PHY 742 Quantum Mechanics II
12-12:50 PM MWF Olin 103

Plan for Lecture 9

1. Continue reading Chapter 14 – Analysis of scattering phenomena
   a. Summary of phase shift analysis and examples
   b. Approximate treatments of scattering – Born approximation

Course schedule for Spring 2022

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	Reading	Topic	HW	Due date
1	Mon: 01/10/2022	Chap. 12	Approximate solutions for stationary states -- The variational approach	#1	01/14/2022
2	Wed: 01/12/2022	Chap. 12 C	Approximate solutions for stationary states -- Perturbation theory	#2	01/19/2022
3	Fri: 01/14/2022	Chap. 12 D	Approximate solutions for stationary states -- Degenerate perturbation theory	#3	01/21/2022
	Mon: 01/17/2022		MLK Holiday -- no class		
4	Wed: 01/19/2022	Chap. 12 C & D	Approximate solutions for stationary states -- Additional tricks	#4	01/24/2022
5	Fri: 01/21/2022	Chap. 13	Examples of of the use of perturbation theory	#5	01/26/2022
6	Mon: 01/24/2022	Chap. 13 & 12 B	Hyperfine perturbation and also the WKB approximation	#6	01/28/2022
7	Wed: 01/26/2022	Chap. 14	Scattering theory		
8	Fri: 01/28/2022	Chap. 14	Scattering theory	#7	02/04/2022
9	Mon: 01/31/2022	Chap. 14	Scattering theory	#8	02/07/2022

PHY 742 -- Assignment #8

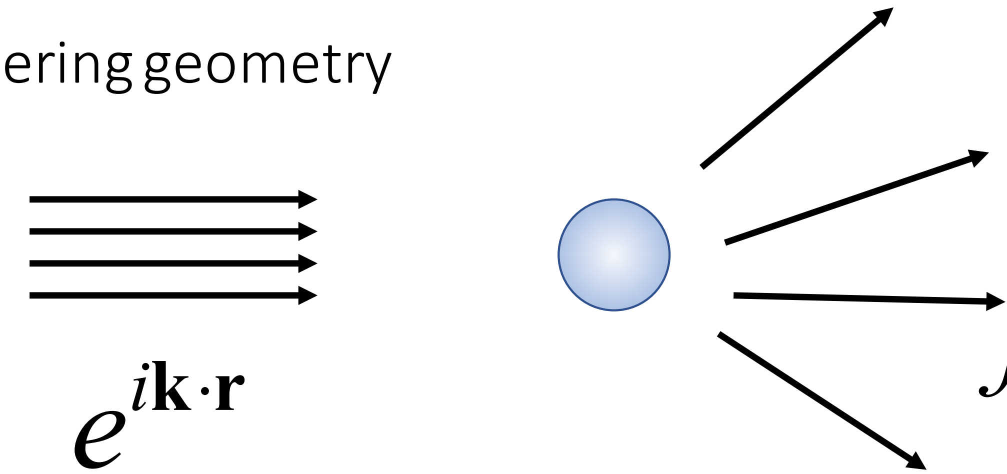
January 31, 2022

Continue reading Chapter 14 in **Carlson's** textbook.

1. Consider the isotropic three-dimensional scattering potential $V(r)$ which is zero for $r < a$ and has value $-V_0$ for $0 \leq r \leq a$, where V_0 is a positive constant.
   a. Write a general expression for the scattering phase shifts $\delta_l(E)$ for $E > 0$.
   b. Evaluate the expression for $l=0$ for two or three values of E/V_0.

Representation of scattering in terms of probability amplitude

Scattering geometry



$\hat{\mathbf{r}}$

$$e^{i\mathbf{k}\cdot\mathbf{r}}$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}})\frac{e^{ikr}}{r}$$

Incident plane wave with wavevector $\mathbf{k}$ and energy $E=\frac{\hbar^2k^2}{2m}$

Scattered spherical wave with scattering amplitude $f(\hat{\mathbf{k}},\hat{\mathbf{r}})$

Summary of analysis for spherical target in terms of scattering phase shifts:

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = \frac{4\pi}{k}\sum_{lm} e^{i\delta_l(E)} \sin(\delta_l(E)) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}})$$

Differential cross section: $\dfrac{d\sigma}{d\Omega} = \left| f(\hat{\mathbf{k}},\hat{\mathbf{r}}) \right|^2$

Total cross section: $\displaystyle\int d\Omega \frac{d\sigma}{d\Omega} = \sigma(E) = \frac{4\pi}{k^2}\sum_{l}\left(2l+1\right)\sin^2(\delta_l(E))$

Summary of analysis for spherical target in terms of scattering phase shifts -- continued:

How to determine phase shifts $\delta_l(E)$ for interaction potential $V(r)$:

