The variable phase method applied to collisions of ultra-cold atoms

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The variable phase method applied to collisions of ultra-cold atoms

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Work done at the Department of Computing Science, University of Glasgow, with Dr. Michael J. Jamieson

Note 1: the following slides were made for various past seminar presentations and put together here; they mostly deal with atomic collisions, but some of them presented in the appendix also show the calculation of 2D exciton wave functions in a screened Coulomb potential.

Note 2: beware of typos! Feedback, if any, is always welcome.

Overview

- notions of potential scattering theory
- little historical detour
- the variable phase method
  - auxiliary functions
  - phase equation
  - Levinson's theorem
- collisions of ultra-cold atoms
  - low-energy expansion: scattering parameters as solutions of Ricatti equations
  - molecular potentials
  - long-range behaviour and corrections to the numerical solutions
- concluding remarks and selection of publications
- appendix, and exciton wave function calculations

OVERVIEW OF SCATTERING THEORY

definitions

Assuming $V(R)$ to be a central potential, the scattering situation is described by a stationary wave function $\Psi(R)$ characterized by the asymptotic boundary condition:

$$\Psi(R) \sim e^{ikz} + f(\theta)\,\frac{e^{ikR}}{R}, \quad R \to \infty$$

$f(\theta)$ is the scattering amplitude and θ the scattering angle.

The differential cross section is defined by: $\dfrac{\mathrm{d}\sigma(\theta)}{\mathrm{d}\Omega} = |f(\theta)|^2$.

The scattering amplitude may be expressed as

$$f(\theta) = \frac{1}{k}\,\sum_{l=0}^{\infty}(2l+1)e^{i\delta_{k,l}}\sin[\delta_{k,l}]P_l(\cos\theta)$$

$P_l(\cos\theta)$ are the Legendre polynomials, $\delta_{k,l}$ is the scattering phase shift and $A_{k,l} = e^{i\delta_{k,l}}\sin[\delta_{k,l}]$ are the partial wave amplitudes.

OVERVIEW OF SCATTERING THEORY

use of the Schrödinger equation

$$\Psi(R) = \frac{1}{R} \sum_{l=0}^{\infty} \psi_l(R) P_l(\cos\theta)$$ (cylindrical symmetry)

where $\psi_l(R)$ satisfies:

$$\left[- \frac{\hbar^2}{2\mu} \frac{\mathrm{d}^2}{\mathrm{dR}^2} + \frac{l(l+1)\hbar^2}{2\mu R^2} + V(R) \right] \psi_l(R) = E\psi_l(R)$$

Behaviour at large $R \longrightarrow$ definition of the scattering phase shift $\delta_{k,l}$:

$$\psi_l(R) \sim \sin(kR - l\pi/2 + \delta_{k,l})$$

BUT with mod$[\pi]$ ambiguity in the definition of $\delta_{k,l}$.

The s-wave scattering length is

$$a_\mathrm{s} = - \lim_{k \to 0} \tan \delta_{k,0}/k$$

PHASE SHIFT CALCULATION

Morse and Allis, Physical Review 44, 269 (1933)

- Scattering of slow electrons from atoms
- Definition of the phase function $\mu(r)$
- $-k\mathrm{d}\mu/\mathrm{d}r = V(r)\sin^2(kr+\mu)$

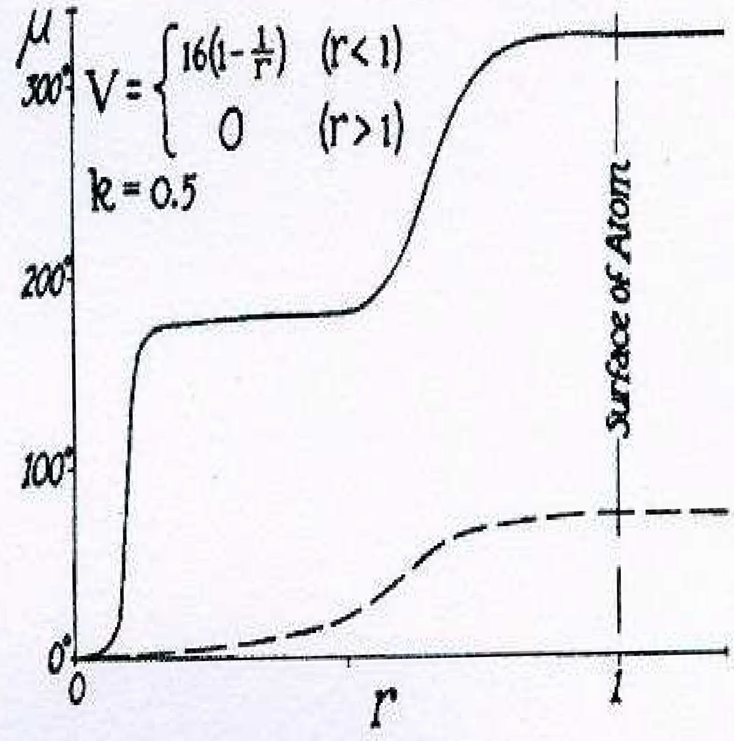


FIG. 1. Phase function $\mu(r)$ for a simple form of potential field. Solid line gives exact solution, dotted line gives corresponding Born approximation.

DIFFERENTIAL ANALYZER

Figure 1: Differential analyzer operated by 3 ladies at the Moore school of Electrical Engineering, University of Pennsylvania, circa 1942 (see wikipedia).

VARIABLE PHASE METHOD

definitions of auxiliary functions

$$\Psi(R) = \frac{1}{R} \sum_{l=0}^{\infty} \psi_l(R) P_l(\cos\theta)$$

and

$$\psi_l(R) = \hat{j}_l(R) - k^{-1} \int_0^R \mathrm{d}R' \left[\hat{j}_l(kR)\hat{n}_l(kR') - \hat{j}_l(kR')\hat{n}_l(kR)\right] V(R')\psi_l(R')$$

Auxilliary functions are defined as

$$s_l = -k^{-1}\int_0^R \mathrm{d}R'\, V(R')\hat{j}_l(kR')\psi_l(R'),\; c_l = 1 - k^{-1}\int_0^R \mathrm{d}R'\, V(R')\hat{n}_l(kR')\psi_l(R')$$

$$\psi_l(R) \sim_{R\to\infty} s_l(\infty)\cos(kR - l\pi/2) + c_l(\infty)\sin(kR - l\pi/2)$$

$\Rightarrow \quad \tan\delta_{k,l} = s_l(\infty)/c_l(\infty),\;\; \delta_{k,l}$ is the scattering phase shift

VARIABLE PHASE METHOD

phase equation

Definition: $t_l(R) = s_l(R)/c_l(R)$ such that $\lim_{R\to\infty} t_l(R) = \tan\delta_{k,l}$ and

$$\frac{\mathrm{d}}{\mathrm{d}R}\, t_l(R) = -k^{-1}V(R)\left[\hat{j}_l(kR) - t_l(R)\hat{n}_l(kR)\right]^2$$

Introducing the *phase function* $\delta_{k,l}(R)$ as $t_l(R) = \tan\delta_{k,l}(R)$ and inserting it in the equation above yields the *phase equation*

$$\frac{\mathrm{d}}{\mathrm{d}R}\,\delta_{k,l}(R) = -k^{-1}V(R)\left[\cos\delta_{k,l}(R)\hat{j}_l(kR) - \sin\delta_{k,l}(R)\hat{n}_l(kR)\right]^2$$

It is a first order non-linear equation of the Riccati type.

