Modal and Nonmodal Perturbations of Monochromatic High-Frequency Gravity Waves: Primary Nonlinear Dynamics

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ABSTRACT

The primary nonlinear dynamics of high-frequency gravity waves (HGWs) perturbed by their most prominent normal modes (NMs) or singular vectors (SVs) in a rotating Boussinesq fluid have been studied by direct numerical simulations (DNSs), with wave scales and values of viscosity and diffusivity characteristic for the upper mesosphere. The DNS is 2.5D in that it has only two spatial dimensions, defined by the direction of propagation of the HGW and the direction of propagation of the perturbation in the plane orthogonal to the HGW phase direction, but describes a fully 3D velocity field. Many results of the more comprehensive fully 3D simulations in the literature are reproduced. So it is found that statically unstable HGWs are subject to wave breaking ending in a wave amplitude with respect to the overturning threshold near 0.3. It is shown that this is a result of a perturbation of the HGW by its leading transverse NM. For statically stable HGWs, a parallel NM has the strongest effect, quite in line with previous results on the predominantly 2D instability of such HGWs. This parallel mode is, however, not the leading NM but a larger-scale pattern, seemingly driven by resonant wave–wave interactions, leading eventually to energy transfer from the HGW into another gravity wave with steeper phase propagation. SVs turn out to be less effective in triggering HGW decay but they can produce turbulence of a strength that is (as that from the NMs) within the range of measured values, however with a more pronounced spatial confinement.

1. Introduction

It has been known for quite a while that the momentum and energy deposition from gravity wave (GW) breakdown is of central importance for the dynamics of the middle atmosphere (Hines 1960; Houghton 1978; Lindzen 1981; Holton 1982, 1983; Garcia and Solomon 1985). An additional potential effect of GW breaking is the generation of turbulence with dissipation rates influencing the mesospheric energy balance (Lübken 1997; Becker and Schmitz 2002). Because of their small scales, GWs, or at least the major part of their spectrum, can be handled in general circulation models only via parameterizations. The uncertainties faced so far by the parameterization attempts are, however, already well documented by the number of different approaches that the available schemes are based upon and the amount of free parameters each of them offers (Fritts and Alexander 2003). Among other reasons, a major problem is the still insufficient understanding of the wave breaking process itself. This process is the focus of the present study.

Linear theory has been used for deriving instability thresholds as well as information on the scales and structures of the most relevant initial perturbations in a breaking wave. Classic results are the criteria of static and dynamic normal-mode (NM) instability, in the present context holding strictly only for monochromatic GWs with exactly vertical phase propagation.1 For the former, one needs local overturning of density and potential temperature contours, while the latter requires a local Richardson number less than 1/4 (Howard 1961; Miles 1961). NM analyses of monochromatic GWs (Mied 1976; Klostermeyer 1991; Lombard and Riley 1996a; Sonmor and Klaassen 1997; Yau et al. 2004) have shown, especially for high-frequency gravity waves (HGWs) with phase propagation at a more or

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less pronouncedly nonvertical inclination angle, instabilities at wave amplitudes well below these thresholds. The orientation of the horizontal direction of propagation of the leading NM with respect to that of the wave depends on the wave amplitude, so that for statically stable HGWs the instability is predominantly 2D (i.e., the NM propagates in the same plane as the HGW, and statically unstable HGWs have leading NMs propagating transversely with respect to the wave).

Mathematically, if the linear dynamics are given by $\frac{dx}{dt} = Ax$, with a state vector $x$ for the perturbations of the GW and a linear operator $A$ determined by the wave properties and the viscous–diffusive parameters, the NMs are simply the eigenmodes of the latter operator. They are thus the solutions $\mathbf{n}_n$ so that $A\mathbf{n}_n = -i(\omega_n + i\gamma_n) \mathbf{n}_n$. An initial perturbation $\mathbf{x}(0) = \sum_{n} a_{n} \mathbf{n}_{n}$ of the GW takes the consecutive time development $\mathbf{x}(t) = \sum_{n} a_{n} \mathbf{n}_{n} \exp(-i\omega_{n}t + i\gamma_{n}t)$, so that the leading NM with the largest growth or damping rate $\gamma_n$ is always approached asymptotically by the perturbation, provided the initial perturbation projects the least onto that NM. While NMs thus characterize the initial instability of a wave subject to infinitesimally small disturbances, optimal perturbations or singular vectors (SVs) are potentially better suited for describing the instability at finite perturbation level. For a given development time $\tau$, to be chosen according to dynamical considerations, SVs are, within the framework of the linear theory, the strongest growing structures [Boberg and Brosa 1988; Farrell 1988a,b; Trefethen et al. 1993; i.e., the optimal perturbation $x(0)$ optimizes the ratio $\|x(\tau)\|^2/\|x(0)\|^2$ for some chosen norm (here the energy norm)]. Because of interference effects, the leading SV is typically not identical to the leading NM. At sufficiently large initial perturbation amplitude, its transient growth can sometimes be quick enough so as to lead the wave into a nonlinear regime before an NM has had time to do so. Moreover, even for comparatively low-amplitude GWs without any unstable NM, considerable optimal growth might still be possible so that optimal perturbation theory also has the potential for extending the range of wave amplitudes allowing a transition to breaking and turbulence. Such has been found to be the case for inertia–gravity waves (IGWs) with nearly vertical phase propagation, while for all inclination angles one finds SVs with stronger growth than NMs and distinctly different properties (Achatz 2005; Achatz and Schmitz 2006a,b). In the case of HGWs, short-term SVs are characterized by predominantly transverse propagation with respect to the wave, and in contrast to the leading NMs they are spatially much more localized and more or less frozen in the flow. The corresponding NMs are typically broader structures moving with the phase of the wave.

