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Semi-canonical quantisation of dissipative equations

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Abstract. In order to avoid the known problems of canonical quantisation of the dissipative equation $m\ddot{x} + \alpha\dot{x}^n + \partial V/\partial x = 0$ a modified approach is proposed. It is based on the classically conserved quantity $E = m\dot{x}^2/2 + V(x) + \alpha \int \dot{x}^n dx$ rather than on a Hamilton function. Linear, quadratic and cubic damping ($n = 1, 2$ and 3) are discussed explicitly. For $n = 1$ and $n = 3$ normalisable (one-particle) states cannot be stable. However, for quadratic friction, which is classically a reversible process, we show by the example of the harmonic oscillator that stable normalisable eigenstates can exist.

1. Introduction

The Lagrange and Hamilton formulations of classical mechanics are important and also of practical interest as they enable the derivation of the equations of motion and conservation laws of more complicated systems. In particular, classical Hamilton functions form the basis of canonical quantisation which, for conservative systems, leads to the well known and, in non-relativistic quantum mechanics, successful Schrödinger equation.

However, the quantisation of even the simplest dissipative equation of motion has not been solved satisfactorily, despite many efforts since the early 1940s [1]. Besides canonical quantisation, non-linear methods (which do not satisfy the superposition principle) have also been used in the attempts to quantise dissipative systems. We mention Kostin's non-linear Schrödinger equation [2] and the articles by Gisin [3] and Razavy [4]. In [3] non-linear terms are added *ad hoc* to the Hamilton operator, and the dissipative system decays into the lowest state excited at time $t = 0$. A nice feature is that all coherent states of the harmonic oscillator decay into the ground state. Razavy arrives at the conclusion [4] 'that there is no consistent way of quantising classical systems in the Hamiltonian form'. Quantising a damped system in a generalised Hamilton-Jacobi formalism, he finds a non-linear wave equation which is identical with the Schrödinger-Langevin equation studied by Kostin [2].

The main goal of this paper is to propose and to study a simple modified model for canonical quantisation of dissipative equations. In § 2 we summarise some known results on Lagrange functions of classical dissipative systems and include a few observations. Section 3 contains the principal part, an attempt to quantise the classically conserved sum of the particle's kinetic and potential energy and its energy 'exchange' with the frictional medium. The resulting Schrödinger equation is studied in § 4 for linear, quadratic and cubic friction. After that, in § 5, Ehrenfest's theorems are discussed. A summary and the principal conclusion are presented in § 6.

2. Classical dissipative Lagrange functions

It is known (probably more among mathematicians than among physicists) that for a single equation of motion

$$G \equiv \ddot{x} + g(x, \dot{x}, t) = 0 \quad (1a)$$

there always exist an integrating function f and a Lagrange function \mathcal{L} such that the equation $fG = 0$ can be derived from \mathcal{L} [5]:

$$fG = \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{x}} - \frac{\partial \mathcal{L}}{\partial x} = 0. \quad (1b)$$

f is a solution of the equation

$$g \frac{\partial \ln f}{\partial \dot{x}} + \frac{\partial g}{\partial x} = \frac{\partial \ln f}{\partial x} \dot{x} + \frac{\partial \ln f}{\partial t}. \quad (1c)$$

For the common example, linear friction, having the equation of motion

$$m\ddot{x} + \alpha\dot{x} + \partial V/\partial x = 0 \quad (2a)$$

one can find

$$f = f_1 = \exp(\alpha t/m) \quad \mathcal{L} = \mathcal{L}_1 = (T - V)f_1 \quad T = m\dot{x}^2/2. \quad (2b)$$

For the equation

$$m\ddot{x} + \alpha\dot{x}^2 + \partial V/\partial x = 0 \quad (3a)$$

with quadratic friction a possible choice of f and \mathcal{L} is

$$f = f_2 = \exp(2\alpha x/m) \quad \mathcal{L} = \mathcal{L}_2 = Tf_2 - \int f_2 \frac{\partial V}{\partial x} dx. \quad (3b)$$

