0 \quad (4.1)$$

The $H^4$-term stems from the vacuum polarization and the $H^2$-term from the Einstein tensor. The remaining ingredients of eq. (4.1) come from the term $R^2$ in the Lagrangian. (Here we only present the tachyonic–free case with $\Lambda = 0$ and $\frac{9}{4}$ in front of $H^4$.) The factor in front of $H^4$ should not influence the weak–field behaviour because for $H \approx 0$ this factor only changes the effective gravitational constant.

From eq. (4.1) the discussion of subsection 3.2 becomes obvious: (4.1) represents a third–order equation for the cosmic scale factor $a$; it is a constraint and not a dynamical equation. (It is only due to the high symmetry, that accidentally the validity of the constraint implies the validity of the dynamical equation.) Supposed, eq. (4.1) would be the true dynamical equation for a theory, then the instability argument of [32] could apply.

The ansatz for solving eq. (4.1)

$$H = \frac{2\dot{s}}{3s}$$

leads to a non–linear third–order equation for $s$

$$2\dot{s}s^{(3)} - \dot{s}^2 + \ddot{s}^2 = 0 \quad (4.2)$$

Derivative with respect to $t$ yields the equation $s^{(4)} + \ddot{s} = 0$ being linear in $s$ and having the solution

$$s = c_1 + c_2 t + c_3 \sin(t + c_4)$$

Inserting this solution into the original equation gives the restriction $|c_2| = |c_3|$. Let us discuss this solution: $c_2 = 0$ leads to the uninteresting flat space–time. So, now let $c_2 \neq 0$. Adding $\pi$ to $c_4$ can be absorbed by a change of
the sign of \( c_3 \). Therefore, \( c_2 = c_3 \) without loss of generality. Multiplication of \( s \) by a constant factor does not change the geometry, so let \( c_2 = 1 \). A suitable time–translation leads to \( c_1 = 0 \). Finally, the cosmic scale factor is calculated as \( a = s^{2/3} \) leading to

\[
a = [t + \sin(t + c_4)]^{2/3} \sim t^{2/3} [1 + \frac{2}{3t} \sin(t + c_4)]
\]

The r.h.s. of eq. (4.3) gives in an elegant way the late–time behaviour already deduced in [46]. The factor \( 1/t \) in front of the "sin"-term shows that the oscillations due to the higher–order terms are damped. The total energy "sitting" in these oscillations, however, remains constant in time (because of the volume–expansion) cf. Suen (1994, ref. [32]) and can be converted into classical matter by particle creation.

Let us mention some further cosmological solutions with higher–order gravity: [47] discusses the \( L(R) \)-stability with a conformally coupled scalar field. Ref. [48] (partial results of it can be found in [49]) deals with fourth–order cosmological models of Bianchi–type I and power–law metrics, i.e.

\[
ds^2 = dt^2 - \sum_{i=1}^{3} t^{2p_i} (dx^i)^2
\]

with real parameters \( p_i \). The suitable notation

\[
a_k = \sum_{i=1}^{3} p_i^k
\]

gives the following: \( a_1 = a_2 = 1 \) is the usual Kasner solution for Einstein’s theory. \( a_1^2 + a_2^2 = 2a_1 \) is the condition to be fulfilled for a solution in \( L = R^2 \). Refs. [50, 51] also discuss \( R^2 \)-models. Brüning, Coule and Xu (1994, ref. [36]) consider inflationary cosmology with a Lagrangian

\[
L = R + \lambda R_{\mu\nu}R^{\mu\nu}/R
\]