Studies of the nonlinear wave breakdown have so far focused on the behavior of a GW subject to a low-level random perturbation. While the first of these studies have been done either for Reynolds numbers well below realistic values or using subgrid-scale models for the small-scale turbulent fluctuations (Winters and D’Asaro 1994; Andreassen et al. 1994; Fritts et al. 1994; Isler et al. 1994; Lombard and Riley 1996b; Lelong and Dunkerton 1998a,b), direct numerical simulations (DNSs) with near-realistic Reynolds numbers and explicitly resolved turbulence have only recently become possible (Fritts et al. 2003, 2006). These investigations are of interest not only because they enable comparisons to measured turbulent dissipation rates and intensities but also since turbulence is instrumental in eventually mixing momentum and potential temperature fluctuations between the GW and the large-scale flow, and thereby in the corresponding deposition. An aspect that has been neglected so far is the nonlinear development resulting from a distinct perturbation of a GW by one of its leading NMs or SVs. One might argue that secondary instabilities will most often lead to the 3D behavior that has been the focus in the studies above. However, conceptually the primary nonlinear interaction between NMs or SVs and the GW remains of interest since it can both serve as a reference to more general studies and can also help in identifying paradigmatic features in GW breakdown that might be useful in interpreting measurements and 3D simulations. A corresponding study has therefore recently been done for IGWs (Achatz 2007), while this study reports work on the nonlinear dynamics of NMs and SVs of HGWs. Major points of interest are the change of the HGW amplitude, the energy exchange between HGW and perturbation, the distribution of perturbation energy between the various dynamical fields in question, its spatial distribution, and the strength and distribution of the occurring turbulent dissipation rates.

With this aim the paper is structured as follows: in section 2 the model is described. Section 3 discusses a way of describing the energetics of the breaking process that facilitates easier comparison to the previous linear studies. The dynamics of HGWs perturbed by their most important NMs are studied in section 4, while section 5 gives an account of the impact of SVs on HGWs. Finally, section 6 summarizes and discusses the main results.

2. Model setup

Since it is the same as used in Achatz (2007), only a very short sketch of the model is given here. For details
the reader is referred to that paper. The equations used are the Boussinesq equations on an f plane. Prognostic variables are the three-dimensional velocity field $\mathbf{v}$ and buoyancy $b$. The $f$ plane is located at 70° latitude. The Brunt–Väisälä frequency is $N = 2 \times 10^{-2}$ s$^{-1}$. The viscosity is $\nu = 1$ m$^2$ s$^{-1}$. The same value is also used for the diffusivity of the model. In the inviscid–nondissipative limit, the equations admit as exact solutions monochromatic GWs with a frequency $\Omega$ satisfying the dispersion relation

$$\Omega = \pm \sqrt{N^2 \cos^2 \Theta + f^2 \sin^2 \Theta},$$

(1)

where $\Theta$ is the inclination angle of the GW wave vector with respect to the horizontal. Following Mied (1976) and Drazin (1977), a coordinate system is introduced in which the representation of the GW is especially simple. Assuming that the GW propagates in the $x$–$z$ plane, this coordinate system is obtained by a rotation about the y axis (so that the new vertical coordinate points in the direction of the wavenumber vector $\mathbf{K}$), a translation along this axis with the phase velocity, and a rescaling of the vertical axis in units of the wave phase $\phi = K \cdot x - \Omega t$. With $K = ||\mathbf{K}||$ the new coordinates are $(\xi, y, \phi)$ with

$$(\xi, \phi) = [x \sin \Theta - z \cos \Theta, K(x \cos \Theta + z \sin \Theta) - \Omega t].$$

(2)

For ease of expression from here on out, any vector components in the plane spanned by the $\xi$ and $y$ axis will be called horizontal, whereas the term truly horizontal will be used for components in the plane spanned by the $x$ and $y$ axes. Likewise, the terms vertical and truly vertical will be used for components parallel to either the $\phi$ or $z$ axis. With the rotated velocity components along the new axes being $u_\xi$, $v_\xi$, and $u_\phi$, the GW takes in this representation the time-independent form

$$(u_\xi, v_\xi, u_\phi, b)_{GW} = -ac \left( \frac{\sin \phi}{\sin \Theta \cos \Theta}, -\frac{f/\Omega}{\cos \Theta} \cos \phi, 0, \frac{N^2/\Omega}{\sin \Theta} \cos \phi \right),$$

(3)

where $c = \Omega/K$. The phase convention (Yau et al. 2004) is such that the buoyancy gradient minimizes (maximizes) at $\phi = 3\pi/2$ ($\pi/2$). The largest shear due to $u_\xi$ occurs at $\phi = 0, \pi$, and the largest shear due to $v$ (negligible for HGWs) is at the extremum of the buoyancy gradient. The nondimensional amplitude $a$ is defined so that the wave is stably unstable for $a < 1$ (i.e., at these values of $a$, one has $N^2 + ab/\partial z > 0$ everywhere).

In the simulations reported here, the initial state for the nonlinear model is always obtained by a superposition of the GW and the state of one of the linear NMs or SVs at $t = 0$. The latter perturbation has the form $(v', b') = \Re\{\hat{u}(\xi, \phi) \exp[(\kappa \xi + \lambda \phi)]\}$, with $(\kappa, \lambda) = (2\pi/\lambda_0)$ (cosa, sina) being the horizontal wave-vector components of the perturbation and $\lambda_0$ and $\alpha$ being the corresponding horizontal wavelength and the azimuth angle between $(\kappa, \lambda)$ and the $\xi$ axis, respectively. The amplitudes $\hat{u}$ and $b$ are periodic in $\phi$ with a period of $2\pi$ (Achatz 2005). The initial state is thus symmetric with respect to the direction in the $\xi$–$y$ plane transverse to the direction of propagation of the perturbation, and the model equations conserve this symmetry. It therefore makes sense to introduce a horizontally rotated system of coordinates

$$(x_\xi, y_\xi) = (\xi \cos \alpha + y \sin \alpha, -\xi \sin \alpha + y \cos \alpha),$$

(4)

respectively pointing in the directions parallel and transverse to the direction of the horizontal wavenumber vector of the perturbation. Here, $(u_\xi, v_\xi)$ are the corresponding velocity components. This is the representation used in the model and also here in the discussion of the results. Moreover, the periodicity of the chosen initial conditions with respect to $\phi$ and $x_\xi$ also implies a conservation of this property in the ensuing time development so that the boundary conditions of the problem can be taken as periodic in all spatial directions.