The results (2b) and (3b) can be easily generalised for mixed, linear and quadratic friction

$$m\ddot{x} + \alpha_1(t)\dot{x} + \alpha_2(x)\dot{x}^2 + \partial V/\partial x = 0 \quad (4a)$$

with t -dependent α_1 and x -dependent α_2 :

$$f = f_{12} = \exp \left[\frac{1}{m} \left(\int \alpha_1(t) dt + 2 \int \alpha_2(x) dx \right) \right] \quad (4b)$$

$$\mathcal{L} = \mathcal{L}_{12} = Tf_{12} - \int f_{12} \frac{\partial V}{\partial x} dx.$$

From (1c) one can see that for frictional terms $\alpha\dot{x}^n$, $n \neq 0, 1, 2$, the integrating function f necessarily depends on \dot{x} .

One problem in canonical quantisation of dissipative equations is that a classical Lagrange function can only be obtained by means of an integrating function f . Apart from the fact that the physical meaning of such a function is not clear, f is not unique, and hence the Lagrange and Hamilton functions are not unique either. For example, for the equation

$$m\ddot{x} + \alpha\dot{x}^n = 0 \quad (5a)$$

one can (with $f = \dot{x}^{-n}$) find the Lagrange function

$$\mathcal{L} = m\dot{x}(\ln \dot{x} - 1) - \alpha x \quad n = 1 \quad (5b)$$

$$\mathcal{L} = -m \ln \dot{x} - \alpha x \quad n = 2 \quad (5c)$$

$$\mathcal{L} = m\dot{x}^{2-n}/[(n-1)(n-2)] - \alpha x \quad n \neq 1, 2 \quad (5d)$$

(equation (5b) is given in [6]). The Lagrangians (5b) and (5c) are not equivalent to the Lagrangians (2b) and (3b) (for $V(x) \equiv 0$).

The Hamilton functions $H = p\dot{x} - \mathcal{L}$, where $p = \partial\mathcal{L}/\partial\dot{x}$, corresponding to all the above Lagrange functions can be readily found. However, (5b), (5c) and (5d) cannot be easily generalised for arbitrary potentials, and it may not always be an easy task to find a Lagrange function, which does not depend explicitly on time, for (2a). (But if V and α do not depend explicitly on time then a not explicitly time-dependent Lagrange function does exist [5].) For the three-dimensional linearly damped harmonic oscillator such a Lagrangian is given in [5].

3. Modified canonical quantisation

Among the principal difficulties in canonical quantisation of dissipative systems we mention (i) contradictions with the uncertainty relation for the mechanical momentum $m\dot{x}$ and (ii) disagreement between the quantum mechanical result for the conservative system ($\alpha = 0$) and that for the dissipative equation in the limit $\alpha \rightarrow 0$. Problem (i) occurs, for example, for the Lagrangian (2b) which leads to an explicitly time-dependent canonical momentum. This problem has been studied extensively for the harmonic oscillator, i.e. the Caldirola-Kanai Hamiltonian [7, 8]. It seems that what is quantised is an oscillator with a time-dependent mass rather than a damped oscillator [9, 10]. Problem (ii) occurs normally for Hamilton functions which, even in the limit $\alpha \rightarrow 0$, do not correspond to the energy of the particle. For example, such Hamilton functions arise from the Lagrange functions (5b)–(5d). We mention also the work of Dekker [11] who factorises the classical equation of motion into two first-order complex differential equations and constructs a complex non-Hermitian Hamiltonian. However, this method has been criticised [4] as the Hamiltonian is not unique and for non-vanishing damping does not correspond to the energy.

Altogether the principal problem is probably that the Lagrangian of a dissipative equation is not the 'physical Lagrangian' [9] and the Hamilton function even in cases where it is a conserved quantity is not the energy. This, in our opinion, makes the use of the corresponding Hamilton operator in the Schrödinger equation (which supposes that the Hamilton operator is the energy operator and $E \rightarrow i\hbar \partial/\partial t$) questionable. The problem may be still worse. Since friction results from the interaction between a 'physical body' (particle) and the particles of the dissipative medium, the *one-particle* Hamilton operator of a quantal dissipative system may not exist at all.

