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STUDY OF SPECTROSCOPIC BINARIES WITH TODCOR. III. APPLICATION TO TRIPLE-LINED SYSTEMS

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ABSTRACT

In a previous paper we introduced TODCOR, a new two-dimensional correlation technique, to analyze spectra of binary stars and derive the Doppler shifts of the two components. We propose here a generalization of TODCOR to analyze spectra of triple-lined stellar systems and derive the Doppler shifts of the *three* components. The algorithm computes the correlation of the observed spectrum against combinations of three template spectra, with all possible shifts. Thus, the correlation is a three-dimensional function in velocity space. The location of the maximum of this function corresponds to the actual shifts of the three components.

We demonstrate the difficulties of the one-dimensional cross-correlation and the advantages of the new algorithm with a simulated example. We also analyze with the algorithm a real test case, HD 100018, and we show that the velocities derived with the new extension of TODCOR solve a long-standing discrepancy between the old orbital elements and the mass estimate for the system.

Subject headings: binaries: spectroscopic — stars: individual (HD 100018) — techniques: spectroscopic

1. INTRODUCTION

In a previous paper (Zucker & Mazeh 1994, hereafter Paper I) we introduced a novel technique to analyze composite spectra of binary stars. The technique, TODCOR, is a two-dimensional correlation scheme to derive the radial velocities of both components of double-lined spectra. TODCOR was introduced as a generalization of the cross-correlation technique (Simkin 1974; Tonry & Davis 1979; Hill 1993) to deal with the difficulties encountered in double-lined spectra, when the lines of the two components cannot be resolved. In Paper II of this series (Mazeh et al. 1995) we applied TODCOR successfully to an extremely eccentric binary, where during most of the orbit the two velocities are very close to each other. The ability to derive the velocities at all phases allows a reduction in the amount of observations required and avoids depending only on observations close to periastron.

In this paper we introduce an extension of TODCOR to analyze spectra of *triple-lined* systems and derive the radial velocities of the *three* components. In cases where the lines of the three stars are well separated, the one-dimensional cross-correlation exhibits three distinct peaks, and therefore the different velocities can be easily derived. The problems arise when two of the velocities are not well separated, leading to blending of the one-dimensional cross-correlation peaks and even blending of the two-dimensional correlation peaks.

The inability to resolve the velocities can occur rather frequently in triple systems for which all three components contribute significantly to the observed spectra. Since a significant fraction of binaries might actually turn out to be triple systems (Duquennoy & Mayor 1991; Mayor & Mazeh 1987), it is important to study the known triples thoroughly. The frequent blending of spectral lines occurring in triple systems limits our ability to study this important part of the population of multiple systems.

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To overcome this problem, we propose to consider any observed triple-lined spectrum as a sum of *three* known templates with unknown shifts. We suggest calculating the correlation between the observed spectrum and combinations of the *three* templates, rendering the correlation a function of the independent shifts of the *three* templates. The location of the maximum in the three-dimensional velocity space will correspond to the actual Doppler shifts of the three components of the observed spectrum.

In order to calculate the correlation in this three-dimensional space, we would need $O(N^4)$ operations, where N is the length of the spectra. However, by using Fourier transform techniques, the number of operations required is reduced to $O(N^3)$. In cases where the spectra have on the order of 10^3 pixels, this amounts to a reduction from about 10^{12} operations to about 10^9 operations, rendering the calculation possible on present workstations.

This paper presents the extension of TODCOR to handle triple-lined spectra. Section 2 briefly explains some of the details of the algorithm, while a more detailed exposition is given in the Appendix. Section 3 demonstrates the new capabilities with a simulated example, while § 4 deals with a specific real test case, HD 100018. Possible applications of the proposed extension are discussed briefly in § 5.

2. THE THREE-DIMENSIONAL CORRELATION

In the one-dimensional cross-correlation technique, one calculates the correlation as a function of the shift between an observed spectrum f and a template g:

$$R^{(1)}\{f, g\} = R^{(1)}\{f, g\}(s) ,$$

where s is the shift between the observed spectrum and the template. For double-lined spectra, TODCOR calculates the correlation between f and a combination of two templates g_1 and g_2, with different shifts and an intensity ratio, denoted by α:

$$g_1(n - s_1) + \alpha g_2(n - s_2) .$$

It can be shown that α is actually the ratio between the intensity of the secondary and the intensity of the primary. The correlation is now a function of s_1, s_2, and α:

$$R^{(2)}\{f, g_1, g_2\} = R^{(2)}\{f, g_1, g_2\}(s_1, s_2, \alpha) .$$

As we have shown in the Appendix to Paper I, we can calculate this function by using only three one-dimensional correlation functions: $R^{(1)}\{f, g_1\}$, $R^{(1)}\{f, g_2\}$, and $R^{(1)}\{g_1, g_2\}$, thus reducing substantially the computational complexity.

