Fitting Potential Energy Curves for Diatomic Molecules. Extrapolation properties of Morse/Long-Range potential

Alketa Sinanaj[1,2] , Asen Pashov[1]

[1]Faculty of Physics, Sofia University, Bul. J. Bourchier 5, 1146 Sofia, Bulgaria

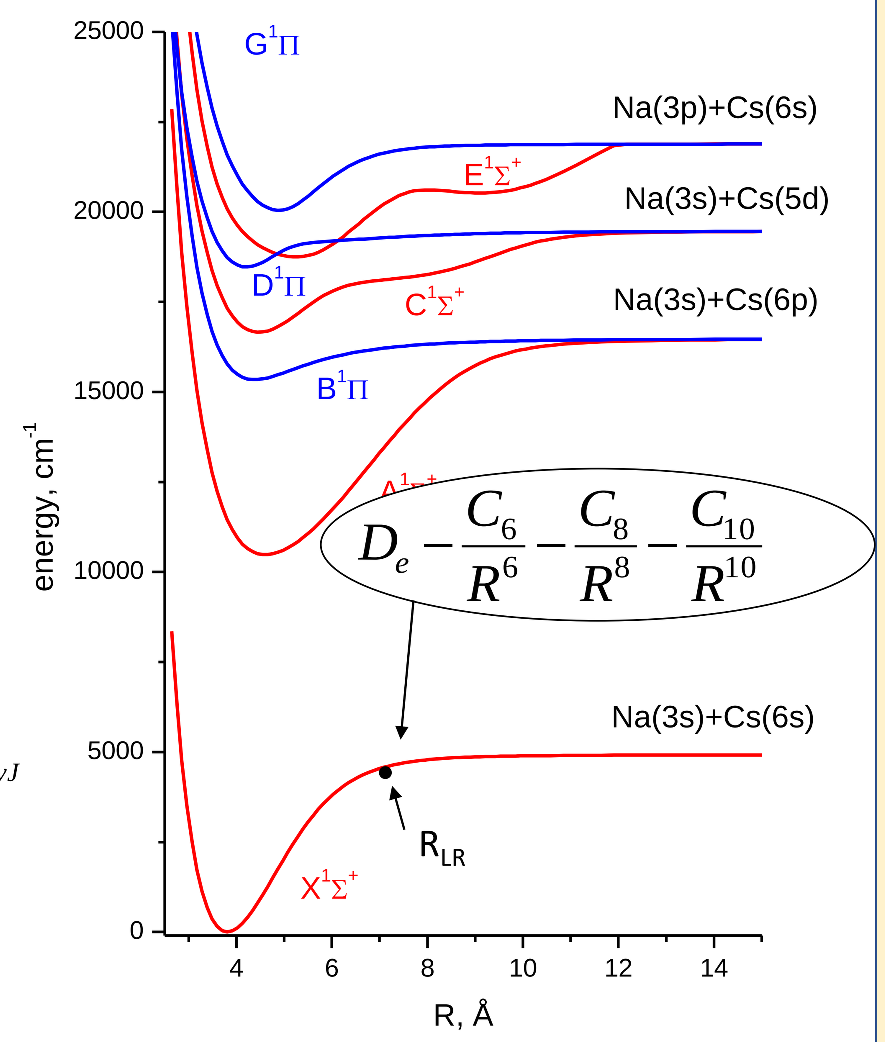
[2] *on leave from* Department of Physics, University "Aleksander Xhuvani" Elbasan, Albania

