

• Matrixelemente des Coulombs-Potentials

21/07/17 -D-

$$V_{nn} = \langle n' | \langle n' | V(\vec{q}) | n \rangle | n \rangle$$

$$= \frac{1}{L^2} \sum_{\mathbf{k}} V_{\mathbf{k}} \langle n' | \langle n' | e^{i \vec{k} \cdot \vec{q}} | n \rangle | n \rangle$$

$$V(\vec{q}) = \frac{1}{L^2} \sum_{\mathbf{k}} e^{i \vec{k} \cdot \vec{q}} V_{\mathbf{k}}$$

Reihenentwicklung in \vec{k} -Basis

$$= \frac{1}{V} \sum_{(2n)} d^2 k (\dots)$$

$$\left(\frac{c_{12}}{a}\right)^d = \delta k$$

$$V_{nn} = \int d^2 q \phi_{nn}^*(\vec{q}) V(\vec{q}) \phi_{nn}(\vec{q})$$

$$= \frac{1}{L^2} \sum_{\mathbf{k}} V_{\mathbf{k}} \int d^2 q \phi_{nn}^*(\vec{q}) e^{i \vec{k} \cdot \vec{q}} \phi_{nn}(\vec{q})$$

$$V(\vec{q}) = \frac{2 \sqrt{\lambda}}{q}$$

$$V_{\mathbf{k}} = \frac{4 \pi \sqrt{\lambda}}{k}$$

(Vgl. FT des 2D Coul.pot.)

• Berechnung der Matrixelemente:

$$e^{i \vec{k} \cdot \vec{q}} = e^{i(k_x q_x + k_y q_y)} = e^{i \frac{k_x}{\sqrt{2}} (a + a^\dagger + b + b^\dagger) + i \frac{k_y}{\sqrt{2}} (a - a^\dagger + b^\dagger - b)}$$

$$= e^{i \frac{K}{\sqrt{2}} a + i \frac{K^*}{\sqrt{2}} a^\dagger + i \frac{K^*}{\sqrt{2}} b + i \frac{K}{\sqrt{2}} b^\dagger}$$

$$= e^{i \frac{K}{\sqrt{2}} a + i \frac{K^*}{\sqrt{2}} a^\dagger} \cdot e^{i \frac{K^*}{\sqrt{2}} b + i \frac{K}{\sqrt{2}} b^\dagger}$$

mit $K = k_x + i k_y$

Baker-Campbell-Hausdorff
Formel

$$e^{A+B} = e^A e^B e^{-\frac{1}{2}[A,B]} \\ = e^B e^A e^{\frac{1}{2}[A,B]}$$

$$(= e^B e^A e^{-\frac{1}{2}[B,A]} \\ = e^{B+A})$$

$$\left[i \frac{K}{\sqrt{2}} a, i \frac{K^*}{\sqrt{2}} a^\dagger \right] = -\frac{|K|^2}{2} [a, a^\dagger] = -\frac{|K|^2}{2}$$

$$\left[i \frac{K^*}{\sqrt{2}} b, i \frac{K}{\sqrt{2}} b^\dagger \right] = -\frac{|K|^2}{2} [b, b^\dagger] = -\frac{|K|^2}{2}$$

$$= e^{i \frac{K}{\sqrt{2}} a^\dagger} e^{i \frac{K}{\sqrt{2}} a} e^{i \frac{K}{\sqrt{2}} b^\dagger} e^{i \frac{K}{\sqrt{2}} b} e^{-\frac{|K|^2}{2}}$$

mit den Eigenzuständen der a -Operatoren folgt

$$F_{nn} = \langle n' | e^{i \frac{K}{\sqrt{2}} a^\dagger} e^{i \frac{K}{\sqrt{2}} a} | n \rangle$$

$$e^{i \frac{K}{\sqrt{2}} a} = \sum_{\ell=0}^{\infty} \frac{(i \frac{K}{\sqrt{2}} a)^\ell}{\ell!}$$

$$= \sum_{m=0}^{n'} \sum_{\ell=0}^n \frac{1}{m! \ell!} \left(\frac{i K^*}{\sqrt{2}} \right)^m \left(\frac{i K}{\sqrt{2}} \right)^\ell$$

$$\bullet \langle n' | (a^\dagger)^m (a)^\ell | n \rangle$$

Vernichtungsop. a
kann nur n -mal
angewendet werden

mit $a^2(n) = \sqrt{\frac{n!}{(n-e)!}}$ $|n-e\rangle$ folgt

$$F_{n|n} = \sum_{m=0}^n \sum_{e=0}^n \frac{1}{m! e!} \left(\frac{iK^*}{\sqrt{2}}\right)^m \left(\frac{iK}{\sqrt{2}}\right)^e \sqrt{\frac{n! m!}{(n-m)! (n-e)!}} \underbrace{\delta_{n-m, n-e}}_{\langle n-m | n-e \rangle}$$

aus der Orthogonalität der EF folgt, daß z.B. m -Summe nur Beitrag für $m = n - n + e$ (falls o.B.d.A. $n \geq n$)

$$F_{n|n} = \sum_{e=0}^n \frac{\sqrt{n! m!}}{(n-n+e)! e! (n-e)!} \left(\frac{iK^*}{\sqrt{2}}\right)^{n-n} \left(-\frac{|K|^2}{2}\right)^e$$

Def: zugeordnete Laguerre-Polynome

Kern OSZ. \rightarrow Laguerre Polynome

$$\sim L_n^{(n-n)}(x) = \sum_{l=0}^n \frac{n!}{(n-n+l)! l! (n-l)!} (-x)^l$$

$$\Rightarrow F_{n|n} = \sqrt{\frac{n!}{n!}} \left(\frac{iK^*}{\sqrt{2}}\right)^{n-n} L_n^{(n-n)}\left(\frac{|K|^2}{2}\right) \quad \text{alles identisch für } b\text{-Operatoren?}$$

Unter Anwendung der gleichen Schritte für die b -Operatoren und zugehörigen Eigenfunktionen folgt

$$\text{Jacobi, Polar koor.} \quad \text{② kommt durch B.C.H.-Formel } e^{A+B} = e^A e^B e^{\frac{1}{2}[A,B]}$$

$$V_{n|n} = \frac{1}{2\pi} \int_0^\infty dk k V_k e^{-\frac{k^2}{2}} [f_{n|n}(k)]^2 \quad \begin{matrix} \text{erlaubt} \\ \text{in ① } K^* \rightarrow k \text{ zu} \\ \text{setzen, da } K^* k = k^2 \end{matrix} \quad k = |K|$$

$$f_{n|n}(k) = \sqrt{\frac{n!}{n!}} \left(-\frac{k}{\sqrt{2}}\right)^{n-n} L_n^{(n-n)}\left(\frac{k^2}{2}\right)$$

$$V_{n|n} = 2\sqrt{\pi} \int_0^\infty dk e^{-\frac{k^2}{2}} \frac{n!}{n!} \left(\frac{k^2}{2}\right)^{n-n} \left[L_n^{(n-n)}\left(\frac{k^2}{2}\right)\right]^2$$

$$\frac{k^2}{2} = x \quad \frac{dx}{dk} = k = \sqrt{x} \quad dk = \frac{dx}{\sqrt{2x}}$$

$$V_{n|n} = 2\sqrt{\pi} \frac{n!}{n!} \int_0^\infty dx \frac{1}{\sqrt{2x}} x^{n-n} e^{-x} \left[L_n^{(n-n)}(x)\right]^2$$

$$x^a \cdot x^{-\frac{1}{2}} = x^{a-\frac{1}{2}}$$

$$V_{n|n} = \sqrt{2\pi} \frac{n!}{n!} \int_0^\infty dx x^{n-n-\frac{1}{2}} e^{-x} \left[L_n^{(n-n)}(x)\right]^2$$

nach Mac Donald & Ritchie folgt hieraus

-F

$$V_{n,n} = \sqrt{2\lambda} \cdot \frac{\Gamma(n-n+\frac{1}{2}) \Gamma(n+\frac{1}{2})}{\Gamma(n-n+1) \Gamma(n+1)} \cdot {}_3F_2 \left[\begin{matrix} \alpha_1, \alpha_2, \alpha_3 \\ \beta_1, \beta_2, \beta_3 \end{matrix} ; 1 \right]$$

• hypergeometr. Reihe (RG 9.100)

$$F(\alpha, \beta; \gamma; z) = 1 + \frac{\alpha \beta}{\gamma \cdot 1} z + \frac{\alpha(\alpha+1) \beta(\beta+1)}{\gamma(\gamma+1) \cdot 1 \cdot 2} z^2 + \frac{\alpha(\alpha+1)(\alpha+2) \beta(\beta+1)(\beta+2)}{\gamma(\gamma+1)(\gamma+2) \cdot 1 \cdot 2 \cdot 3} z^3 + \dots$$

