原子過程理論－電子衝突散乱断面積の解析

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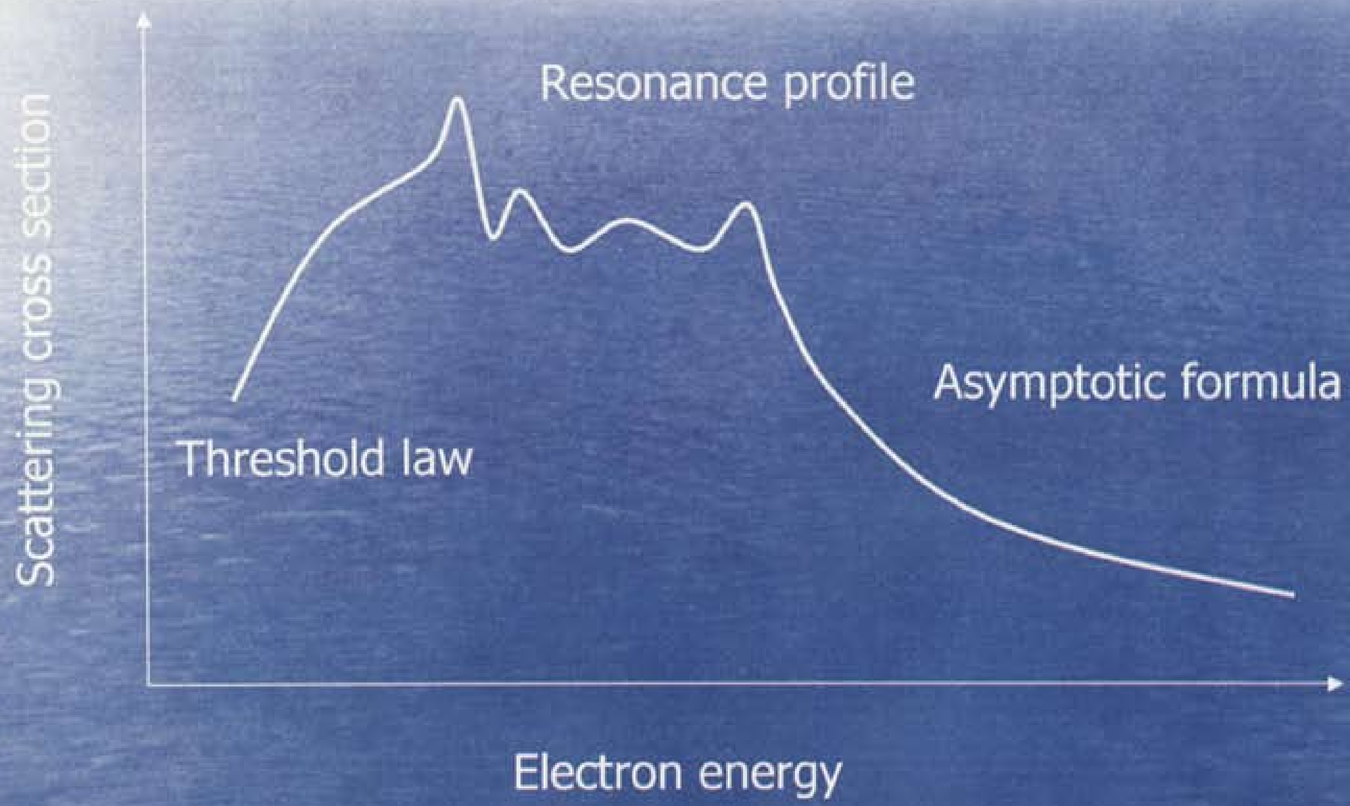
OUTLINE