and mention that it is unclear under which circumstances the existence of the Weyl term in anisotropic models allows the de Sitter space–time to be an attractor solution. Ref. [52] deals with anisotropic Bianchi–type IX solutions for \( L = R^2 \). They look for chaotic behaviour analogous to the mixmaster
model in Einstein’s theory. Ref. [53] gives exact solutions for $L = R^2$ and a closed Friedmann model, ref. [54] discusses the bounce in closed Friedmann models for $L = R - \epsilon R^2$. Supplementing the discussion of [54, eq.(1)] let us mention: In the non–tachyonic case, there exist periodically oscillating models with an always positive scale factor $a$. Ref. [55] looks for chaos in isotropic models, e.g. by conformally coupled massive scalar fields in the closed universe. The papers [56, 57] consider the stability of power–law inflation for $L = R^m$ within the set of spatially flat Friedmann models. Refs. [58] give overviews on higher–order cosmology, especially chaotic inflation as an attractor solution in initial–condition space. [59] deals with quantum gravitational effects in the de Sitter space–time, and [60] gives a classification of inflationary Einstein–scalar–field–models via catastrophe theory. Ref. [61] considers Chern–Simon terms in Bianchi cosmologies and the cosmic no-hair conjecture. The axion with field strength $H_{ijk}$ puts an extra hair on black holes. Its energy-momentum tensor does not fulfil the energy conditions, and so one gets both recollapsing solutions and ever-expanding solutions which are essentially anisotropic also for late times.

4.2 Kantowski–Sachs models

Before we come to the fourth–order solution by Accioly let us mention some results on Kantowski–Sachs models in general.

The solution found in 1950, cf. ref. [62] - now it is called Nariai solution - is the only static spherically symmetric solution of the Einstein equation with positive $\Lambda$-term which cannot be written in Schwarzschild coordinates. It has a six-dimensional isometry group and is of Kantowski–Sachs type; it represents the direct product of two two–dimensional spaces of equal and non–vanishing constant curvature (in short: $S^2 \times S^2$). One of the many possibilities to present it is

$$ds^2 = (1 - \Lambda r^2)dt^2 - \frac{dr^2}{1 - \Lambda r^2} - \frac{1}{\Lambda^2}(d\theta^2 + \sin^2 \theta d\phi^2)$$ (4.4)

Ref. [63] discusses the stability of the Bertotti–Robinson (also the direct product of two two–dimensional spaces of non–vanishing constant curvature,
but with vanishing 4–curvature scalar, in short $\tilde{S}^2 \times S^2$) and Nariai solutions. Ref. [64] is an obituary to H. Nariai, it especially mentions the Nariai solution. Kofman, Sahni and Starobinsky (1983, ref. [65]) get the result that there is no particle production in the Nariai solution. [66] discusses the analogous question for the Bertotti–Robinson metric, the authors of ref. [67] consider the Nariai metric and its decay into de Sitter and Kasner–like space–times. They consider essentially Einstein’s vacuum theory with positive $\Lambda$–term and Kantowski–Sachs metric.

Torrence and Couch (1988, ref. [68]) showed how the de Sitter space–time can be presented locally as a Kantowski–Sachs cosmological model. Moreover, no other Robertson–Walker space–time can be presented as Kantowski–Sachs model, cf. also [69] for this question.

Moniz (1993, ref. [70]) discussed the Kantowski–Sachs models in Einstein’s theory with positive $\Lambda$–term in relation to the no–hair conjecture and got the following result. The majority of solutions is asymptotically de Sitter, a small number recollapses: infinite to finite measure if $dBd\dot{B}$ is taken as measure in the initial condition space, and $B$ is the radius of the $S^2$ of the model:

$$ds^2 = dt^2 - A^2(t)dv^2 - B^2(t)(d\theta^2 + \sin^2 \theta d\phi^2)$$

Accioly (1987/88, refs. [71, 72]) found an exact cosmological solutions of the Gödel type for higher–order gravity, the new solution he found is the direct product of a 3–space of non–vanishing constant curvature with the real line in space–like direction (see [72, eq. (18)]). This gives a 7–dimensional isometry group.

Comment: Because of the high symmetry, this exact solution belongs both to the Gödel and to the Kantowski–Sachs classes of metrics (with $A = \text{const.}$ and $B = \cosh t$). The latter class is more popular, so we classify it here and not primarily as Gödel model.