For a numerical treatment, the model equations have been discretized on a standard staggered C grid with periodic boundary conditions. The model domain extends from 0 to $2\pi$ in $\phi$ and from $\lambda_0$ in $x_\xi$. Consistent with these chosen initial states there is no dependence on $y_\xi$. The model might be called 2.5D since it describes buoyancy and a 3D velocity field depending on two spatial coordinates. Moreover, in contrast to traditional 2D approaches, the treatment of perturbations with $a \neq 0$ is also possible. The model resolution was always chosen finely enough to resolve both the inertial and the viscous subrange of the resulting turbulence spectra. Corresponding details, including the model resolution, are provided in Table 1. It shall be stressed that the 2.5D approach with periodic boundary conditions, as convenient as it might be for computational reasons, is also a desired simplification for better conceptual insight. Only with reference to the results from such an idealized study can more complex behavior, such as from local nonperiodic initial perturbations or the full 3D behavior after secondary perturbations with a spatial dependence in $y_\xi$ direction, be understood most clearly.

3. Energetics

The basic HGW is horizontally symmetric, that is, with respect to $x_\xi$ and $y_\xi$. One can therefore analyze the
interaction between HGW and perturbation in terms of the energy exchange between the horizontal mean \((\mathbf{v}, \mathbf{b})\) and the horizontally dependent deviations \((\mathbf{v}', \mathbf{b}') = (\mathbf{v} - \mathbf{v}_0, \mathbf{b} - \mathbf{b}_0)\) (for simplicity, hereinafter called the “eddy” part). From the model equations one finds the following budget equations for the kinetic energy densities \(\mathcal{R} = |\mathbf{v}|^2/2\) and \(\mathcal{K}' = |\mathbf{v}'|^2/2\) and the densities of available potential energy \(\mathcal{A} = \mathcal{B}'^2/2\mathcal{N}^2\) and \(\mathcal{A}' = \mathcal{B}'^2/2\mathcal{N}^2\):

\[
\frac{\partial \mathcal{R}}{\partial t} + K \frac{\partial \mathcal{R}}{\partial \phi} = \mathcal{W} - P_s - \mathcal{E} \tag{5}
\]

\[
\frac{\partial \mathcal{K}'}{\partial t} + K \frac{\partial \mathcal{K}'}{\partial \phi} = \mathcal{W}' - P_s - \mathcal{E}' \tag{6}
\]

\[
\frac{\partial \mathcal{A}}{\partial t} + K \frac{\partial \mathcal{A}}{\partial \phi} = -\mathcal{W} - C - \mathcal{D} \tag{7}
\]

\[
\frac{\partial \mathcal{A}'}{\partial t} + K \frac{\partial \mathcal{A}'}{\partial \phi} = \mathcal{W}' + C - \mathcal{D}' \tag{8}
\]

The contributing terms on the right-hand sides are the shear production \(P_s = -\mathcal{W} - \mathcal{K}'\), the convective production \(C = -\mathcal{W} - \mathcal{K}'\), the dissipation \(\mathcal{E} = -\mathcal{W} - \mathcal{K}'\), the eddy dissipation \(\mathcal{E}' = -\mathcal{W} - \mathcal{K}'\), the diffusive losses \(\mathcal{D} = \mathcal{W} + \mathcal{K}\), and the diffusive losses \(\mathcal{D}' = \mathcal{W}' + \mathcal{K}'\) of the eddy available potential energy. For a definition of the viscous–diffusive loss terms see Achatz (2007), as well as for the flux divergence terms on the left-hand sides of (5)–(8), which serve to redistribute energy between different GW type directions but do not contribute to the budget of the mean of all reservoirs in phase direction. The equation \(\mathcal{E} = -\mathcal{W} - \mathcal{K}'\) with an instantaneous amplification rate \(\Gamma = \Gamma_{b} + \Gamma_{a} + \Gamma_{b} + \Gamma_{d} + \Gamma_{e}\), where the amplification rate parts

\[
(\Gamma_{b}, \Gamma_{a}, \Gamma_{b}, \Gamma_{d}, \Gamma_{e}) = (\gamma_{b}, \gamma_{a}, \gamma_{b}, \gamma_{d}, \gamma_{e}) = -\left(\mathcal{W}_b, \mathcal{W}_a, \mathcal{W}_b, \mathcal{W}_d, \mathcal{W}_e\right)2(E)\tag{9}
\]

as in the linear dynamics (Achatz 2005) describe consecutively the impact of the eddy fluxes of momentum in \(\gamma_{b}\) and \(\gamma_{a}\) direction against the corresponding gradients in the horizontal mean, as well as the effect of the countergradient buoyancy fluxes and of diffusive and viscous damping. The relative strengths of \(\Gamma_{b}, \Gamma_{a}, \Gamma_{b}, \Gamma_{d}, \Gamma_{e}\) indicate which part of the gain (or loss) of \(\langle E' \rangle\) can be attributed to respective direct changes in \(\langle K_{b} \rangle = \langle \mathcal{W}_b^2/2 \rangle\), \(\langle K_{a} \rangle = \langle \mathcal{W}_a^2/2 \rangle\), and \(\langle A' \rangle\). The respective contributions to \(\mathcal{W}_b^2/2(E')\), that is, \(-\mathcal{W}_b - \mathcal{K}_b\)}
and corresponding \( P \) between \( a \). The corresponding \( a \) and \( \frac{1}{2} \) from the HGW between 0.7 and 1.4) after a perturbation by one \( a \) and \( \frac{1}{2} \) of the HGW. For an explanation of the terminology “horizontal” vs “truly horizontal” and “vertical” vs “truly vertical”, see the main text.