In the case of s-waves, $l = 0$:

$$\frac{\mathrm{d}}{\mathrm{d}R}\,\delta_{k,0}(R) = -k^{-1}V(R)\sin^2\left[kR + \delta_{k,0}(R)\right]$$

VARIABLE PHASE METHOD

number of bound states

Knowledge of the s-wave phase shift, $\delta_{k,0}$, solution of the phase equation for $R \to \infty$

$$\frac{\mathrm{d}}{\mathrm{d}R}\,\delta_{k,0}(R) = -k^{-1}V(R)\sin^2\left[kR + \delta_{k,0}(R)\right]$$

yields *directly* the number of bound states supported by the potential $V(R)$, via Levinson's theorem:

$$N_{\mathrm{b}} = \frac{1}{\pi}\lim_{k\to 0}\delta_{k,0}$$

VARIABLE PHASE METHOD

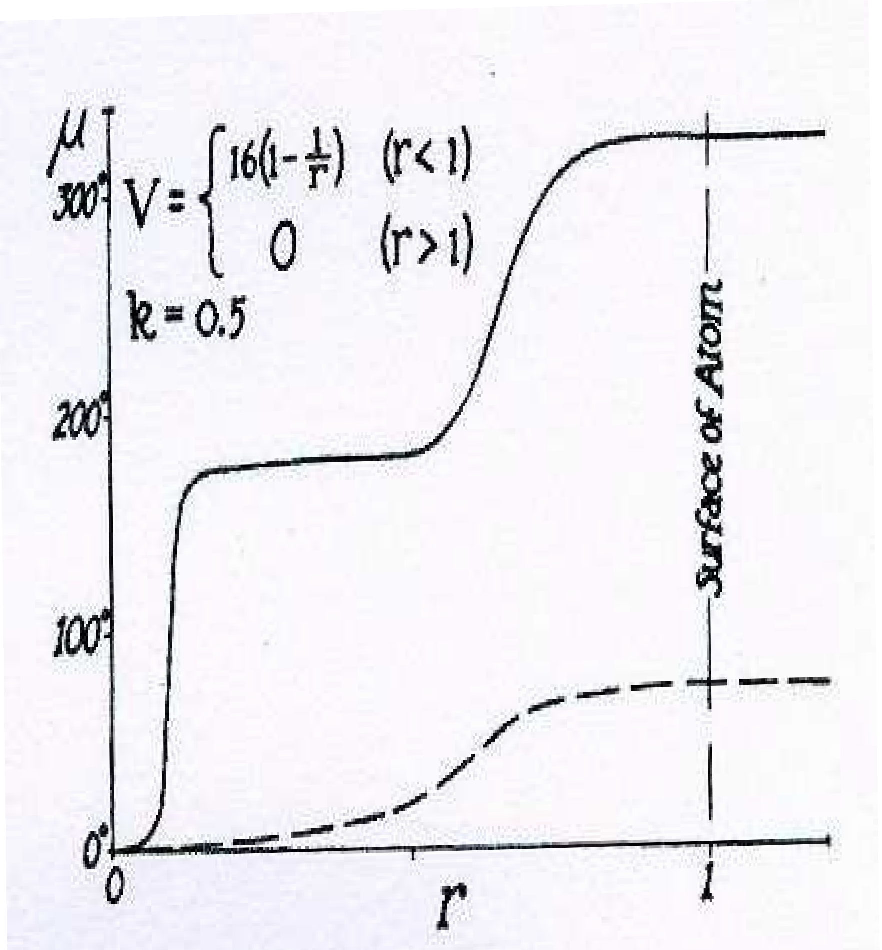
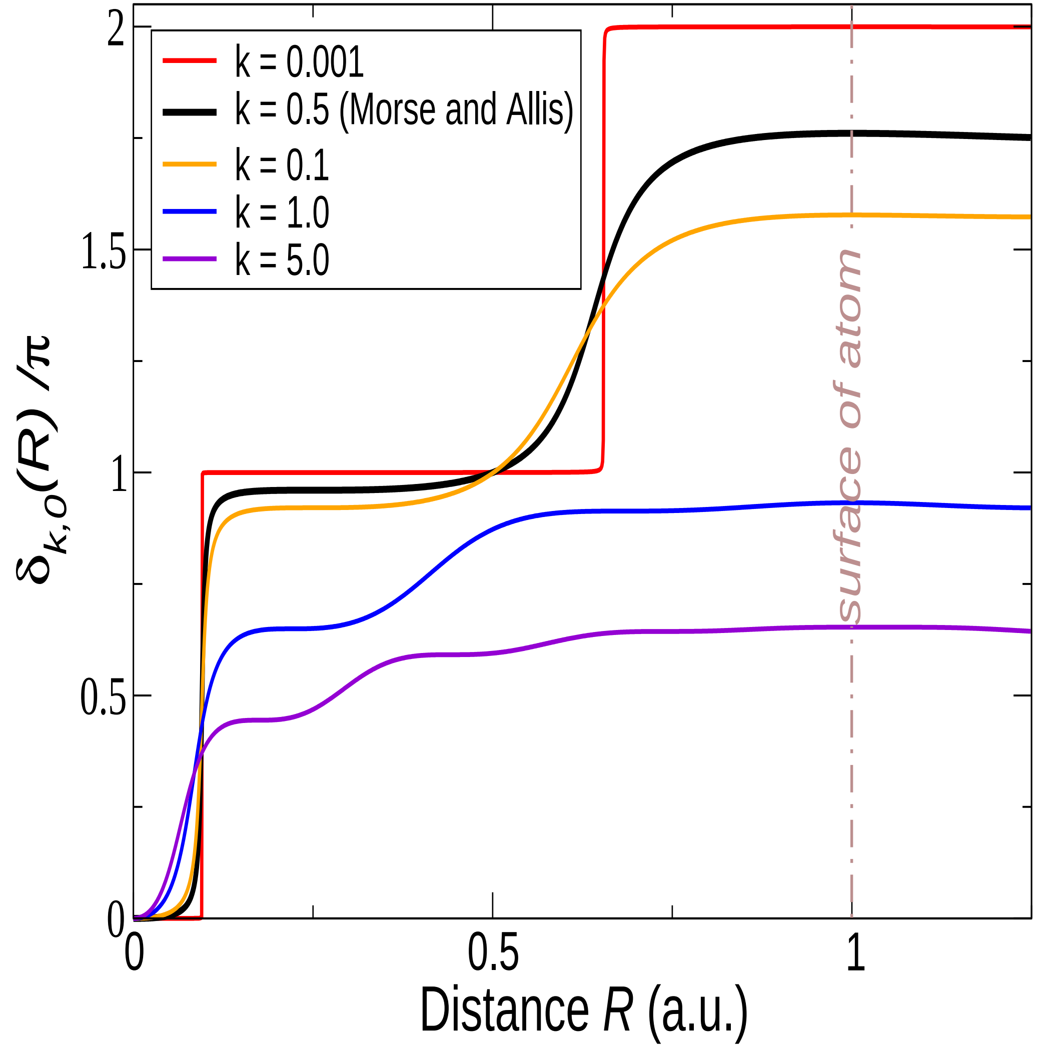


FIG. 1. Phase function $\mu(r)$ for a simple form of potential field. Solid line gives exact solution, dotted line gives corresponding Born approximation.



Application to

ultra-cold collisions of alkali atoms

(computation of the scattering length).

