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Fourier disentangling of spectra in observational surveys

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Abstract. The usage of the Fourier disentangling of component spectra and orbital parameters of multiple stars is advantageous in follow-up campaigns to big photometric surveys. The perspectives of its applications in spectroscopic surveys are outlined.

Key words: stars: fundamental parameters – binaries: spectroscopic – stars: atmospheres

1. Introduction

The observations of binary and multiple stars reveal the fundamental parameters of stars, which are crucial not only for testing the theory of structure and evolution of stars, but also of stellar systems, galaxies, and of chemical evolution of the universe. Specifically, the spectroscopic observations of binaries provide an information about their absolute sizes and physical parameters of their atmospheres (T_{eff}, $\log g$, abundances etc.). Due to the multiplicity of the stellar systems, the spectra of component stars are blended. In order to determine the atmospheric parameters of the components we need to separate their individual spectra from the observations. This can be done numerically (e.g. using the method of tomographic separation by Bagnuolo & Gies, 1991) if the Doppler shifts of the component spectra at different exposures are known. However, to recognize the dynamics of the system and the consequent Doppler shifts, it is desirable to have the component spectra separated (in order to measure their Doppler shifts similarly to the method of cross-correlation by Simkin, 1974). Thus, the mutually conditioned information about the dynamics and the spectra of the component stars is entangled in the sets of observed spectra and therefore must be sought in parallel. Methods of such a simultaneous search for the component spectra and the orbital parameters are called the disentangling of spectra. They were introduced by Simon & Sturm (1994), who solved the separation of spectra by means of the singular-value decomposition in the wavelength domain, and by Hadrava (1995) using a solution in the Fourier domain. (It should be noted that the term 'disentangling' is sometimes used also for procedures which do not solve the problem in its complexity.)

To get a complete information about the dynamics of a multiple stellar system, it is desirable to combine the spectroscopy with a photometry or interferometry which are sensitive to the inclination of the orbit. Moreover, as the photometry is less observationally demanding than the spectroscopy, it is usually available for a longer period of time. The light curves are thus more suitable for determining the orbital periods. Typically the photometric variability indicates targets worth of a spectroscopic follow-up. With the increasing number and extent of the space- and ground-based photometric surveys, the chances to find in their archives light curves needed to complement the spectra obtained in a campaign dedicated to objects of interest are growing. Disentangling is then an efficient method to interpret the observations.

There are also available spectroscopic surveys of stars. Because the method of disentangling is much less laborious than the classical procedure of measuring the radial velocities (RVs) and subsequent solution of RV-curves, it is more suitable for an automated search for orbital parameters from the observed spectra of multiple stars.

2. Disentangling in context of interpreting observations

Progress in science can generally only be achieved through a combination of theory and observation (experiment). A theory which is not based on empirically found facts and is not experimentally verified can be an interesting thought exercise, but in the end it may mislead from an understanding of nature. On the other hand, an observation that is not motivated by an actual theoretical question and whose results and consequences are not interpreted theoretically is useless. It may seem that the most reliable confirmation of a theory and the best interpretation of the observations would be a detailed theoretical prediction of the experimental results that agrees within the errors with the observations. However, any theoretical model is biased by our assumptions about importance of the various effects which may play a role in physics of the investigated object. Even a good agreement of a sophisticated theoretical model with a set of observations thus cannot guarantee that an alternative model would not fit a wider set better.

For example, it is used to model spectra of close binaries as a superposition of synthetic spectra radiated by small elements of the surfaces of the component stars. Each spectrum is computed from a non-LTE plane-parallel model atmosphere with local values of $T_{\rm eff}$ and $\log g$ which, according to the von Zeipel's theorem, correspond to the Roche model of the equipotential of a tidally distorted stellar surface. But, the Roche model is based on an assumption of hydrostatic equilibrium, which is inconsistent with the diffusion approximation of radiative transfer presumed by the von Zeipel's theorem. Such a sophisticated computation thus need not give a better result than a more pragmatic approximation using a single synthetic spectrum corresponding to a mean temperature and gravity acceleration. This simple model is also often used as a template for RV measurements using the cross-correlation method. However, the components of binaries are often peculiar (for instance if they are fast rotators with a decretion disc), so that it is safer to avoid a use of any template or any assumption on structure of their atmospheres. This is what the disentangling enables.