Partial wave differential equation:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}\right)+V(r)-E\right)R_{El}(r)=0$$

Spherical Bessel function

Spherical Neumann function

Continuity conditions at $r=D$: $\quad R_{El}(D)=\mathcal{N}_l\left(\cos\delta_l\, j_l(kD)-\sin\delta_l\, y_l(kD)\right)$

$$\frac{dR_{El}(D)}{dr}=\mathcal{N}_l\left(\cos\delta_l\frac{dj_l(kD)}{dr}-\sin\delta_l\frac{dy_l(kD)}{dr}\right)$$

$$\tan\delta_l(E)=\frac{L_l(E)j_l(kD)-kj_l{}'(kD)}{L_l(E)y_l(kD)-ky_l{}'(kD)} \quad \text{where} \quad \frac{d\ln\left(R_{El}(r)\right)}{dr}=\left.\frac{\dfrac{dR_{El}(r)}{dr}}{R_{El}(r)}\right|_{r=D}\equiv L_l(E)$$

Slight simplification in functions --

Define slightly more convenient radial function: $R_{El}(r) \equiv \frac{P_{El}(r)}{r}$

Partial wave differential equation for $P_{El}(r)$:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2}\right) + V(r) - E\right)P_{El}(r) = 0$$

Similarly, we can define the scaled spherical Bessel and Neumann functions:

$jj_l(x) = xj_l(x)$ and $yy_l(x) = xy_l(x)$

Continuity conditions at $r = D$: $P_{El}(D) = \mathcal{N}_l\left(\cos\delta_l\, jj_l(kD) - \sin\delta_l\, yy_l(kD)\right)$

$$\frac{dP_{El}(D)}{dr} = \mathcal{N}_l\left(\cos\delta_l \frac{djj_l(kD)}{dr} - \sin\delta_l \frac{dyy_l(kD)}{dr}\right)$$

$$\tan\delta_l(E) = \frac{LL_l(E)\, jj_l(kD) - kjj_l\,'(kD)}{LL_l(E)\, yy_l(kD) - kyy_l\,'(kD)} \quad \text{where} \quad \left.\frac{d\ln\left(P_{El}(r)\right)}{dr}\right|_{r=D} \equiv LL_l(E)$$

Slight simplification in functions – continued (Note: This notation is not standard.)

Scaled Bessel and Neumann functions:

$$jj_0(x) = \sin(x) \qquad yy_0(x) = -\cos(x)$$

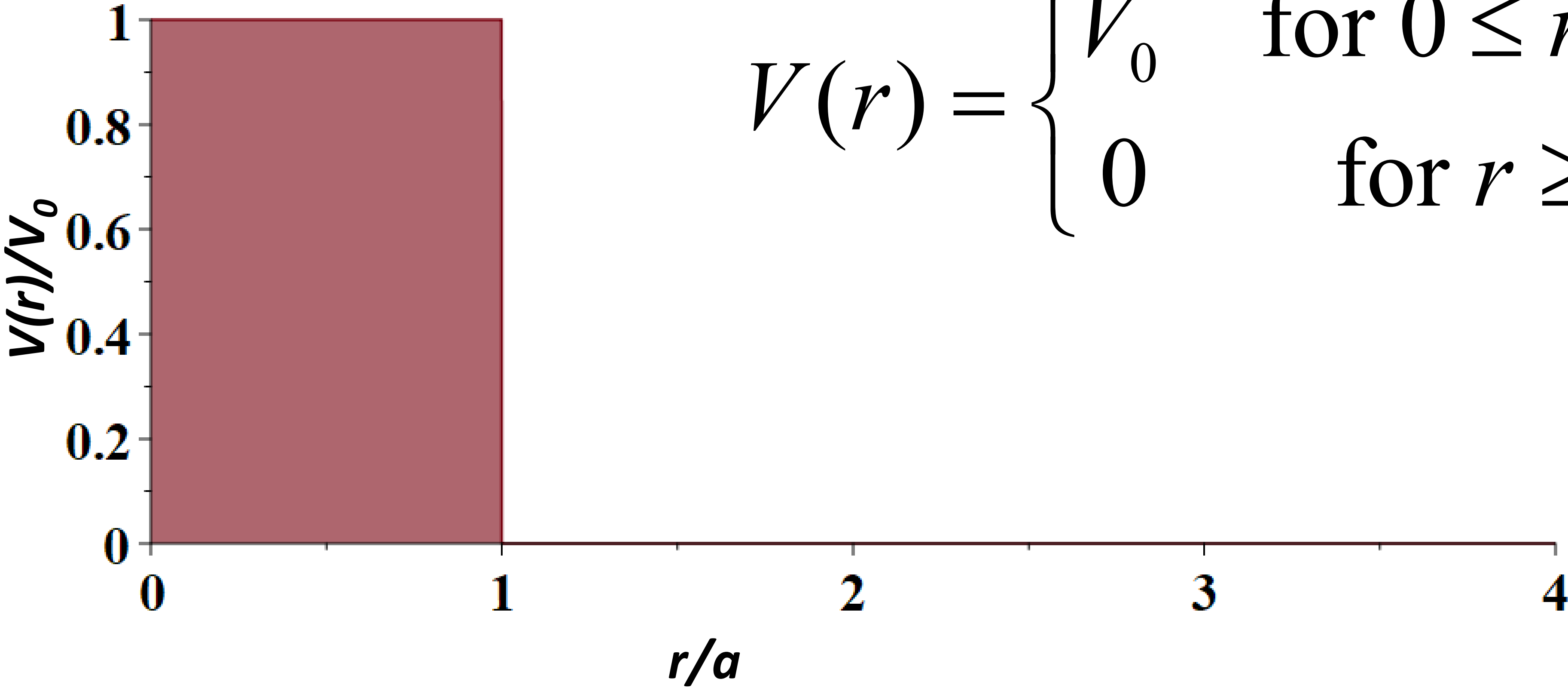
$$jj_1(x) = \frac{\sin(x)}{x} - \cos(x) \qquad yy_1(x) = -\frac{\cos(x)}{x} - \sin(x)$$