ULTRA-COLD ATOMIC COLLISIONS

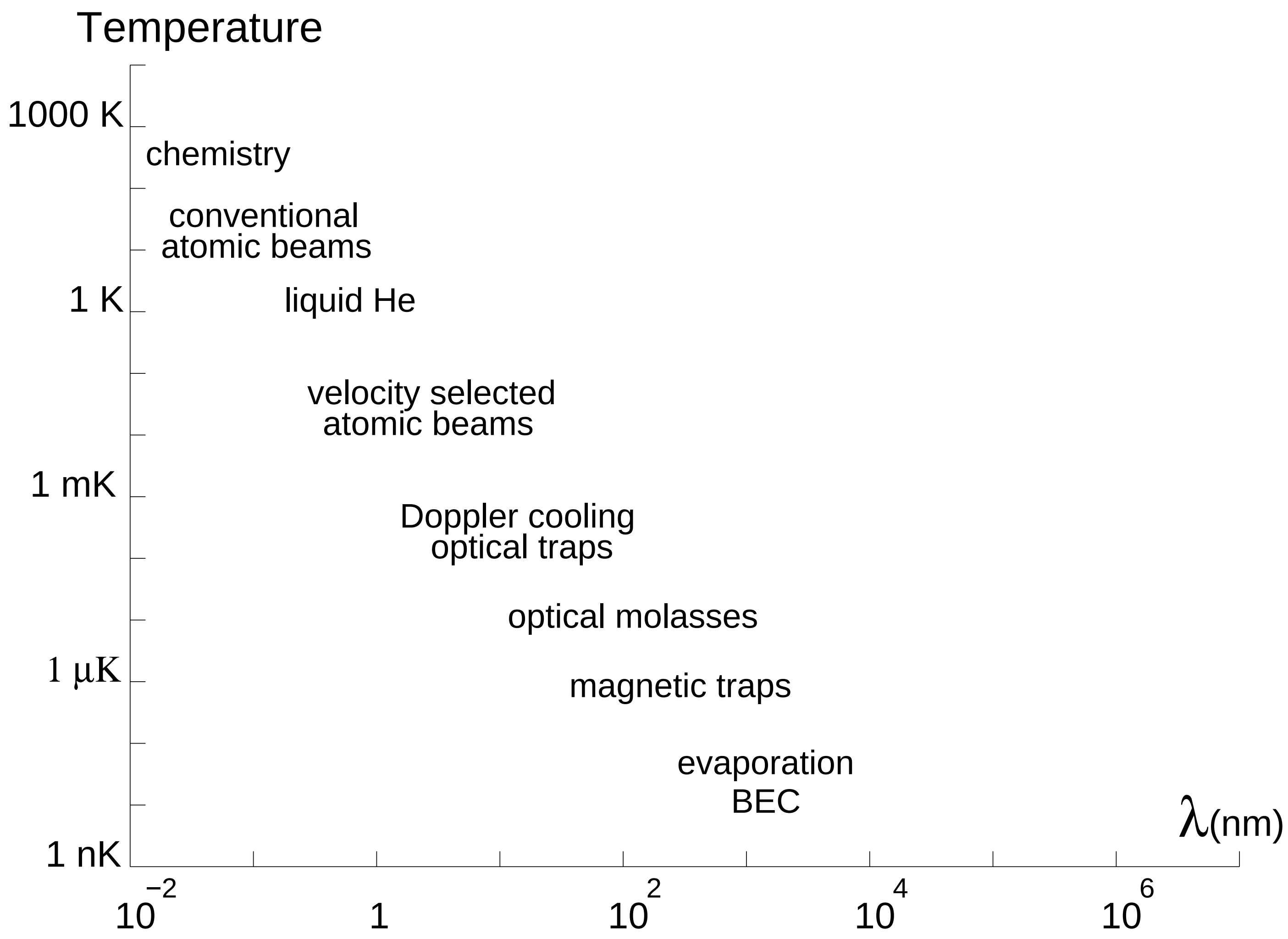


Figure 2: Temperature regimes vs de Broglie wavelength. Adapted from J. Weiner *et al*, Rev. Mod. Phys. **71**, 1 (1999).

ULTRA-COLD ATOMIC COLLISIONS

low energy expansion - scattering parameters

$\longrightarrow$ low energy expansion $k \to 0$

$$t_l(R) \sim k^{2l+1} \left[a_l(R) + k^2 b_l(R) + \mathcal{O}(k^4) \right]$$

$\longrightarrow$ Riccati equation for the scattering length, $l = 0$

$$\frac{\mathrm{d}a_0(R)}{\mathrm{d}R} = \left[R - a_0(R) \right]^2 V(R)$$

$\longrightarrow$ Riccati equation for the scattering volume, $l = 1$

$$\frac{\mathrm{d}a_1(R)}{\mathrm{d}R} = \left[\frac{R^3}{3} - a_1(R) \right]^2 R^{-2} V(R)$$

MOLECULAR POTENTIALS

- Short range potential: *ab initio* calculations or experimental data.

- Long range potential:

  – exchange energy $V_X(R)$ given by Smirnov and Chibisov

$$V_X(R) = \pm J_{A,B,\alpha,\beta}(R) \times R^{\frac{2}{\alpha}+\frac{2}{\beta}-\frac{1}{\alpha+\beta}-1} \exp^{-(\alpha+\beta)R}$$

  – Van der Waals dispersion $V_d(R)$

$$V_d(R) = -C_6 R^{-6} - C_8 R^{-8} - C_{10} R^{-10}$$

NUMERICAL METHODS
change of variables

$$a_l(R) = \tan\theta(R) \quad \text{and} \quad R = \tan\phi(R)$$

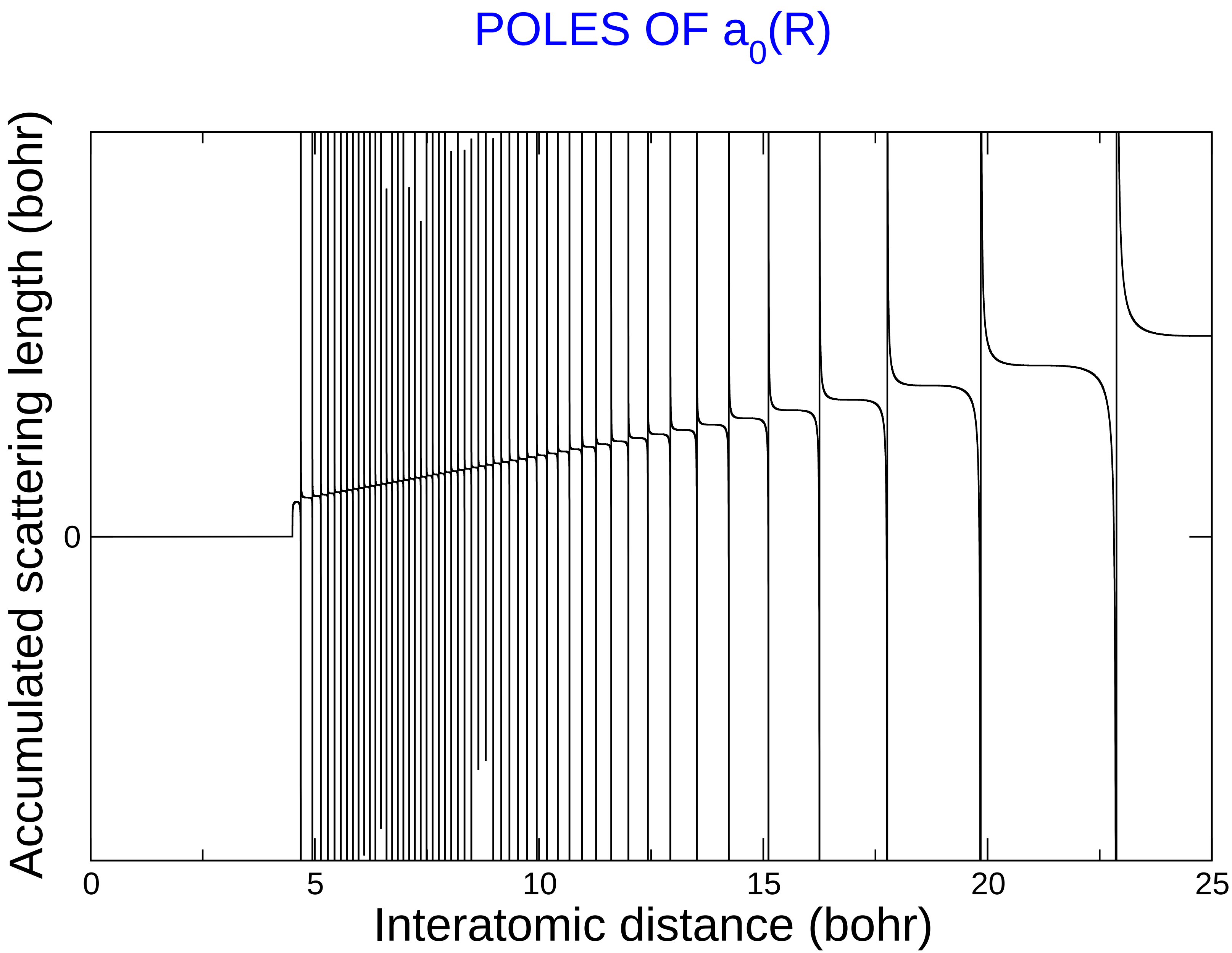
The Riccati equation for the scattering length becomes

$$\frac{\mathrm{d}\theta(\phi)}{\mathrm{d}\phi} = \sec^4\phi\,\sin^2\left[\theta(\phi) - \phi\right] V[\tan(\phi)]$$