3. Basic features of the disentangling

In its standard version, the method of disentangling assumes, that the only change in the spectra of binary components is their Doppler shift due to the orbital motion, but the method does not impose any restrictive presumption on their shape. Instead of templates needed in alternative methods to determine the Doppler shifts in individual exposures, the exposures in other orbital phases are used in disentangling to find the relative changes of RVs between the exposures and to solve for the orbital parameters. Naturally, the systemic velocity of the multiple system cannot be determined, unless some line in spectrum of a component is identified and the total value of its Doppler shift is measured. The spectra of components separated in the disentangling are their mean shapes over the period of observation. The separation of the component spectra has to be overdetermined, i.e. more exposures in different orbital phases are needed than is the number of components to be separated, in order to have a residual least squares, which are then minimized by the search for the parameters. The residual noise of the separated spectra decreases with the square root of the number of exposures, what makes their subsequent comparison with synthetic spectra easier and more reliable than an independent fit of individual exposures.

Because the Doppler shift of the continua is in practice unmeasurable, the disentangling is usually performed in limited regions of spectra normalized with respect to the continua. The contributions of the individual component stars to the continuum cannot therefore be separated and the line depths in the separated spectra are related to the level of continuum of the whole system. Consequently, a comparison of the disentangled spectra with theoretical models must take into account unknown multiplicative line-strength factors, together with the parameters of the rotational broadening and the Doppler shift due to the systemic velocity. Successful fit of one component by a synthetic spectrum decreases uncertainties in separating of other components. Hence, if there is an indication that the spectrum of some of the components is of a type for which we have reliable synthetic model (e.g. when the component is a main-sequence star), it is advantageous to perform the template-constrained disentangling, in which the spectrum of the one component is chosen from a set of the synthetic spectra and only the other(s) is computed as an unknown (see Hadrava, 2016, for explanation).

Possible changes of component spectra during the orbit or on a longer time scale can be investigated from differences between individual exposures and their synthetic model computed as a superposition of the separated spectra Doppler shifted according to the corresponding RVs. The disentangling can be generalised to treat also changes of line profiles of individual components. The line-profile variations can often be expressed or at least approximated using a convolution of the intrinsic line profile with a time-variable broadening function dependent on a few parameters. The values of these parameters can be then found in the same way as the orbital parameters on which the broadening function of the Doppler shift (i.e. a shifted delta function) depends. The simplest case is the variation of line strength parametrized by a multiplicative factor. Another example are pulsations of a component star (see Hadrava et al., 2009). Fourier transform turns the convolution into multiplication and it thus splits the high-dimension linear problem of the separation of spectra into independent low-dimension solutions of each Fourier mode. This makes the Fourier disentangling fast and capable of further generalisations.

Any such generalisation should, however, be possible in both versions of disentangling – in the wavelength and in the Fourier domain. There appear sometimes claims (often misleading) in the literature about advantages and disadvantages of both methods. One alleged disadvantage should be a need to rebin the input spectra into an equidistant logarithmic scale. Regarding the wavelength dependence of the Doppler effect, it is a constant shift just in the logarithmic wavelength-scale, which is thus needed in both methods of disentangling as well as in any correct method of separation. Naturally, the difference from a linear wavelength-scale can be negligible in a narrow region of wavelengths, but it would be already an inaccuracy. If the Doppler shift should be represented by a unit off-diagonal matrix in the wavelength domain, then the input and output must be equidistant. It is possible to multiply this matrix from both sides by matrices performing the interpolation from the sampling of the input data and to the desired sampling of the output, but the outcome is the same as in subsequent interpolation, solution, and an additional resampling. The constant shift is given by a diagonal matrix (of unit complex numbers) in the Fourier representation, but the game takes place in the direct and inverse Fourier transform. It could also be adapted to any sampling of the input and output, but it is facilitated by a two-step procedure of interpolation into an equidistant sampling and then a use of Fast Fourier Transform (FFT). In any case, the overal procedure of spectra separation is in fact a linear interpolation from the input to output spectra. To minimize a smoothing by subsequent interpolations, it is recommendable to resample the input data into a finer scale than is the original resolution of the input spectra.