Similarly, we have scaled modified Bessel and Neumann functions

$$ii_0(x) = \sinh(x) \qquad kk_0(x) = \frac{\pi}{2} e^{-x}$$

$$ii_1(x) = -\frac{\sinh(x)}{x} + \cosh(x) \qquad kk_1(x) = \frac{\pi}{2} e^{-x} \left(\frac{1}{x} + 1 \right)$$

Example --



$$V(r) = \begin{cases} V_0 & \text{for } 0 \le r \le a \\ 0 & \text{for } r \ge a \end{cases}$$

For the case that $E < V_0$, define $\kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ and $k = \sqrt{\frac{2mE}{\hbar^2}}$

Example -- continued

Partial wave differential equation for $P_{El}(r)$:

$$\left(-\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}\right)+V(r)-E\right)P_{El}(r)=0$$

Focusing on the solution for $l=0$: For $r \le a$:

$$\left(\frac{d^2}{dr^2}-\kappa^2\right)P_{E0}(r)=0 \qquad \text{Physical solution:} \quad P_{E0}(r)=\sinh(\kappa r)$$

$$\text{where } \kappa=\sqrt{\frac{2m(V_0-E)}{\hbar^2}} \text{ and } k=\sqrt{\frac{2mE}{\hbar^2}}$$

$$LL_0(E)=\kappa\frac{\cosh\kappa a}{\sinh\kappa a}\equiv\frac{1}{\lambda_0} \qquad \tan\delta_0(E)=\frac{\sin(ka)/\lambda_0-k\cos(ka)}{-\cos(ka)/\lambda_0-k\sin(ka)}$$

Example -- continued

$$\tan\delta_0(E) = \frac{\sin(ka)/\lambda_0 - k\cos(ka)}{-\cos(ka)/\lambda_0 - k\sin(ka)} \qquad \lambda_0 = \frac{\sinh\kappa a}{\kappa\cosh\kappa a}$$

$$\text{For } ka \ll 1, \quad \tan\delta_0(E) \approx \delta_0(E) \approx \frac{ka/\lambda_0 - k}{-1/\lambda_0} = -k(a-\lambda_0)$$

Note that for infinite potential well, $\lambda_0 \to 0$ as derived previously.

More generally, for $ka \ll 1$ $\qquad \sigma \approx 4\pi(a-\lambda_0)^2$

Even more generally, this approach can be used to determine the exact cross section for this model from scattering amplitude:

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = \frac{4\pi}{k}\sum_{lm} e^{i\delta_l(E)}\sin(\delta_l(E))Y^*_{lm}(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}})$$

Some famous examples and extensions of phase shift analysis

1. **Ramsauer-Townsend effect -- scattering of electrons from spherical atoms**
2. **Xray absorption fine structure**

Ramsauer-Townsend effect -- Review article:
https://doi.org/10.1103/RevModPhys.5.257