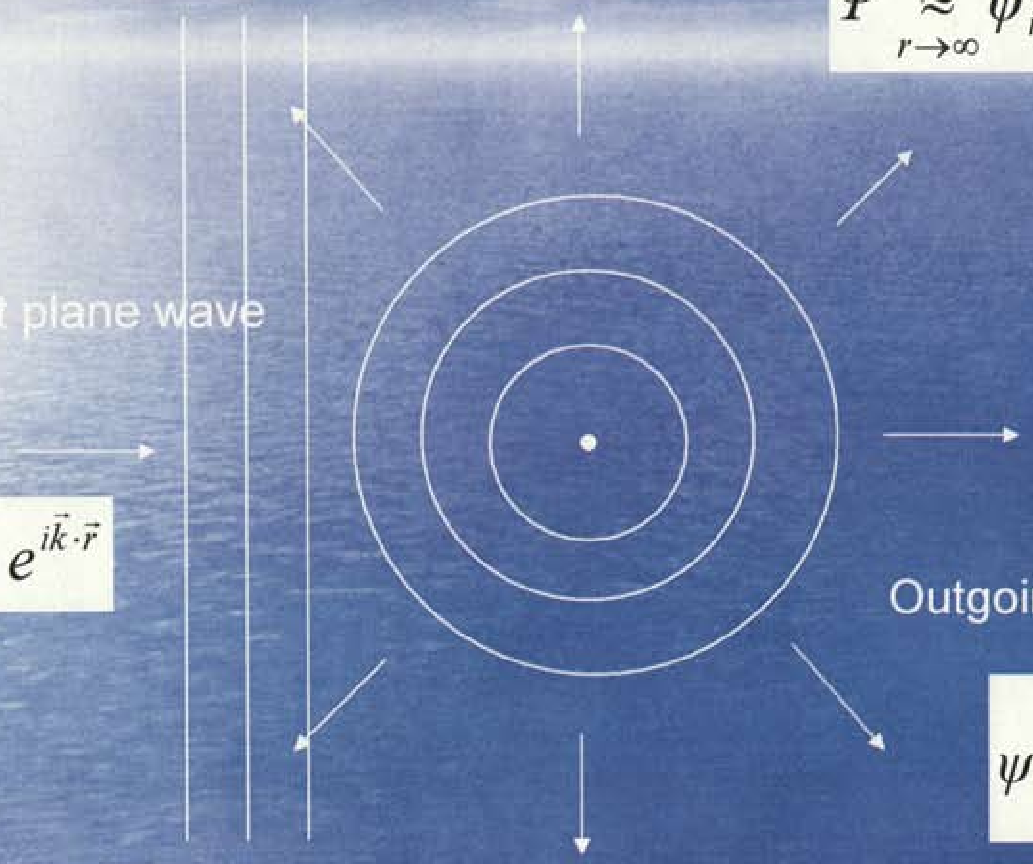
- Basic theories for scattering cross sections
- Scattering cross sections near threshold
- Resonance profile
- Inelastic scattering cross section at high energies (asymptotic formula)

Overall picture of scattering cross section



Electron wave scattering

$$\Psi \underset{r\to\infty}{\approx} \psi_{inc} + \psi_{sc}$$



Incident plane wave

$$\psi_{inc} = e^{i\vec{k}\cdot\vec{r}}$$

Outgoing wave

$$\psi_{sc} = f(k,\theta,\phi)\frac{e^{ikr}}{r}$$

Integral equation for potential scattering
(Lippmann-Schwinger equation)

Schroedinger equation :

$$\left(\nabla^2 + k^2\right)\Psi = U(\vec{r})\Psi$$

A general solution is written formally as,

$$\Psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \int G_0^{(+)}(k,\vec{r},\vec{r}')U(\vec{r}')\Psi(\vec{r}')d\vec{r}'$$

Green's function of outgoing wave :

$$\left(\nabla^2 + k^2\right)G_0^{(+)} = \delta(\vec{r} - \vec{r}')$$

$$G_0^{(+)} = -\frac{1}{4\pi}\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r} - \vec{r}'|}$$

Born series of scattering amplitude

Iterative solution :

$$\Psi_0 = e^{i\vec{k}\cdot\vec{r}}$$

$$\Psi_1 = e^{i\vec{k}\cdot\vec{r}} + \int G_0^{(+)} U \Psi_0 d\vec{r}'$$

$$\vdots$$

$$\Psi_n = e^{i\vec{k}\cdot\vec{r}} + \int G_0^{(+)} U \Psi_{n-1} d\vec{r}'$$

Born series for the scattering amplitude :

$$f = -\frac{1}{4\pi}\left\langle e^{-i\vec{k}'\cdot\vec{r}} \middle| U + UG_0^{(+)}U + UG_0^{(+)}UG_0^{(+)}U + \cdots \middle| e^{i\vec{k}\cdot\vec{r}} \right\rangle$$

Partial-wave expansion of scattering amplitude and phase shift

For spherical potential

Radial Schroedinger equation of each partial - wave :

$$\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}-U(r)+k^2\right]R_l(k,r)=0$$

Partial - wave expansion of f and phase shift δ_l :

$$f(k,\theta)=\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)\left[\exp\left(2i\delta_l(k)\right)-1\right]P_l(\cos\theta)$$

Integral representation of phase shift :

$$\tan\delta_l=-k\int_0^{\infty}j_l(kr)U(r)R_l(k,r)r^2dr$$

Differential cross section :

$$\frac{d\sigma}{d\Omega}=\frac{k}{k}|f|^2$$

Integrated cross section :

$$\sigma(\mathrm{k})=2\pi\int_0^{\pi}|f|^2\sin\theta d\theta=\frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l(k)$$