Another reservation about the Fourier disentangling repeated in a literature is that it does not allow to assign different weights to individual bins of input spectra. Usually it is not mentioned that the wavelength-domain disentangling does not enable to assign different weights to different Fourier modes, which is a more useful option. Possible dead pixels or cosmics in the input spectra can and should be eliminated in both methods during preprocessing of the data before the resampling into the equidistant scale. On the other hand, a suitable weighting of different Fourier modes, i.e. of features on a long and short scale, enables to minimize an influence of unevenesses of continua and to strengthen the impact of narrow lines on solution of orbital parameters, or to combine the disentangling of spectra with different resolution. It is especially important in use of echelle spectra, where merging of the orders complicates finding of the continuum (see Hensberge, 2007). In some cases, like the Hα emission, the lines can be wider than the width of the order. It would be thus ideal to have to each high-resolution echelle spectrum also a simultaneous single-order low-resolution spectrum in wide region of wavelengths for flux normalisation.

A real advantage of the wavelength-domain disentangling is that it enables to separate the component spectra in a range enlarged on both sides of the input region for a short interval which enters the region only in some exposures due to non-zero Doppler shifts of the components. The solution in these intervals suffers more from the noise, but it is important that its absence does not violate the solution inside the sampled region. The choice of the region is equivalent to a multiplication of the whole spectrum by characteristic function of its interval, which means a convolution with its transform in the Fourier domain. In particular, the usage of FFT assumes a periodical repeating of the region, so that a line which disappears behind one edge of the region should appear at the other one. Its neglecting may disturb the solution at the region edges in a width comparable to the amplitude of the Doppler-shift. It is thus preferable to cut the regions of sampling in wavelengths where are no prominent lines (which is usually easy for early-type stars), or to choose a wider region and to skip a vicinity of its edges.

4. Disentangling in spectroscopic surveys

Disentangling of spectra obtained in follow-up campaigns focused on targets indicated in photometric surveys as possible binaries is a common practice. The recent development of space- and ground-based spectroscopic surveys opens a new option for study of multiple stars. As pointed out by Seeburger et al. (2024), the disentangling is a powerful technique to interpret the observed spectra, however, it may encounter slightly different problems when applied to spectroscopic surveys. In particular, spectra from such surveys can be of low resolution and available only from too few epochs. Low S/N and unsuitable distribution of the observations over the phases of orbital motion of individual objects can also be a problem. This is not necessarily always the case (see, e.g., Guo et al., 2022, who used more than six observations at resolving power $R \simeq 7500$ of each star). All these problems depend on the instrumentation used, strategy of the observations, as well as on duration of the survey, and they may diminish in a more distant future. If the survey has to yield a statistics of multiplicity of the stars, then its insufficient quality and completeness requires a careful treatment of

Table 1. Orbital parameters of 68 u Her (P in days, T in HJD-2400000, $K_{1,2}$ in $\mathrm{km\,s^{-1}}$).

Solution	Kolbas+	43 spectra	4 spectra	$R \simeq 2000$
P	2.05102685(68)	2.050966(4)	2.050933(11)	2.050936(22)
T	47611.5007(15)	52302.226(2)	52302.227(3)	52302.221(7)
K_1	94.6±2.3	99.10(6)	97.98(16)	97.66±1.42
K_2	267.4±3.3	273.16	268.99	261.45
$q = K_1/K_2$	0.354	0.363(8)	0.364(2)	0.374(5)

selection effects. Nevertheless, Seeburger et al. (2024) present their implementation of disentangling, which should avoid the problem of few-epochs spectra replacing the search for orbital parameters by computation of the RVs only.

Considering simple double-lined spectroscopic binaries (SB2), it is true that three exposures are sufficient to separate the two spectra of components if their RVs are to be also disentangled, while at least five exposures are needed to disentangle all spectroscopic orbital parameters (i.e. the period P, periastron passage T, eccentricity e, longitude of periastron ω, and RV amplitudes $K_{1,2}$). In a review of existing codes for disentangling in their Tab. 1, Seeburger et al. (2024) claim that the Korel code can solve only for orbital parameters and not RVs, what is not true. Any of these options can be chosen for any component, but the computation of RVs is rarely used because the choice of orbital parameters is more valuable. Although the authors justify the superiority of the template-independent methods, they are using templates to combine their disentangling with cross-correlation.

In order to test correctness and reliability of the operation of disentangling in a case of few-epochs data expected in spectroscopic surveys, it is advantageous to treat a subset selected from a large set of spectra. This makes it possible to check the reliability of results obtained from a limited data set against the results from a richer data set. As an example, let us take the eclipsing binary 68 u Her studied in detail by Kolbas et al. (2014). By analysing *Hipparcos* photometry and 43 high-resolution spectra (with $R \simeq 40000$) obtained at Calar Alto Observatory in 2008, the authors arrived at orbital parameters given here in the first column of Tab. 1.