OCTOBER, 1933 REVIEWS OF MODERN PHYSICS VOLUME 5

The Quantitative Study of the Collisions of Electrons with Atoms

ROBERT B. BRODE, *University of California*

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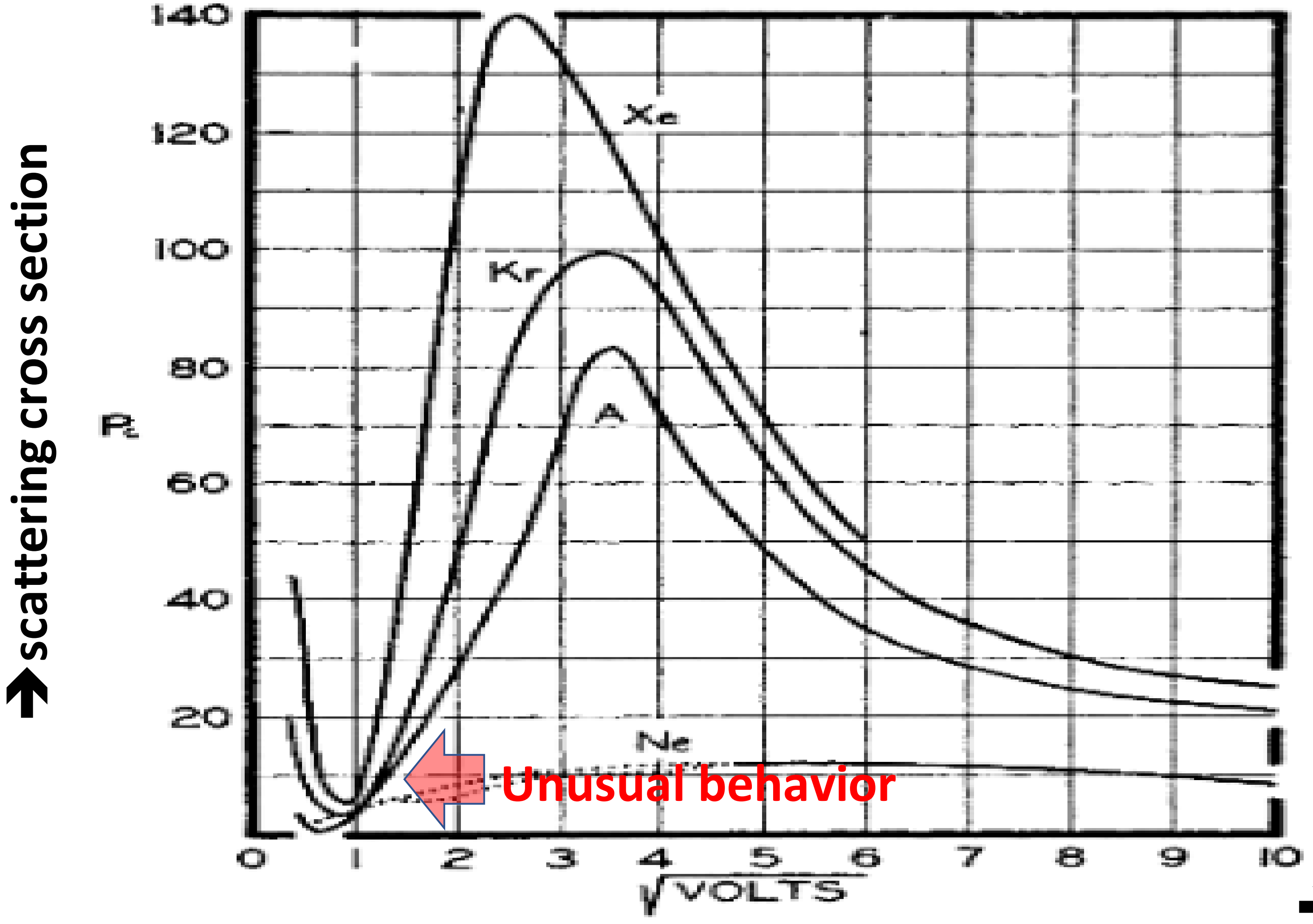


FIG. 8. Probability of collision in Ne, A, Kr and Xe.

Unusual effect caused by interaction potential

$$V(r) = -\frac{1}{2}\frac{\alpha e^2}{r^4}$$

➔increasing electron energy

Extended X-ray fine structure absorption spectroscopy (XAFS or EXAFS)

See for example:
https://www.lehigh.edu/imi/teched/GlassCSC/SuppReading/Tutorials.pdf

X-ray causes excitation of core electron which scatters from neighboring atoms causing absorption spectrum to show interference pattern related to local structure.

