Comparison of different separability approximations (complete and partial) for the case of near Fermi resonance

The hamiltonian of our model system is

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - \frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{\omega_x^2}{2}x^2 + \frac{\omega_y^2}{2}y^2 + \frac{\omega_z^2}{2}z^2 + \lambda\eta x^3 + \mu\varsigma y^3 + \lambda x y^2 + \mu y z^2 .$$

where $\omega_x = 1.31$, $\omega_y = 1.3$, $\omega_z = 1.0$, $\lambda = \mu = -0.10$, and $\eta = \varsigma = 0.10$ (the first frequency is almost equal to the second frequency, another parameters are the same as for the model of [K. M. Christoffel, J. M. Bowman, Chem. Phys. Lett. **85**, 220, 1982]). This problem is solved perturbatively by introducing a small parameter δ:

$$H_\delta = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - \frac{1}{2}\frac{\partial^2}{\partial z^2} + \frac{\omega_x^2}{2}x^2 + \frac{\omega_y^2}{2}y^2 + \frac{\omega_z^2}{2}z^2 + \delta^{1/2}(\lambda\eta x^3 + \mu\xi y^3 + \lambda x y^2 + \mu y z^2)$$

and expanding the energy in powers of δ:

$$E(\delta) = \sum_{k=0}^{\infty} E_k \delta^k$$

The initial hamiltonian corresponds to $\delta = 1$.

We used five methods: complete separability ($x-y-z$), partial separability ($xy-z$, $zx-y$, and $yz-x$), and exact perturbation theory (all modes xyz are coupled). The results are listed in a following table. Since $zx-y$ approximation is identical to $x-y-z$ approximation for our potential (generally, it holds for any potential of the form $V_1(x,y)+V_2(y,z)$), $zx-y$ approximations are not listed.

State *n n n*	Method	$\lvert E\ \ \rvert$	Result	Relative error, %	Earlier results
000	x - y - z	$-8.939\cdot10^{-37}$	1.8031265072	0.049	
	xy - z	$-4.741\cdot10^{-30}$	1.8028310783	0.033	
	yz - x	$-1.107\cdot10^{-25}$	1.8025318479	0.016	
	xyz	$\mathbf{-1.279\cdot10^{-24}}$	**1.8022353217**		
100	x - y - z	$-5.881\cdot10^{-36}$	3.1123544721	0.048	
	xy - z	$5.232\cdot10^{-8}$	3.1115828743	0.023	
	yz - x	$-1.343\cdot10^{-25}$	3.1117591345	0.029	
	xyz	$\mathbf{6.164\cdot10^{-6}}$	**3.1108536646**		
010	x - y - z	$-3.702\cdot10^{-32}$	3.0981721726	0.18	
	xy - z	$-3.800\cdot10^{-8}$	3.0965602390	0.13	
	yz - x	$-1.793\cdot10^{-22}$	3.0941115727	0.048	
	xyz	$\mathbf{-6.164\cdot10^{-6}}$	**3.0926236502**		
001	x - y - z	$-4.911\cdot10^{-29}$	2.7964258505	0.077	
	xy - z	$-1.496\cdot10^{-27}$	2.7961102986	0.065	
	yz - x	$-4.742\cdot10^{-23}$	2.7946065153	0.011	
	xyz	$\mathbf{-4.324\cdot10^{-22}}$	**2.7942872954**		
200	x - y - z	$-3.387\cdot10^{-35}$	4.4213265959	0.050	
	xy - z	$8.226\cdot10^{-3}$	4.4199071275	0.018	
	yz - x	$-1.630\cdot10^{-25}$	4.4207305776	0.036	
	xyz	**-0.2312**	**4.4191321750**		
110	x - y - z	$-1.456\cdot10^{-31}$	4.4063614343	0.16	
	xy - z	$-7.449\cdot10^{-3}$	4.403484444	0.099	
	yz - x	$-2.105\cdot10^{-22}$	4.4023012291	0.072	
	xyz	**0.2294**	**4.3991458624**		

Coefficients of the perturbation series are calculated up to the 20th order for complete separability, up to the 20th order for partial separability, and up to the 20th order for the exact problem. The 20th order coefficients are given in the third column of the table to compare different methods regarding feasibility of summation of the series. Smaller coefficients, easier summation of the series.

To sum this constant-sign series, we use quadratic Padé approximants. We give only stable digits.