Born−Oppenheimer approximation
Adiabatic approximation

Radial Schrödinger equation

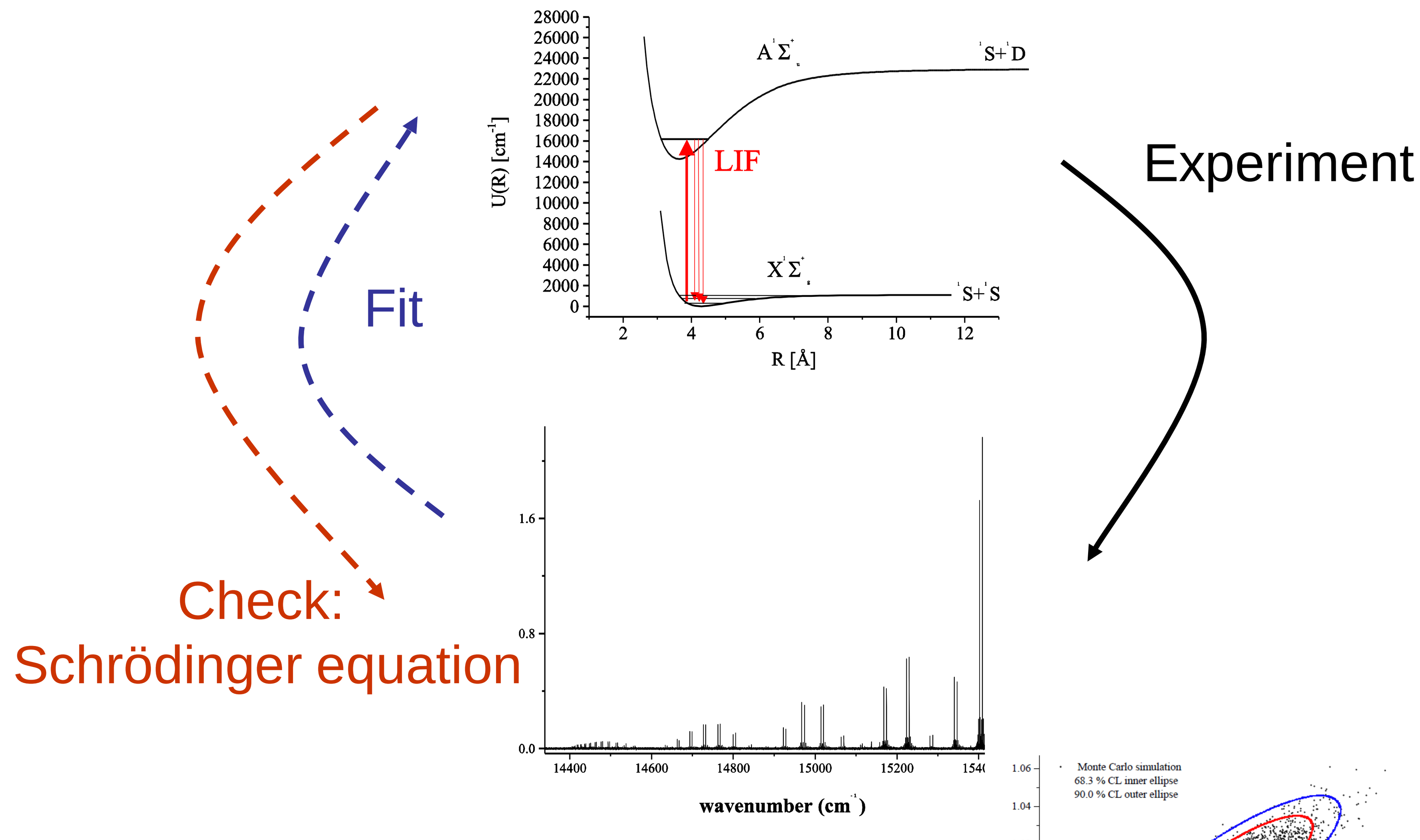
$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dR^2}+\frac{\hbar^2}{2mR^2}J(J+1)+U(R)\right]\Psi_{vJ}=E_{vJ}\Psi_{vJ}$$

No general model available!

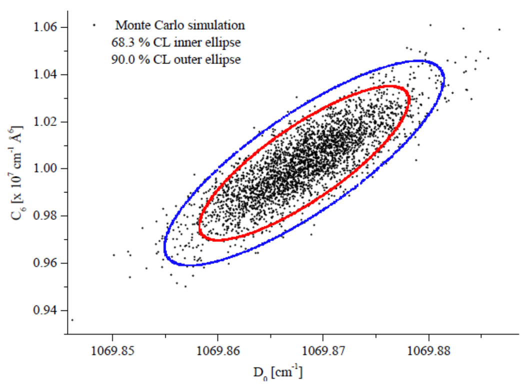


Korek et al. *Can. J. Phys.* **78**, 977 (2000)

Inverse Problem in spectroscopy



Example: Ca_2. Allard et al. Eur. Phys. J. D **26**, 155–164 (2003)
About 3600 transition frequencies.



Morse/Long-Range (MLR) potential

$$V_{\mathrm{MLR}}(r) = \mathfrak{D}_e\left(1 - \frac{u_{\mathrm{LR}}(r)}{u_{\mathrm{LR}}(r_e)}\, e^{-\beta(r)\cdot y_p^{\mathrm{eq}}(r)}\right)^2 \qquad \beta(r) = \beta_{\mathrm{MLR}}(r) = y_p^{\mathrm{ref}}(r)\,\beta_\infty + \left[1-y_p^{\mathrm{ref}}(r)\right]\sum_{i=0}\beta_i\left[y_q^{\mathrm{ref}}(r)\right]^i$$

$$V_{\mathrm{MLR}}(r) \simeq \mathfrak{D}_e - u_{\mathrm{LR}}(r) + \mathcal{O}\left(\frac{u_{\mathrm{LR}}^2}{4\,\mathfrak{D}_e}\right) \qquad u_{\mathrm{LR}} = \frac{C_{m_1}}{r^{m_1}} + \frac{C_{m_2}}{r^{m_2}} + \ldots \qquad \frac{r^p-(r_e)^p}{r^p+(r_e)^p} \equiv y_p^{\mathrm{eq}}(r)$$

R. J. Le Roy Chapter 6, pp. 159-203, of ***Equilibrium Structures of Molecules*****, J. Demaison and A. G. Csaszar editors, Taylor & Francis, London (2011).**

Simulations

We study the extrapolation properties of MLR

- MLR potentials fitted with various combination of R_{ref}, p and q.
- β_i, C_6, C_8, C_{10}, D_e – fitted.
- Experimental data limited to
  - $v_{max} \leq 25$,
  - $v_{max} \leq 30$,
  - $v_{max} \leq 35$,
  - $v_{max} \leq 38$.
- A total of 123 PEC fitted. Dimensionless standard deviation 0.62-0.67
- Present results show very good extrapolation properties of the MLR form.
- Original study (Allard. et al.) C6=(1.034±0.033)x 10^7 $cm^{-1}Å^6$, D0=(1069.868±0.010) cm^{-1}

1069.868(10)

Results