Hypergeom. Reihe bricht ab, falls α od. β ganzzahlig neg oder null

verallg. hypergeom. Reihe (RG 9.14)

$$\begin{aligned} {}_pF_q (\alpha_1, \alpha_2, \dots, \alpha_p; \beta_1, \beta_2, \dots, \beta_q; z) & \text{Was meint dieser Indiz?} \\ = {}_pF_q \left[\begin{matrix} \alpha_1, \dots, \alpha_p \\ \beta_1, \dots, \beta_q \end{matrix}; z \right] & = \sum_{k=0}^{\infty} \frac{(\alpha_1)_k (\alpha_2)_k \dots (\alpha_p)_k}{(\beta_1)_k (\beta_2)_k \dots (\beta_q)_k} \frac{z^k}{k!} \end{aligned}$$

$$\text{mit } {}_2F_1 (\alpha, \beta; \gamma; z) = F(\alpha, \beta; \gamma; z)$$

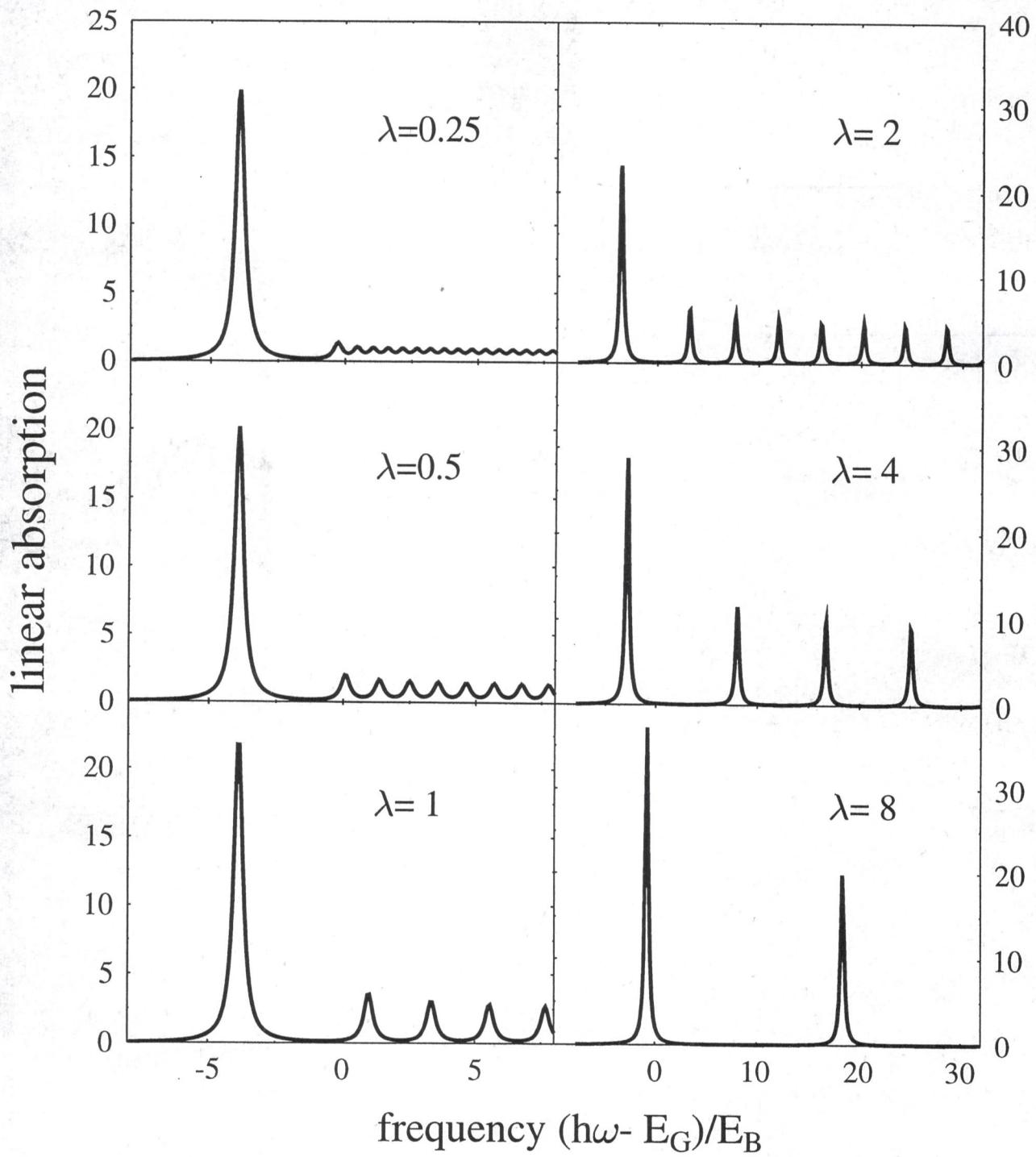
• für die T-Funktion gilt $(n, n \in \mathbb{N})$

$$T(n+1) = n!$$

$$T(n-n+1) = (n-n)!$$

$$\begin{aligned} \frac{T(x_1) T(x_2)}{T(x_3) T(x_4)} &= \frac{e^{\ln T(x_1)} e^{\ln T(x_2)}}{e^{\ln T(x_3)} e^{\ln T(x_4)}} \\ &= e^{\ln T(x_1) + \ln T(x_2) - \ln T(x_3) - \ln T(x_4)} \end{aligned}$$

Two-Dimensional Magnetoexcitons



Opt. Suszeptibilität für Magnetooxizitonen

24/07/17

- inhomogene Exzitongleichung (im Ortsraum, ohne Magnetfeld)

$$\text{Naug} \Rightarrow \left[-\frac{\hbar^2}{2\mu} \Delta - V(\vec{r}) + E_g - \hbar\omega - i\delta \right] \psi(\vec{r}) = dE(\omega) \delta(\vec{r})$$

im k -Raum werden die zu einem Term verbunden

Emstrahlfrequenz ω physikalischer Parameter, fällt weg bei Hartree-Fock

H_r^{ex} ... Hamiltonian für Exziton - Relativbewegung \rightarrow Zentrale Dämpfung

Folge aus Trafo? Ja!

- verallg. Gleichung für Magnetooxizitonen

hat keine Bandlücke drin, normale Form abh von Relativkoord. $\vec{r} = \vec{r}_e - \vec{r}_h$

$$[H_r^{\text{ex}} + E_g - \hbar\omega - i\delta] \psi(\vec{r}) = dE(\omega) \delta(\vec{r})$$

Physikalisch: Rekombination $\vec{r} = 0$!

- entwickeln $\psi(\vec{r})$ nach Eigenfunktionen $\phi_\alpha(\vec{r})$ zu H_r^{ex} (weitergef. für Mag. e)

$$\psi(\vec{r}) = \sum_\alpha b_\alpha \phi_\alpha(\vec{r}) \quad H_r^{\text{ex}} \phi_\alpha(\vec{r}) = E_\alpha \phi_\alpha(\vec{r})$$

einsetzen in inh. Magnetooxgl. und $\int d^3r \phi_\alpha^*(\vec{r})$

$$\sum_\alpha b_\alpha [E_\alpha + E_g - \hbar\omega - i\delta] \underbrace{\int d^3r \phi_\alpha^*(\vec{r}) \phi_\alpha(\vec{r})}_{\delta_{\alpha\alpha} \rightarrow \text{eliminiert Summe}} = dE(\omega) \phi_\alpha^*(0)$$

$$b_\alpha = -\frac{dE(\omega)}{\hbar\omega + i\delta - E_\alpha - E_g} \phi_\alpha^*(\vec{r}=0)$$

$$\psi(\vec{r}) = -dE(\omega) \sum_\alpha \frac{\phi_\alpha^*(\vec{r}=\vec{0})}{\hbar\omega + i\delta - E_g - E_\alpha} \phi_\alpha(\vec{r})$$

$$\chi = \frac{\gamma}{E} \text{ oder } \frac{\gamma}{dE} \text{ (Definitionssache)}$$

- mater. Interband-Pol. / opt. Spektrum

$$\text{Naug Rock} \Rightarrow P(\omega) = d^* \psi(\vec{r}=\vec{0}, \omega) + d \psi^*(\vec{r}=\vec{0}, -\omega)$$

Ch. 5
<er>, wie schon EW in 2. Quant. aus?

$$= -d\Gamma^2 E(\omega) \sum_\alpha \frac{|\phi_\alpha(\vec{r}=\vec{0})|^2}{\hbar\omega + i\delta - E_g - E_\alpha}$$

wie genau, wo ω abh.?

- "nichtrenon."