The Riccati equation for the scattering volume becomes

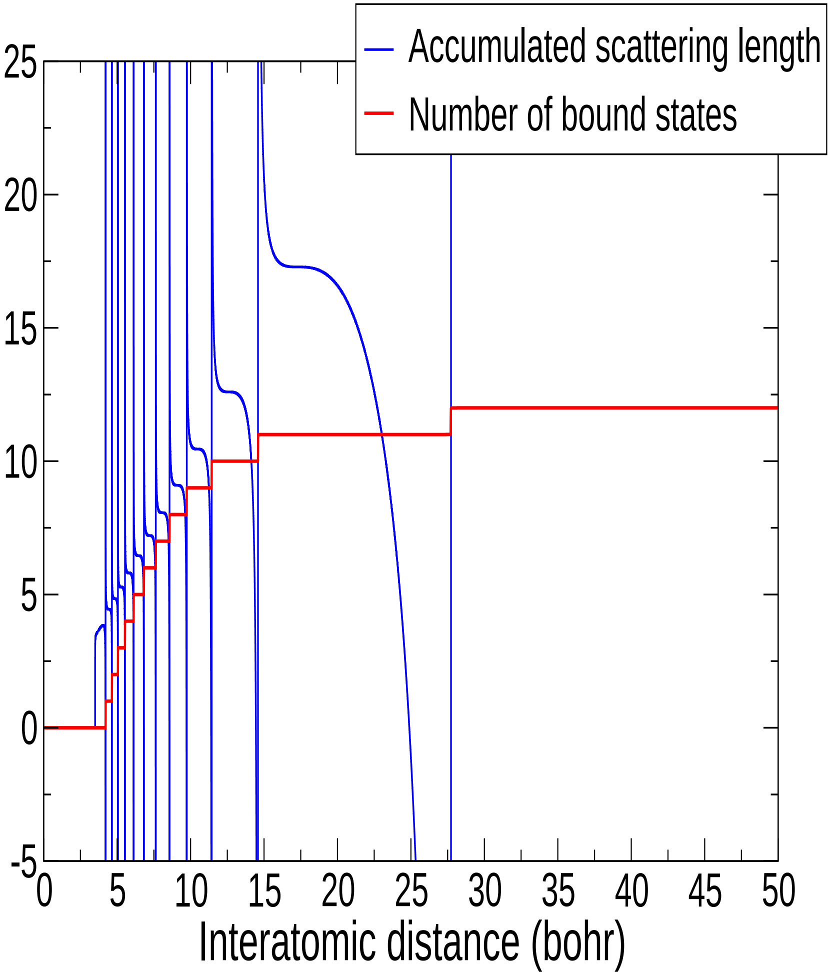
$$\frac{\mathrm{d}\theta(\phi)}{\mathrm{d}\phi} = \frac{\cos^2\theta}{\sin^2\phi}\left[\frac{\tan^3\phi}{3} - \tan\theta\right]^2 V[\tan\phi]$$

solved by the Runge-Kutta method over a range $[0, \phi_c]$, with $\phi_c \to \pi/2$.

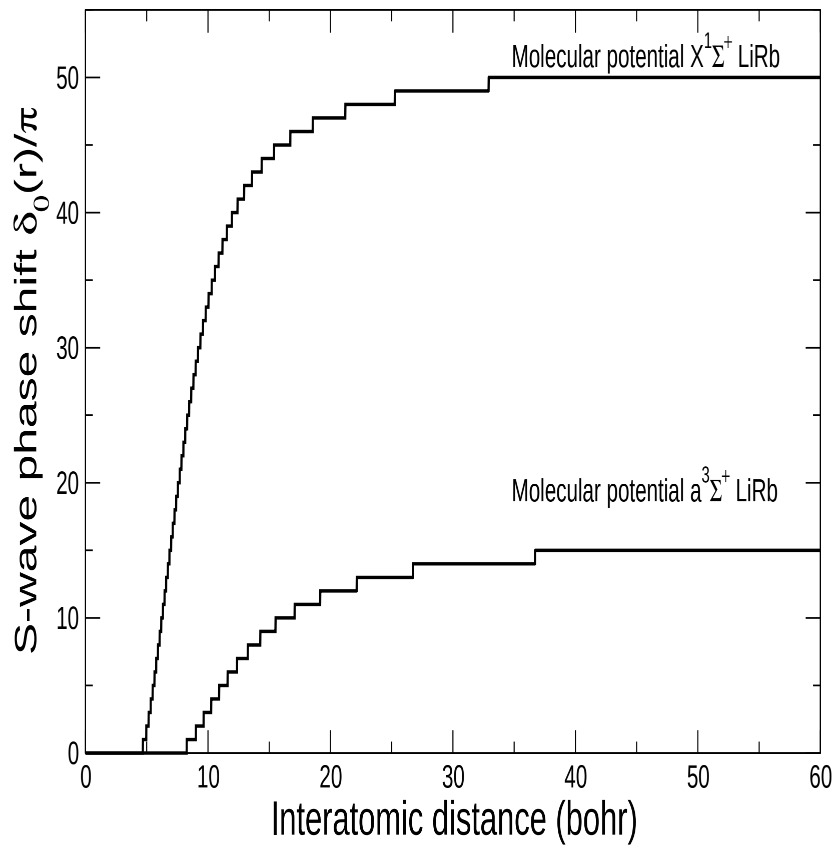


POLES OF a0(R)
Accumulated scattering length (bohr)
0
Interatomic distance (bohr)
0
5
10
15
20
25

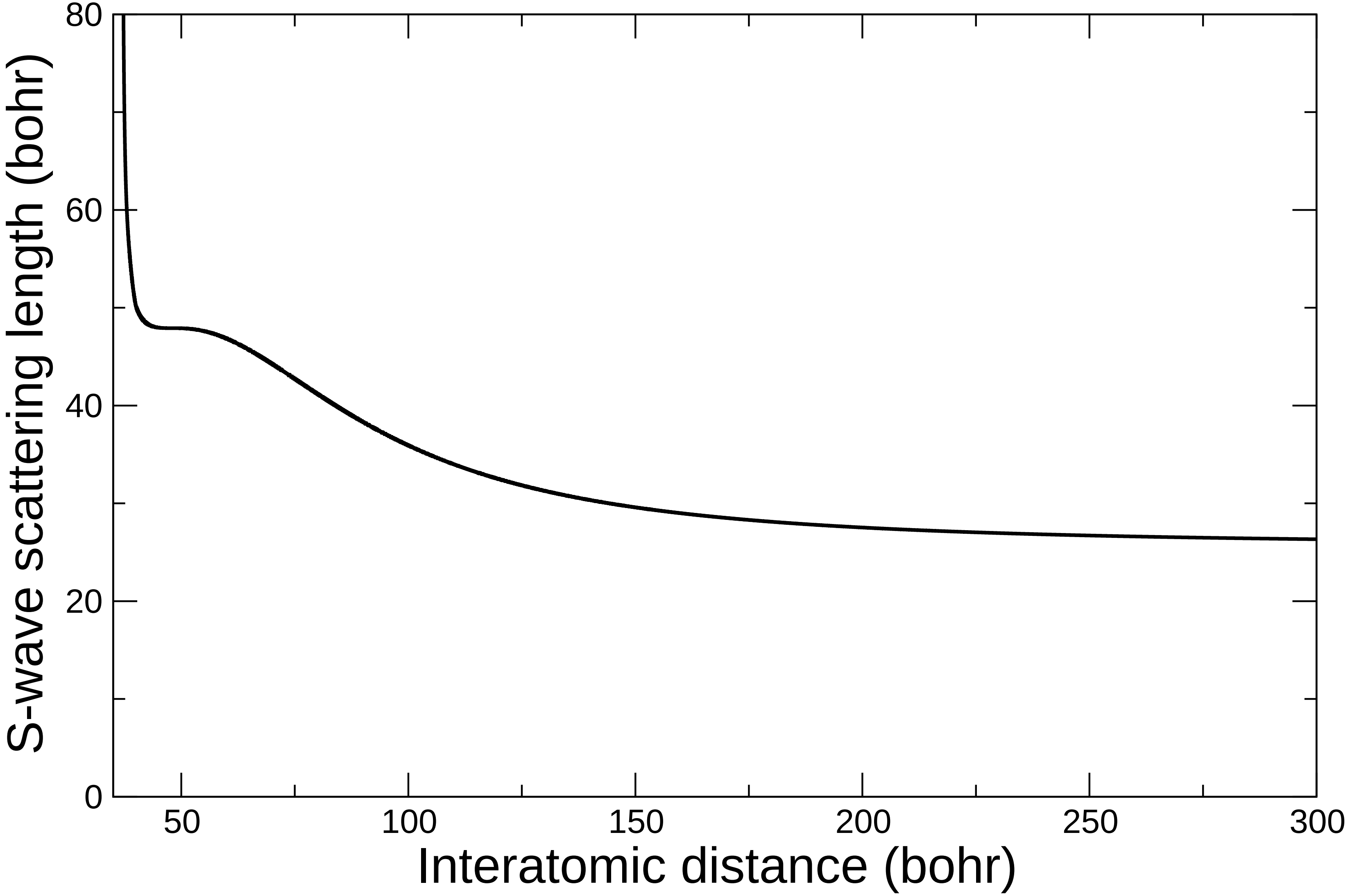
BOUND STATES



LEVINSON'S THEOREM



LONG RANGE BEHAVIOUR OF $a_0(R)$



CORRECTIONS TO THE SCATTERING PARAMETERS

The Riccati equation for the scattering parameters is

$$\frac{\mathrm{d}}{\mathrm{d}R}\, a_l(R) = \left[\alpha_l^{(+)} R^{l+1} - \alpha_l^{(-)} R^{-l} a_l(R)\right]^2 V(R)$$