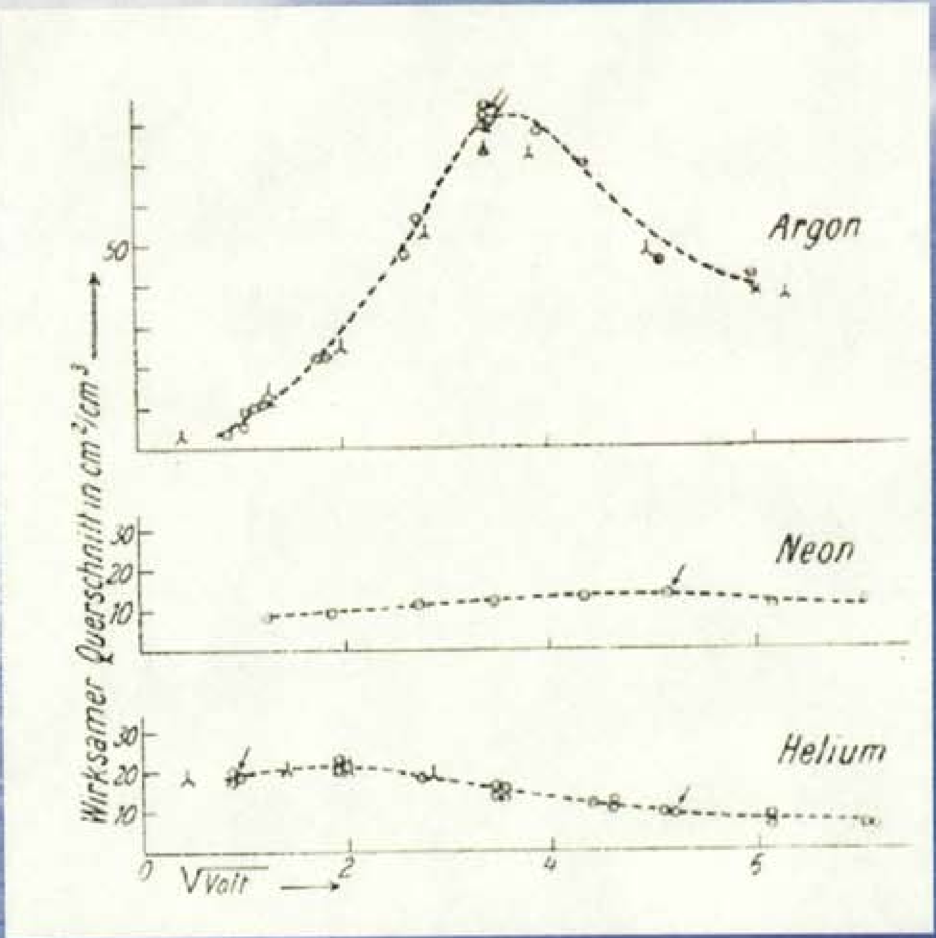
Convergence of partial-wave expansion

Impact parameter for particle momentum (p) and orbital angular momentum (L) :

$$b = \frac{L}{p}$$

Particles with orbital angular momentum $L > pa$
are not scattered by potential which vanishes beyond a certain distance a.

Ramsauer effect in slow electron scattering by noble gas atom



C. Ramsauer, Ann. d. Phys. 66, 546 (1921).

Cross section of s - wave:

$$\sigma \approx \frac{4\pi}{k^2}\sin^2\delta_0(k) = 0 \quad \text{at} \quad \delta_0(k) = n\pi.$$

In Jena I was particularly interested in a paper of Ramsauer that I am not able to believe, though I cannot show any mistake in the experiment. Ramsauer obtained the result that in argon the free path lengths are tremendously large at very low velocity of electrons....If this result is right, it seems to me fundamental.

J. Franck（フランク－ヘルツの実験のフランク）がN. Bohrに宛てた手紙の抜粋

原子衝突協会誌「しょうとつ」第3巻第3号（2006年）“原子衝突実験の歩み” 市川行和 より転載

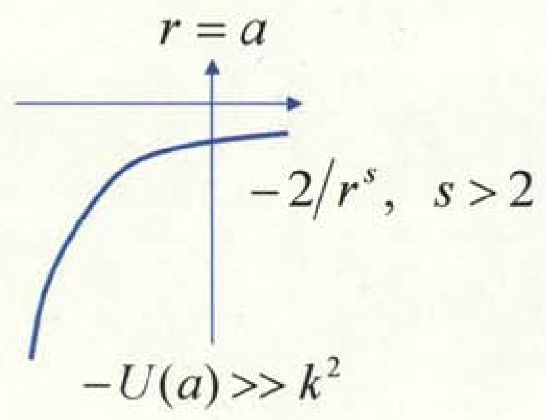
Zero-energy behavior of phase shift and scattering length

External solution by linear combination of spherical Bessel functions $\{j_l, n_l\}$:

$R_l(k,r) \approx j_l(kr) - \tan\delta_l n_l(kr)$ for $r > a$.