Having these problems in mind (and despite the eventual non-existence of the desired Hamilton operator) one can try to tackle the problem from another direction. Instead of a Hamilton function for the equation of motion

$$m\ddot{x} + \alpha\dot{x}^n + \partial V/\partial x = 0 \quad (6a)$$

one may search for a classically conserved energy which governs the motion of the particle in the frictional medium. Due to the frictional interaction the particle loses

to (or, more generally, exchanges with) the frictional medium the energy

$$\Delta E = \alpha \int^t \dot{x}^{n+1} dt = \alpha \int^x \dot{x}^n dx. \quad (6b)$$

The sum of ΔE and the particle's kinetic and potential energies

$$E = \frac{1}{2}m\dot{x}^2 + V(x) + \Delta E \quad (6c)$$

should be a conserved quantity. This is easily verified from

$$dE/dt = \dot{x}(m\ddot{x} + \partial V/\partial x + \alpha \dot{x}^n) = 0. \quad (6d)$$

Since E is not related to a Lagrange function we have to define a momentum p which is to be quantised. The simplest ansatz is to quantise the mechanical momentum

$$p = m\dot{x}. \quad (7a)$$

Since

$$\partial E/\partial x = \partial V/\partial x + \alpha \dot{x}^n \quad (7b)$$

the choice (7a) ensures that the equation

$$-\dot{p} = \partial E/\partial x \quad (7c)$$

yields the correct equation of motion (6a). In principle, one could add a function $f(x, p)$ to the right-hand side of (7a). Then (7c) would yield (6a) only if $\dot{p} \partial f/\partial p = 0$, reducing f to a function of x only. But such a function cannot help to satisfy the equation $\dot{x} = \partial E/\partial p = p/m$ which corresponds to the second Hamilton equation. This incompatibility might be related to many-particle effects. We shall come back to this point in § 5 when discussing Ehrenfest's theorems.

Quantising (6c) and (7a) by

$$p \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x} \quad (8a)$$

one obtains the 'energy operator' for the quantum mechanical motion of the particle

$$H_e = H_0 + \alpha H_i \quad (8b)$$

where

$$H_0 = \frac{p^2}{2m} + V(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (8c)$$

is the Hamilton operator of the corresponding conservative system and αH_i , obtained from (6b), (7a) and (8a), gives the frictional interaction

$$\Delta E \rightarrow \alpha \int \left(\frac{\hbar}{im} \frac{\partial}{\partial x} \right)^n dx = \alpha \left(\frac{\hbar}{im} \right)^n \frac{\partial^{n-1}}{\partial x^{n-1}} =: \alpha H_i. \quad (8d)$$

One observes first that H_i is a non-Hermitian operator. (A mathematically consistent formulation of quantal dissipation in terms of non-Hermitian complex operators has been discussed by Dekker [11].) Secondly, in the approach above the quantisation of the dissipative term is independent of $V(x)$. This is quite different from and much simpler than in canonical quantisation. Finally, since the mechanical momentum $m\dot{x}$ is equal to the quantised momentum p , (7a) and (8a), the uncertainty relation will always be satisfied.

In § 4 we shall examine the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = H_e \psi = \left[H_0 + \alpha \left(\frac{\hbar}{im} \right)^n \frac{\partial^{n-1}}{\partial x^{n-1}} \right] \psi \quad n = 1, 2, 3 \quad (9a)$$

for the existence of separable solutions

$$\psi(x, t) = \varphi(x) \exp(Et/i\hbar) \quad (9b)$$

which correspond to the stationary solutions (bound states) of real energy E in conservative systems.

4. Examples

4.1. Linear friction

From (9a) and (9b) one obtains the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m} \frac{d^2 \varphi}{dx^2} + \left(V(x) + \frac{\alpha \hbar}{im} \right) \varphi = E \varphi. \quad (10a)$$

Due to linear friction the real conservative potential gets a constant imaginary part. A corresponding imaginary part, up to a constant positive factor, has been obtained by Dekker [4, 11] for the damped harmonic oscillator by a quite different method, in which, however, linear friction also changes the Hermitian part of the Hamiltonian.