Regarding the intensity ratio α, the algorithm can be used either in cases where α is known a priori, or in cases where it is unknown. In the first case, TODCOR simply calculates the correlation using the known α. In the second case, TODCOR eliminates the α dependency by finding analytically the α which maximizes the correlation for each pair of shifts. In both cases, the correlation turns out to be a function only of s_1 and s_2:

$$R^{(2)}\{f, g_1, g_2\} = R^{(2)}\{f, g_1, g_2\}(s_1, s_2) .$$

Now we extend the technique to the triple-lined case. We have three templates, g_1, g_2, and g_3, and we calculate the correlation against a combination of the three templates with three different shifts:

$$g_1(n - s_1) + \alpha g_2(n - s_2) + \beta g_3(n - s_3) .$$

Here α is the ratio between the intensity of the secondary and the intensity of the primary, while β is the ratio between the intensity of the tertiary and that of the primary. The correlation is now a function of the three shifts and the two intensity ratios α and β:

$$R^{(3)}\{f, g_1, g_2, g_3\} = R^{(3)}\{f, g_1, g_2, g_3\}(s_1, s_2, s_3, \alpha, \beta) .$$

We show in the Appendix that, as in the two-dimensional case, this expression can also be computed using only one-dimensional cross-correlation functions, in this case six correlations between the four spectra. Using these six one-dimensional correlations, we calculate the correlation for a grid of values for the shifts and then locate the maximum in this three-dimensional grid. The shifts at the maximum are the estimates for the actual velocities of the three components of the system.

Regarding the intensity ratios, we consider four possible cases: (*a*) both α and β are known a priori, (*b*) both α and β are unknown, (*c*) α is known and β is unknown, and (*d*) α is unknown and β is known.

The first case requires only substitution of the known α and β in the formula. The three other cases are handled by finding the unknown ratios which maximize the correlation for each set of shifts s_1, s_2, and s_3. In all cases, the correlation turns out to be a function only of s_1, s_2, and s_3.

3. TESTING THE ALGORITHM

We have performed numerous tests in which the new algorithm was applied to simulated triple-lined spectra, prepared in the same way as those presented in Paper I. All tests showed a very good agreement between the input values and the estimates obtained with the extension of TODCOR.

We present here the results obtained for a simulated triple system composed of a calculated G5 V spectrum and two identical calculated K0 V spectra. The calculated spectra are taken from a grid of synthetic spectra computed by Jon Morse from model stellar atmospheres developed by Kurucz (1992a, b). They cover a 45 Å spectral band centered at 5187 Å, the standard window for routine stellar work at the Center for Astrophysics (Latham 1985). Since the spectra in the grid are characterized by their effective temperature, we chose a temperature of 5500 K for the G5 V spectrum and 5000 K for the K0 V spectrum. The intensity ratio between the K0 V secondary and the G5 V primary was chosen to be 0.5, and the ratio between the K0 V tertiary and the G5 V primary was taken to be 0.4. To mimic real observed spectra, we added normally distributed noise with a signal-to-noise ratio (S/N) of 85.

The first example we show here is a triple-lined spectrum in which we combined the templates with well-separated velocities of -50 km s^{-1} for the primary, 0 km s^{-1} for the secondary, and $+50$ km s^{-1} for the tertiary. The combined spectrum is displayed in Figure 1*a*, and a close examination reveals three sets of lines. Figure 1*b* shows the classical one-dimensional cross-correlation against the G template, where one can see clearly the three peaks corresponding to the three velocities. This is a simple case where the standard one-dimensional technique can give satisfactory results because the three peaks are sufficiently separated.

In the second example, we combined the spectra in a way that causes the peaks of the two K stars to blend, with velocities of $+20$ km s^{-1} for the primary star, -15 km s^{-1} for the secondary, and -25 km s^{-1} for the tertiary. Figure 2*a* displays this combined spectrum, where only two sets of lines can be seen. In Figure 2*b* we display the one-dimensional cross-