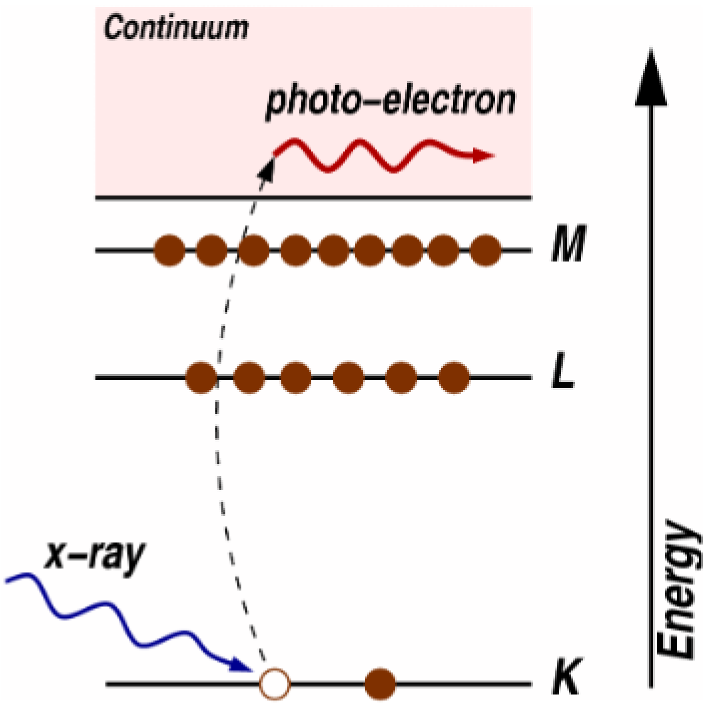


Figure 2.1: The photoelectric effect, in which an x-ray is absorbed and a core-level electron is promoted out of the atom.

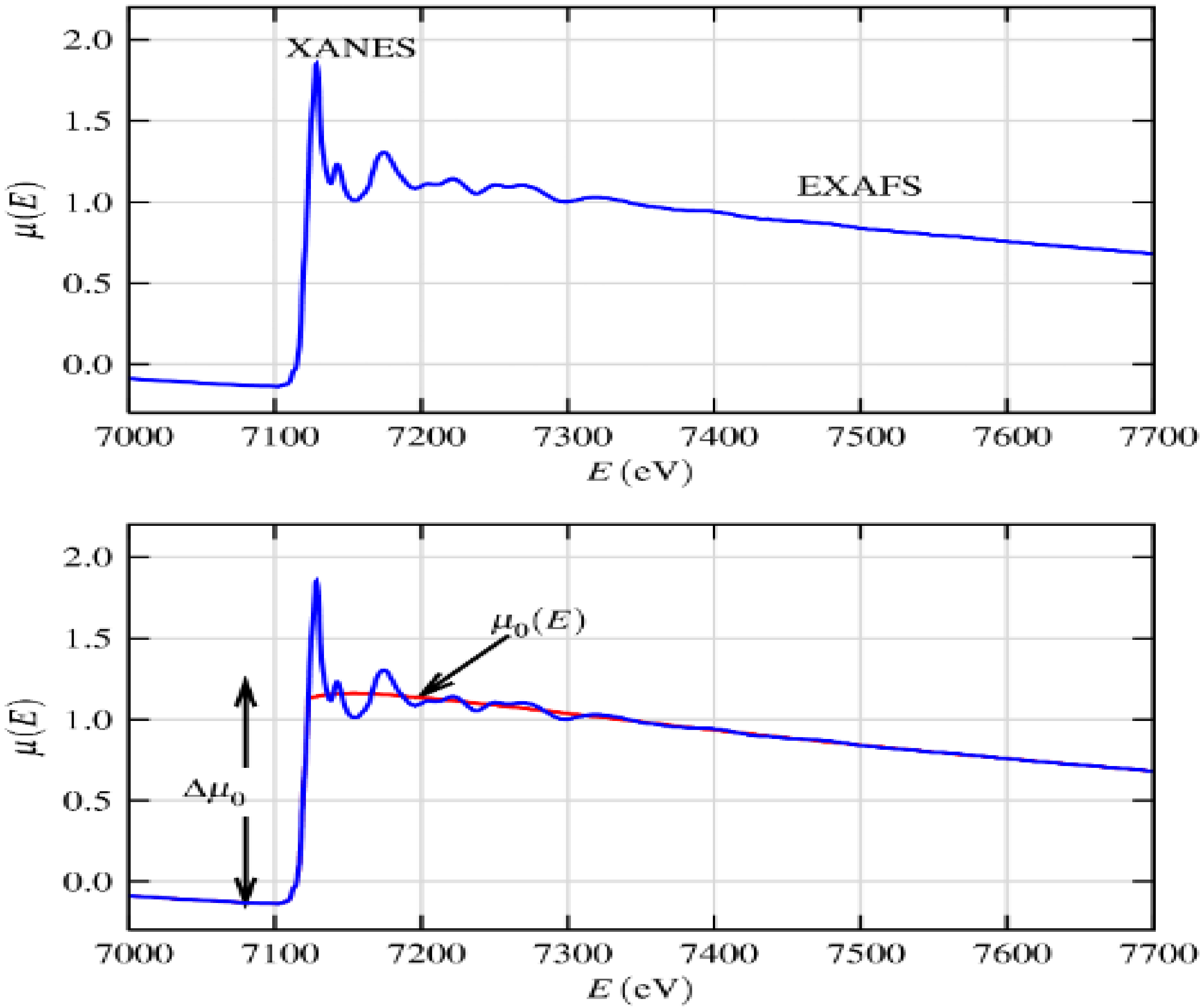


Figure 2.6: XAFS $\mu(E)$ for FeO. On top, the measured XAFS spectrum is shown with the XANES and EXAFS regions identified. On the bottom, $\mu(E)$ is shown with smooth background function $\mu_0(E)$ and the edge-step $\Delta\mu_0(E_0)$.