4. Perturbation of the wave by normal modes

All simulations of the respective HGW either perturbed by an NM or an SV have been done with an HGW at \( \Theta = 70^\circ \). With a period of \( P = 920 \) s (i.e., approximately 3 Brunt–Väisälä periods), this is the lowest-frequency HGW analyzed by Achatz (2005), and it also comes close to the wave studied by Fritts et al. (2003, 2006) that has \( \Theta = 72^\circ \). The linear analysis shows that the leading NMs are at either \( \alpha = 0^\circ \) (parallel NMs) or \( \alpha = 90^\circ \) (transverse NMs). The corresponding growth rates are shown in Fig. 1 for various \( a \) between 0.2 and 1.4. Note that these growth rates are identical to the instantaneous amplification rates at \( t = 0 \) in the nonlinear case and for all times in the linear limit (Achatz 2005). One sees that for \( a > 1 \), the most quickly growing NM of all is transverse. As shown below (Figs. 4, 10), this results from a positive contribution of both shear production and convective production to the growth of the transverse NM.\(^2\) The parallel NM, however, is fuelled by convective production, but there is a damping contribution from shear production. For \( a < 1 \), the parallel NMs take the lead since for these NMs the especially positive impact of the convective production is stronger than for the transverse NMs, while in both modes the shear production does not act as a damping term. At \( a \approx 0.6 \), transverse NM growth is negligible, so that for these HGWs the instability seems to be predominantly determined by 2D wave–wave interactions (McComas and Bretherton 1977; Klostermeyer 1991; Lombard and Riley 1996a; Achatz 2005). The reader should also note the secondary growth rate peak for parallel NMs at large wavelengths. As will be seen below, the corresponding NMs can be quite relevant for low-amplitude HGWs.

The ratio between eddy energy and horizontal-mean energy from model integrations of the HGW (with initial \( a \) between 0.7 and 1.4) after a perturbation by one of the NMs is shown in Fig. 2. In all cases, the amplitude of the NM was chosen so that the peak ratio between its local energy density \( e'(x_0, \phi) = (u_x'^2 + u_z'^2 + u_c'^2 + b_{ig}^2/N^2)/2 \) and the corresponding field \( \bar{e} \) from the HGW is \( A_{NM} = \max_{x,\phi} \bar{e}'(x_0, \phi)/\bar{e} = 10^{-2.3} \). As initial perturbation of the HGW, the leading NM was taken, or the leading large-scale NM for \( a = 0.7 \) (see also Table 1). In agreement with the linear theory, the initial growth is at initial amplitude \( a > 1 \) strongest for \( \alpha = 90^\circ \), leading to a transient phase with more eddy energy than energy in the horizontal mean, followed by eddy energy decay, so

\(^2\) As discussed by Klostermeyer (1991) and Lombard and Riley (1996a), the oscillating peaks of the growth rates can be interpreted in terms of higher-order resonances between free normal modes of the Boussinesq equations.

\(^3\) From (3) one can also see that \( r \) is at \( t = 0 \), uniform, and identical to \( \bar{E} = \bar{K} + \bar{A} \), which is \( \bar{E}(t = 0) = (a^2/2)c^2/(\sin \Theta \cos \Theta)^2 \).
that the final state is again dominated by its horizontal-mean contribution. At initial amplitude $a < 1$, the strongest growth is observed for the parallel NMs. Only for $a = 0.7$ does the eddy energy rise over that of the horizontal mean, which is a temporary effect for the transverse leading NM but permanent for the large-scale parallel NM. As will be seen below, the latter permanent effect results from the energy of the HGW being non-linearly scattered into another HGW with a steeper inclination angle.4

Following a procedure outlined in the appendix, the horizontal mean has been decomposed into its contributions from GWs with upward and downward moving phase (among the latter, the basic GW) and vortical modes. The time-dependent amplitude of the basic GW with respect to its overturning threshold is shown in Fig. 3. Not surprisingly, strong wave damping is found for the simulation of the HGW at initial amplitude $a \approx 1$ perturbed by its leading transverse NM. In all these cases a final wave amplitude $a_w \approx 0.3$ is reached. It is interesting that this is in good agreement with the results of Fritts et al. (2003, 2006), who have done fully 3D simulations of a randomly perturbed HGW. Apparently essential aspects of the breaking process are also captured in a 2.5D DNS here. One should also note that the final HGW amplitude cannot really be derived from the linear instability analysis, since the wave instability to transverse perturbations is already virtually halted near $a = 0.5$ (not shown, but see Fig. 1 where the growth rates for $a = 0.6$ are already very small and those for $a = 0.4$ are all negative or neutral). Seemingly there is an overshooting beyond this linear threshold that is completely due to non-linear dynamics. Another interesting aspect is that wave decay is quite ubiquitous, even for initial amplitude $a < 1$. These cases are characterized by a predominant impact from the parallel NMs. The respective 2D behavior leads for initial $a = 0.7$ to a rather strong damping down to $a_w \approx 0.2$ if the initial perturbation is chosen to be the leading large-scale NM. Also this is in interesting agreement with the results from Fritts et al. (2006). Notably, however, the leading transverse NM also has a strong effect on the HGW by leading to a wave decay down to $a_w \approx 0.2$

4 Though not shown, the slow rise of the eddy energy in the case of the perturbation of the HGW by the secondary transverse NM continues until $t \approx 12P$, after which it starts decaying again from a moderate level. In comparison to the other NMs with a more rapid and stronger impact, this specific NM seems to be of rather minor importance.

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![Fig. 2. From simulations of the nonlinear development of HGWs with initial amplitude $a$ between 0.7 and 1.4 after a perturbation by the (left) leading (and leading secondary, for $a = 0.7$) parallel or (right) transverse NM, the time development of the total energy of the eddies (i.e., the deviations from the horizontal mean) normalized by the horizontal-mean energy. Here the wave period $P = 920$ s. For easier comparison, time has also been normalized by the SV optimization time $\tau = 5$ min used below.](image-url)
shear production. After about half an HGW period \( P \),
the linear growth phase ends, followed by comparatively strong viscous–diffusive damping of the eddies. While quite soon a new state of equilibration has been reached for \( \alpha = 90^\circ \), the other case shows even by \( t = 4P \) a rather strong variability in the total amplification rate. One recognizes an especially positive impact from the convective production, as in the initial NM. Indeed, given the transient HGW amplitude in Fig. 3 and the corresponding positive growth rates in Fig. 1 for parallel NMs at \( \lambda = 1 \) km, one expects continuing eddy growth at larger scales. At the same time the increased viscous–diffusive damping indicates that some eddy energy has cascaded down to smaller scales where it can be dissipated. Thus the late amplification-rate decomposition for \( \alpha = 0^\circ \) indicates a continuing competition between linear growth at large eddy scales and nonlinear energy transfer to smaller scales where viscosity and diffusion remove the eddy energy, hence the transient equilibration at \( a > 0 \), although NM instabilities still exist there. This is further borne out by Fig. 5 where the vertically averaged horizontal spectra of the total eddy energy are shown for four characteristic time instances. Clearly in the case \( \alpha = 0^\circ \) at later times (between \( t = 3P \) and \( t = 4P \)) the spectrum is rather stable with dissipation at fixed scales, whereas in the other case the energy in the inertial range decays and the viscous dissipation range moves successively to larger scales, as would be expected from decaying turbulence.