It can be recast as

$$a_l(\infty) = \int_0^{R_\mathrm{c}} \left[\alpha_l^{(+)} R^{l+1} - \alpha_l^{(-)} R^{-l} a(R)\right]^2 V(R)\mathrm{d}R + \int_{R_\mathrm{c}}^{\infty} \left[\alpha_l^{(+)} R^{l+1} - \alpha_l^{(-)} R^{-l} a(R)\right]^2 V(R)\mathrm{d}R$$

The scattering parameters may then be written as

$$a_l(\infty) = a_{l,\mathrm{c}} + E_\mathrm{c}^{(1)} + E_\mathrm{c}^{(2)} + \ldots$$

where $a_{l,\mathrm{c}} = a_l(R_\mathrm{c})$.

CORRECTIONS TO THE SCATTERING PARAMETERS

first order correction

$$E_\mathrm{c} = E_\mathrm{c}^{(1)} + 2\int_{R_\mathrm{c}}^{\infty} \left[B_l R^{2l+1} - a_l(R)\right]^2 A_l R^{-2l} V(R) \times \left\{\left[B_l R^{2l+1} - a_l(R)\right] W_l(R) - X_l(R)\right\} \mathrm{d}R$$

where $E_\mathrm{c}^{(1)}$ is the first order correction

$$E_\mathrm{c}^{(1)} = -(B_l R_\mathrm{c}^{2l+1} - a_{l,\mathrm{c}})^2 W_{l,\mathrm{c}} + 2(B_l R_\mathrm{c}^{2l+1} - a_{l,\mathrm{c}}) X_{l,\mathrm{c}} - 2Y_{l,\mathrm{c}}$$

and

$$W_l(R) = \int^R A_l R^{-2l} V(R) \mathrm{d}R, \;\; X_l(R) = \int^R (2l+1) B_l R^{2l} W(R) \mathrm{d}R, \;\; Y_l(R) = \int^R (2l+1) B_l R^{2l} X(R) \mathrm{d}R$$

Assuming an attractive potential

$$a_l(\infty) = a_{l,\mathrm{c}} + E_\mathrm{c} < a_\mathrm{c} + E_\mathrm{c}^{(1)} = a^{(\mathrm{U})}$$

CORRECTIONS TO THE SCATTERING PARAMETERS

higher order correction

$$\mathcal{E}_{\rm c} = 2\int_{R_{\rm c}}^{\infty} \left[B_l R^{2l+1} - a_l(R)\right]^2 A_l R^{-2l} V(R) \times \left\{\left[B_l R^{2l+1} - a_l(R)\right] W_l(R) - X_l(R)\right\} \mathrm{d}R$$

Integrating by parts leads to

$$\mathcal{E}_{\rm c} = E_{\rm c}^{(2)} + \text{higher order terms}$$

where

$$E_{\rm c}^{(2)} = -(B_l R_{\rm c}^{2l+1} - a_{l,{\rm c}})^3 W_{l,{\rm c}}^2 + 2X_{l,{\rm c}}Y_{l,{\rm c}} + 3(B_l R_{\rm c}^{2l+1} - a_{l,{\rm c}})^2 W_{l,{\rm c}} X_{l,{\rm c}}$$

$$- 2(B_l R_{\rm c}^{2l+1} - a_{l,{\rm c}})(X_{l,{\rm c}}^2 + W_{l,{\rm c}} Y_{l,{\rm c}})$$

takes account of some of the second order terms.

$$\mathcal{E}_{\rm c} > E_{\rm c}^{(2)} \quad \longrightarrow \quad a > a_{\rm c} + E_{\rm c}^{(1)} + E_{\rm c}^{(2)} = a^{(\rm L)}$$

CORRECTIONS TO THE SCATTERING PARAMETERS

inverse powers series potential

The asymptotic potential has the form

$$V_{\mathrm{d}}(R) = -C_6 R^{-6} - C_8 R^{-8} - C_{10} R^{-10}$$

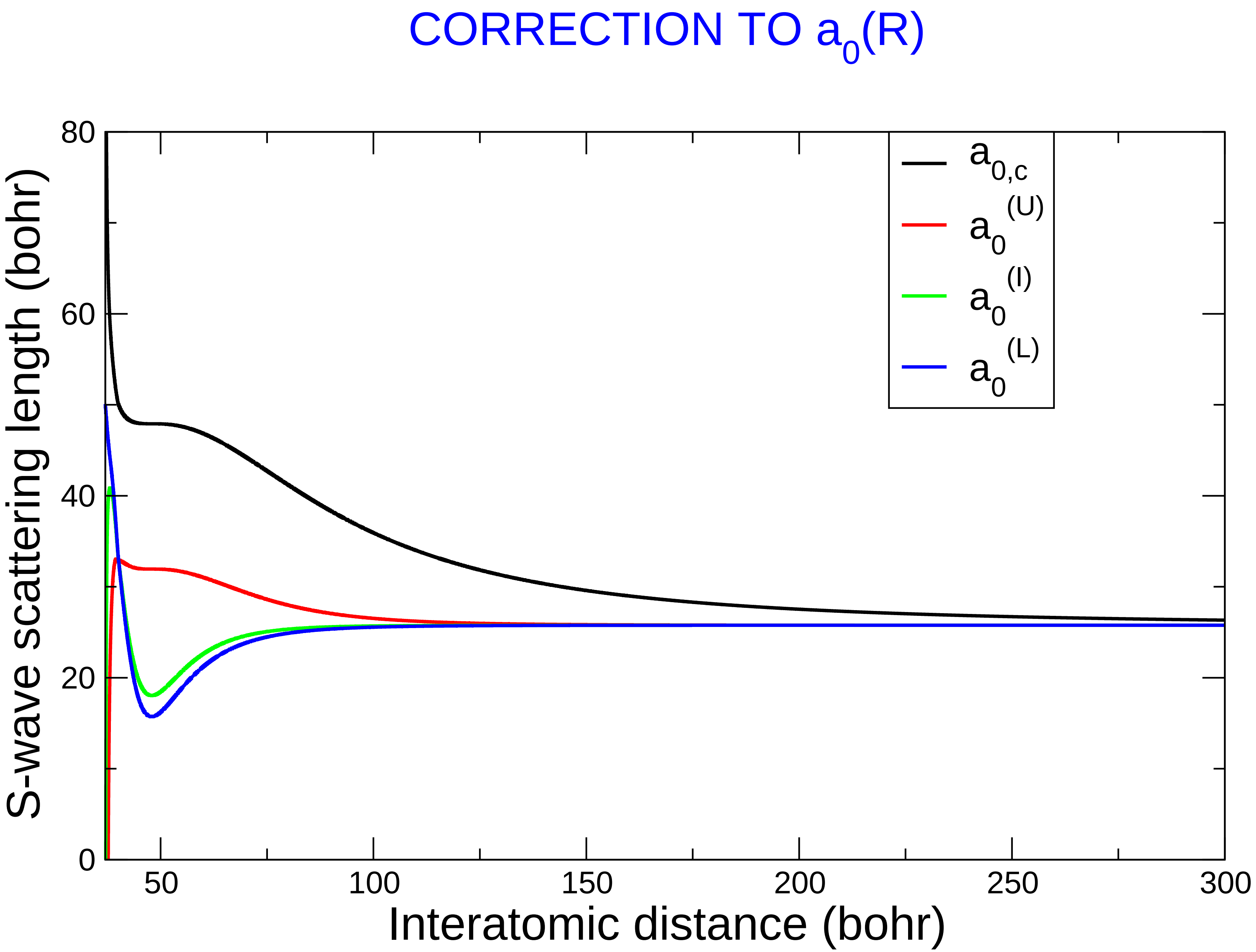
The corrections to $a_0^{(\mathrm{U})}$ and $a_0^{(\mathrm{L})}$ are asymptotically

$$\tilde{\mathcal{E}}_0^{(U)} = -2 \frac{\tilde{\alpha}_n^{2n-4}}{(n-2)(2n-5)} \text{ and } \tilde{\mathcal{E}}_0^{(\mathrm{L})} = \frac{\tilde{\alpha}_n^{2n-4}}{(n-2)(n-3)(2n-5)} = -\frac{\tilde{\mathcal{E}}^{(\mathrm{U})}}{2(n-3)}$$