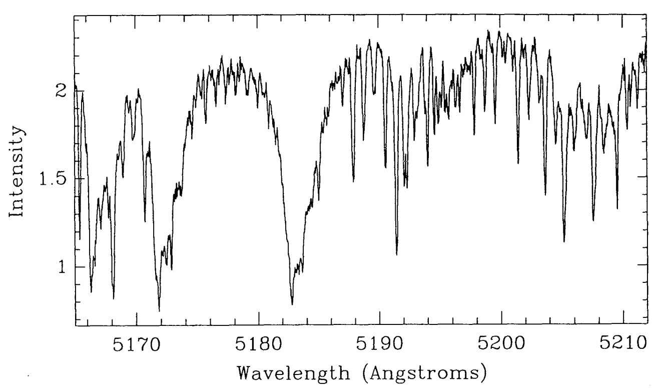

FIG. 1*a*

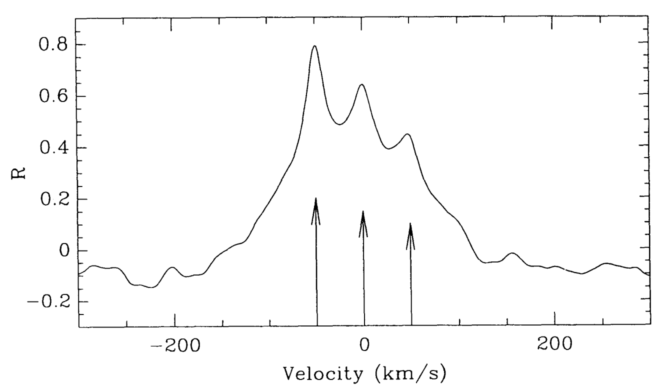

FIG. 1*b*

FIG. 1.—(*a*) Simulated spectrum composed of three templates with velocities of -50 km s^{-1} for the G5 V primary, 0 km s^{-1} for the K0 V secondary, and 50 km s^{-1} for the K0 V tertiary. (*b*) One-dimensional cross-correlation function against the G5 spectrum. Arrows indicate the velocities used in the simulation.

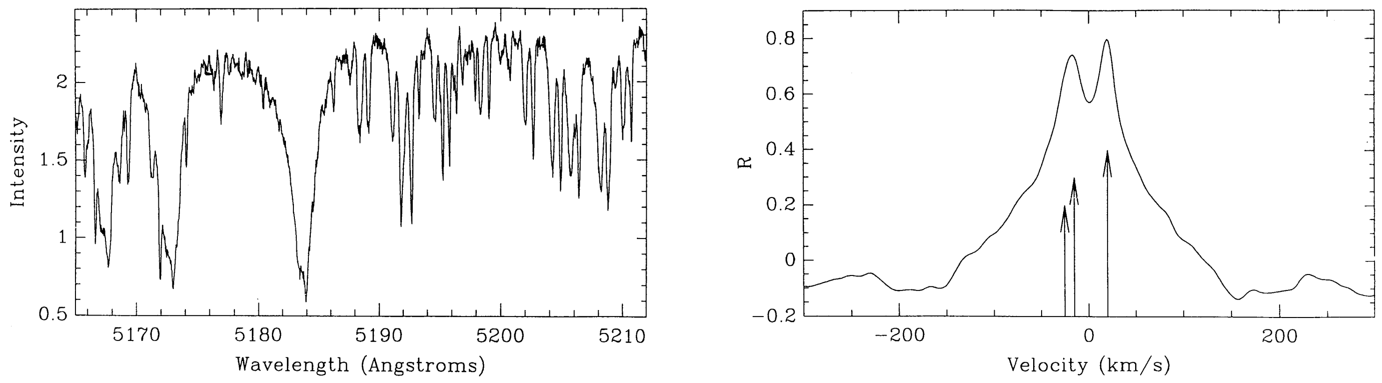

FIG. 2a FIG. 2b

FIG. 2.—(a) Simulated spectrum composed of three templates with velocities 20 km s^{-1} for the G5 V primary, -15 km s^{-1} for the K0 V secondary, and -25 km s^{-1} for the K0 V tertiary. (b) One-dimensional cross-correlation function against the G5 spectrum. Arrows indicate the velocities used in the simulation.

correlation function of the spectrum against the G5 V template. The peak corresponding to the velocity of the G5 V stars is clearly separated and located at the correct velocity, whereas the two K0 V stars have blended into one peak.

Severe line blending poses a major difficulty to the classical cross-correlation techniques, and such spectra can be successfully resolved only in special cases (e.g., Fekel et al. 1994). In the second simulated example, we were indeed unable to measure the velocities of the two K0 V stars, either with classical cross-correlation techniques or by using TODCOR. However, applying the new algorithm allows the problem to be readily solved. The velocities derived with the new extension of TODCOR are 19.98 ± 0.06 km s^{-1}, -15.0 ± 0.1 km s^{-1}, and -25.2 ± 0.2 km s^{-1}, with intensity ratios of $\alpha = 0.51 \pm 0.02$ and $\beta = 0.38 \pm 0.02$. To illustrate the solution, we show in Figure 3 the three-dimensional correlation function, projected onto three axes. The second curve, for example, represents the correlation as a function of the second velocity, leaving the first and the third fixed at the value of the maximum. The most striking features are the enhancement of the relevant peak in each graph and the attenuation of the other two. All three velocities are easily derived.

We applied the algorithm to a broad set of simulated spectra, with a variety of intensity ratios, velocities, and S/Ns. We were able to measure correctly the three velocities (with uncertainties of up to 3 km s^{-1}) even at S/Ns of 3 and when the tertiary star is 10 times fainter than the primary ($\beta = 0.1$). For an S/N of 100, we were able to detect a tertiary with $\beta = 0.03$. It is obvious that a brighter tertiary and a higher S/N improve the results.