Wie kann man $\phi_\alpha(\vec{r}=\vec{0}) = \langle \vec{r}=\vec{0} | \alpha \rangle = \sum_{nn'} \langle \vec{r}=\vec{0} | \{n\} \langle n'|\} \{n'| \langle n|\} | \alpha \rangle$ diesen Schritt nachvollziehen?

$$\phi_{nn'}(\vec{r}=\vec{0}) = \langle \vec{r}=\vec{0} | \{n\} \langle n'|\} \sim r^{1/n-n'}$$

(Vollständigkeit der Landau-EF)

\Rightarrow nur für $n=n'$ nicht verschwindender Beitrag zur opt. Suszeptibilität

zu erwarten auch aus Symmetriegründen

$$\phi_{nn}(\vec{r}=\vec{0}) = \frac{1}{2\pi R^2} = \frac{1}{2\pi a_s^2} \quad \text{mit } l^2 = \frac{\hbar}{eB} \text{ und } \frac{\hbar a_s}{2\pi B} = \frac{a_s^2}{e^2} \quad (\text{ist prop.})$$

$$\boxed{\chi(\omega) \sim \frac{1}{2\pi} \sum_\alpha \frac{\sum_n |\langle \alpha | \{n\} \langle n'|\}|^2}{\hbar\omega + i\delta - E_\alpha - E_n}}$$

-- Oszillatortextur ist direkt prop. zu a_s für $n=n'$

$$\left(h\nu_c \left(n + \frac{1}{2} \right) + V'_c + E_c - E_\alpha - i\Gamma \right) \sum_n c_{an} \phi_{nn}^{(i)} = dE \delta(\vec{r}) \quad \text{wir befinden uns im w-Raum}$$

$\mathcal{Y}(\vec{r}) \leftarrow \text{Fouriertransf. von } \langle v_k^+ c_k \rangle = \mathcal{Y}_k \quad (\text{mikr. Polarisation})$

$$\langle \phi_{nn'} | \cdot \Rightarrow \sum_n \left[\left(\hbar\omega \left(n + \frac{1}{2} \right) + E_b - E_\alpha - i\Gamma \right) \delta_{nn'} + \underbrace{\langle \phi_{nn'} | V_c | \phi_{nn'} \rangle}_{S_{nn'} \leftarrow \text{analytisch gelöste}} \right] c_{an} = dE \underbrace{\phi_{nn'}(0)}_{\rightarrow 1}$$

$$\text{Lösungsvektor: } \vec{\chi} \stackrel{(2)}{=} \frac{\vec{c}_\alpha}{dE} \quad \begin{pmatrix} c_{an_1} \\ c_{an_2} \\ \vdots \\ c_{an_i} \\ \vdots \\ c_{an_N} \end{pmatrix} =: \vec{c}_\alpha$$

$$\Rightarrow \mathcal{Y}(\vec{r}) = \sum_n c_{an} \phi_{nn}^{(i)} \quad \text{nicht Funktion?} \quad \mathcal{P} = \sum_k d^* q_k + d^* \chi^* = d^* \mathcal{Y}(r \rightarrow 0, \omega) + d^* \mathcal{Y}(r \rightarrow \infty, \omega)$$

$$\text{darauf: } \chi = \frac{p}{E} = \lim_{\vec{r} \rightarrow 0} \frac{\left(d^* \sum_n c_{an} \phi_{nn}^{(i)} + d^* \sum_n c_{an} \phi_{nn}^{(r)} \right)}{E} \quad \begin{matrix} \downarrow \\ \langle c^\dagger v \rangle \end{matrix} \quad \text{das was ich ausrechnete ①}$$

$$\text{ergenommen, dass null} \quad \hookrightarrow = \frac{2}{E} \frac{d \sum_n c_{an}}{n} = 2d^2 \sum_i X_i \quad \leftarrow \text{Summe des Lösungssatzes entspricht Suszeptibilität } \chi \text{ Skalierung?}$$

Was rechne ich in eigentlich aus?

```

C === 2D-MX-SPEKTRUM
COMMON /PARA /PHI, GA, PI, RLAMB, IN
*      /GLS /ZA(0:1000,0:1000), ZB(0:1000), ZY(0:1000)
*      /COUL /VVC(0:1000,0:1000)
REAL DAT(3,500)

C . . . KONSTANTEN
PI=4.*ATAN(1.)
EBDHQ=6.373

C . . . PARAMETER
IN=200
GA=0.2
RLAMB=2.

C . . .
CALL COUPOT
Rechenung 201

NPHI=500
PHIU=-8.
PHIO=32. I*0.+8.
DO 1 IPHI=1,NPHI
    PHIU=PHIU + (PHIO-PHIU)*IPHI/NPHI

CALL MATRIX
CALL GLSYS

ZCHI=CMLPX(0.,0.)
DO 2 I=0,IN
    ZCHI =ZCHI + ZY(I)
CONTINUE
ZCHI=ZCHI/PI *RLAMB
FORMAT(3F12.5)
WRITE(*,100) PHI,ZCHI
100
FORMAT(3F12.5)
CONTINUE

DAT(1,IPHI)=PHI
DAT(2,IPHI)=REAL(ZCHI)
DAT(3,IPHI)=AIMAG(ZCHI)
1
CONTINUE

OPEN(1,FILE='mexc.dat', STATUS='unknown')
DO 10 I=1,NPHI
    WRITE(1,200) DAT(1,I), DAT(2,I), DAT(3,I)
200
FORMAT(3E12.4)
CLOSE(1)

C ===-
END
SUBROUTINE MATRIX
COMMON /PARA /PHI, GA, PI, RLAMB, IN

```

Diag
out
var A

```

C----- SUBROUTINE GLSYS
      IMPLICIT COMPLEX (Z)
      COMMON /PARA /PHI, GA, PI, RLAMB,
      *           /GLS /ZA(0:1000, 0:1000), ZB(0:1000), ZY(0:1000)
      *           /VVC /VC(0:1000, 0:1000)
      DO 1 L=0, N
      DO 2 I=0, N
          IF (I .NE. L) THEN
              ZF=ZA(I, L)/ZA(L, L)
              ZB(I)=ZB(I)-ZB(L)*ZF
          DO 3 J=L, N
              ZA(I, J)=ZA(I, J)-ZA(L, J)*ZF
          CONTINUE
      ENDIF
      CONTINUE
      RETURN
 2 CONTINUE
 1 DO 4 I=0, N
      ZY(I)=ZA(I)/ZA(I, I)
 4 CONTINUE
      RETURN
END

C----- SUBROUTINE COUPOT
      IMPLICIT COMPLEX (Z)
      COMMON /PARA /PHI, GA, PI, RLAMB, IN
      *           /GLS /ZA(0:1000, 0:1000), ZB(0:1000), ZY(0:1000)
      *           /COUL /VVC(0:1000, 0:1000)
      DO 1 I=0, IN
          DO 2 J=0, I
              print *, i,j
              CALL HYPSER(-J, 0.5+I-J, 0.5, 1.0+I-J, 0.5-J, F32)
              print *, f32
 2      VC(I, J)=SQRT(2.*RLAMB/PI)
      *           *EXP( GAMMLN(0.5+I-J)+GAMMLN(0.5+J)
      *           -GAMMLN(1.0+I-J)-GAMMLN(1.0+J)) *F32
      VC(J, I)=VC(I, J)
 1      END
ENDDO
      END

C----- SUBROUTINE hyperser(a, b, c, d, e, series)
      INTEGER n, a, a
      REAL b, c, d, e, series, bb, cc, dd, ee, fac, temp
      fac=1.
      temp=fac
      aa=a
      bb=b

```

Okt 27, 04 15:55

spek_magex.f

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```

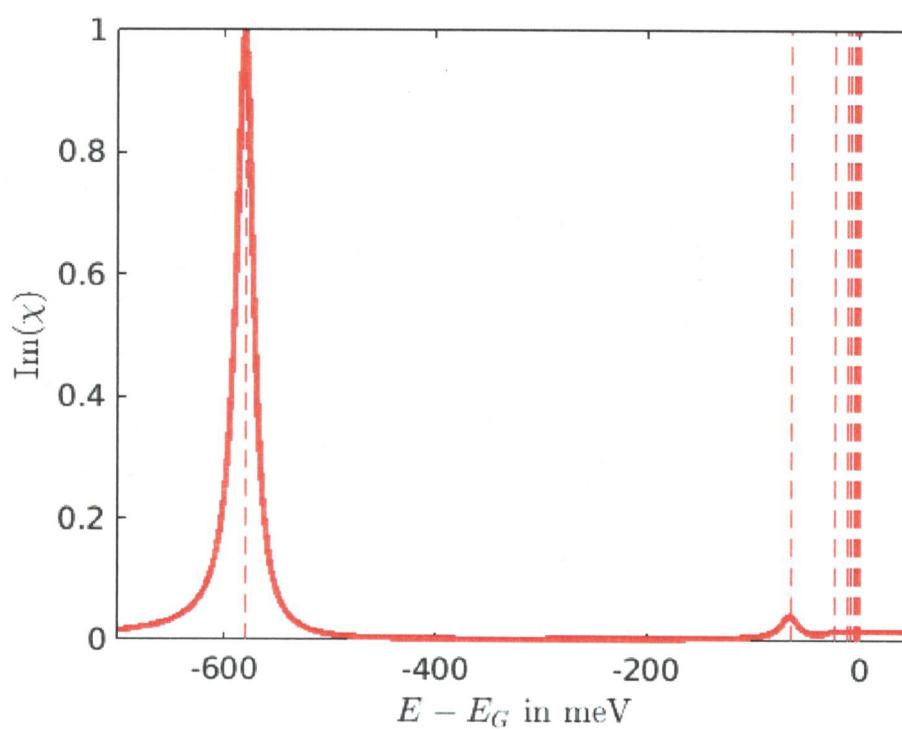
cc=c
dd=d
ee=e
do 1 n=1, 1000
    fac=fac*aa*bb*cc/dd/ee/n
    series=series+fac
    if (series.eq.temp) return
    temp=series
    aa=aa+1
    bb=bb+1.
    cc=cc+1.
    dd=dd+1.
    ee=ee+1.
1  continue
pause' convergence failure in hypers'
END
C-----
```

