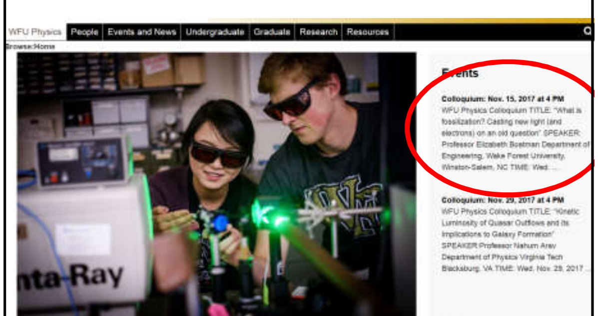
PHY 741 Quantum Mechanics
12-12:50 AM MWF Olin 103

Plan for Lecture 31:

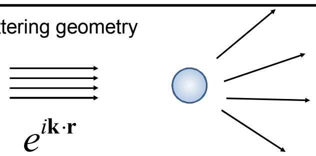
Chap. 19 in Shankar: Scattering theory

1. **Scattering cross section in terms of phase shifts**
2. **Optical theorem**
3. **Born approximation**

22	Mon, 10/23/2017	Chap. 15	Multi-electron atoms	#13	10/25/2017
23	Wed, 10/25/2017	Chap. 15	Multi-electron atoms	#14	10/30/2017
24	Fri, 10/27/2017		Effects of nuclear motion		
25	Mon, 10/30/2017	Chap. 17	Time-independent perturbation theory	#15	11/3/2017
26	Wed, 11/01/2017	Chap. 17	Time-independent perturbation theory		
27	Fri, 11/03/2017		Effects of a static magnetic field		
28	Mon, 11/06/2017	Chap. 18	Time-dependent perturbation theory	#16	11/10/2017
29	Wed, 11/08/2017	Chap. 18	Time-dependent perturbation theory		
30	Fri, 11/10/2017	Chap. 19	Scattering theory	#17	11/15/2017
	Mon, 11/13/2017		*Class cancelled*		
31	Wed, 11/15/2017	Chap. 19	Scattering theory		
32	Fri, 11/17/2017	Chap. 20	Dirac Equation		
33	Mon, 11/20/2017	Chap. 20	Dirac Equation		
	Wed, 11/22/2017		*Thanksgiving Holiday -- No class*		
	Fri, 11/24/2017		*Thanksgiving Holiday -- No class*		
34	Mon, 11/27/2017	Chap. 20	Dirac Equation		
35	Wed, 11/29/2017	Chap. 20	Dirac Equation		
36	Fri, 12/01/2017	Chap. 1-20	Review		
	Mon, 12/04/2017		Presentations I		
	Wed, 12/06/2017		Presentations II		
	Fri, 12/08/2017		Presentations III		



Scattering geometry



$$e^{i\mathbf{k}\cdot\mathbf{r}} \qquad f(\hat{\mathbf{k}})\frac{e^{ikr}}{r}$$

Differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{\text{Probability of particle scattering}}{\text{Incident flux of particles}}$$

$$= \left| f(\hat{\mathbf{k}}, \hat{\mathbf{r}}) \right|^2$$

$$= \left(\frac{4\pi}{k}\right)^2 \left| \sum_{lm} e^{i\delta_l(E)} \sin(\delta_l(E)) Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \right|^2$$

Some details:

It can be shown that: $e^{i\mathbf{k}\cdot\mathbf{r}} = 4\pi \sum_{lm} i^l j_l(kr) Y_{lm}{}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}})$

In presence of spherically symmetric interaction potential $V(r)$:

$$\Psi_E(\mathbf{r}) = \sum_{lm} R_{El}(r) Y_{lm}(\hat{\mathbf{r}})$$

Differential equation for radial function

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

Outside the range of $V(r)$; when $V(r) \approx 0$:

$$R_{El}(r) = A_l j_l(kr) + B_l y_l(kr) = \mathcal{N}_l \left(\cos\delta_l j_l(kr) - \sin\delta_l y_l(kr) \right)$$

Denote by D a radius outside the range of $V(r)$.