The spatial distribution of the eddy energy in the simulation of the HGW with \( \alpha = 1.4 \) perturbed by its leading transverse NM is shown in Fig. 6. The corresponding spatially dependent exchange terms are given in Figs. 7 and 8. Most prominent in the kinetic energy is the temporary accumulation of \( K_r \) near \( \phi = \pi \), resulting from a corresponding shear production. This shear production is due to a transient sharp edge in \( v_l = \bar{v}_l \) near this location (not shown). One also sees that the energy flux divergence [i.e., the residual between the \( \partial K'/\partial t \) and the right-hand side of (6)] and the buoyant

![Fig. 3. Same integrations as in Fig. 2 but for the amplitude of the basic HGW with respect to its overturning threshold.](image1)

![Fig. 4. Same integrations as in Figs. 2 and 3 with initial \( a = 1.4 \), but for the decomposition of the total amplification rate \( \Gamma \) into its contributions from convective production \( \Gamma_v \), shear production \( \Gamma_P = \Gamma_s + \Gamma_v \), and viscous–diffusive damping \( \Gamma_D + \Gamma_v \).](image2)
exchange term tend to smoothen the final distribution. Similarly the main growth of $A^\prime$ is between $\phi = 0.6\pi$ and $0.8\pi$, due to a temporary deformation of the buoyancy field in the horizontal mean, with shifts of the leading gradients into this region (also not shown), so that the convective production also mainly acts there. The corresponding turbulent diffusion rate $D^\prime$ and dissipation rate $\epsilon'$ (the latter especially of interest for comparisons to the available observations) are shown in Fig. 9. Downstream of the regions of largest turbulent energy, $D^\prime$ and $\epsilon'$ also maximize, with values of several $10^2$ mW kg$^{-1}$. Both terms contribute nearly equally to the total energy sink for the turbulence, however with an especially strong transient peak in $D^\prime$. A feature reminiscent of the behavior of SVs (see below) is that in the turbulent phase the main structures move upward at a velocity very close to minus the phase velocity of the HGW (i.e., by $2\pi$ in one HGW period $P$). Remembering that the coordinate is moving downward at exactly this velocity, one can conclude that the turbulent structures seem to be frozen in the flow while the HGW moves over them.

b. Statically stable HGWs

The energetics of the integrations of the perturbed HGW with initial amplitude $a = 0.7$ resulting in the strongest decay of that wave (i.e., after a perturbation by the leading large-scale parallel NM or the leading transverse NM) are shown in Fig. 10. Initially, both shear production and convective production act as instability sources. In the case of the perturbation by the parallel NM, the convective production acts especially strongly so that the resulting amplification rate is larger. The transition to the turbulent phase with strong viscous–diffusive losses is later (near $t = P$ or $t = 4P$) than for initial amplitude $a > 1$. The local analysis analogous to Figs. 6–8 gives similar results, however with a stronger impact from the energy flux divergence (not shown) so that the dynamics of the corresponding NMs are of a more global kind.

Perhaps a better understanding can be derived by getting back [similar to Fritts et al. (2006)] to the findings from the classic linear analyses (e.g., Klostermeyer 1991) that at low HGW amplitude the dynamics of its NMs can be interpreted via resonant wave–wave interactions. For this purpose the data have been decomposed into the free NMs of the Boussinesq equations, with two GWs (with positive or negative intrinsic frequency) and a vortical mode for each combination of horizontal wavenumber $k_\parallel$ and vertical wavenumber $\mu$. Details are also given in the appendix. The decomposition of the parallel NM($k_{\parallel} = k_1$) is shown in the upper panel of Fig. 11. One sees contributions from both GW types at wavenumbers between $\mu = -4K$ and $\mu = K$. A resonant first-order wave–wave interaction between any two of these modes (labeled by the indices 1 and 2) and the basic HGW is possible if they have wavenumbers $k_{1,2}$ and frequencies $\omega_{1,2}$, so that

$$k_1 \pm k_2 = (0, 0, K)$$

$$\omega_1 \pm \omega_2 = 0,$$

remembering that in the reference system chosen the basic HGW has zero frequency. The respective modal frequencies are shown in Fig. 12. One sees two possible pairs of modes allowing a resonant difference interaction. These are the GW with positive intrinsic frequency (GW+) at $\mu = -3K$ and the GW with negative intrinsic frequency (GW−) at $\mu = -2K$, and GW+ at $\mu = -2K$ and GW− at $\mu = -K$. Their eigenfrequencies are also sufficiently close to that of the unstable parallel NM (0.016 s$^{-1}$) to allow an interpretation of the dynamics of the NM via resonant wave–wave interactions. Similar findings also apply to the leading transverse NM, with the dominant effect there, however, coming from resonant interactions between a free GW, a vortical mode, and the basic HGW (not shown).

The structural development of the buoyancy fields in the two integrations is shown in Fig. 13. In the case of
Fig. 6. The dependence of the four energy densities on time and HGW phase from the simulation of the HGW with $a = 1.4$ perturbed by its leading transverse NM. Shown is the ratio between the respective energy density and the initial total energy density of the HGW. Contour interval (CI) = 0.1, with the lowest contour at 0.1.