The direct product of a 3–space of positive constant curvature with the real line in time–like direction is known as Einstein’s static universe. So, by imaginary coordinate transformations, both metrics can be mapped onto each other locally. This implies that Accioly’s solution is conformally flat (because Einstein’s universe carries this property). In the set of conformally flat space–times, the term $R_{ij}R^{ij}$ gives the same variational derivative as $\frac{1}{3}R^2$, 

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so Accioly’s paper has to be classified in the set of non-linear Lagrangians $L = F(R)$; he assumes $F$ to be a quadratic function of $R$. As one knows there is a critical value of the curvature scalar in such theories, it is defined by $\frac{dF}{dR} = 0$. (Cf. subsection 3.2 above: there the Cauchy problem is not well-posed.)

At these values, the fourth-order differential equation reduces to the second order one $F = 0$; it turns out that Accioly’s solution obeys this critical value so it is unstable similar to Einstein’s static universe. More directly: Let $L = (R - R_0)^2$ with a constant $R_0$, then each solution of the second-order equation $R = R_0$ solves also the fourth-order field equation following from $L$. So a lot of solutions (including Accioly’s one) can be found, but they all live in the region where the Cauchy problem is ill-posed.

5 Summary

The scope of this paper was to present the foundations necessary to deduce the Wheeler–de Witt equation for a cosmological minisuperspace model in fourth-order gravity.

The method (sporadically developed in [51] for $L = R^2$ and a spatially flat Friedmann model) to handle with eqs. (1.3 - 1.6) was systematically generalized in sct. 2 to give a Hamiltonian formulation of a general fourth-order theory. The possibility of deducing this method makes it clear that the method of ref. [51] is not restricted to highly symmetric models. The alternate Hamiltonian formulation has some advantages in comparison with Ostrogradski’s one: No constraint is needed, the Hamiltonian is typically a quadratic function in the momenta. (Ostrogradski’s approach leads always to a Hamiltonian linear in the momenta which gives artificial factors $i$ in the Schrödinger equation.) The calculation of the momenta from the Lagrangian follows the usual equations (2.8) whereas the Ostrogradski approach needs some additional terms. Our approach is less ambiguous, cf. eq. (2.7).

One could pose the question whether both approaches are equivalent on another level, this is not fully excluded, but even if it is the case, the approach deduced here is more directly applicable to fourth–order quantum cosmology.
The fact that the Jacobian eq. (2.28) is always negative excludes the possibility to get a positive definite Jacobi metric in eq. (1.2). This is one of the many possibilities to say what is meant by the phrase "fourth-order theories are always unstable". The Jacobi metric plays the role of the conformally transformed superspace–metric used in quantum cosmology. And here the circle can be closed: In Einstein’s theory (both for Lorentzian and Euclidean signature of the underlying manifold) the superspace–metric has Lorentzian signature and cannot be positive definite. So we get once more the result of subsection 3.2: Fourth–order gravity contains some instabilities, but only those which it has in common with General Relativity.

To decide the quantum instability of the Minkowski or de Sitter space–times in fourth–order gravity one must solve the corresponding Wheeler–de Witt equations (Mazzitelli and Rodrigues [33] deduced them for the spatially flat Friedmann model and the Lagrangian $L = R - \epsilon R^2$) and has to interpret them carefully. This has to be done yet.

In [50] it is mentioned that a classical theory with higher derivatives has instabilities: "At the quantum level, the difference is even more dramatic. Noncommuting variables in the lower–derivative theory, such as position and velocities, become commuting in the higher–derivative theory." Remark of U. Kasper to this sentence: "The uncertainty relation is primarily between positions and momenta. If the momentum is independent of the velocity then commuting position and velocity need not bother."

The duality theorem deduced in subsection 3.1 is a method to construct new solutions of fourth–order gravity from known solutions of a (possibly other) fourth–order theory. It gives non–trivial results only for solutions with a non–constant curvature scalar, e.g. the Chimento solution [44] which has been rewritten in subsection 4.1. Kantowski–Sachs models (whose quantum cosmology is considered in [73]) have begun to discuss in subsection 4.2; this shall be completed elsewhere.

Acknowledgement. I thank Dr. U. Kasper and Dr. M. Rainer for making some clarifying remarks. Financial support from the Wissenschaftler–Integrations–Programm under contract Nr. 015373/E and from the Deutsche Forschungsgemeinschaft under Nr. Schm 911/5-2 is gratefully acknowledged.
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