So that

$$a_0' = \frac{a_0^{(\mathrm{U})} + 2(n-3) a_0^{(\mathrm{L})}}{2n-5}$$

The quantity $\alpha_n = \left[2\mu C_n / \hbar^2\right]^{1/(n-2)}$ is a length characteristic of the potential (scaled to R_c).


CORRECTION TO $a_0(R)$
S-wave scattering length (bohr)
Interatomic distance (bohr)
$a_{0,c}$
$a_0^{(U)}$
$a_0^{(I)}$
$a_0^{(L)}$
0
20
40
60
80
50
100
150
200
250
300

CONCLUDING REMARKS

- ◇ scattering parameters are found as solutions of the Riccati type equations in the asymptotic region.
- ◇ the scattering phase shift is found unambiguously.
- ◇ the variable phase method is very effective for the calculations of low-energy scattering phase shifts.
- ◇ the number of bound states is given by the simplest formulation of Levinson's theorem.
- ◇ Riccati equations are readily employed to derive corrections arising from long range interactions.
- ◇ the variable phase method has been succesfully applied to a wide variety of problems: multichannel scattering, scattering on nonlocal potentials, complex potentials etc . . .

PUBLICATIONS RELATED TO COLD COLLISIONS AND VPM

1. M. J. Jamieson, H. Sarbazi-Azad, **H.Ouerdane**, G.-H. Jeung, Y. S. Lee and W. C. Lee, *Elastic scattering of cold rubidium and caesium atoms*. **Journal of Physics B**: Atomic, Molecular and Optical Physics **36**,1085 (2003).

2. **H. Ouerdane**, M. J. Jamieson, D. Vrinceanu et M. J. Cavagnero, *The variable phase method used to calculate and correct scattering lengths*. **Journal of Physics B**: At. Mol. and Opt. Phys. vol. **36**, 4055 (2003).

3. **H. Ouerdane**, M. J. Jamieson, *Scattering parameters for ultra-cold alkali atoms derived from variable phase theory*. **Physical Review A** vol. **70**, 022712 (2004).

4. **H. Ouerdane**, M. J. Jamieson, *A note on the calculation of the effective range*. **Journal of Physics B**: At. Mol. and Opt. Phys. vol. **37**, 3765 (2004)

5. M. J. Jamieson, A. S.-C. Cheung, **H. Ouerdane**, G.-H. Jeung and N. Geum, *S-wave scattering lengths and effective ranges for collisions of ground state Be atoms*, **Journal of Physics B**: Atomic, Molecular and Optical Physics vol. **40**, 3497 (2007).

6. **H. Ouerdane**, M. J. Jamieson, *S-wave and p-wave scattering in a cold gas of Na and Rb atoms*. **The European Physical Journal D 53**, 27 (2009).

7. M. J. Jamieson, A. S.-C. Cheung, and **H. Ouerdane**, *Dependence of the scattering length for hydrogen atoms on effective mass*. **The European Physical Journal D 56**, 181 (2010).

PUBLICATIONS RELATED TO COLD COLLISIONS AND VPM

8. **H. Ouerdane** and M. J. Jamieson, *Comment on "Scattering length for fermionic atoms"*. **The European Physical Journal D 57**, 325 (2010).

9. M. J. Jamieson and **H. Ouerdane**, *Error cancellation in the semiclassical calculation of the scattering length*. **The European Physical Journal D 61**, 373 (2011).

10. M. J. Jamieson and **H. Ouerdane**, *Parameters for cold collisions of lithium and caesium atoms*. **Chinese Physics Letters 28**, 060308 (2011).

Publications related to VPM in semiconductor physics

1. P. Bogdanski and **H. Ouerdane**, *Scattering states of coupled valence bands holes in point defect potential derived from variable phase theory*. **Physical Review B** vol. **74**, 085210 (2006).

2. **H. Ouerdane**, R. Varache, M. E. Portnoi and I. Galbraith, *Photon emission induced by elastic exciton−carrier scattering in semiconductor quantum wells*. **European Physical Journal B** vol. **65**, 195 (2008).

3. P. Bogdanski and **H. Ouerdane**, *Coulomb singularities in scattering wave functions of spin-orbit-coupled states.* **Journal of Mathematical Physics 52**, *073515 (2010).*

SOME PUBLICATIONS RELATED TO VPM BY OTHER AUTHORS

— M. E. Portnoi and I. Galbraith, *Variable phase method and Levinson's theorem in two dimensions: application to a screened Coulomb potential*. **Solid State Communications** vol. **103**, 325 (1997).

— M. E. Portnoi and I. Galbraith, *Levinson's theorem and scattering phase shift contributions to the partition function of interacting gases in two dimensions*. **Physical Review B** vol. **58**, 3963 (1998).

— M. E. Portnoi and I. Galbraith, *Ionization degree of the electron-hole plasma in semiconductor quantum wells*. **Physical Review B** vol. **60**, 5570 (1999).

— D. A. Stone, C. A. Downing, and M. E. Portnoi, *Searching for confined modes in graphene channels: The variable phase method*, **Physical Review B** vol. **86**, 075464 (2012).

— C. A. Downing, A. R. Pearce, R. J. Churchill, M. E. Portnoi, *Optimal traps in graphene*, **Phys. Rev. B** vol. **92**, 165401 (2015).

“THE” REFERENCE

F. Calogero

Variable Phase Approach to Potential Scattering

(Academic Press, New York, 1967).

OTHER EXCELLENT REFERENCE ON SCATTERING THEORY

J. R. Taylor

SCATTERING THEORY

The quantum theory of nonrelativistic collisions

(Dover Publications Inc., Mineola, New York, 2006).

My heartfelt thanks go to

Dr. Michael J. Jamieson

APPENDIX 1

Additional definitions and calculation details

RICCATI EQUATIONS
definition

Consider the *first order* differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x,y)$$

To solve the above equation, $f(x,y)$ may be expressed as the expansion

$$f(x,y) = P(x) + Q(x)y + R(x)y^2 + \ldots$$

for a given x. Riccati studied the approximation to the second degree:

$$\frac{\mathrm{d}y}{\mathrm{d}x} = P(x) + Q(x)y + R(x)y^2$$

The above equation is a Riccati equation . It is a *first-order* and *non-linear* differential equation.

VARIABLE PHASE METHOD

amplitude equation

An *amplitude function* $\alpha_l(r)$ is introduced as:

$$\psi_l(R) = \alpha_l(R)\left[\cos\delta_{k,l}(R)\hat{j}_l(kR) - \sin\delta_{k,l}(R)\hat{n}_l(kR)\right]$$

Lengthy algebra yields the *amplitude equation*

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}R}\,\alpha_l(R) &= -k^{-1}\alpha_l(R)V(R)\left[\cos\delta_{k,l}(R)\hat{j}_l(kR) - \sin\delta_{k,l}(R)\hat{n}_l(kR)\right] \\ &\quad \times\left[\sin\delta_{k,l}(R)\hat{j}_l(kR) + \cos\delta_{k,l}(R)\hat{n}_l(kR)\right] \end{aligned}$$

VARIABLE PHASE METHOD

bound states calculations

Bound states have negative energy $\Longrightarrow k = i\kappa,\ \kappa > 0$.