In the present work we shall use another 43 spectra of Hα region secured in the years 2002-2007 using the CD700 camera ($R \simeq 13000$) at 2m Perek Telescope of Ondřejov Observatory. The Korel disentangling shown in Fig. 1 separates the line profiles of the primary and secondary component and the water telluric lines, which are significant in this region (see the bottom three green lines). The disentangled orbital parameters are given in the second column of Tab. 1. The distribution of Bayesian probability of the parameters is shown in Fig. 2 by the error ellipse and isocontours corresponding to 1, 2, and 3-σ probability (see Hadrava, 2016, for explanation). The couples of parameters $P - T$ and $K_1 - q$

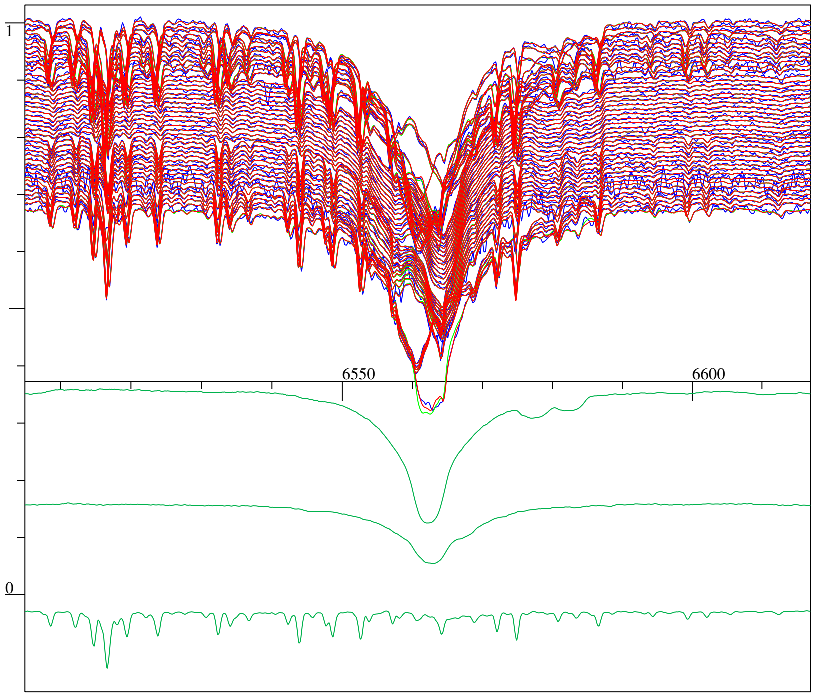

Figure 1. KOREL-disentangling of 43 Ondřejov spectra in Hα region of 68 u Her.

are anticorrelated with correlation coefficients -0.863 and -0.571, respectively.

If the initial conditions for the convergence of parameters contain a non-zero eccentricity, it quickly converges to zero in the case of 68 u Her. The longitude of periastron is thus chosen 90° to set the periastron passage identical with conjunction of the components (and a centre of eclipse). A negligible excentricity is a common case in short-period binaries due to their tidal circularization. An assumption of a circular orbit may thus simplify the search for orbital parameters and to decrease the number of needed exposures in short-lasting surveys. Unprecise initial estimates of velocity amplitudes also usually converge quite smoothly to the correct values. The orbital period which we obtained by adjusting an initial estimate to our spectroscopic data agrees with a relative error 2.97×10^{-5} with the ephemeris derived from the *Hipparcos* photometry. This is a satisfactory result regarding the fact that appart of the last exposure taken about 926 periods after the first one, all others are obtained within 604 periods. The search for period is, however, very sensitive to the initial conditions and often leads to a false local minimum.