From (9a) one finds the continuity equation

$$\frac{\partial \rho}{\partial t} + \text{div } j = -\frac{2\alpha}{m} \rho \quad (10b)$$

where $\rho(x, t) = |\psi(x, t)|^2$ and $j(x, t)$ stand for the common one-particle density and current, respectively. Integrating (10b) over x one gets

$$\frac{d}{dt} \int_{-\infty}^{\infty} \rho(x, t) dx = -\frac{2\alpha}{m} \int_{-\infty}^{\infty} \rho(x, t) dx. \quad (10c)$$

Then the probability $w(t)$, that the particle is in a state (9b) or a linear combination of such states, is given by

$$w(t) = \int_{-\infty}^{\infty} \rho(x, t) dx = w(0) \exp(-2\alpha t/m). \quad (10d)$$

A normalisable eigenstate of the Hamilton operator (8c) becomes unstable ($\alpha > 0$) in the presence of (8d), i.e. to the real eigenvalues E of H_0 there correspond complex eigenvalues $E + \alpha \hbar/im$ of (8b).

Complex potentials are used in nuclear physics to describe damping or absorptive effects when the target is excited to higher complicated configurations [12]. Thus the damping effect in (10d) is no surprise, but it may be surprising that the ground state to H_0 also decays in the presence of $\alpha H_i = \alpha \hbar/im$. This can be explained in the following way. Let the particle at $t = 0$ be in an eigenstate of H_0 and switch on damping. Then the particle will be absorbed by the dissipative medium, i.e. at large times it will no longer be in an eigenstate to H_0 or H_e , but in an eigenstate to the full Hamilton operator H_t of the particle and the dissipative medium. The eigenstates of H_t may be completely different from those of H_e since H_e does not contain the mutual interaction between the particles of the medium. Of course, this interpretation implies that quantal linear friction cannot be treated consistently in a one-particle theory.

4.2. Quadratic friction

The stationary Schrödinger equation is

$$\frac{\hbar^2}{2m} \frac{d^2\varphi}{dx^2} + \frac{\alpha\hbar^2}{m^2} \frac{d\varphi}{dx} + (E - V(x))\varphi = 0. \tag{11a}$$

The first derivative $d\varphi/dx$ in (11a) will change the eigenvalues and eigenstates of H_0 , but, in contrast to linear friction, (11a) can have stable normalisable eigenstates. This will now be shown for the oscillator potential

$$V(x) = \frac{1}{2}m\omega^2x^2. \tag{11b}$$

The general solution of (11a) and (11b) is [13]†

$$\begin{aligned} \varphi(x) &= x^{-1/2} \exp(-\alpha x/m) (C_1 M_{k,1/4}(z^2) + C_2 M_{k,-1/4}(z^2)) \\ k &= \frac{2E/\hbar - \alpha^2\hbar/m^3}{4\omega} \quad z = \left(\frac{m\omega}{\hbar}\right)^{1/2} x. \end{aligned} \tag{11c}$$

C_1 and C_2 are arbitrary constants and $M_{k,\pm 1/4}$ are Whittaker functions whose asymptotic behaviour for $\text{Re } z^2 \rightarrow +\infty$ (see formulae (13.1.32) and (13.1.4) of [14]) is

$$M_{k,1/4}(z^2) \sim \frac{\Gamma(\frac{3}{2})}{\Gamma(\frac{3}{4}-k)} \exp(z^2/2) z^{-2k} (1 + O(z^{-2})) \quad \frac{3}{4}-k \neq 0, -1, -2, \dots \tag{12a}$$

$$M_{k,-1/4}(z^2) \sim \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{4}-k)} \exp(z^2/2) z^{-2k} (1 + O(z^{-2})) \quad \frac{1}{4}-k \neq 0, -1, -2, \dots \tag{12b}$$

Therefore the solution (11c) will not be square integrable unless $k = l + \frac{1}{4}$ or $k = l + \frac{3}{4}$, $l = 0, 1, 2, \dots$, when the Whittaker function is related to the Hermite polynomials [13]

$$M_{l+3/4,1/4}(z^2) = (-1)^{l+1} \frac{l!}{2(2l+1)!} \exp(-z^2/2) z^{1/2} H_{2l+1}(z) \tag{13a}$$

$$M_{l+1/4,-1/4}(z^2) = (-1)^l \frac{l!}{(2l)!} \exp(-z^2/2) z^{1/2} H_{2l}(z). \tag{13b}$$