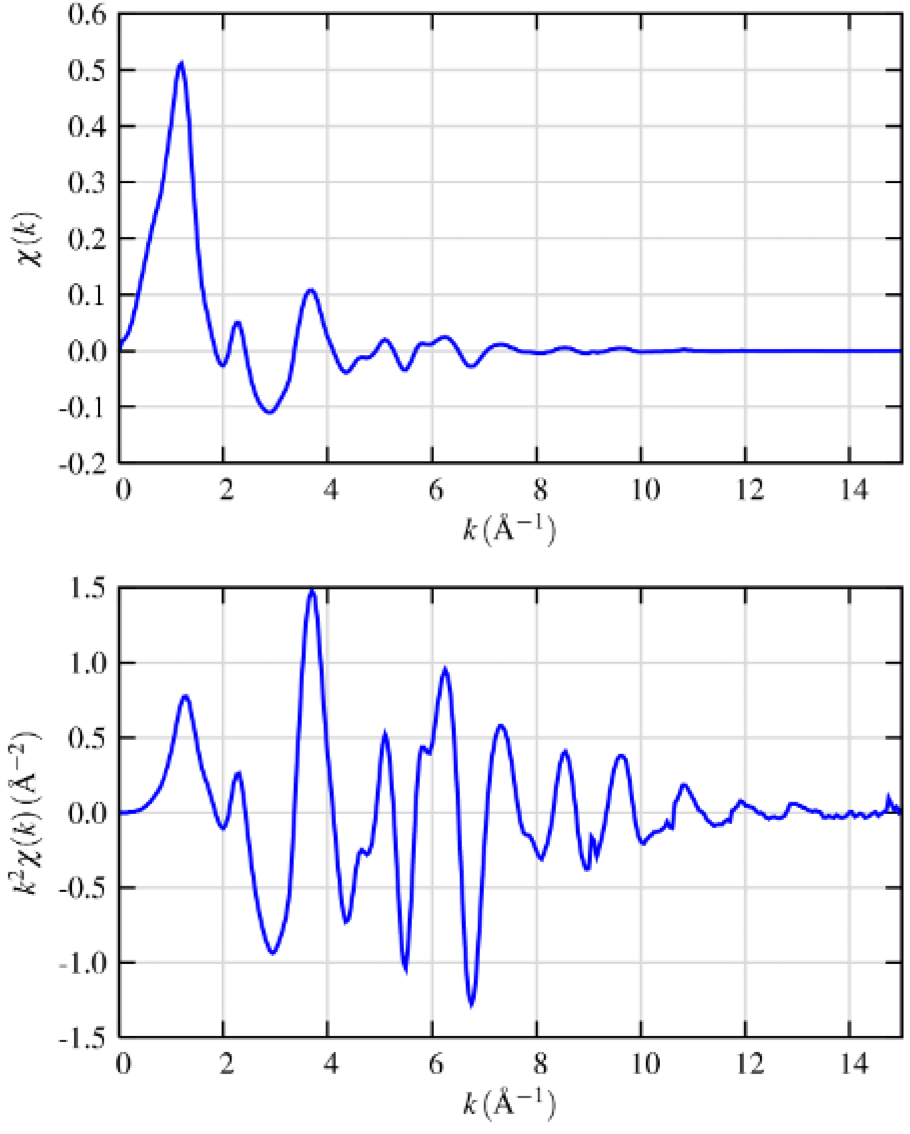


Figure 2.7: Isolated EXAFS $\chi(k)$ for FeO (top), and the k-weighted XAFS, $k^2\chi(k)$ (bottom).