To simulate data from a few-epochs survey, we can choose 4 exposures, which

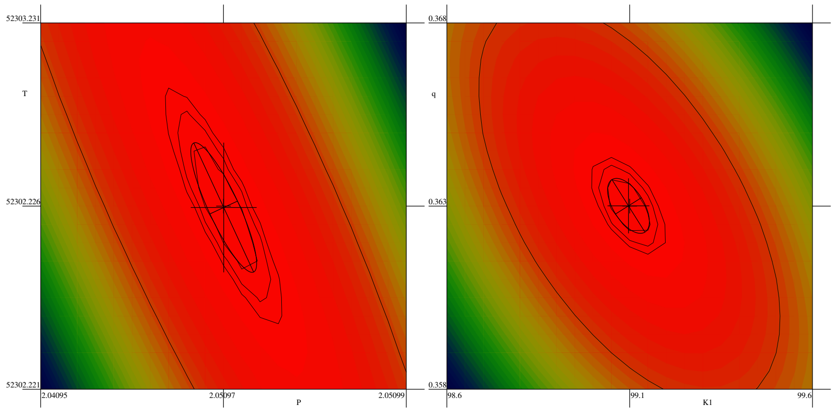

Figure 2. Distribution of probability of disentangled parameters in the plane $P-T$ (left panel) and K_1-q (right panel).

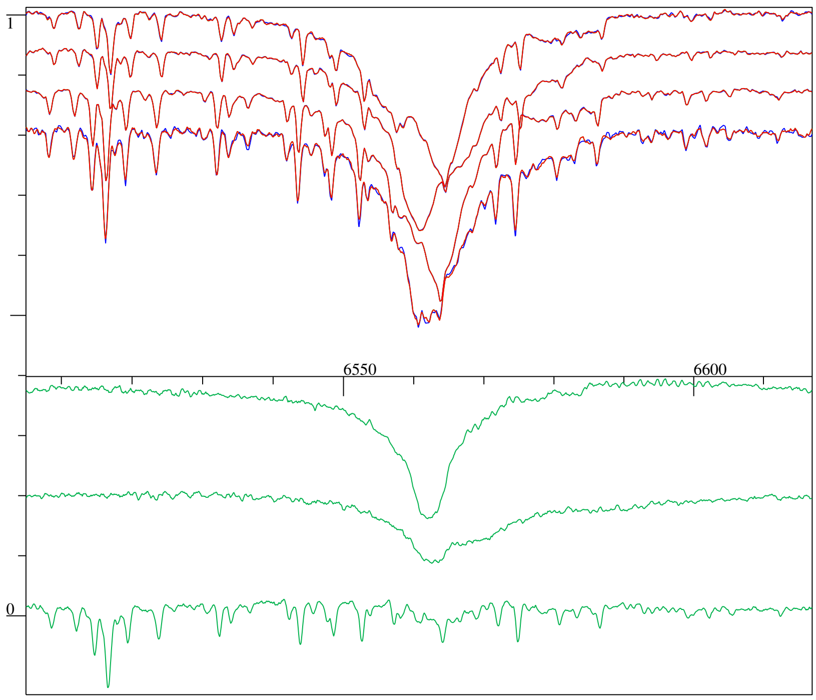

Figure 3. KOREL-disentangling of four Ondřejov spectra in Hα region of 68 u Her.

are a minimum needed to disentangle the three component spectra and RVs or the orbital parameters without e and ω. Because the second exposure in our set of spectra began immediately after the end of the first one, we shall choose the exposures 2-5. The disentangling of these four spectra shown in Fig. 3 reveals basically the same features as the results obtained from the whole set of 43 spectra (e.g. the C II doublet 6578 and 6582Å in the more massive primary), but naturally in a more noisy form. Because of a lower overdeterminacy, the input spectra are fitted more precisely than in the disentangling of the whole set (compare the input spectra displayed in blue lines with their fit in red), but their noise is more imprinted onto the separated spectra. The disentangled orbital parameters shown in the third column of Tab. 1 also agree with the previous solutions but with a higher error. For example, the relative error of the period with respect to the photometric ephemeris is 3.71×10^{-5} while the data span 292 periods. However, the period cannot be determined reliably from such scarce data. In our case, the first two exposures were taken at the beginning of the year 2002 and the next two in the summer 2003, so that periods shorter or longer for about $P/292 \simeq 0.007$d can give nearly the same orbital phases with one more or one less cycle. It can be seen from the distribution of residuals after the disentangling which is displayed in Fig. 4. Zooming in the vicinity of the central peak of the probability distribution, we can find that it has a fine structure. It is due to an interference of the sampling epochs. The central peak gets more compact and pronounced with increasing number of exposures, while the side lobes of the probability distribution diminish. For a disentangling of orbital parameters from a few-epochs spectroscopy, it is thus desirable to have an estimate of the orbital period (and possibly also the epoch of conjunction) from a photometric survey.