We can calculate the log-derivative:

$$\frac{d\ln\left(R_{El}(r)\right)}{dr} = \left. \frac{\dfrac{dR_{El}(r)}{dr}}{R_{El}(r)} \right|_{r=D} \equiv L_l(E)$$

It follows that:

$$\tan\left(\delta_l(E)\right) = \frac{L_l(E) j_l(kD) - k j_l'(kD)}{L_l(E) y_l(kD) - k y_l'(kD)}$$

From the assymptotic form of the Bessel functions:

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

$$\frac{d\sigma}{d\Omega} = \left| f(\hat{\mathbf{k}},\hat{\mathbf{r}})\right|^2$$

Total scattering cross section:

$$\sigma(E) = \int d\Omega \frac{d\sigma}{d\Omega} = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2(\delta_l(E))$$

Interesting identities; "optical theorem"

Note that: $\sum_{m=-l}^{l} Y_{lm}{}^*(\hat{\mathbf{k}})Y_{lm}(\hat{\mathbf{r}}) = \frac{2l+1}{4\pi}P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})$

where $P_l(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})$ is a Legendre polynomial where $P_l(1) = 1$

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

$$\sigma(E) = \frac{4\pi}{k^2}\sum_l (2l+1)\sin^2(\delta_l(E))$$

Note that:

$$\Im\left(f\left(\hat{\mathbf{k}}=\hat{\mathbf{r}}\right)\right) = \frac{k}{4\pi}\sigma(E)$$

Imaginary part of forward scattering is proportional to the total scattering cross section.

The phase shift analysis of scattering theory provides a convenient mechanism to relate experiment to the interaction potential

Example --

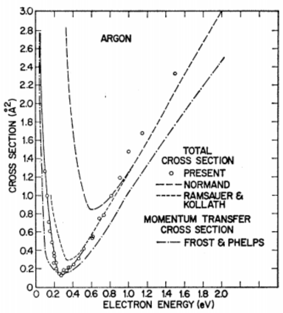
PHYSICAL REVIEW VOLUME 149, NUMBER 1 9 SEPTEMBER 1966

Low-Energy e^--Ar Total Scattering Cross Sections: The Ramsauer-Townsend Effect*

D. E. GOLDEN AND H. W. BANDEL
Lockheed Palo Alto Research Laboratories, Palo Alto, California
(Received 25 April 1966)

The Ramsauer technique has been used to measure absolute total e^--Ar scattering cross sections from 0.1 to 21.6 eV with an estimated probable error of ±3%. A phase-shift analysis of the data (for the l=0,1,2 partial waves) has been made using "modified effective range" theory which yields a scattering length of $-1.65\ a_0$ and a minimum total cross section of 0.125 Å² at 0.285 eV.

FIG. 2. e^--Ar scattering cross sections versus electron energy 0–2 eV.



This minimum in σ is not seen in e-He and e-Ne scattering.

It can be explained by $V(r) \approx -\frac{\alpha e^2}{2r^4}$ due to atom polarization.

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

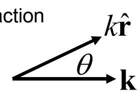
$$\left|\Psi\right\rangle \approx e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{2m}{4\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r' e^{-ik\hat{\mathbf{r}}\cdot\mathbf{r}'} V(r') e^{i\mathbf{k}\cdot\mathbf{r}'}$$

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

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



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

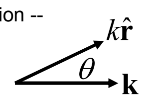
$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'} V(r')$$

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

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

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

Example – screened Coulomb interaction -- continued



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

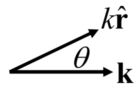
$$V(r) = -\frac{Ze^2}{r}e^{-\gamma r}$$

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

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 – spherical well



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

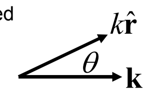
$$f(\hat{\mathbf{k}},\hat{\mathbf{r}}) = -\frac{2m}{4\pi\hbar^2}\int d^3r' e^{i(\mathbf{k}-k\hat{\mathbf{r}})\cdot\mathbf{r}'}V(r')$$

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

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

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

Example – spherical well – continued



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

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

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

Differential cross section:

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

Beyond the Born approximation

Equation for full wavefunction:

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

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

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

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

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

$$+\ldots$$