```

FUNCTION gammln (xx)
REAL gammln, xx
INTEGER j
DOUBLE PRECISION ser, stp, tmp, x, y, cof(6)
SAVE cof, stp
DATA cof, stp /76.18009172947146d0, -86.50532032941677d0,
*24.01409824083091d0, -1.231739572450155d0, .1208650973866179d-2,
x-5395239384953d-5, 2.5066282746310005d0/
x=xx
y=x
tmp=x+5.5d0
tmp=(x+0.5d0)*log(tmp)-tmp
ser=1.000000000190015d0
do 11 j=1, 6
    y=y+1.d0
    ser=ser+cof(j)/y
11  continue
gammln=tmp+log(stp*ser/x)
return
END
C-----
```

E/S
2²
//
2/2²

Exzitonenspektrum



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```

function [out1, out2] =
    Exzitonenanregung(Input,Method,Potential,Energies)
% Konstanten bestimmen
c                      = constants ;
me                     = 0.46*c.me ;
mh                     = 0.41*c.me ;
mu                     = (me*mh)/(me+mh) ;
C                      = - (c.e^2)/(8*pi^2*c.eps0*c.eps) ;

% Dimension der k Matrix und St#tzstellen f#r das phi-Integral muss
in
% Input Struktur gespeichert sein.
% z.B.:
%   Input = struct('I_k', [0 1 10 100], 'N_k', [10 10 10], ...
%                   'I_phi', [-pi pi], 'N_phi', [50])
[I_k, N_k, I_phi, N_phi] = deal(Input.I_k, Input.N_k, Input.I_phi,
Input.N_phi) ;

[k , g_k ]           = integrate(I_k,N_k,4) ;
[phi, g_phi]         = integrate(I_phi,N_phi,6) ;
dim                  = length(k) ;

% Erzeugen des 3D Gitters (k',k,phi)
[K1,K,PHI]           = meshgrid(k,k,phi);
kk1                  = K1(:,:,1) ;
kk                  = K(:,:,1) ;
weight_k             = repmat(g_k',[dim, 1]) ;

% Integration #ber Phi f"r beliebige Funktionen F(k,k',phi)
weight_phi           = permute(repmat(g_phi,[1,dim,dim]),[3,2,1]) ;
PHIntegrate          = @(k,k1,phi,fcn) sum((fcn(k,k1,phi) .* ...
weight_phi), 3) ;

% g_c                  : Konvergenzfaktor g(k,k')
% veff                 : Integrand in Veff(k,k'); Veff(k,k') = veff dphi
% in [0,2pi]
% veff_ii              : Integrand in Diagonalelementen
% veff_ij              : Integrand in Nicht-Diagonalelementen
% t_ii                 : Funktion f"r kinetische Energie

g_c                  = @(k,k1)      4*k.^4 ./ (k.^2 + k1.^2).^2 ;
switch Potential
    case{'Coulomb'}
        veff            = @(k,k1,phi) (C*k1 ./ sqrt(k.^2 ...
+k1.^2 - 2*k.*k1.*cos(phi))).*(k~=k1) ;
        I               = 12.0015;
    case{'Keldysh'}
        % Hier muss das zum Keldyshpotential gehoerende veff/I rein
        veff            = 1 ;
        I               = 1;
    otherwise
end

```

LGS: $\underline{A} \vec{x} = \vec{b}$

```

veff_ij          = veff;
veff_ii          = @(k,k1,phi) g_c(k,k1) .*veff_ij(k,k1,phi) ;
t_ii             = @(k,k1)      1/2/mu *(c.hbar*k).^2 .*eq(k,k1);

% Erstellen der verschiedenen Anteile der Hamiltonmatrix
T_ii             = t_ii(kk,kk1);
V_ii             = C*I*(kk==kk1).*kk -
diag(PHIntegrate(K,K1,PHI,veff_ii)*g_k);
V_ij             = PHIntegrate(K,K1,PHI,veff_ij) .* weight_k;

% Hamiltonmatrix zusammenfuegen
H = T_ii + V_ij + V_ii ;

switch Method
    case{'Spektrum'}
        disp('Spektrum')
        out1      = [] ;
        b         = ones(dim,1) ;
        for E = Energies
            H_const   = (c.E_G - E - 1i*c.Gamma)*(kk==kk1); ← zusätzliches Matrixterm
            A         = H + H_const ;
            x_k       = linsolve(A,b) ;
            x         = 1/(2*pi)*g_k'*(k.*x_k); ←  $\chi = \frac{1}{(2\pi)^2} \int d^2 k \chi_k$ 
            out1      = [out1 x] ;
            out2      = Energies ;
            end
        case{'Eigenwerte'}
            disp('Eigenwerte')
            % Bestimmung der Eigenwerte (eig_val) samt Normierung der Wellenfunktionen
            % (states). Beides beginnend mit dem Grundzustand (sort).
            [states, EW] = eig(H, 'vector') ;
            [EW, idx]   = sort(EW) ;
            states      = states(:,idx) ;
            norm        = sqrt(2*pi*(states.^2)'*(k.*g_k));
            for i=1:dim; states(:,i) = states(:,i)*1/
            norm(i)*sign(states(1,i)); end

            % Anzeigen der Grundzustandsenergie
            disp(EW(1))
            out1      = EW ;
            out2      = states ;
        end
    end

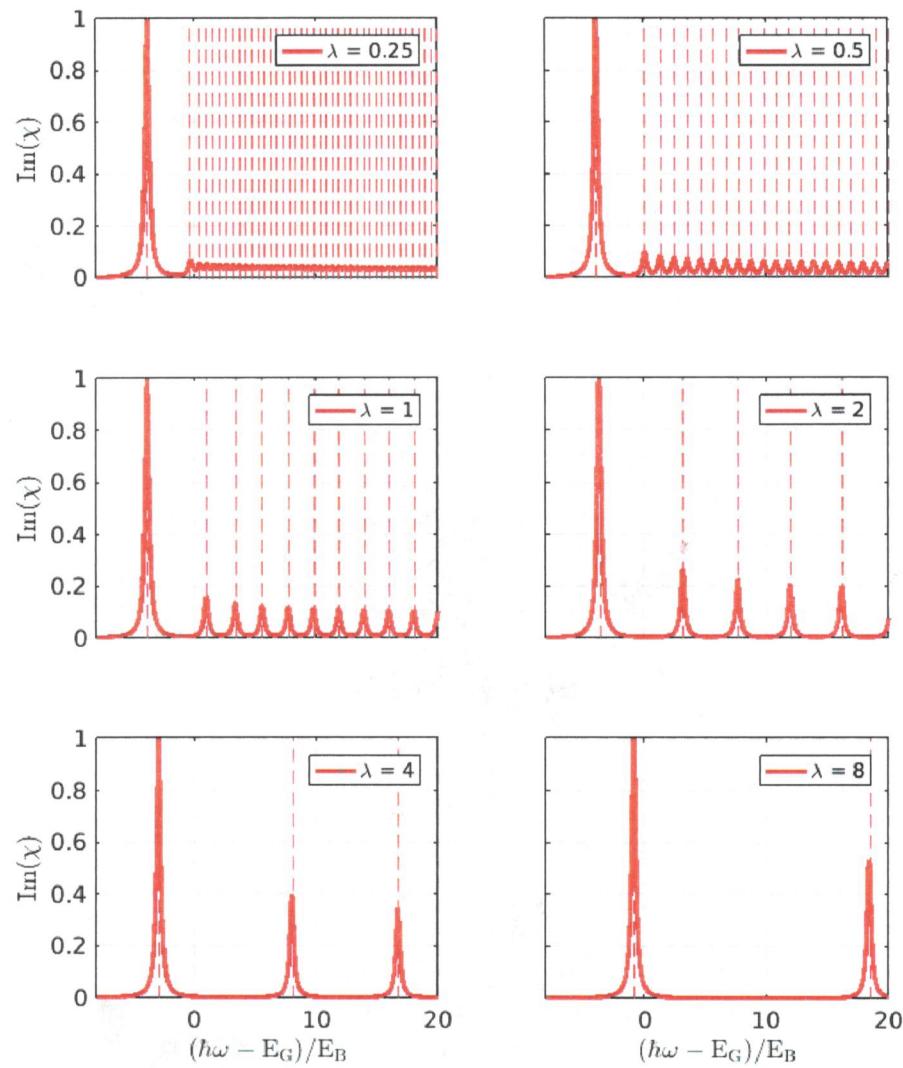
```

