Dunker and Gordon potential [1] can be written in the form

$$V(r,\theta) = V_A(r,\theta) + V_R(r,\theta), \tag{1}$$

where the attractive and repulsive parts are expanded as

$$V_A(r,\theta) = -\varepsilon \frac{\alpha}{\alpha - 6} \left(\frac{r_m}{r}\right)^6 \left[1.00 + 0.32 \left(\frac{r_m}{r}\right) P_1(\cos\theta) + 0.24 P_2(\cos\theta)\right], \tag{2}$$

and

$$V_R(r,\theta) = \varepsilon \frac{6}{\alpha - 6} \exp\left[\alpha \left(1 - \frac{r}{r_m}\right)\right] \left[1.00 + 0.51 P_1(\cos\theta) + 0.78 P_2(\cos\theta)\right]. \tag{3}$$

Таблица 1: Physical constants and potential energy parameters used in the calculation of bound states of ^{40}Ar-H^{35}Cl.

$\mu = 34505.15$ a.u.
$B_0 = 10.44019$ cm^{-1}
$\varepsilon = 140.39566$ cm^{-1}
$\alpha = 13.50$
$r_m = 3.930$ Å
1 a.u. of energy = 219475.797 cm^{-1}
1 a.u. of length = 0.529177 Å

Таблица 2: Ro-vibrational energy levels of Ar-HCl on the Dunker-Gordon potential (in cm^{-1})

J = 0 [2]	J = 0 (our)	J = 1 [2] odd parity	J = 1 (our) odd parity	J = 1 [2] even parity (M=0)?	J = 1 (our) even parity(M=1)?
-132.5012	-132.5012	-132.3882	-132.3881		
		-113.6419		-113.6393	-113.5213
-111.3839	-111.3838	-111.2705	-111.2720		
-92.2126	-92.2125	-92.1075	-92.1079		
-86.6109	-86.6108	-86.5974	-86.5029		
		-85.4678		-86.5614	-86.4487
-67.4835	-67.4834	-67.3864	-67.3865		
-62.8488	-62.8486	-62.7528	-62.7456		
		-61.9661		-61.9721	-61.8663
		-57.4417		-57.4282	-60.6106
-53.9889	-53.9886	-53.8709	-53.8841		
-47.1472	-47.1471	-47.0560	-47.0566		
-41.6786	-41.6785	-41.5876	-41.5829		
		-40.2178		-40.2220	-40.1237
-33.1305	-33.1303	-33.0471	-33.0458		
		-29.6137		-29.6063	-29.5017
-25.5940	-25.5938	-25.4958	-25.5026		
-23.9208	-23.9207	-23.8357	-23.8327		
		-22.1597		-22.1633	-22.0733
-19.7022	-19.7021	-19.6264	-19.6267		
-12.1013	-12.1012	-12.0370	-12.0366		
-9.8526	-9.8524	-9.7773	-9.7736		
		-7.9985		-7.9998	-7.9176
-6.6103	-6.6102	-6.5642	-6.5545		
		-6.2461		-6.2525	-6.1558
-3.3323	-3.3322	-3.2768	-3.2795		
-1.4769	-1.4768	-1.4303	-1.4320		
-0.4111	-0.4110	-0.3832	-0.3836		
	-0.0185		-0.0095		

Надо бы применить граничные условия по ВКБ для ренормализованного метода Нумерова. Манолополус отмечает их важность для log-derivative метода. Жесткие граничные условия: на -1.0 от левой поворотной точки, на +15.0 от правой поворотной точки. 15 каналов, 5.000 точек.

1 Список литературы

1. Dunker, A. M., Gordon, R. G. (1976). Calculations on the HCl–Ar van der Waals complex. The Journal of Chemical Physics, 64(1), 354-363.

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