Instead of disentangling the orbital parameters, we can also disentangle independently RVs of all components in all exposures as suggested by Seeburger et al. (2024). In a template independent disentangling we have to fix RV of one exposure of each component to prevent the ambiguity in an additive constant to RVs of the component and the corresponding Doppler shift of its separated spectrum. In our present case of Hα region we can retain orbital parameters for the telluric lines, which are calculated from the coordinates of the star and to solve only for the strengths of these lines. If we start the convergence of RVs from values close to the solution found using disentangling of orbital parameters, we arrive at solution which is very similar in both the separated spectra and the RVs (see Tab. 2). Residual noise σ of the spectra in units of the continuum level is even slightly smaller compared to the disentangling of the orbital parameters (see the last line of Tab. 2) owing to a higher number of free parameters (6 RVs instead of P, T, and $K_{1,2}$). However, if the initial conditions of some RVs deviate significantly from this correct solution, the disentangling converges to a false minimum, separated spectra are distorted, and RVs of other components are also wrong. While in the disentangling of orbital parameters the RVs of each component in each exposure are bound to be consistent with other exposures, in

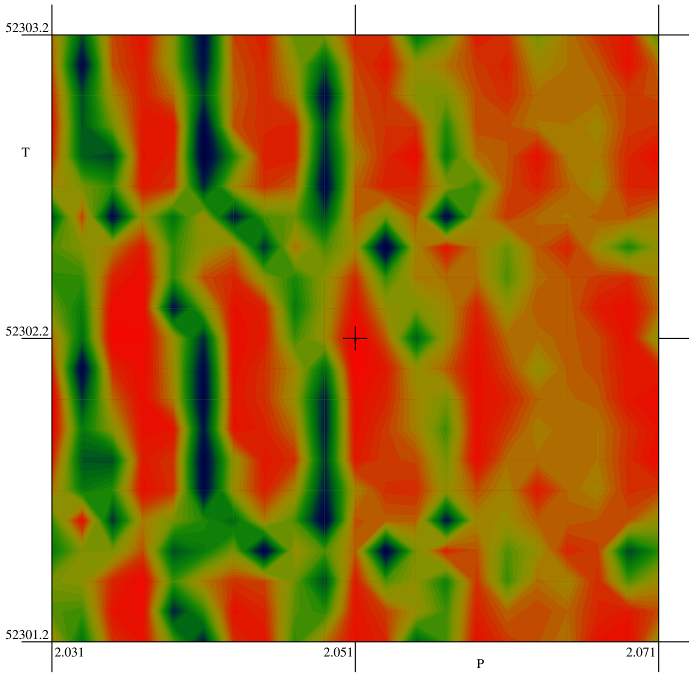

Figure 4. Distribution of residuals in the $P-T$ plane at disentangling of four spectra.

Table 2. Radial velocities disentangled in various solutions.

Spectra/parameters HJD-2400000	43/orbit RV_1	4/orbit RV_1	4/RVs RV_1	43/orbit RV_2	4/orbit RV_2	4/RVs RV_2
52303.6811	96.8	94.9	97.6	−267.6	−259.9	−263.2
52308.6665	−77.0	−75.4	−81.0	204.6	206.9	199.5
52841.3914	70.5	63.6	62.4	−183.5	−176.2	−182.8
52903.3475	−53.4	−55.4	−56.0	148.8	152.7	149.2
$\sigma \times 10^3$	1.99	1.07	1.05			

their direct disentangling they are prone to fall into a false local minimum or to confuse to which component they belong. If there are available more exposures than the very minimum of three, then the disentangling of RVs has more free parameters than the disentangling of orbital parameters (especially if the period is known), which causes a higher instability of the solution. Regarding also the fact that the whole solution of orbital parameters offers more information about the observed systems, the decision to limit the disentangling to RVs is not much suitable.