Spectra fit to scattering theory based expression for neighboring atoms at R_j

$$\chi(k) = \sum_j \frac{N_j e^{-2k^2\sigma_j^2} f_j(k)}{kR_j^2} \sin[2kR_j + \delta_j(k)]$$

Approximate treatment of scattering – Born approximation

In this treatment, we use the notions of perturbation theory

$$H = H^0 + H^1$$

$$H^0 = -\frac{\hbar^2}{2m}\nabla^2$$

$$H^1 = V(r)$$

In this case, the relevant eigenstates of H^0 are plane waves.

$$H^0\left|\Psi_E^0\right\rangle = E\left|\Psi_E^0\right\rangle \qquad \left|\Psi_E^0\right\rangle = e^{i\mathbf{k}\cdot\mathbf{r}} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Equation for first order wavefunction:

$$\left(H^0(\mathbf{r})-E\right)\left|\Psi^1\right\rangle=-V(r)\left|\Psi^0\right\rangle$$

Note that for

$$\left(-\frac{\hbar^2}{2m}\nabla^2-E\right)G(\mathbf{r},\mathbf{r}',E)=-\delta\left(\mathbf{r}-\mathbf{r}'\right)$$

$$G(\mathbf{r},\mathbf{r}',E)=-\frac{2m}{\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

$$\left|\Psi^1\right\rangle=-\int d^3r'G(\mathbf{r},\mathbf{r}',E)V(r')\Psi^0(\mathbf{r}')$$

$$\left|\Psi\right\rangle\approx e^{i\mathbf{k}\cdot\mathbf{r}}-\frac{2m}{4\pi\hbar^2}\int d^3r'\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}V(r')e^{i\mathbf{k}\cdot\mathbf{r}'}$$

$$\left|\Psi\right\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\int d^3r' \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} V(r')e^{i\mathbf{k}\cdot\mathbf{r}'}$$

For $r \gg r'$, $|\mathbf{r}-\mathbf{r}'| \approx r - \mathbf{r}'\cdot\hat{\mathbf{r}}$

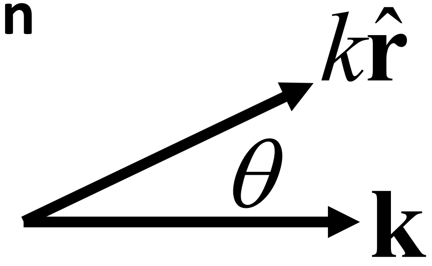
$$\left|\Psi\right\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(r')e^{i\mathbf{k}\cdot\mathbf{r}'}$$

$$\approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

Scattering amplitude in the Born approximation:

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

Example – screened Coulomb interaction



$$V(r) = -\frac{Ze^2}{r} e^{-\gamma r}$$

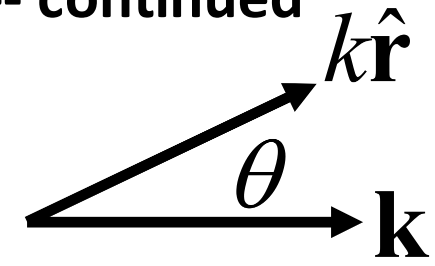
$$f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2} \int d^3r' e^{i(\mathbf{k} - k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

$$= \frac{2m}{\hbar^2} \frac{Ze^2}{K} \int_0^\infty dr' \; e^{-\gamma r'} \sin(Kr')$$

$$= \frac{2m}{\hbar^2} \frac{Ze^2}{\left(K^2 + \gamma^2\right)}$$

where $\quad K = \left|\mathbf{k} - k\hat{\mathbf{r}}\right| = 2k \sin(\theta / 2)$

Example – screened Coulomb interaction -- continued



$$V(r) = -\frac{Ze^2}{r}e^{-\gamma r}$$

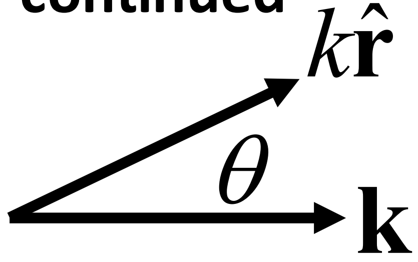
$$K = \left|\mathbf{k} - k\hat{\mathbf{r}}\right| = 2k\sin(\theta/2)$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = \frac{2m}{\hbar^2}\frac{Ze^2}{\left(K^2+\gamma^2\right)}$$

Differential cross section:

$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2 = \left(\frac{2mZe^2}{\hbar^2}\right)^2 \left|\frac{1}{\left(K^2+\gamma^2\right)}\right|^2$$

Example – screened Coulomb interaction -- continued



$$V(r) = -\frac{Ze^2}{r} e^{-\gamma r}$$

$$K = \left|\mathbf{k} - k\hat{\mathbf{r}}\right| = 2k\sin(\theta/2)$$

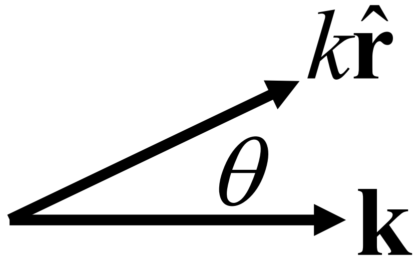
Differential cross section:

$$\frac{d\sigma}{d\Omega} = \left| f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) \right|^2 = \left(\frac{2mZe^2}{\hbar^2} \right)^2 \left| \frac{1}{\left(K^2 + \gamma^2\right)} \right|^2$$