$$= \frac{1}{(2\pi)^2} \sum_k g_k \cdot k \cdot \chi_k$$

num. Integral

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Magnetoexziton



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GaAs $a_0 = 12.4 \text{ nm}$
 $E_B = 4.2 \text{ meV}$

$$\text{GaN: } 12,4 / 125 \text{ nm} \quad \mu = 0,0584 \text{ m}^2 \frac{\text{V}}{\text{s}}$$

$$\text{MoS}_2: 1 \text{ nm} \quad \mu = 0,2168 \text{ m}^2 \frac{\text{V}}{\text{s}}$$

$$E_0 = \frac{\hbar^2}{2m_a}$$

$$5d, 5791 \text{ meV}$$

λ	B in T
$\frac{1}{4}$	1,07
0,15	2,14
1	4,28
2	8,56
4	17,12
8	34,24
GaAs	

λ in $\frac{\text{nm}}{1000}$	B in T
$\frac{1}{2}$	0,33
1	0,66
2	1,32
4	2,63
8	5,27
16	10,53

$$\lambda = \frac{a_0^2}{e^2} = \frac{a_0^2 \cdot eB}{\hbar}$$

$$[B] = \frac{\text{meVps}}{(\text{nm})^2 \text{pAps}} = \frac{\text{meV}}{(\text{nm})^2 \text{pA}}$$

$$= 2 \cdot 10^3 \text{ T}$$

$$\lambda = \hbar \omega_c / 2t_B$$

$$\lambda = \frac{a_0^2}{e^2} = \frac{a_0^2 e B}{\hbar}$$

$$1 \text{ V} = 2 \cdot 10^{-24} \text{ J}$$

$$B = \frac{\hbar \lambda}{a_0^2 e}$$

$$1 \text{ meV} = 10^3 \text{ eV} = 2 \cdot 10^{-27}$$

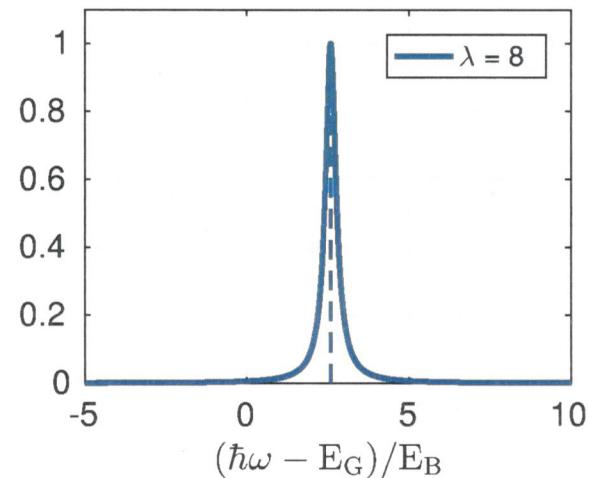
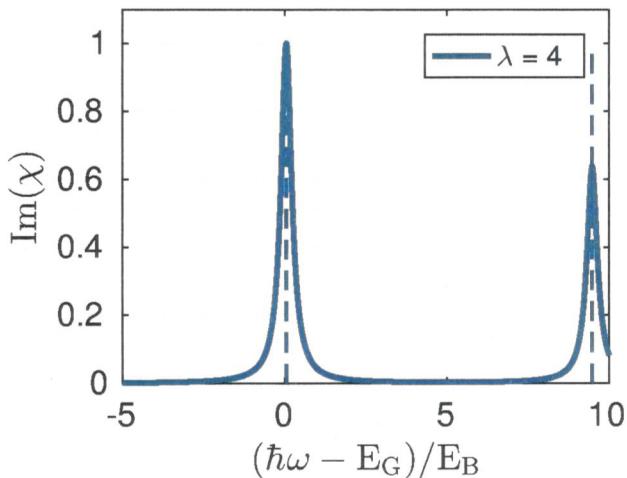
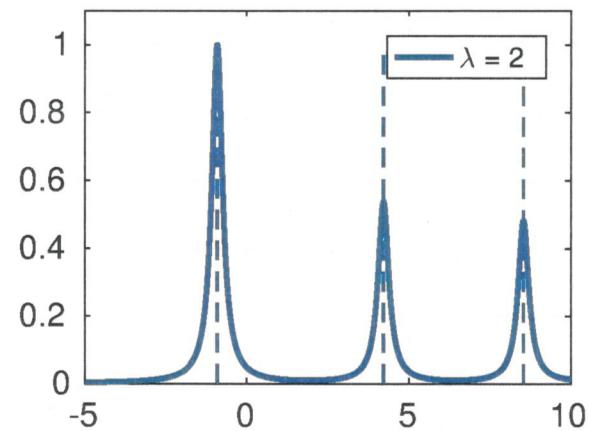
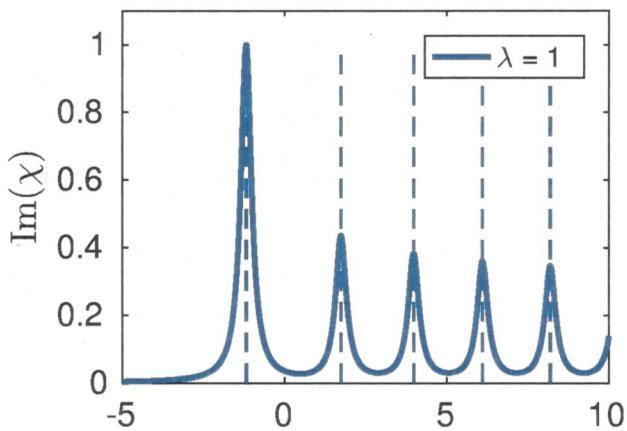
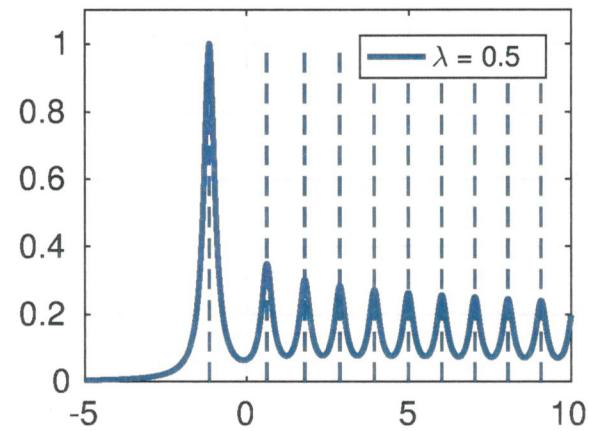
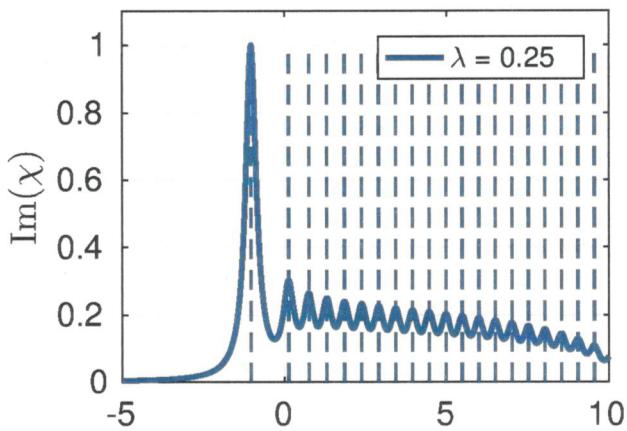
$$\frac{\text{meVps}}{(\text{nm})^2 \text{pAps}} = \frac{2 \cdot 10^{-27} \text{ J}}{10^{-18} \cdot 10^{-12} \text{ m}^2 \text{ A}}$$

$$= 2 \cdot 10^3 \text{ T}$$

Keldysh-Potential

$n=20$ (geringe Auflösung)

$$\chi(q) \sim \frac{1}{a + bq} \quad ; \quad \left\{ \begin{array}{l} b \text{ sehr klein gewählt} \rightarrow \text{Modell bestätigen} \\ a \text{ erst einmal } 1 \end{array} \right.$$



- genügen Stützstellen?

$$\text{für } \frac{x^m}{1+x^{\frac{m}{2}}}; \quad \frac{d^m}{dx^m} \left(\frac{x^{2n}}{1+x^{\frac{m}{2}}} \right) = \sum_{k=0}^m \binom{m}{k} \left(x^{2n} \right)^{(k)} \left(\frac{1}{1+x^{\frac{m}{2}}} \right)^{(m-k)}$$

Term $\max(|\mathcal{E}(x)|) := \tilde{\mathcal{E}}(\xi)$ möglichst klein? $x \in \mathbb{R}^+$

$$E \propto \int^{(m)} x^m dx, \text{ wenn } L_x^\beta(a) = 0 \text{ gesucht}$$

\Rightarrow also # Stützstellen

Material!