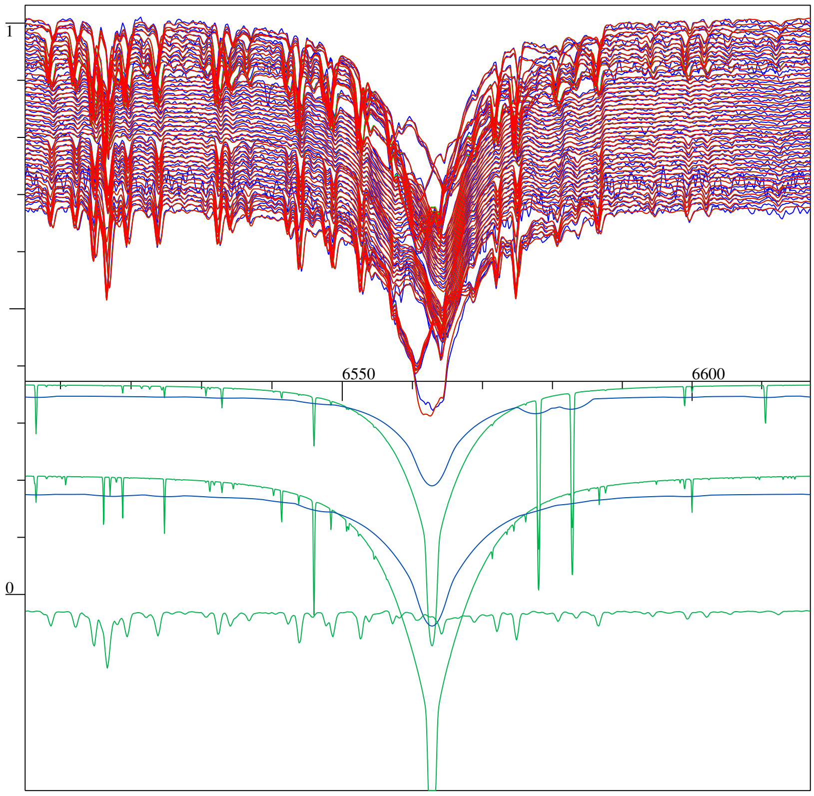

Figure 5. KOREL-disentangling of 68 u Her constrained by synthetic templates for 21000 K and 11750 K.

When we find that the disentangled spectra agree sufficiently with spectra of main-sequence stars or another type of objects for which model spectra are available, we can use for their further analysis a template-constrained disentangling. In the present case of 68 u Her we can use synthetic spectra computed using the code SPECTRUM, version 2.75, by Gray (1999), applied to the grid of LTE model atmospheres by Castelli & Kurucz (2003). If the spectra of one component and of the telluric lines are fixed to the result from the free disentangling, while the template of the other component is chosen from the set of synthetic spectra, and we converge its line strengths, rotational broadening, and systemic velocity, we find the best fit for the primary component at the temperature 21000 K and for the secondary at 11750 K. Disentangling constrained by both these templates is displayed in Fig. 5; here the green lines show the input synthetic spectra and the cyan their rotational broadening rescaled in depth. This solution has a residual noise $\sigma = 3.09 \times 10^{-3}$, that is only for a half higher than that of the free disentangling. However, it does not show, e.g., the drop in red wing of Hα of the secondary which can be seen even in the disentangling of the subset of four spectra in Fig. 3. Using a quadratic fit also to three neighbouring synthetic templates for each component, we arrive at estimate of the temperatures of the component stars 21350 K and 11900 K, for which Kolbas et al. (2014) found 21600 ± 220 K and 12600 ± 550 K. The mean line-strength factors indicate the continuum of the primary to be at 0.750 and of the secondary at 0.232 of the total continuum, which is close to the *Hipparcos* photometric light ratio 0.739 ± 0.026 according to Kolbas et al. (2014). The systemic velocity of the primary is $\gamma_1 = -22.0\,\mathrm{km\,s^{-1}}$ and of the secondary $\gamma_2 = -6.2\,\mathrm{km\,s^{-1}}$.

The template-constrained disentangling of RVs can be performed even for a single exposure. This procedure can also select the templates which fit the observed spectrum best and it could be applied if a survey does not contain more than one exposure of a star. However, due to a higher noise, it is less sensitive than the disentangling of multiple exposures. This method is practically equivalent to a two-dimensional cross-correlation, with a difference that the rotational broadening is also obtained in this way.

To test the performance of the Fourier disentangling in a case of low signal-to-noise ratio and low-resolution spectra, we can add to our data an artificial noise and to blur them by convolving them with a Gaussian function or another kernel imitating the instrumental profile of the spectrograph in use. Our spectra of 68 u Her can be degraded to a resolution $R \sim 2000$ using a convolution with Gaussian of half-with 1.5 Å. Applying it to the above selected four spectra, we arrive by disentangling to the orbital parameters given in the fourth column of Tab. 1 and to the separated spectra shown in Fig. 6. As we can see, these results are still qualitatively consistent with those obtained from the spectra with a higher resolution. Naturally, the tinny telluric lines cannot be clearly distinguished, what may cause problems also in a case of binaries with late-type stars.