4. A REAL TEST CASE: HD 100018

After applying the algorithm successfully to numerous simulations, we went on to try it on a well-known triple-lined system, HD 100018 (ADS 8189, $\alpha_{2000} = 11^{\rm h}30^{\rm m}49\overset{\rm s}{.}9$, $\delta_{2000} = +41°17'12''$). This object has long been known as a visual binary with a period of about 85 yr (Riechert 1923). The variability of the radial velocity of one of the components of the visual pair was discovered in 1918 by Adams, Joy, & Sanford (1924), who also discovered double lines in its spectra. Petrie & Laidler (1952) found that the star is a spectroscopic triple; sometimes they could see three sets of lines. They identified the third set of lines as coming from the visual secondary B, which could not be resolved from A, the visual primary, upon their slit head. They determined a 7.4 day orbit for the close pair (Aa, Ab). Their findings were confirmed by Petrie & Batten (1969), who studied the system further and succeeded in measuring the radial velocities of the three components in some of their spectra. In all the old solutions of the spectroscopic pair, one can see the absence of measurements close to conjunction, where the velocities of Aa and Ab are close to the center-of-mass velocity of A. Since the relative velocity between A and B is small, the velocities of Aa and Ab at conjunction are also close to the velocity of B, which means that all *three* lines are blended.

Petrie & Batten used the center-of-mass velocity of the close pair and the velocity of B to calculate the relative velocity of the visual pair. The value they obtained was 5.8 ± 0.7 km s^{-1}. Combining this result with the visual orbit of Couteau (1965), they were able to estimate the amplitude of the relative velocity curve, $K_A + K_B$, and from there they were able to estimate the semimajor axis. The value they derived was 14.1 AU, which, together with an orbital period of 86.44 yr (Couteau 1965), corresponds to a total mass of the system of 0.38 $M_\odot$. This is *inconsistent* with the spectral classification of Petrie & Batten, who classified Aa, Ab, and B as F2, F5, and F2, respectively. This classification of the components suggests a total mass of about 4 $M_\odot$. We repeated their calculations using the more recent orbit by Couteau (1989) and obtained very similar results. This puzzling disagreement has remained unsolved for the past 25 years.

We observed HD 100018 between 1986 and 1989 with the digital speedometer (Latham 1985, 1992) operated by the Center for Astrophysics (CfA) with the 1.5 m Wyeth Reflector at the Oak Ridge Observatory in Harvard, Massachusetts. The spectral resolution of the observations is $\lambda/\Delta\lambda = 30{,}000$. Altogether, we have secured 42 spectra of HD 100018, spanning over 1000 days. We also included in our analysis an additional spectrum obtained approximately 2000 days later, during 1994.

To derive the three velocities, we selected templates from the same grid of synthetic spectra from which we took the spectra for the simulations. The synthetic spectra cover a 45 Å spectral band centered around 5187 Å, identical to the observed spectral range (Latham 1985). Using the spectral classification of Petrie & Batten (1969), we started with templates calculated for stars with temperatures of 7000 K, 6500 K, and 6750 K for components Aa, Ab, and B, respectively, metallicity $[m/H] = 0.0$, $\log g = 4.5$, and $v \sin i = 0.0$. Deriving the three

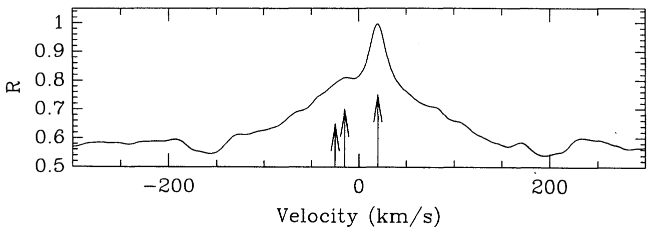

FIG. 3*a*

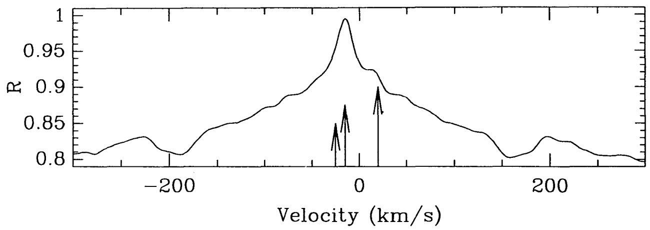

FIG. 3*b*

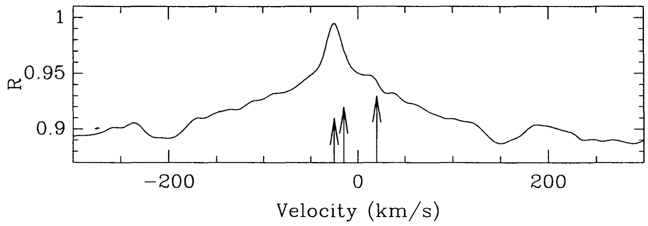

FIG. 3*c*

FIG. 3.—Cross sections of the three-dimensional correlation function, taken at the peak of this function. Spectrum is the same as in Fig. 2. (*a–c*) the correlation function as a function of the primary, secondary, and tertiary velocity, respectively, with the other two velocities fixed at the value of the maximum. Arrows indicate the velocities used in the simulation.

velocities for each spectrum took about 35 s on a 33 MHz SPARC workstation.