Bound states are given by the poles of the S matrix function:

$$S_l(\kappa, R) = 2\kappa A_l(\kappa, R) - 1$$

In the case of s-waves, $l = 0$:

$$A_0(\kappa, R) \propto \tan \eta_0(\kappa, R)$$

$$\Longrightarrow \text{bound states} \Longleftrightarrow \begin{cases} \lim_{R\to\infty} \eta_0(\kappa, R) = (2n+1)\frac{\pi}{2} \\[2ex] \dfrac{\mathrm{d}\eta_0(\kappa, R)}{\mathrm{d}R} = -RV(R)\left(\cos \eta_0(\kappa, R) + \sin \eta_0(\kappa, R)\right)^2 \end{cases}$$

NUMERICAL METHODS
log-derivative method

Substituting

$$w(R) = [R - a(R)]^{-1}$$

the Riccati equation for the scattering length becomes

$$\frac{\mathrm{d}w(R)}{\mathrm{d}R} + w^2(R) - V(R) = 0$$

the Riccati equation for the log-derivative of the radial wave function at zero energy. The evaluation is done with the propagator

$$\left[1 - hw(R+h) + \frac{1}{3}\,h^2V(R+h)\right]^{-1} + \left[1 + hw(R-h) + \frac{1}{3}\,h^2V(R-h)\right]^{-1}$$

$$= 2\left[1 - \frac{1}{6}\,h^2V(R)\right]^{-1}\left[1 + \frac{1}{2}\,h^2V(R)\right]$$

with the initial condition that $w(0)$ is very large, and h is the step length.

APPENDIX 2

Exciton wave functions in

two-dimensional screened Coulomb potential

2D EXCITON WAVE FUNCTIONS

→ Thomas-Fermi attractive 2D screened Coulomb potential:

$$V_s(\rho) = -\frac{e^2}{\epsilon}\int_0^\infty \frac{qJ_0(q\rho)}{q+q_s}\,\mathrm{d}q = -\frac{e^2}{\epsilon}\left\{\frac{1}{\rho} - \frac{\pi}{2}\,\left[\mathbf{H}_0(q_s\rho) - N_0(q_s\rho)\right]\right\}$$

N_0 and $\mathbf{H}_0$ are the Neumann and Struve functions respectively.

→ "Electron-hole" part of the partition function:

$$Z_{\text{int}} = \sum_m \sum_\nu e^{-\beta E_{m,\nu}} + \frac{1}{\pi}\int_0^\infty \left(\sum_{m=-\infty}^{\infty} \frac{\mathrm{d}}{\mathrm{d}q}\,\delta_m(q)\right)\, e^{-q^2/q_T^2}\mathrm{d}q$$

which is the 2D analog of the Bethe-Uhlenbeck formula.

2D EXCITON WAVE FUNCTIONS

The Schrödinger equation for the radial wavefunction of the relative motion:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \frac{1}{\rho}\frac{\mathrm{d}}{\mathrm{d}\rho} + k^2 - U(\rho) - \frac{m^2}{\rho^2}\right] R_{m,\kappa}(\rho) = 0 \text{ with } U(\rho) = 2m_\mathrm{r} V_\mathrm{s}(\rho)/\hbar^2$$

$$\rightarrow k^2 = -\kappa^2 = 2m_\mathrm{r} E/\hbar^2 < 0$$

$$R_{m,\kappa}(\rho) = A_m \left(I_m(\kappa\rho)\cos\eta_m + \frac{2}{\pi} K_m(\kappa\rho)\sin\eta_m \right)$$

$I_m(\kappa\rho)$ and $K_m(\kappa\rho)$: modified Bessel functions of the 1st and 2nd kinds.

$$\rightarrow k^2 = 2m_\mathrm{r} E/\hbar^2 > 0$$

$$R_{m,\kappa}(\rho) = A_m \left(J_m(\kappa\rho)\cos\delta_m - N_m(\kappa\rho)\sin\delta_m \right)$$

$J_m(\kappa\rho)$ and $N_m(\kappa\rho)$: Bessel and Neumann functions.

2D EXCITON WAVEFUNCTIONS

scattering states

Phase equation:

$$\frac{\mathrm{d}}{\mathrm{d}\rho}\,\delta_{m,k}(\rho) = -\frac{\pi}{2}\,\rho\,U(\rho) \times \left(J_m(k\rho)\cos\delta_{m,k}(\rho) - N_m(k\rho)\sin\delta_{m,k}(\rho)\right)^2$$

Amplitude:

$$\frac{\mathrm{d}}{\mathrm{d}\rho}\,A_{m,k}(\rho) = A_{m,k}(\rho)\,\frac{J_m(k\rho)\sin\delta_{m,k}(\rho) + N_m(k\rho)\cos\delta_{m,k}(\rho)}{J_m(k\rho)\cos\delta_{m,k}(\rho) - N_m(k\rho)\sin\delta_{m,k}(\rho)} \times \frac{\mathrm{d}}{\mathrm{d}\rho}\,\delta_{m,k}(\rho)$$

2D EXCITON WAVE FUNCTIONS

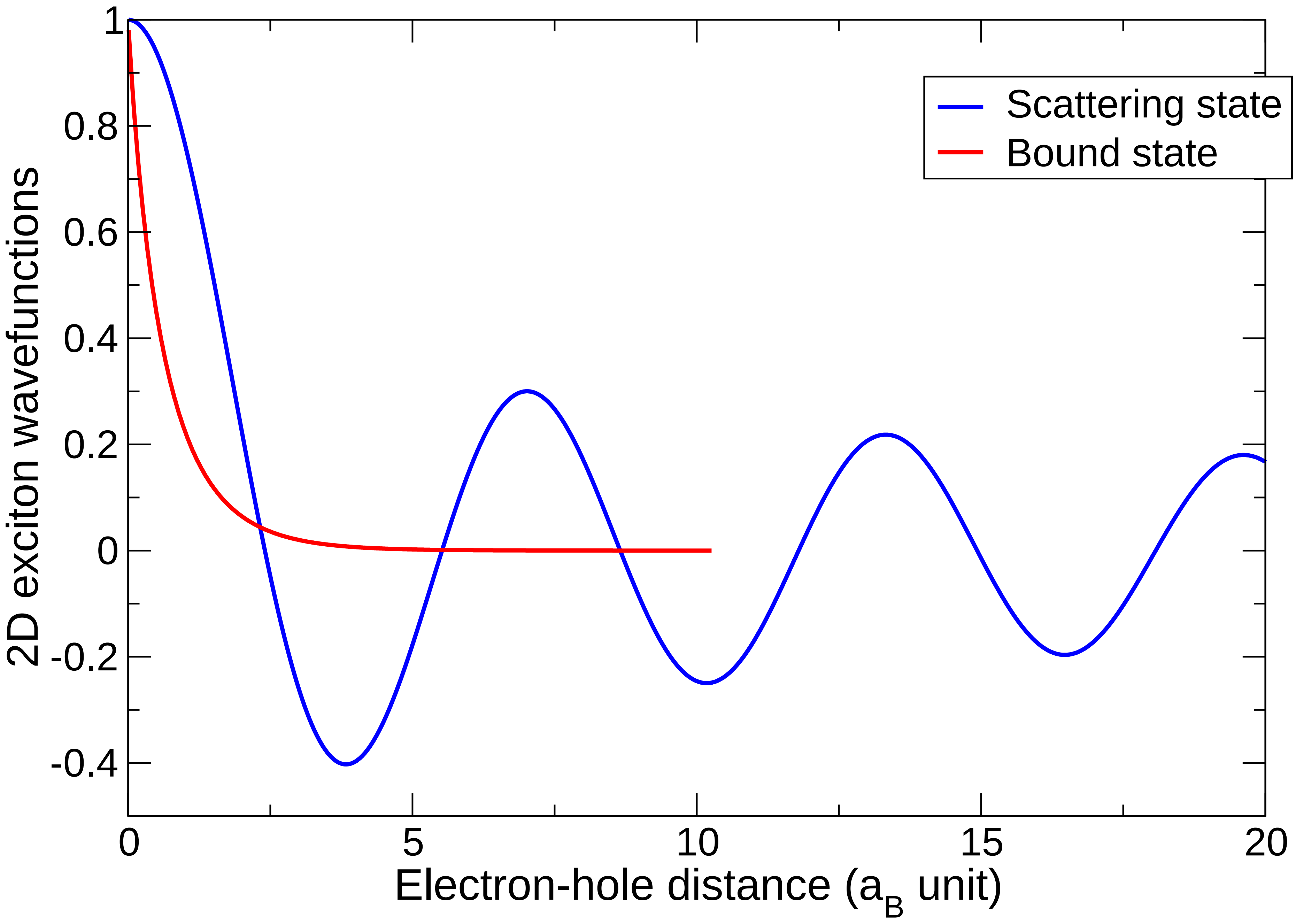
bound states

Phase equation:

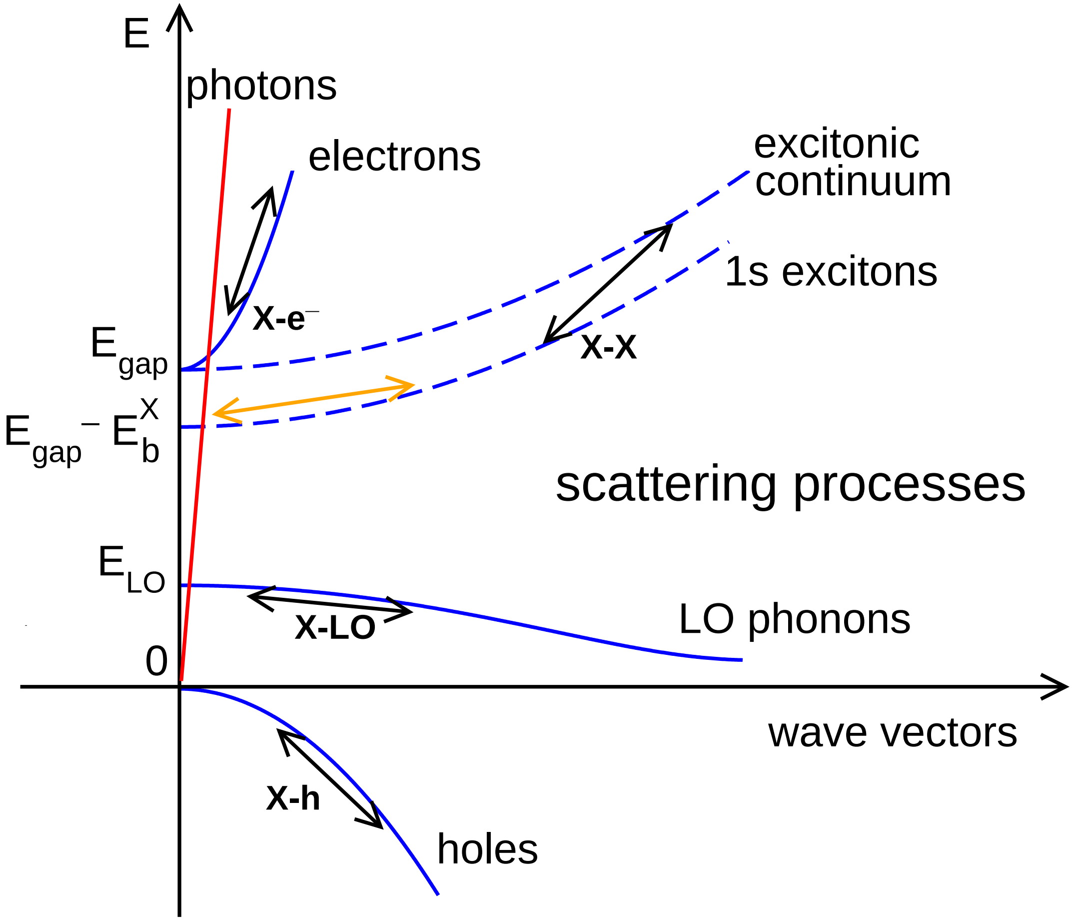
$$\frac{\mathrm{d}}{\mathrm{d}\rho}\,\eta_{m,\kappa}(\rho) = -\frac{\pi}{2}\,\rho\,U(\rho) \times \left(I_m(\kappa\rho)\cos\eta_{m,\kappa}(\rho) + \frac{2}{\pi}\,K_m(\kappa\rho)\sin\eta_{m,\kappa}(\rho) \right)^2$$

Amplitude:

$$\frac{\mathrm{d}}{\mathrm{d}\rho}\,A_{m,\kappa}(\rho) = A_{m,\kappa}(\rho)\,\frac{I_m(\kappa\rho)\sin\eta_{m,\kappa}(\rho) - \frac{2}{\pi}\,K_m(\kappa\rho)\cos\eta_{m,\kappa}(\rho)}{I_m(\kappa\rho)\cos\eta_{m,\kappa}(\rho) + \frac{2}{\pi}\,K_m(\kappa\rho)\sin\eta_{m,\kappa}(\rho)} \times \frac{\mathrm{d}}{\mathrm{d}\rho}\,\eta_{m,\kappa}(\rho)$$


Scattering state
Bound state
2D exciton wavefunctions
Electron-hole distance (a_B unit)
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
0
5
10
15
20

SCATTERING PROCESSES IN QW



scattering induced excitonic recombination

2D EXCITON WAVE FUNCTIONS

→ exciton wave function:

$$\Psi_{m,\kappa,\boldsymbol{k}_{\rm cm}}(\mathbf{R},\rho,\varphi) = A_m(\rho,\kappa)\left(I_m(\kappa\rho)\cos\eta_m(\rho,\kappa) + \frac{2}{\pi}K_m(\kappa\rho)\sin\eta_m(\rho,\kappa)\right)e^{im\varphi}\times\exp(-i\boldsymbol{k}_{\rm cm}\cdot\mathbf{R})/\sqrt{\mathcal{A}}$$

→ carrier-exciton scattering matrix elements:

$$V^{\rm eX}_{\rm scat}(\boldsymbol{k}_{\rm cm},\boldsymbol{k}_2) = \frac{1}{2}\int {\rm d}\boldsymbol{r}_1{\rm d}\boldsymbol{r}_2{\rm d}\boldsymbol{r}_{\rm h}\;\left(\phi^\dagger_{\boldsymbol{k}_2+\boldsymbol{k}_{\rm cm}}(\boldsymbol{r}_2)\Psi^\dagger_{0,\kappa,\vec{0}}(\vec{0},\rho_{1\rm h}) - \phi^\dagger_{\boldsymbol{k}_1+\boldsymbol{k}_{\rm cm}}(\boldsymbol{r}_1)\Psi^\dagger_{0,\kappa,\vec{0}}(\vec{0},\rho_{2\rm h})\right)$$
$$\times\left(V_{\rm s}(\rho_{1\rm h}) + V_{\rm s}(\rho_{2\rm h}) + V_{\rm s}(\rho_{12})\right)\;\left(\Psi_{0,\kappa,\boldsymbol{k}_{\rm cm}}(\boldsymbol{R}_1,\rho_{1\rm h})\phi_{\boldsymbol{k}_2}(\boldsymbol{r}_2) - \Psi_{0,\kappa,\boldsymbol{k}_{\rm cm}}(\boldsymbol{R}_2,\rho_{2\rm h})\phi_{\boldsymbol{k}_1}(\boldsymbol{r}_1)\right),$$

→ rates of photon emission induced by carrier-exciton scattering:

$$R_{\rm eX}(\hbar\Omega) = \frac{2\pi}{\hbar}\frac{4\pi\xi\hbar\Omega/E_{\rm g}}{(1-\hbar^2\Omega^2/E_{\rm g}^2)^2 + 4\pi\xi}\sum_{\boldsymbol{k}_{\rm cm}}\frac{2\pi\beta\hbar^2}{M}(1-\alpha)n\;\exp\left(-\beta\frac{\hbar^2k_{\rm cm}^2}{2M}\right)$$
$$\times\sum_{\boldsymbol{k}_2}\frac{2\pi\beta\hbar^2}{m_{\rm e}}\alpha n\;\exp\left(-\beta\frac{\hbar^2k_2^2}{2m_{\rm e}}\right)\;|V_{\rm scat}(\boldsymbol{k}_{\rm cm},\boldsymbol{k}_2)|^2\;\delta\left(E_{\rm g} - E^{\rm X}_{\rm b} + \frac{\hbar^2k_{\rm cm}^2}{2M} - \hbar\Omega - \frac{\hbar^2}{2m_{\rm e}}(k_{\rm cm}^2 + 2\boldsymbol{k}_{\rm cm}\cdot\boldsymbol{k}_2)\right)$$