- Welche Werte für $\chi_{20}; \delta$?

$$\text{wobei } \chi_{20}(q) = \frac{\epsilon^2}{2\epsilon_0} \left(\frac{1}{aq + bq^2} \right) = \underbrace{\frac{\epsilon^2}{2\epsilon_0} \cdot \frac{b}{a} \left(\frac{1}{bq} - \frac{1}{a+bq} \right)}_{\text{gut für qualitatives Verständnis}}$$

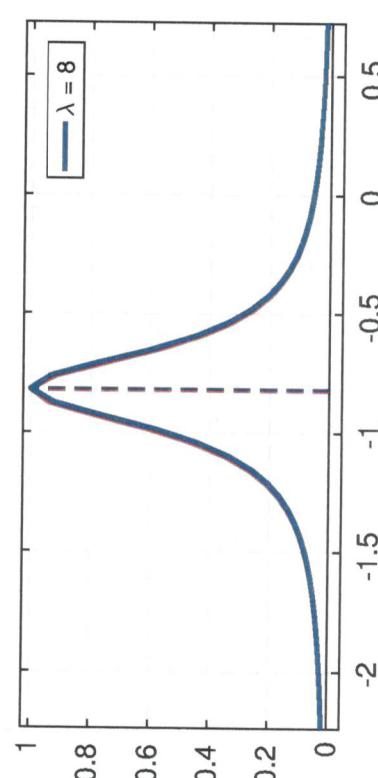
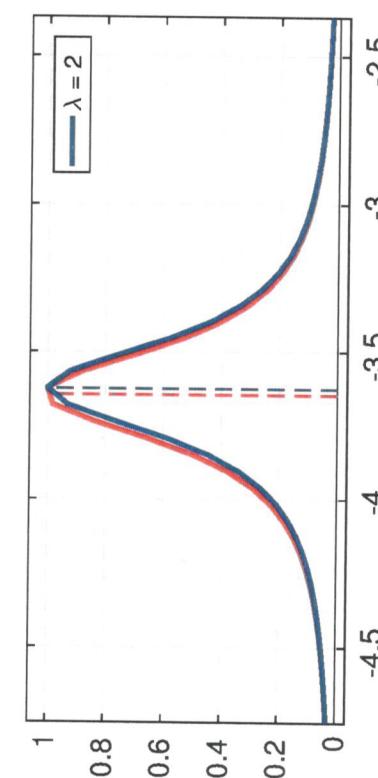
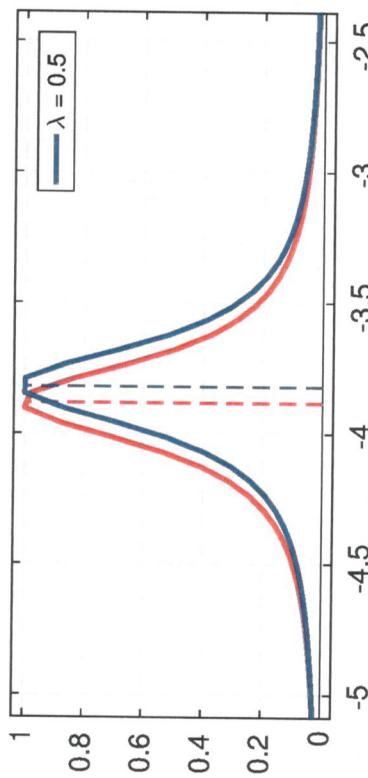
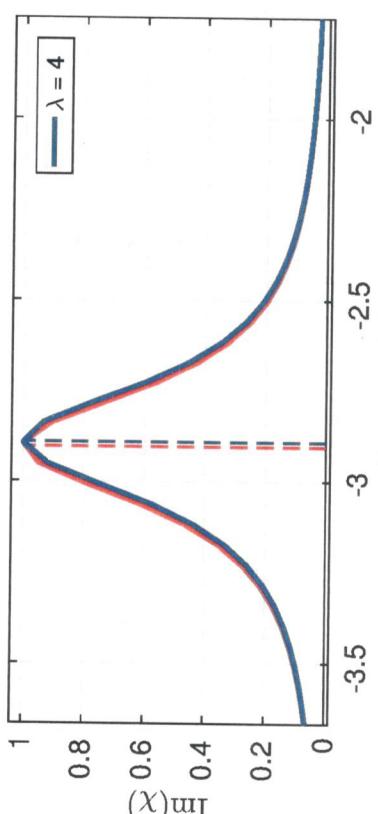
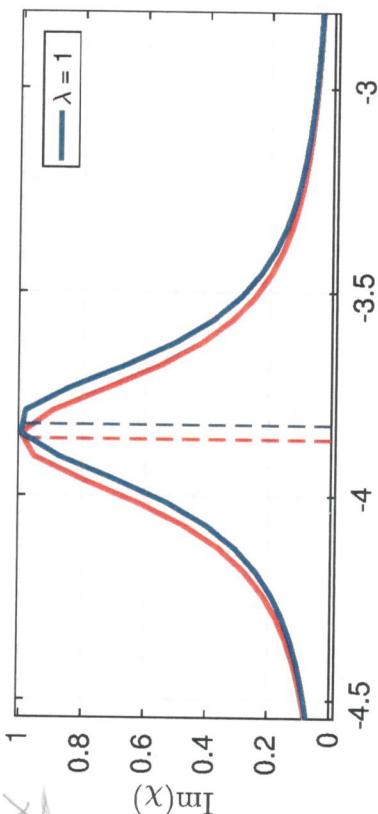
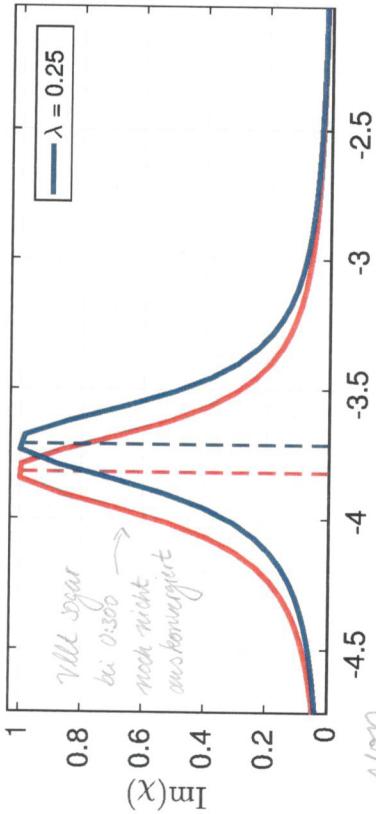
für ①:

$$\alpha = \delta \quad / \text{hier an von? ②}$$

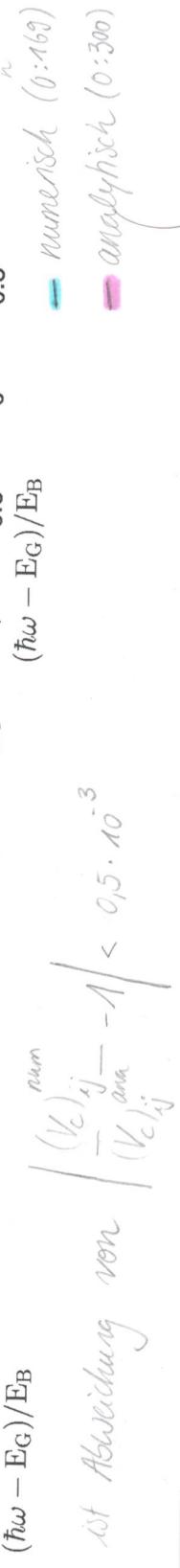
$$\frac{b}{a} = r_0 = 2\pi \frac{\chi_{20}}{\delta}$$

- Gleichungen für χ ? Eigentlich dim. los, aber nicht in ②!