We performed an iterative search in the parameter space defined by the characteristics of the templates. At each iteration we solved the orbit of the spectroscopic pair using ORB18 (Mazeh, Krymolowski, & Latham 1993), a code which takes special care to find the global minimum of the χ^2 statistic in the orbital elements space. Then we changed the parameters of the various templates, looking for the combination which gave the best fit of the velocities to the radial velocity curve for the close pair. We also changed the rotational broadening of the templates by convolving them with a rotational profile (Gray 1976). The final values we adopted from this procedure for the temperatures are 7000 K, 6500 K, and 6750 K for the components Aa, Ab, and B, respectively. The final value for the rotational velocity is $v \sin i = 8$ km s^{-1} for all three components, although this value probably does not correspond to the true rotational velocity of the stars, since part of the line broadening is caused by instrumental effects. The intensity ratios we obtained are $\alpha = 0.55$ between the secondary and the primary and $\beta = 1.05$ between the tertiary and the primary. We estimate the uncertainties of these ratios to be 0.05 at a confidence level of 1 σ.

For the final parameters stated above, the velocities we derived are listed in Table 1. Figure 4 depicts the radial velocity curve for the close spectroscopic pair together with the velocities of the third star, and Table 2 presents the orbital elements of this solution. The elements are very similar to those obtained by the previous studies, except for minor differences.

Assuming the masses for Aa and Ab corresponding to spectral types F2 and F5 are 1.3 ± 0.2 $M_\odot$ and 1.2 ± 0.2 $M_\odot$ (Habets & Heintz 1981), we arrive at an estimate for $\sin i_1$ of the close pair of 0.9 ± 0.1. This means $i_1 = 76° \pm 9°$. Couteau (1989) determined an inclination angle for the visual pair of $i_2 = 56.7°$, which means that the minimal angle between the two orbital planes is $19° \pm 9°$.

All our observations were made roughly at the same phase of the long orbit, which is 0.239 ± 0.015 according to the orbital elements by Couteau (1989). The center-of-mass velocity of A is -2.1 ± 0.1 km s^{-1}, and the average velocity of B is -7.4 ± 0.2 km s^{-1}. Therefore, the relative velocity of the components of the visual pair is $V_{BA} = -5.3 \pm 0.2$ km s^{-1}. Using Couteau's orbit, we find that this value of V_{BA} implies that $K_A + K_B = 9.5 \pm 0.8$ km s^{-1}, and the semimajor axis of the visual binary is 31 ± 3 AU. This value for the semimajor axis

TABLE 1

DERIVED RADIAL VELOCITIES OF HD 100018

HJD (−2,440,000)	V_{Aa} (km s^{-1})	V_{Ab} (km s^{-1})	V_B (km s^{-1})
6438.816..........	−27.89	27.25	−7.76
6459.765..........	−56.54	59.00	−5.34
6597.675..........	76.81	−94.65	−8.11
6757.839..........	−2.99	3.99	−9.18
6771.949..........	−22.84	23.82	−6.82
6803.820..........	55.84	−66.92	−6.53
6812.813..........	24.49	−32.60	−6.32
6813.875..........	−59.99	61.84	−6.72
6819.703..........	74.30	−90.12	−5.56
6837.924..........	−39.30	41.83	−7.61
6842.830..........	−25.96	23.58	−7.39
6860.887..........	−19.73	16.99	−6.18
6900.737..........	79.79	−96.74	−6.25
7104.936..........	−22.22	21.91	−7.22
7115.928..........	57.80	−66.58	−7.09
7144.963..........	81.00	−96.13	−7.17
7163.884..........	−29.19	29.60	−8.40
7167.917..........	31.35	−43.66	−6.92
7172.746..........	17.70	−21.13	−5.77
7198.720..........	−61.96	66.22	−6.58
7202.845..........	35.19	−44.10	−7.64
7214.789..........	−50.01	54.86	−6.88
7217.737..........	3.30	−5.75	−9.31
7218.901..........	80.97	−92.29	−6.65
7220.763..........	−60.50	61.01	−9.15
7222.845..........	−36.16	38.10	−8.05
7226.773..........	68.36	−79.55	−7.24
7227.750..........	−40.02	37.41	−7.59
7228.728..........	−63.30	67.97	−8.08
7229.761..........	−46.18	45.36	−7.35
7232.829..........	51.67	−60.79	−7.39
7310.668..........	−56.18	59.70	−7.47
7320.586..........	11.46	−18.20	−6.14
7347.660..........	−58.20	58.04	−7.54
7481.896..........	−32.46	31.35	−8.60
7495.933..........	−50.99	54.91	−7.87
7511.797..........	−24.31	23.19	−8.97
7517.820..........	−58.23	61.80	−7.65
7526.982..........	−15.10	11.08	−6.36
7538.953..........	−59.94	63.71	−7.19
7544.767..........	76.24	−92.36	−7.63
7550.820..........	43.57	−53.17	−7.53
9535.559..........	38.93	−49.41	−9.44