Note that for $\gamma \rightarrow 0$:

$$\frac{d\sigma}{d\Omega} = \left| f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) \right|^2 = \left(\frac{2mZe^2}{\hbar^2} \right)^2 \frac{1}{K^4} = \left(\frac{Ze^2}{4E} \right)^2 \frac{1}{\sin^4\left(\frac{\theta}{2}\right)}$$

Example – spherical well



$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

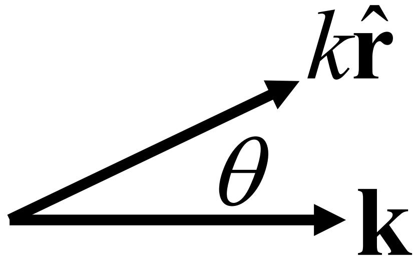
$$f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2} \int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

$$= -\frac{2m}{4\pi\hbar^2} \frac{4\pi V_0}{K} \int_0^a dr'\; r' \sin(Kr')$$

$$= -\frac{2m}{\hbar^2} \frac{V_0}{K^3} \left(\sin(Ka) - Ka\cos(Ka) \right)$$

where $\quad K = \left| \mathbf{k} - k\hat{\mathbf{r}} \right| = 2k\sin(\theta/2)$

Example – spherical well – continued



$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

$$K = \left|\mathbf{k} - k\hat{\mathbf{r}}\right| = 2k\sin(\theta/2)$$

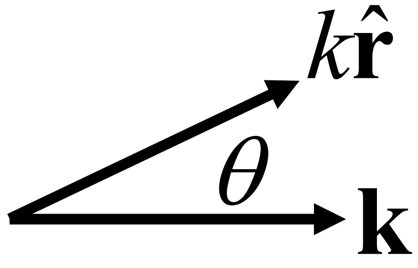
$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{\hbar^2}\frac{V_0}{K^3}\left(\sin(Ka) - Ka\cos(Ka)\right)$$

Differential cross section:

$$\frac{d\sigma}{d\Omega} = \left|f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2 = \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{K^6}\left|\sin(Ka) - Ka\cos(Ka)\right|^2$$

Total cross section: $\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \frac{2\pi}{k^2}\int_0^{2k} \frac{d\sigma}{d\Omega} K dK$

Example – spherical well – continued
(Ref. Landau and Lifshitz)



$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

$$K = \left|\mathbf{k} - k\hat{\mathbf{r}}\right| = 2k\sin(\theta/2)$$

$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{\hbar^2}\frac{V_0}{K^3}\left(\sin(Ka) - Ka\cos(Ka)\right)$$

$$\text{Total cross section: } \sigma = \int \frac{d\sigma}{d\Omega}d\Omega = \frac{2\pi}{k^2}\int_0^{2k}\frac{d\sigma}{d\Omega}KdK$$

$$\text{When the dust clears: } \sigma = \frac{2\pi}{4k^2}\left(\frac{2mV_0a^2}{\hbar^2}\right)^2\left(1 - \frac{1}{(2ka)^2} + \frac{\sin(4ka)}{(2ka)^3} - \frac{\sin^2(2ka)}{(2ka)^4}\right)$$

$$\text{For } ka \ll 1 \quad \sigma \approx \frac{4\pi a^2}{9}\left(\frac{2mV_0a^2}{\hbar^2}\right)^2 \qquad ka \gg 1 \quad \sigma \approx \frac{\pi}{2k^2}\left(\frac{2mV_0a^2}{\hbar^2}\right)^2$$

(Not generally consistent with phase shift analysis.)

Beyond the Born approximation

Equation for full wavefunction:

$$\left(H^0(\mathbf{r}) - E\right)\left|\Psi\right\rangle = -V(r)\left|\Psi\right\rangle$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)G(\mathbf{r},\mathbf{r}',E) = -\delta\left(\mathbf{r}-\mathbf{r}'\right) \qquad G(\mathbf{r},\mathbf{r}',E) = -\frac{2m}{\hbar^2}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}$$

$$\left|\Psi\right\rangle = \int d^3r' G(\mathbf{r},\mathbf{r}',E)V(r')\Psi(\mathbf{r}')$$

$$\left|\Psi\right\rangle \approx \left|\Psi^0\right\rangle + \int d^3r' G(\mathbf{r},\mathbf{r}',E)V(r')\Psi^0(\mathbf{r}')$$

$$+\int d^3r'' G(\mathbf{r},\mathbf{r}'',E)V(r'')\Psi^0(\mathbf{r}'')\int d^3r' G(\mathbf{r}'',\mathbf{r}',E)V(r')\Psi^0(\mathbf{r}')$$

$$+\ldots$$