For $k = l + \frac{1}{4}$ and $C_1 = 0$ the solution (11c) is normalisable as well as for $k = l + \frac{3}{4}$ and $C_2 = 0$, $l = 0, 1, 2, \dots$. From (11c) one finds the energy eigenvalues

$$E = \begin{cases} (2l + \frac{1}{2})\omega\hbar + \frac{1}{2}\alpha^2\hbar^2m^{-3} & \text{if } k = l + \frac{1}{4} \\ (2l + \frac{3}{2})\omega\hbar + \frac{1}{2}\alpha^2\hbar^2m^{-3} & \text{if } k = l + \frac{3}{4} \end{cases} \tag{13c}$$

which can be written as only one formula

$$E_l = (\hat{l} + \frac{1}{2})\omega\hbar + \frac{1}{2}\alpha^2\hbar^2m^{-3} \quad \hat{l} = 0, 1, 2, \dots \tag{13d}$$

The energies are shifted against the eigenvalues of the undamped oscillator by a constant term. Due to the factor $\exp(-\alpha x/m)$ in (11c) the corresponding eigensolutions $\varphi(x)$ are damped slightly more for positive x and slightly less for negative x ($\alpha > 0$) than the solutions for $\alpha = 0$. In the limit $\alpha \rightarrow 0$ the eigenvalues (13d) and the corresponding normalisable eigenstates agree with those of the undamped harmonic oscillator.

† Note that the argument in the solution [2.273 (11)] given in [13] should be cx^2 instead of cx .

That stable bound states in the potential $V(x)$ are possible for quadratic friction can be understood from the following analogy with classical mechanics. The term $\alpha\dot{x}^2$, $\alpha > 0$, is dissipative only if $\dot{x} > 0$. For negative velocities it adds energy to the particle. Quadratic friction is reversible and stable quantum mechanical bound states can exist, provided the binding potential is strong enough.

From the results of this and the foregoing section one can easily predict the behaviour of a harmonic oscillator with both linear and quadratic friction $\alpha_1\hbar/im - \alpha_2\hbar^2m^{-2}\partial/\partial x$. The eigenstates and eigenvalues are determined by quadratic friction, but the eigenstates decay as $\exp(-\alpha_1t/m)$.

4.3. Cubic friction

For $n = 3$ one obtains from (8d)

$$\alpha H_i = -\frac{\alpha\hbar^3}{im^3} \frac{\partial^2}{\partial x^2} \tag{14a}$$

and the continuity equation

$$\frac{\partial\rho}{\partial t} + \text{div } j = \frac{\alpha\hbar^3}{m^3} \left(\frac{\partial^2\rho}{\partial x^2} - 2 \left| \frac{\partial\psi}{\partial x} \right|^2 \right). \tag{14b}$$

Without investigating how the eigenspectrum and eigenstates of H_0 are changed by (14a) one can conclude from (14b) that the density ρ of a normalisable one-particle state decays:

$$\frac{d}{dt} \int_{-\infty}^{+\infty} \rho \, dx = -2 \frac{\alpha\hbar^3}{m^3} \int_{-\infty}^{+\infty} \left| \frac{\partial\psi}{\partial x} \right|^2 dx < 0 \quad \text{if } \alpha > 0. \tag{14c}$$

In contrast to linear friction, the decay (14c) depends explicitly on the eigenstate since the integrand is $|\partial\psi/\partial x|^2$. Apart from this detail the decay can be interpreted as for linear damping in § 4.1.

For frictional terms x^n with exponents $n > 3$ the operator (8d) would yield a differential equation of higher than second order in x . We shall not discuss such a situation here.