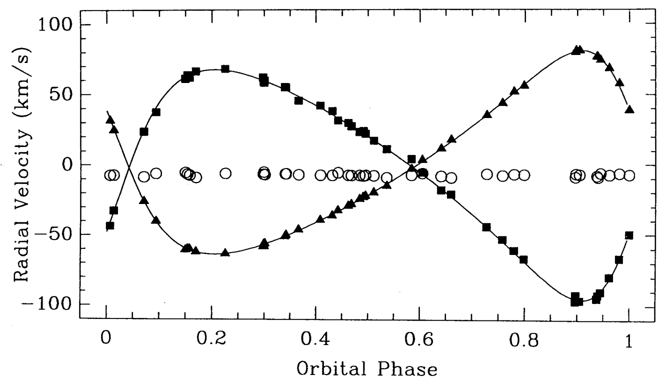

FIG. 4.—The orbital solution of HD 100018 as a function of the orbital phase of the close pair. Triangles, squares, and circles represent the velocities of the primary (Aa), secondary (Ab), and tertiary (B), respectively. The two continuous lines display the calculated radial velocity of the close pair.

leads to a total mass of $4 \pm 1\ M_\odot$, in very good agreement with the assumed spectral types. This is a substantial improvement over the result of Petrie & Batten, who obtained an estimate of 0.38 $M_\odot$ for the total mass of the system. Their erroneous result stems from their value of V_B, which is incorrect for that phase of the wide binary.

From the semimajor axis reported by Couteau, 0".41, we derive a parallax for the system of 0".013 ± 0".001. Halliwell (1981) summarized a long controversy regarding the parallax of the system and suggested the true value lies in the range between 0".009 and 0".042. He concluded that the most probable value is 0".013, which we can now confirm.

It is interesting to note that Petrie & Batten (1969), referring to the possible source of the discordance between the various estimates of the parallaxes and the masses, wrote: "*The most likely cause of systematic error in the radial velocities is blending of the profiles of each line triplet. The stronger lines, used for radial velocity measurement, are not completely resolved.... Therefore, the measured position of all three lines will be affected by the blending of their profiles.*" Since our work is intended to deal precisely with this effect, it is gratifying to see that it has solved the problem in exactly the way foreseen by Petrie & Batten.

5. DISCUSSION

We have shown in this paper that the extension of TODCOR is capable of deriving reliable radial velocities of the three components of triple systems. Admittedly, the simulations we presented are free of any complications which arise in real cases, mainly mismatches between the templates and the actual stars, which restrict the capability of any correlation technique. However, our algorithm does improve the ability to eliminate the error caused by blending of the peaks or spectral differences between the components. Using this algorithm, one actually correlates each component of the triple system with a specific template tailored to its spectral type, rather than using the same template for all components. The real system we analyzed here demonstrates the applicability of the algorithm to real stellar spectra. It also illustrates how major improvements in velocity measurement have solved a long-standing discrepancy between the old measurements and the mass estimate for the system.

It may be possible to use TODCOR to obtain estimates of various parameters of the components of binary systems affecting the spectra besides the velocity, such as the spectral types itself, the rotational velocity, and also the magnitude difference between the system components. This can be done by searching for the best correlation, or by searching for the best orbital solution, as was done here in the case of HD 100018.

Analysis by any correlation technique requires the availability of templates, either synthetic or observed, which should be as close as possible to the real spectra. Among the techniques aimed at generating templates directly from the observed spectra, we mention here the tomographic method of Bagnuolo & Gies (1991), and the recent disentanglement procedure of Simon & Sturm (1994). Suitable extensions of those techniques to the case of triples, together with the extension of TODCOR presented here, may prove to be fruitful in analyzing triple-lined spectra.

Measuring the complete set of velocities in triple and other multiple systems may contribute to our understanding of triple systems, their interesting dynamical behavior (Mazeh & Shaham 1976; Mazeh & Mayor 1983; Söderhjelm 1984; Bailyn 1987; Mazeh 1990; Mazeh et al. 1993), and the statistics of their various characteristics (Fekel 1981). The next paper in this series will deal with a specific triple-lined system—HD 98800 (Torres et al. 1995). We intend in the future to apply the algorithm to other known triple systems, such as Gliese 644 and Gliese 866, and to report our findings in subsequent works. Another advantage of the algorithm is the improved ability to detect faint third comparisons to known spectroscopic binaries. As we demonstrated in a previous work (Mazeh & Zucker 1994), TODCOR is capable of detecting very faint companions and measuring their velocities. This may prove to be true also in the triple-lined case.