✓ schlechte Basis, da Magnetfeld zu klein



Negligible von
Nummerik &
Analytik



bei gleicher Auflösung ist Abweichung von $\left| \frac{(V_c)_{\text{num}} - (V_c)_{\text{ana}}}{(V_c)_{\text{ana}}} \right| < 0,5 \cdot 10^{-3}$

Numerische Berechnung der Coulomb-Matrix-Elemente

01/08/17

$$V_{nn} = 2\sqrt{\lambda} \int dk \frac{n!}{n'!} V(k) k \left(\frac{k^2}{2} \right)^{n-n'} \left[L_n \left(\frac{k^2}{2} \right) \right]^2$$

$$= 2\sqrt{\lambda} \int_0^\infty \frac{dx}{\sqrt{2x}} e^{-x} \frac{n!}{n'!} V(\sqrt{2x}) \cdot \sqrt{2x} \cdot x^{n-n'} \left[L_n(x) \right]^2$$

Keldysh hat

$$\text{stochastischen Vorfaktor } \frac{n!}{n'!} \int_0^\infty x^{n-n'} \frac{1}{\sqrt{2x}(a+b\sqrt{2x})} \cdot e^{-x} \left[L_n(x) \right]^2$$

$$= 2\sqrt{\lambda} \frac{n!}{n'!}$$

richtiger Vorfaktor, \mathcal{C}

$$= \underbrace{\sqrt{\lambda} \frac{n!}{n'!}}_{=: \mathcal{C}} \int_0^\infty x^{n-n'-\frac{1}{2}} e^{-x} \underbrace{\frac{\left(L_n(x) \right)^2}{a+b\sqrt{2x}}}_{f(x)}$$

$$\mathcal{H}_k: \text{Gauß-Laguerre - Gewicht}$$

$$\mathcal{H}_k = \sum_{k=1}^n \mathcal{H}_k f(a_k)$$

$$a_k: \text{Nullstellen von } L_n(x) \\ k=1, \dots, n \quad (\beta \text{ null}, \beta > -1)$$

$$E: \text{Fehlerterm } \propto \int f(x)$$

$$\boxed{= \mathcal{C} \int_0^\infty x^\beta e^{-x} f(x)}$$

- Abweichen muss das \mathcal{H} vom Potenzial? Beim $\mathcal{L} \rightarrow \frac{1}{(2m)a} \int dk \rightarrow$ Fourier ist nicht eindeutig, daher aus Dimensionengründen Schraw vor die k -I zu schreiben! ($\frac{1}{\sqrt{2\pi}} \int_k V_k e^{ikx} = V(x)$)

- ① bei analytisch noch $\frac{1}{\sqrt{\pi}}$ drin, folge der analytischen Auswertung

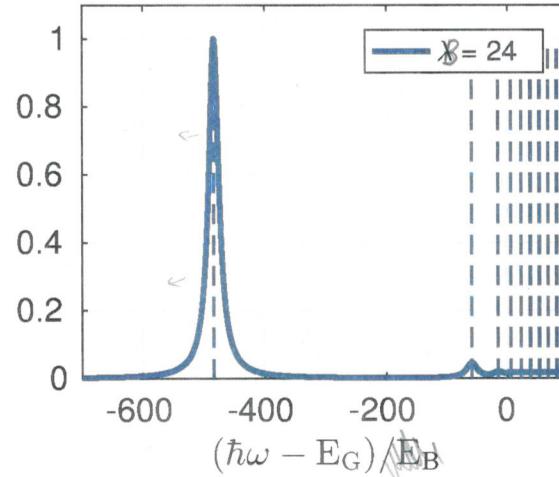
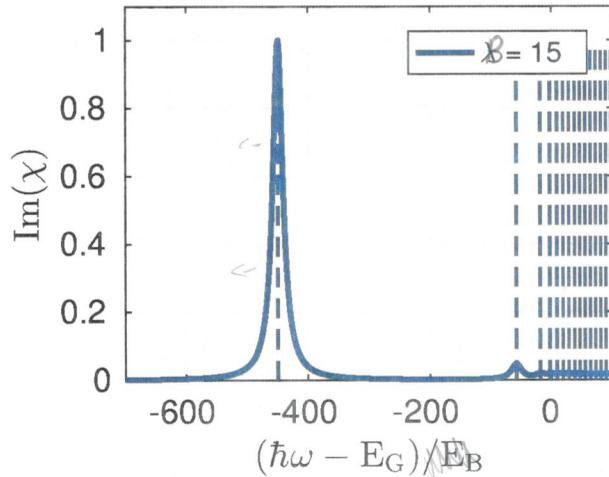
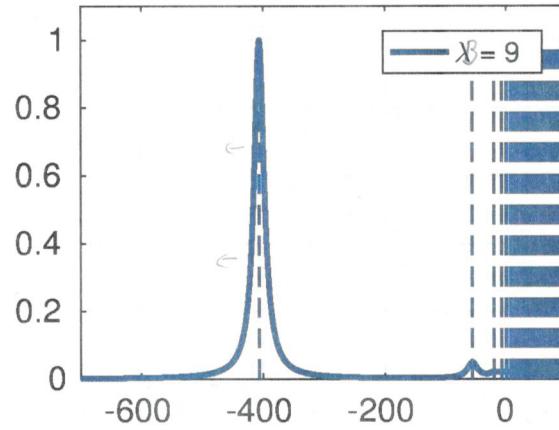
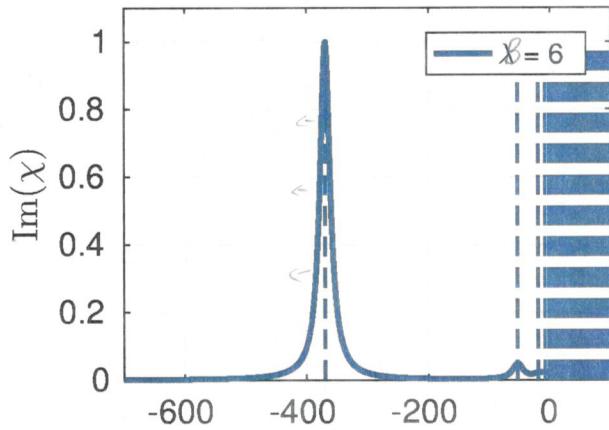
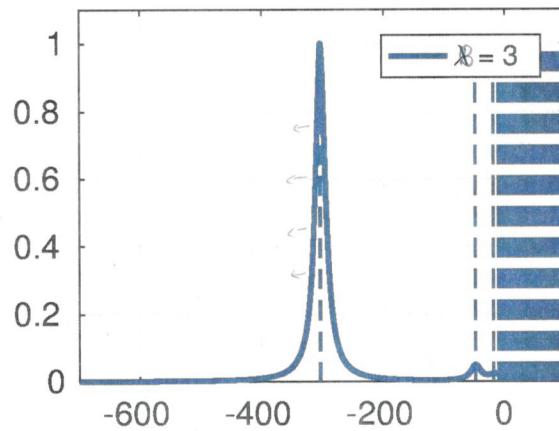
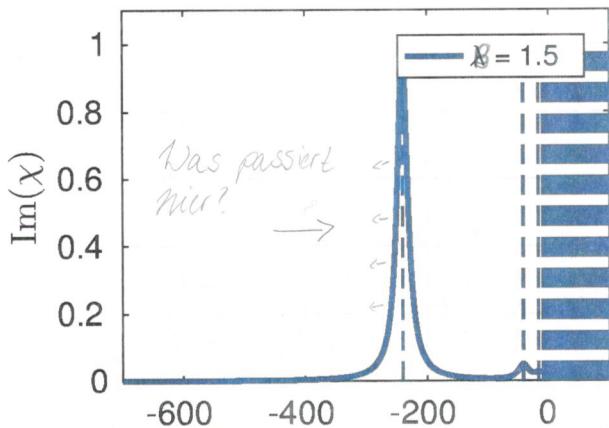
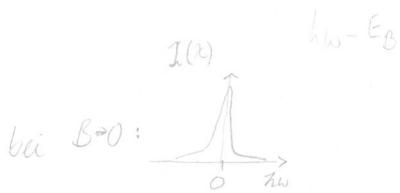
Umschrieb auf SI-Einheiten

Die Suche nach ϵ_r

03/08/17

MoS_2 - Coulomb

$$(V(r) = \frac{1}{4\pi\epsilon_0} \frac{1}{r}) \text{, analytisch } n=0:300$$



Bohr-Radius:

$$\left(\frac{h^2}{2m\alpha^2} - \frac{1}{4\pi\epsilon_0 \alpha} \right)^{\frac{1}{2}} = -\frac{2h^2}{2ma^3} + \frac{1}{4\pi\epsilon_0 \alpha^2} \cdot \frac{e^2}{a} = 0 \quad \Rightarrow \quad \frac{1}{a^2} \left[\frac{h^2}{ma} - \frac{e^2}{4\pi\epsilon_0} \right] = 0$$

① rausgezogen

$$\frac{h^2}{2m} \cdot \frac{1}{\ell^2} = \frac{h^2}{3\mu} \cdot \frac{eB}{\hbar} = \frac{1}{2} k \frac{eB}{\mu} = \frac{1}{2} \hbar \omega_c$$

$$\left(\frac{1}{\ell^2} = \frac{eB}{\hbar} \right) ; \omega_c = \frac{eB}{\mu} ; \quad r = \ell \cdot \beta$$