Fig. 7. Same integration as in Fig. 6 but for the dependence on time and HGW phase of the tendency of the (top left) total eddy kinetic energy density, (bottom left) total shear production, (top right) truly vertical buoyancy flux, and (bottom right) sum of all contributions to $\partial K'/\partial t$ up to the energy flux divergence. All fields have been divided by $<E'>$). CI = $2 \times 10^{-3}$ s$^{-1}$. The zero contour is not drawn. Negative values are indicated by dashed contours and shading.
the HGW perturbed by the large-scale parallel NM, one sees a transition from the highly turbulent phase into a late state that is characterized by a dominance of the horizontal and vertical wavenumbers $k_{||} = \pm k_y = \pm 2\pi/\lambda_y$ and $\mu = \pm 2K$, respectively. The decomposition of the horizontal wavenumber part at $k_{||} = k_y$ into the various free NMs at the respective vertical wavenumbers (lower panel of Fig. 11) identifies as the dominant structure GW at $\mu = -2K$, which seemingly survives as the dominant component from the various contribu-

![Graph](image1)

**Fig. 8.** Same as in Fig. 6 but for the (top left) total eddy available potential energy density, (bottom left) total convective production, (top right) negative truly vertical buoyancy flux, and (bottom right) sum of all contributions to $\dot{\mathcal{A}}/\dot{\tau}$ up to the energy flux divergence. All fields have been divided by $\langle 2E' \rangle$. CI = $2 \times 10^{-3}$ s$^{-1}$. The zero contour is not drawn. Negative values are indicated by dashed contours and shading.

![Graph](image2)

**Fig. 9.** Same as in Fig. 6 but for the dependence on time and HGW phase of (left) $\log_{10}[D'(mW/kg)]$ and (right) $\log_{10}[\varepsilon'(mW/kg)]$. CI = 1, beginning at 1.
tors in the resonant triads in the initial NM, followed by a contribution from GW at $\mu = -K$, while the initially especially prominent GW+ at $\mu = -3K$ has virtually disappeared. Transforming the results back into the geostationary reference frame, one can find that the resulting wave (GW+ at $\mu = -2K$) has an inclination angle $\Theta = 83^\circ$, and thus has a steeper phase propagation than the original HGW. Seemingly the initial NM structure can only give limited clues on the final outcome of the wave–wave interactions here. Also, the turbulent diffusive losses shall finally be documented, which is done in Fig. 14. One sees that also here, both the eddy dissipation and the eddy diffusion reach values of several $10 \text{mW kg}^{-1}$, which is for the turbulent dissipation rates quite typical for turbulence measured in the middle atmosphere (Lübken 1997; Müllemann et al. 2003).

5. Perturbation of the wave by singular vectors

For an overview of the possible impact of SVs on HGWs, the latter have at initial amplitude $a = 0.7$ or 1.4 been perturbed by their leading parallel or transverse SVs for an optimization time $\tau = 5$ min (i.e., about one Brunt–Väisälä period $2\pi/N$). As shown in Achatz (2005), the most prominent optimal growth for this $\tau$ is found for $\alpha = 90^\circ$. The horizontal wavelength of all SVs, identical to the respective horizontal domain extension in the simulation, is given in Table 1. For larger $\tau$, the leading SV converges more and more toward the leading NM. In the present cases the SVs have much shorter horizontal scales than the leading NMs so that the NM behavior, to which they might finally converge as $t \to \infty$, cannot as be as vigorous as shown above. As an oversight, the initial strength of the SVs has been chosen so that its peak relative energy density $A_{SV}^2$, defined in analogy to $A_{NM}^2$ above, was either $10^{-2}$, $10^{-1}$, or 1.

The time-dependent HGW amplitude obtained in the simulations is shown in Fig. 15. Clearly the SV impact on the HGW is weaker than that from the leading NMs. There are several reasons why. One is that the SV itself has not only smaller horizontal but also smaller...
vertical scales. As also shown in Achatz (2005), all SVs have more or less the form of sharply peaked pulses with a very narrow extent in HGW phase that are frozen in the flow as the HGW propagates over them, thus repeatedly invigorating or weakening them as they get into contact with regions of favorable or unfavorable shear or stratification. Therefore their impact on the HGW can also only be very local, all the more so since the convergence of the SV toward the leading NM (at the horizontal wavelength of the SV) is usually very slow (Achatz 2005). Typically the SV impact is hampered by nonlinear processes before it can show a major effect. An example is shown in Fig. 16, where one can see the time development of the amplification-rate decomposition from the simulation of the HGW with $a = 1.4$ perturbed by its leading parallel and transverse SV. The feature of interest here is the rather early departure from the regular behavior characterizing the linear growth phase documented by Achatz (2005), especially the early impact from the viscous–diffusive damping. The rapid HGW decay as obtained above from NM perturbations is prevented by the specific initial conditions that are horizontally periodic over a wavelength of the SV. This wavelength is much shorter than that of the relevant NMs (see Table 1) so that the latter are excluded from the simulation by definition.

The nonlinear dynamics of the SVs, however, have a measurable effect. As an example, Fig. 17 shows the dependence of $\epsilon'$ and $D'$ on time and HGW phase from the integration of the HGW perturbed by its leading parallel SV. The feature of interest here is the rather early departure from the regular behavior characterizing the linear growth phase documented by Achatz (2005), especially the early impact from the viscous–diffusive damping. The rapid HGW decay as obtained above from NM perturbations is prevented by the specific initial conditions that are horizontally periodic over a wavelength of the SV. This wavelength is much shorter than that of the relevant NMs (see Table 1) so that the latter are excluded from the simulation by definition.

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transverse SV with $A_{SV}^{2} = 10^0$. One sees that values of several 100 mW kg$^{-1}$ are reached. As was to be expected from the linear dynamics, both are also confined to sharply peaked pulses. These pulses are apparently moving through the model domain at the negative phase speed of the HGW (i.e., in reality they seem to be frozen in the flow while the HGW moves over them). Perhaps interesting to see is that repeated periods of

Fig. 14. The dependence of the (left) turbulent eddy diffusion rate $D'$ and (right) turbulent dissipation rate $\epsilon'$ on time and HGW phase from the integrations shown in Fig. 10 after a perturbation of the HGW with $a = 0.7$ by the (top) leading large-scale parallel NM or (bottom) leading transverse NM. Shown is $\log_{10}$ of these quantities in units of mW kg$^{-1}$. CI = 1, beginning at 1.