TABLE 2

ORBITAL ELEMENTS OF THE CLOSE PAIR

Parameter	Value
$P(d)$	7.39905 ± 0.00002
γ(km s^{-1})	−2.1 ± 0.1
K_1(km s^{-1})	72.3 ± 0.2
K_2(km s^{-1})	81.6 ± 0.4
e	0.356 ± 0.002
ω	65°.6 ± 0°.4
T(JD −2,440,000)	7182.67 ± 0.01
$a_1 \sin i(10^9$ m)	6.87 ± 0.02
$a_2 \sin i(10^9$ m)	7.76 ± 0.04
$M_1 \sin^3 i(M_\odot)$	1.21 ± 0.01
$M_2 \sin^3 i(M_\odot)$	1.072 ± 0.008
M_2/M_1	0.886 ± 0.005
σ_1(km s^{-1})	0.82
σ_2(km s^{-1})	1.84

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APPENDIX

Both the stellar spectrum and the template are assumed to be given as a function of n, where

$$n = A \ln \lambda + B .$$

Thus, the Doppler shift results in a uniform linear shift of the spectrum.

The one-dimensional cross-correlation function of Tonry & Davis (1979) is

$$R^{(1)}\{f, g\}(s) = \frac{\sum_n f(n)g(n-s)}{N\sigma_f \sigma_g} , \tag{A1}$$

where N is the number of bins in the spectra, and σ_f and σ_g are the intensity standard deviations of the spectra:

$$\sigma_f^2 = \frac{1}{N} \sum_n f(n)^2 .$$

Actually, since the sums do not include exactly N summands, but rather the number of overlapping bins, N in the denominators should be changed to the overlap length. The calculations do not differ much, so we choose to keep N for simplicity.

As Tonry & Davis point out, one can compute the numerator in equation (A1) effectively with the fast Fourier transform (FFT) algorithm. We denote the discrete Fourier transforms (DFTs) of $f(n)$ and $g(n)$ by $F(k)$ and $G(k)$, respectively. The DFT of $\sum_n f(n)g(n-s)$ is

$$F(k)G(k)^* ,$$

where $G(k)^*$ denotes the complex conjugate of $G(k)$. Using FFT, we can calculate the complete cross-correlation function in an $O(N \log N)$ process, instead of $O(N^2)$.

Within the new three-dimensional algorithm, we correlate $f(n)$ against a combination of *three* templates, with three *different* Doppler shifts:

$$g_1(n-s_1) + \alpha g_2(n-s_2) + \beta g_3(n-s_3) ,$$

where α and β are the intensity ratios of the system, which we assume are known. We relax this assumption later.

As a direct extension of equation (A1), we obtain

$$R^{(3)}\{f, g_1, g_2, g_3\}(s_1, s_2, s_3, \alpha, \beta) = \frac{\sum_n f(n)[g_1(n-s_1) + \alpha g_2(n-s_2) + \beta g_3(n-s_3)]}{N\sigma_f \sigma_g(s_1, s_2, s_3)} , \tag{A2}$$

in which

$$\sigma_g^2(s_1, s_2, s_3) = \frac{1}{N} \sum_n [g_1(n-s_1) + \alpha g_2(n-s_2) + \beta g_3(n-s_3)]^2 .$$

The numerator in equation (A2) can be written as:

$$\sum_n f(n)g_1(n-s_1) + \alpha \sum_n f(n)g_2(n-s_2) + \beta \sum_n f(n)g_3(n-s_3) ,$$

that is, three summands which can be computed efficiently using FFT, just like the numerator of equation (A1). However, the denominator in equation (A2) includes σ_g, which is a function of s_1, s_2, and s_3, unlike the denominator in equation (A1), which is constant. To compute σ_g, we note that

$$\sigma_g^2(s_1, s_2, s_3) = \sigma_{g1}^2 + \alpha^2\sigma_{g2}^2 + \beta^2\sigma_{g3}^2 + 2\alpha\sigma_{12} + 2\beta\sigma_{13} + 2\alpha\beta\sigma_{23} ,$$

where

$$\sigma_{ij}(s_j - s_i) \equiv \frac{1}{N} \sum_n g_i(n-s_i)g_j(n-s_j) .$$

The first three terms include the standard deviations of the individual templates. The other three have exactly the same form as the numerator of equation (A1), which makes them easy to compute via FFT. For simplicity, let us define