Umsschreiben in SI

Eigenwertgleichung:

von $e^- \& h$

$$\textcircled{2} \quad \left[\hbar \omega_c \left(a^\dagger a + \frac{1}{2} \right) - \frac{e^2}{4\pi\epsilon_0} \frac{1}{\ell^2} \right] \psi = \mathcal{H} \rightarrow \sum_n \left[\hbar \omega_c \left(a^\dagger a + \frac{1}{2} \right) \delta_{nn} - \int d\beta \phi_{nn} \left(\frac{e^2}{4\pi\epsilon_0} \beta \right) \phi_{nn} \right] \psi_n = E_n \psi_n \quad (*)$$

$$\left(\frac{h^2}{2m\alpha^2} - \frac{1}{4\pi\epsilon_0 \alpha} \right)^{\frac{1}{2}} = -\frac{2h^2}{2ma^3} + \frac{1}{4\pi\epsilon_0 \alpha^2} \cdot \frac{e^2}{a^2} = -\frac{h^2}{2ma^2} - \frac{h^2}{ma^2} = -\frac{h^2}{2ma^2} = -E_B$$

algebraisch gelöst
→ Legendre-Polynome

in $(**)$: $E_{min} = \frac{h^2}{2ma^2} - \frac{h^2}{ma^2} = -\frac{h^2}{2ma^2}$

④ Hooke'sche-Blast-Gleichungen

$$\textcircled{4} \quad \left[2E_B \left(\frac{a}{\ell} \right)^2 \left(n + \frac{1}{2} \right) - 2E_B \left(\frac{a}{\ell} \right) \hat{V}(s) - \hbar \omega - i\Gamma \right] \chi = 1 \quad | : \overline{E_B}$$

$$\boxed{\begin{aligned} & \left[2E_B \left(\frac{a}{\ell} \right)^2 \left(n + \frac{1}{2} \right) - 2E_B \left(\frac{a}{\ell} \right) \hat{V}(s) - \hbar \omega - i\frac{\Gamma}{E_B} \right] \chi = 1 \\ & \rightarrow E_B \left[2\lambda \left(n + \frac{1}{2} \right) - \frac{2\sqrt{\lambda}}{\ell} \hat{V}(s) - \frac{\hbar \omega}{E_B} - i\frac{\Gamma}{E_B} \right] \chi = 1 \end{aligned}}$$

↖ Das habe ich gerechnet

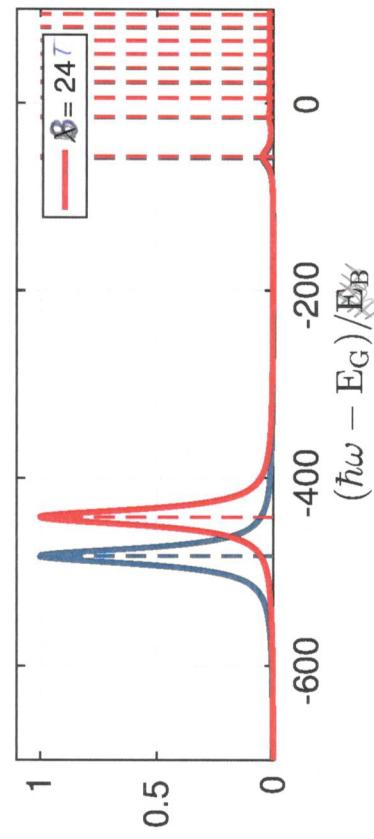
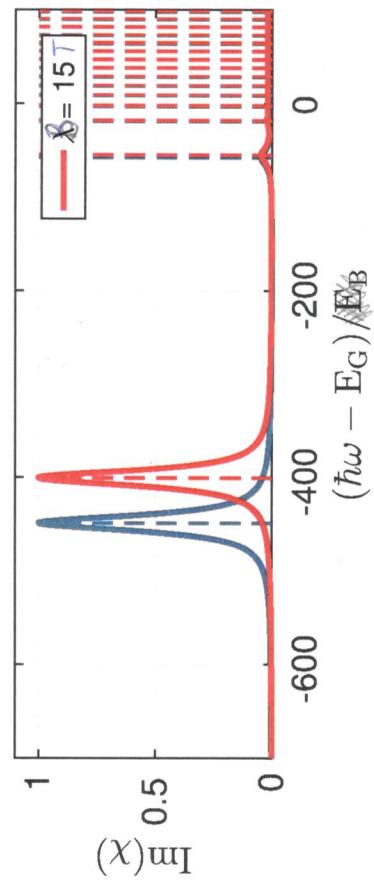
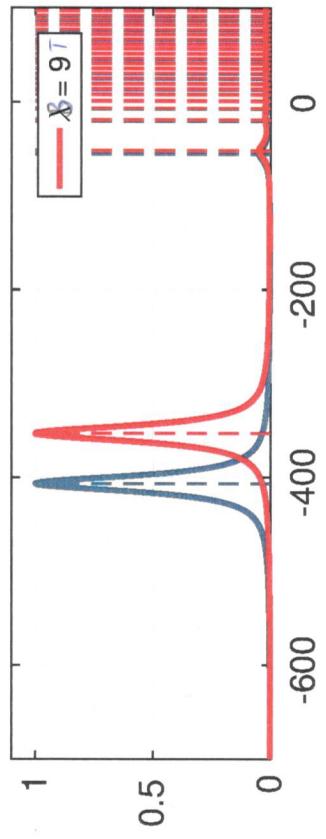
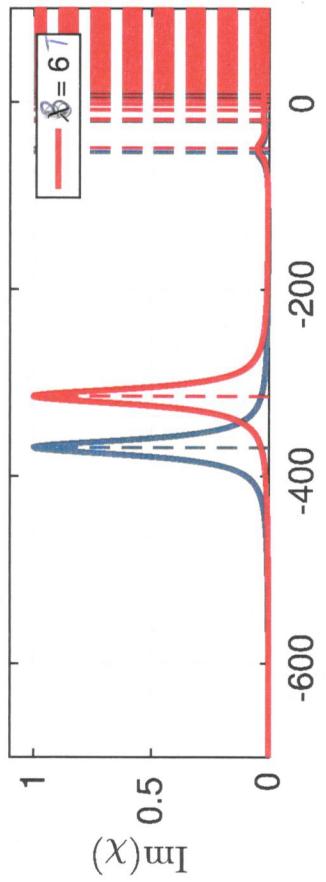
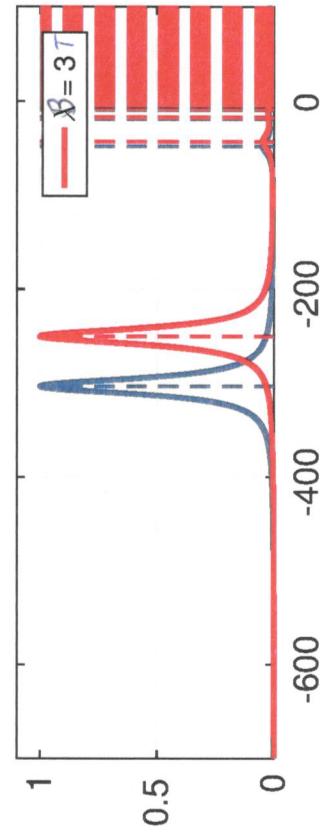
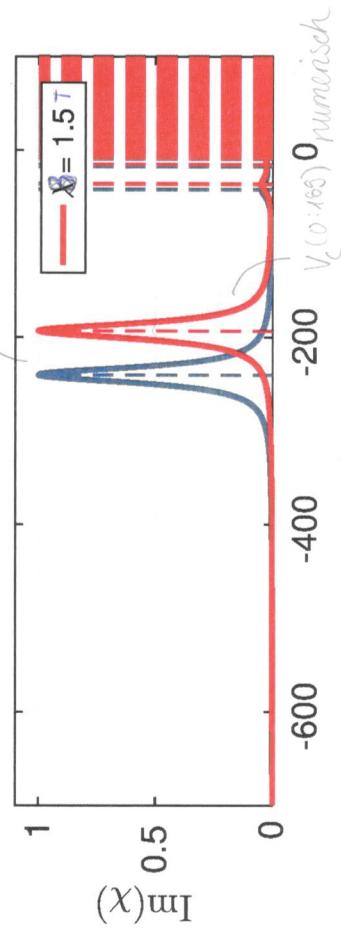
$$\text{wegen Entwicklung in } \lambda : 2\sqrt{\lambda} \rightarrow \sqrt{2\lambda}$$

⑤ Für Coulomb sind λ -Werte bekannt

→ ändert sich $a_0 \rightarrow \beta$ muss sich ändern ; Was bei $\hbar \omega$?

MoS_2 - Coulomb

$V_c(0:300)$ analytisch



→ Vorfaktor identisch, obwohl $\frac{1}{\sqrt{n}}$ nur bei analytischer Rechnung auftauchen sollte → Antwort: \sqrt{n} wird in gausssagtem dargestellt

↖ Landau-Basis nur keine gute Wahl, da β noch zu klein für $n_{0,2}$