Fig. 15. The time dependence of the HGW amplitude developing after the perturbation from the simulations of an HGW with an initial amplitude with respect to the overturning threshold $a = 0.7$ (black lines) or 1.4 (gray) perturbed by its (left) leading parallel or (right) transverse SV (for optimization time $\tau = 5$ min) with relative peak energy density $A_{SV}^{2}$ of either $10^{-2}$, $10^{-3}$, or $10^0$. Here the wave period $P = 920$ s.
little viscous–diffusive damping, when the SV is near $\phi = \pi$, alternate with periods of stronger damping, when the SV is near $\phi = 0, 2\pi$. Returning to Fig. 16, one sees that the stronger active phases are preceded by a positive energy input from mainly convective production, when the SV “passes” $\phi = 3\pi/2$ but also shear production near $\phi = 2\pi$. Similar results are obtained for the HGW with initial amplitude $a = 0.7$, however

![Graph](image.png)

**Fig. 16.** The decomposition of the instantaneous amplification rate $\Gamma$ according to (9) into its contributions from convective production $\Gamma_c$, shear production $\Gamma_s = \Gamma_{\perp} + \Gamma_{\parallel}$, and viscous–diffusive losses $\Gamma_v$ from the integrations in Fig. 15 of the HGW with $a = 1.4$ perturbed by its (top) leading parallel or (bottom) transverse SV with initial relative peak energy density $A_{2V}$ of either (left) $10^{-2}$ or (right) $10^0$.

![Graph](image.png)

**Fig. 17.** The dependence of the (left) turbulent eddy diffusion rate $D'$ and (right) turbulent dissipation rate $\epsilon'$ on time and HGW phase from the integration of an HGW with $a = 1.4$, perturbed by its leading transverse SV for $\tau = 5$ min (initial relative peak energy density $A_{2V} = 10^0$) as also in Figs. 15 and 16. Shown is log$_{10}$ of these quantities in units of mW kg$^{-1}$. CI = 1, beginning at 1.
with values for $\epsilon'$ and $D'$ on the order of several $10 \text{ mW kg}^{-1}$ (not shown). SVs thus seem to be of minor importance for the problem of HGW damping, but they can still lead to considerable turbulent dissipation rates. Especially, the fact that the mesosphere turbulence is often observed in rather thin layers (Müllemann et al. 2003; Strelnikov et al. 2003) indicates that SVs there might still be of relevance for the problem of turbulence onset. One should also note that the range of dissipation rates measured there is between $1$ and $10^3 \text{ mW kg}^{-1}$, which the simulations seem to be consistent with.

6. Summary and conclusions

The primary nonlinear dynamics resulting from a perturbation of an HGW by its most important NMs or SVs have been studied by direct numerical simulations (DNSs). Since the effect of possible secondary instabilities has been neglected, the DNS could be restricted to two spatial dimensions (the direction along the phase propagation of the HGW and the direction of propagation of the perturbation in the plane orthogonal to that). Nonetheless, the simulated velocity field was 3D, and in contrast to traditional 2D simulations, cases with $\alpha \neq 0$ can also be treated so that the present simulations can be classified as 2.5D. Viscosity and diffusivity, as well as the HGW wavelength, were given values typical for the upper mesosphere.

Similarly to the results from Fritts et al. (2003, 2006), it is found that both statically unstable and statically stable HGWs can decay considerably after a perturbation by NMs. For statically unstable HGWs, the NM of greatest impact is the leading transverse NM, which is driven both by shear and convective production but more by the former. Interestingly the same final HGW amplitude $a_{\infty} \sim 0.3$ is reproduced in the 2.5D approach, as identified by the authors above in their 3D simulations. One might thus hope that 2.5D simulations can be a tool helpful in the studies of GW breaking, which might supplement the most comprehensive analyses using 3D DNS.

Also in agreement with Fritts et al. (2006), the instability of a statically stable HGW ends in the transfer of energy from that wave into another parallel wave ($\alpha = 0^\circ$) that has (in the present case) half the wavelength in the direction of the HGW phase propagation and about twice the wavelength in the direction orthogonal to that, yielding an inclination angle near $\Theta \approx 83^\circ$. The turbulent, seemingly resonant, wave–wave interaction thus results in energy transfer from the HGW (with $\Theta = 70^\circ$) into another wave with steeper phase propagation. The present study teaches us that this process is not due to the impact of the leading parallel NM but to a larger-scale parallel NM. A comparison between the impact of the two patterns indicates that the former is, due to its smaller scales, impeded earlier in its growth by nonlinear secondary instabilities, resulting in rapid energy transfer to even smaller scales and viscous–diffusive losses (not shown). Interestingly, for statically stable HGWs, the initial instability is driven more by convective production than by shear production, while the opposite is the case for statically unstable HGWs.

As for the impact of the most prominent short-term SVs, it is found that these are considerably less effective in initiating HGW decay. The main reason for this is the smaller scale of the SVs in comparison to the NMs, so that their effect on the HGW is only local and thus slower (as the HGW propagates over the SV). This effect is rather soon blocked by the nonlinear decay of the SV, resulting in turbulent dissipation and diffusion rates of magnitudes that are (as well as those obtained from the NM integrations) often in the range of values (between $1$ and $10^3 \text{ mW kg}^{-1}$) observed in the mesosphere (Lübken 1997; Müllemann et al. 2003). Also here, however, a similar caveat as in Achatz (2007) applies in that the spectra exhibit a considerable anisotropy between the horizontal and vertical flow field components (not shown), which is inconsistent with the basic assumptions behind the retrieval of the turbulent dissipation rates from relative density fluctuations measured by in situ rocket soundings. There it is assumed that density can be considered a passive tracer in isotropic turbulence. Beyond that, perhaps an interesting aspect is that the turbulence from SV decay is typically, as with the SV itself, more locally confined. SVs might thus be helpful in explaining the layering often observed in mesospheric turbulence.

So what have we learned so far that might be relevant for parameterizations? Perhaps the most important message, already partly obtained from the linear theory, is that wave breaking sets in earlier (below the static and dynamic instability thresholds) and that the HGW deposits much more of its momentum than typically assumed nowadays. Unfortunately, a major problem remaining is the question as to whether it is possible to understand and predict the final amplitude of the HGW, and whether and which other GWs arise in the course of the process. Next to the HGW properties, this also seems to be sensitively dependent on the specific initial perturbations and their strength. Much work remains to be done here.