$$C_1(s_1) \equiv \frac{1}{N\sigma_f \sigma_{g1}} \sum_n f(n)g_1(n-s_1) ,$$

$$C_2(s_2) \equiv \frac{1}{N\sigma_f \sigma_{g2}} \sum_n f(n)g_2(n-s_2) ,$$

$$C_3(s_3) \equiv \frac{1}{N\sigma_f \sigma_{g3}} \sum_n f(n)g_3(n-s_3) ,$$

$$C_{12}(s_2 - s_1) \equiv \frac{1}{N\sigma_{g1}\sigma_{g2}} \sum_n g_1(n) g_2[n - (s_2 - s_1)] ,$$

$$C_{13}(s_3 - s_1) \equiv \frac{1}{N\sigma_{g1}\sigma_{g3}} \sum_n g_1(n) g_3[n - (s_3 - s_1)] ,$$

$$C_{23}(s_3 - s_2) \equiv \frac{1}{N\sigma_{g2}\sigma_{g3}} \sum_n g_2(n) g_3[n - (s_3 - s_2)] .$$

Now we have

$$\begin{aligned}\sigma_g^2 &= \sigma_{g1}^2 + \alpha^2\sigma_{g2}^2 + \beta^2\sigma_{g3}^2 + 2\alpha\sigma_{g1}\sigma_{g2} C_{12} + 2\beta\sigma_{g1}\sigma_{g3} C_{12} + 2\alpha\beta\sigma_{g2}\sigma_{g3} C_{23} \\ &= \sigma_{g1}^2(1 + \alpha'^2 + \beta'^2 + 2\alpha' C_{12} + 2\beta' C_{13} + 2\alpha'\beta' C_{23}) ,\end{aligned}$$

in which $\alpha' \equiv (\sigma_{g2}/\sigma_{g1})\alpha$ and $\beta' \equiv (\sigma_{g3}/\sigma_{g1})\beta$. The final expression is

$$R^{(3)}\{f, g_1, g_2, g_3\}(s_1, s_2, s_3, \alpha, \beta) = \frac{C_1 + \alpha' C_2 + \beta' C_3}{\sqrt{1 + \alpha'^2 + \beta'^2 + 2\alpha' C_{12} + 2\beta' C_{13} + 2\alpha'\beta' C_{23}}} . \tag{A3}$$

We see that the final expression includes only six cross-correlations: three between the observed spectrum and the templates, $C_1(s_1)$, $C_2(s_2)$, and $C_3(s_3)$, and three between the templates, $C_{12}(s_2 - s_1)$, $C_{13}(s_3 - s_1)$, and $C_{23}(s_3 - s_2)$. This fact preserves the $O(N \log N)$ nature of the calculation. In fact, since we can obtain a rough estimate of the three shifts using the usual cross-correlation or other dynamical considerations, we can evaluate equation (A3) only for a small domain of the (s_1, s_2, s_3) space.

In order to obtain error estimates for each of the shifts, say s_2, we can fix the other two shifts, s_1 and s_3, to their values at the maximum, $\hat{s}_1$ and $\hat{s}_3$, and look at the function:

$$P(s_2) = R^{(3)}\{f, g_1, g_2, g_3\}(\hat{s}_1, s_2, \hat{s}_3, \alpha, \beta) .$$

Careful examination of this function of s_2 shows that it is closely related to the cross-correlation of f against g_2, after subtracting g_1 and g_3 from f with the appropriate weights. Thus, an error estimate can be obtained using the error analysis of the one-dimensional cross-correlation (e.g., Kurtz et al. 1992).

So far we have assumed that the relative weights of the templates, α and β, are known. We move now to discuss the case where at least one of them is unknown. We wish to choose, for each s_1, s_2, and s_3, the value of the unknown weight which maximizes the correlation between $f(n)$ and the linear combination of g_1, g_2, and g_3. The dependence of the correlation on α and β is analytic and can be explored in all cases by the most basic means; the expressions for both weights and the corresponding correlation values can be calculated easily. Finally, in the case where both light ratios are unknown, their values may be computed by the expressions

$$\alpha = \left(\frac{\sigma_{g1}}{\sigma_{g2}}\right) \frac{(C_{13}C_{23} - C_{12})C_1 + (1 - C_{13}^2)C_2 + (C_{12}C_{13} - C_{23})C_3}{(1 - C_{23}^2)C_1 + (C_{13}C_{23} - C_{12})C_2 + (C_{12}C_{23} - C_{13})C_3} ,$$

$$\beta = \left(\frac{\sigma_{g1}}{\sigma_{g3}}\right) \frac{(C_{12}C_{23} - C_{13})C_1 + (C_{12}C_{13} - C_{23})C_2 + (1 - C_{12}^2)C_3}{(1 - C_{23}^2)C_1 + (C_{13}C_{23} - C_{12})C_2 + (C_{12}C_{23} - C_{13})C_3} .$$

These values can be substituted in the formula for the correlation to obtain the value of the correlation for the best α and β for each set of velocities.

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