5. Ehrenfest's theorems

From (9a) one finds for the time derivative $\dot{\bar{A}}$ of the expectation value \bar{A} of a physical observable A (with $\partial A/\partial t = 0$) [11] that

$$\dot{\bar{A}} = \frac{d}{dt} \int_{-\infty}^{+\infty} \psi^* A \psi \, dx = \frac{i}{\hbar} \int_{-\infty}^{+\infty} \psi^* ([H_0, A]_- - [\alpha H_i, A]_+) \psi \, dx. \tag{15a}$$

The anticommutator of A with αH_i stands because H_i is not Hermitian. For $A = x$ one gets

$$\dot{\bar{x}} = \frac{\bar{p}}{m} - \frac{\alpha}{m^n} \overline{(xp^{n-1} + p^{n-1}x)} \tag{15b}$$

and for $A = p$

$$\dot{\bar{p}} = -\frac{\partial \bar{V}}{\partial x} - \frac{2\alpha}{m^n} \bar{p}^n. \quad (15c)$$

In order that (15c) corresponds with the classical law of motion it seems necessary to substitute $\alpha \rightarrow \alpha/2$ in the quantisation (8d). The factor $\frac{1}{2}$ compensates some 'double counting' in the anticommutator. Since the classical equation $\dot{x} = \partial E / \partial p$ is not satisfied, deviations of (15b) from $\dot{x} = \bar{p}/m$ can be expected in principle. Indeed, for odd n the eigenstates of H_e are only quasistationary and their decay in time will lead to additional terms in $\dot{\bar{A}}$. For example, for $n = 1$ one finds $\dot{\bar{x}}_0 = \bar{p}_0/m$ where $\dot{\bar{x}}_0$ is the time derivative of the expectation value \bar{x}_0 in an eigenstate ψ_0 of H_0 . In consequence, with respect to the eigenstate $\psi = \psi_0 \exp(-\alpha t/m)$ of H_e one finds

$$\dot{\bar{x}} = \frac{\bar{p}_0 \exp(-2\alpha t/m)}{m} - \frac{2\alpha \bar{x}_0 \exp(-2\alpha t/m)}{m}$$

in agreement with (15b); \bar{p}_0 is the expectation value of p in the state ψ_0 . For the oscillator potential (as for other potentials symmetric with respect to $x = 0$) one finds $\bar{x}_0 = 0$ such that for $n = 1$ the classical equation $\dot{x} = \bar{p}/m$ is fulfilled by (15b). On the other hand, for $n = 2$ (and all even n), where stationary states can exist, one can show by $n - 1$ partial integrations that $p^{n-1}x = -xp^{n-1}$, and (15b) has the classically correct form $\dot{x} = \bar{p}/m$. These results support the choice (7a) of the momentum p to be quantised. Equations similar to (15b) and (15c) were obtained for the linearly damped harmonic oscillator in [3] and apparently also in [11]. (Note that in this case $\partial \bar{V} / \partial x \sim \bar{x}$.)

6. Summary and conclusion

In classical conservative one-particle systems the Hamilton function is equal to the energy of the particle. This does not hold for dissipative systems. Therefore we argue that in principle two candidates for 'canonical quantisation' of dissipative equations exist: the class of (mathematical) Hamilton functions of the equation, and the class of quantities (or the quantity) related to the physically relevant energy of the system. We name the latter method 'semicanonical quantisation'.

Canonical quantisation of classical Hamilton functions has been studied extensively and has met with serious difficulties that cannot yet be resolved. In view of this the energy-based alternative offered above should be examined seriously, and the classically conserved quantity (6c) seems to be a reasonable basis for this purpose. In order to obtain an energy operator the pure Lagrange and Hamilton formulation has been relinquished. In consequence, one must also define which is the classical momentum to be quantised. The choice (7a) is the simplest possibility. Anyhow, this heuristic method avoids the problems of canonical quantisation and yields plausible physical results for linear, quadratic and cubic friction. It is certainly interesting that our results show some correspondence with [11] as regards the non-Hermitian quantal frictional operator and the complex absorptive potential for linear damping.

The principal result of our quantisation method is the indication that irreversible friction ($n = 1, 3$) cannot be described consistently within a one-particle quantum theory. Namely, H_i simulates absorptive effects, and the eigenstates of $H_e = H_0 + \alpha H_i$ dissipate into eigenstates of H , the total Hamiltonian of the particle and the dissipative medium. For this reason the ground state of H_e also decays. On the other hand,

classically reversible friction ($n = 2$) can be considered quantum mechanically as the motion of a single particle in the external potential $V(x)$ and the 'average frictional potential' αH_1 .

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