Nonetheless, it is the author’s belief that the systematic approach taken here, from the linear theory to the
2.5D DNS, was already able to shed more light on the GW stability problem. It seems worthwhile to continue following this path. An important aspect to be studied systematically is secondary instabilities, to all expectations leading to a full three-dimensionalization of the turbulent fields (Klaassen and Peltier 1985; Winters and D’Asaro 1994; Andreassen et al. 1994; Fritts et al. 1994). Another task that deserves attention in the future is the certainly difficult one of the parameterization of turbulence in breaking GWs. The available DNS data might be used for testing and improving corresponding subgrid-scale schemes (e.g., Germano et al. 1991; Lilly 1992; Ferziger 1996; Meneveau et al. 1996) that might then be available for the application of large-eddy simulations to this problem. This might improve our options for studies of whole spectra of GWs developing both in space and time, a scenario that is presumably of great relevance. Once that is possible, but probably only then, we might gather new hope for more trustworthy GW parameterization schemes than the ones we have at present.

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## APPENDIX

### Projection onto Free Normal Modes

For a meaningful analysis of the horizontal mean and the eddies in the simulations one can use an orthogonality property of the respective free normal modes of the Boussinesq equations. Linearizing these equations with identical viscosity and diffusivity about a fluid at rest with zero buoyancy and taking for the perturbation fields the ansatz \((\mathbf{v}', \mathbf{b}')(x, y, z, t) = (\mathbf{v}, \mathbf{b}) \exp[\mathbf{i}(\kappa_\parallel x_\parallel + \mu_\parallel y + \mathbf{b} \cdot \mathbf{k} - \omega t)]\), that is, with wavenumbers \(\kappa_\parallel\) and \(\mu\) parallel to the horizontal direction of propagation of the perturbation pattern and in GW phase direction, respectively, and frequency \(\omega\), one obtains (similar to Achatz 2005)

\[
-i\omega u_\parallel - f(\sin\Theta v_\parallel - \sin\alpha \cos\Theta u_\phi) + ik_\parallel p + b \cos\alpha \cos\Theta = 0
\]  
\[
-i\omega u_\parallel + f(\sin\Theta u_\parallel) + \cos\alpha \cos\Theta u_\phi - b \sin\alpha \cos\Theta = 0
\]  
\[
-i\omega u_\phi - f(\sin\alpha \cos\Theta u_\parallel) + \cos\Theta u_\phi + i\mu p - b \sin\Theta = 0
\]  
\[
-i\omega b + N^2 (\cos\alpha \cos\Theta u_\parallel + \sin\Theta \sin\phi u_\parallel + \sin\Theta u_\phi) = 0
\]

\[
 i\kappa_\parallel u_\parallel + i\mu u_\phi = 0,
\]

where \(\hat{\omega} = \hat{\omega} + \Omega \mu / k \) and \(i \nu (\kappa_\parallel^2 + \mu^2)\) is the inviscid-nondiffusive part of the intrinsic frequency. The resulting eigenmodes are best obtained by first transforming the equations back into the geostationary \((x, y, z)\) coordinate system. One obtains three solutions for each combination of \(\kappa_\parallel\) and \(\mu\). One of these is the vortical mode with \(\hat{\omega} = 0\) and structure

\[
(u, v, w, b) = \frac{\sqrt{2Nf}}{\sqrt{\beta^2 + N^2(k^2 + l^2)}} \times \left( -i \frac{l}{f}, \frac{k}{f}, 0, 0 \right),
\]

where \((u, v, w)\) and \((k, l, m)\) are, respectively, the velocity and wavenumber vector in the geostationary reference frame. The wavenumber vector can be obtained from \(\kappa_\parallel\) and \(\mu\) via

\[
k = \kappa \sin\Theta + \mu \cos\Theta
\]

\[
l = \kappa_\parallel \sin\alpha
\]

\[
m = -\kappa \cos\Theta + \mu \sin\Theta
\]

\[
\kappa = \kappa_\parallel \cos\alpha.
\]

The other solutions are free GWs with \(\hat{\omega} = \hat{\omega}_\pm = \pm \sqrt{\beta^2 + N^2(k^2 + l^2)} / (k^2 + l^2 + m^2)\) and structure

\[
(u, v, w, b) = \frac{m}{\sqrt{k^2 + l^2 + m^2}} \left( \frac{k + ilf/\hat{\omega}}{\sqrt{k^2 + l^2}}, \frac{l - ikf/\hat{\omega}}{\sqrt{k^2 + l^2}}, \frac{\sqrt{k^2 + l^2}}{m}, iN \frac{N \sqrt{k^2 + l^2}}{m} \right).
\]  

\[
\frac{\sqrt{k^2 + l^2 + m^2}}{\sqrt{k^2 + l^2 + m^2}} \left( \frac{k + ilf/\hat{\omega}}{\sqrt{k^2 + l^2}}, \frac{l - ikf/\hat{\omega}}{\sqrt{k^2 + l^2}}, \frac{\sqrt{k^2 + l^2}}{m}, iN \frac{N \sqrt{k^2 + l^2}}{m} \right).
\]
The representation of the modes in the coordinate system used here can be obtained via the rotations

\[ u_\theta = u_\ell \cos \alpha + u \sin \alpha \]  
\[ v_\perp = -u_\ell \sin \alpha + v \cos \alpha \]  
\[ u_\phi = u \cos \theta + w \sin \theta \]  
\[ u_\ell = u \sin \theta - w \cos \theta . \]

Having defined an energy-metric scalar product

\[ \left( v_1, v_2 \right) = \frac{v_1 \cdot v_2}{2} + \frac{b_1 b_2}{2N^2} \]

for any two modes \((\mathbf{v}, \mathbf{b})_1,2\) (the overbar denotes complex conjugation), one can easily check that the normal modes are orthonormal (most easily in the geostationary coordinate system). Among these modes, the GW with \((\kappa_\ell, \mu) = (0, K)\) and downward-directed phase velocity is the basic GW of the problem. A decomposition into the contributions from the various free modes, and thus also extraction of that of the basic GW, can be so done by Fourier decomposition (into the contributions from the different \(\kappa_\ell\) and \(\mu\)) and straightforward projection.

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