Matching logarithmic derivative of internal solution $\gamma_l \equiv \left[R_l^{-1}(dR_l/dr)\right]$ $(r < a)$ external solution $(r > a)$ at $r = a$:

$$\tan\delta_l = \frac{(dj_l/dr)_{r=a} - \gamma_l(k)\, j_l(ka)}{(dn_l/dr)_{r=a} - \gamma_l(k)\, n_l(ka)}$$



As $\lim_{k\to 0} \gamma_l$ does not depend on k, $\tan\delta_l \underset{k\to 0}{\approx} k^{2l+1}$.

Defining scattering length $\alpha = -\lim_{k\to 0} \frac{\tan\delta_0}{k}$,

scattering amplitude becomes $f \underset{k\to 0}{\approx} -\alpha$, and total cross section $\sigma \underset{k\to 0}{\approx} 4\pi\alpha^2$.

Zero-energy behavior for scattering with Coulomb potential

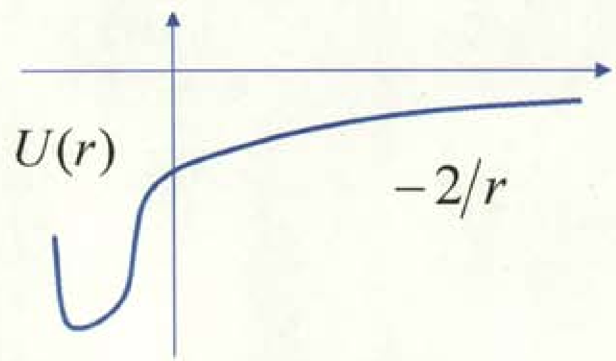
$$\tan\delta_l^C = -k\int_0^\infty \psi_l^C(kr)U(r)R_l^C(k,r)r^2dr$$

Regular Coulomb function F_l :

$$\psi_l^C(kr) = k^{-1}F_l(-1/ka_0, kr)$$

$$\lim_{k\to 0}\psi_l^C(kr) \propto k^{-1/2}, \text{ as } \lim_{k\to 0}F_l(-1/ka_0, kr) \propto k^{1/2}.$$

Scattering amplitude $f \propto k^{-1}$, and cross section $\sigma \propto k^{-2}$ that is consistent with Rutherford formula.



Zero-energy behavior of inelastic scattering

Differential cross section for inelastic scattering :

$$\frac{d\sigma_{q0}}{d\Omega} = \frac{k_q}{k_0}\left|f_q\right|^2$$

$$\tan\delta_{l,q} = -k_q \int_0^\infty \psi_l(k_q r) U_{q0}(r) R_l(k_0, r) r^2 dr$$

$$f_q \underset{k\to 0}{\approx} \frac{\tan\delta_{0,q}}{k_q}$$

For excitation of neutral atom (no long - range potential) :

$$\frac{d\sigma_{q0}}{d\Omega} \propto k_q$$

For excitation of ion (long - range potential) :