5. Discussion and conclusion

In addition to the few epochs of exposures and their random distribution in orbital phase, the low S/N ratio can also be an obstacle to a successful disentangling in spectroscopic surveys. As already mentioned, the residual noise of the separated spectra decreases with a number of the input exposures, but in a few-epochs data it cannot be reliably diminished. The limiting factor is not the absolute value of S/N, which is given by the ratio of (mostly photon) noise to the level of continuum, but its relation to the depth and width of the spectral lines, which are the carrier of information about the multiplicity of the stellar system. The same S/N can thus be sufficient to separate the components in

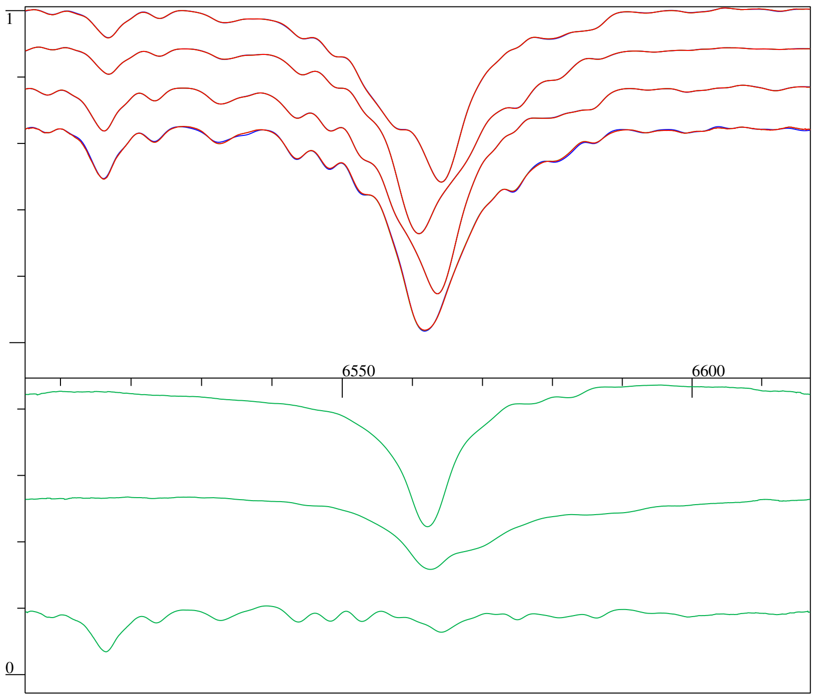

Figure 6. KOREL-disentangling of 68 u Her spectra with $R \sim 2000$.

some SB2 system, it may fail to detect a companion in some other system, or it may be completely unable to find RV-changes in yet another system.

Similarly, the applicability of a particular method of disentangling is not given by resolving power of the used spectrograph alone, but it also depends on the amplitude of RVs in the observed system and on the spectra of its components. Fourier disentangling enables to reach a sub-pixel precision in the determination of the Doppler shift (see Hadrava, 2009), but it does not mean a possibility to resolve and to separate dense narrow lines of late-type stars if they are below the resolution of the detector. The residual noise may mimic intrinsic spectral features in low resolution and low S/N spectra and no method can then yield a reliable disentangling of a low number of exposures.

Finally, the success of disentangling and reliability of its results for a particular system also depends on its possible intrinsic variability, e.g. due to pulsations, mass loss, spots etc. An automated application of disentangling to large spectroscopic surveys should thus be combined with a more sophisticated clasification and pre-selection of the targets like in the work by Škoda et al. (2020). Statistical conclusions from such studies should take into account the selection effects of the detectability of the companion stars.

In spite of these complications, the disentangling of spectra is a method appropriate for treatment of multiple stars observed in spectroscopic surveys. The template-independent version is capable to interpret also spectra of systems with some peculiarities and the template-constrained disentangling can find parameters of stellar atmospheres of common stars. The disentagling of orbital parameters is preferable to the disentangling of radial velocities. It is desirable to combine the disentangling of spectra with a light-curve solution of data from photometric surveys.

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