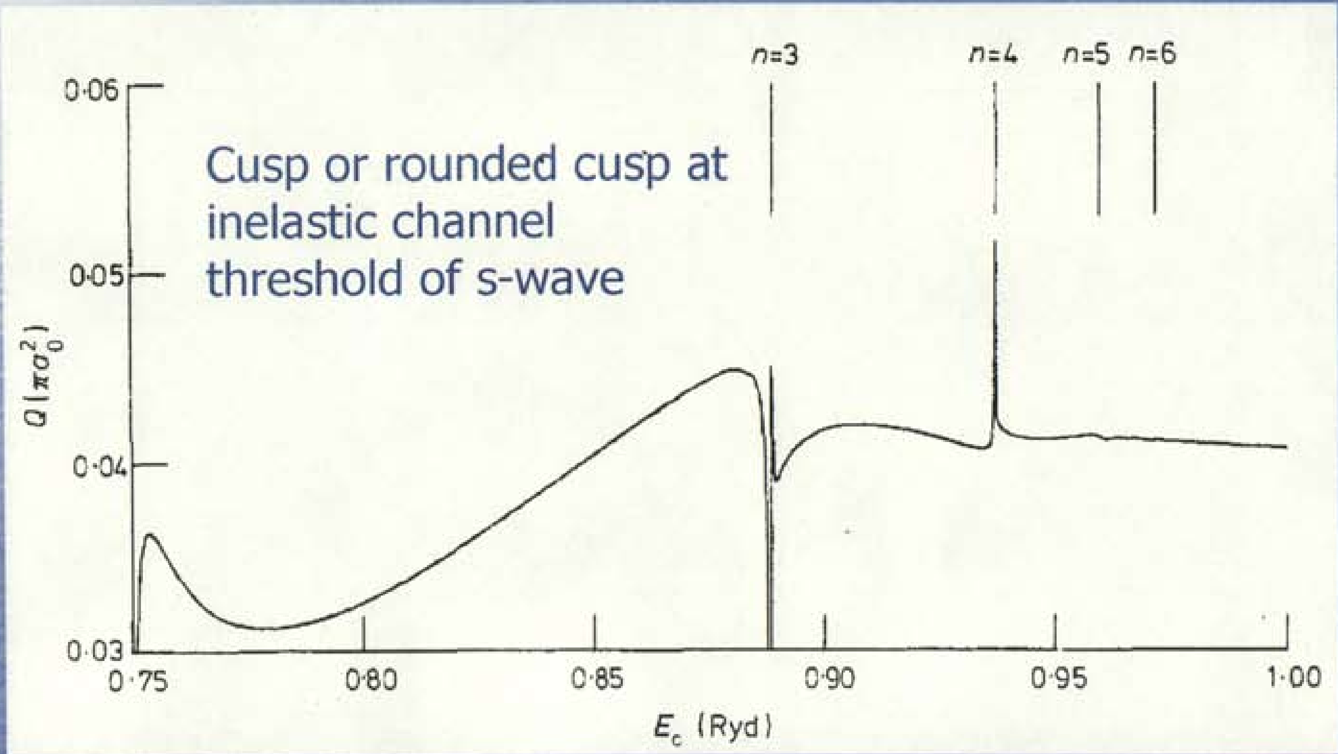
$$\frac{d\sigma_{q0}}{d\Omega} \propto k_q^0 \ \text{(constant)}$$

Singularities in integrated cross section

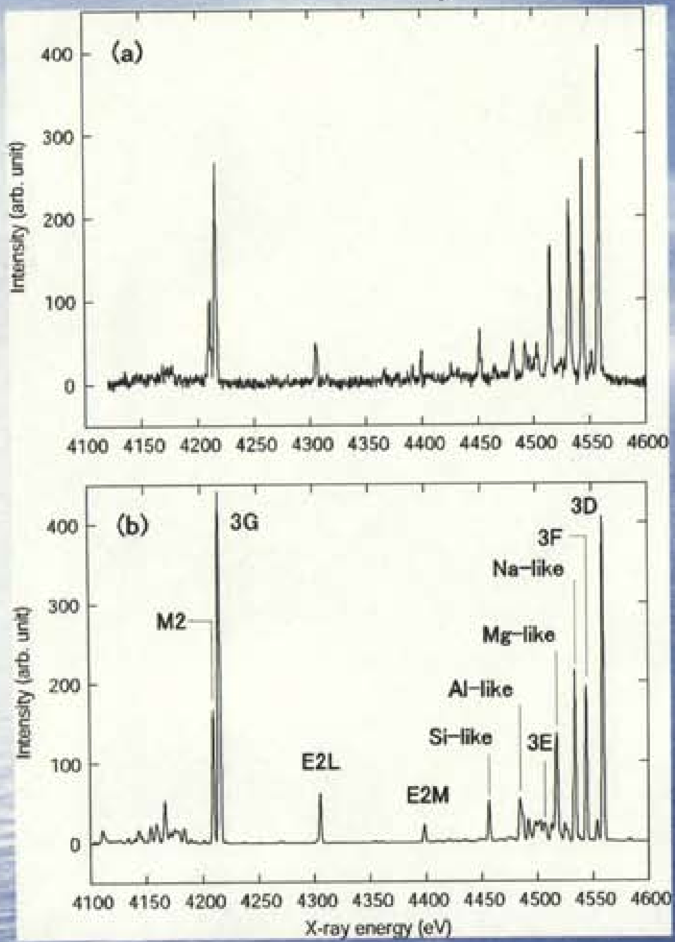
Temkin - Poet model (s^2 model):

$$\left(\nabla_1^2 + \nabla_2^2 + \frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{\max(r_1, r_2)} + E\right)\Psi = 0$$

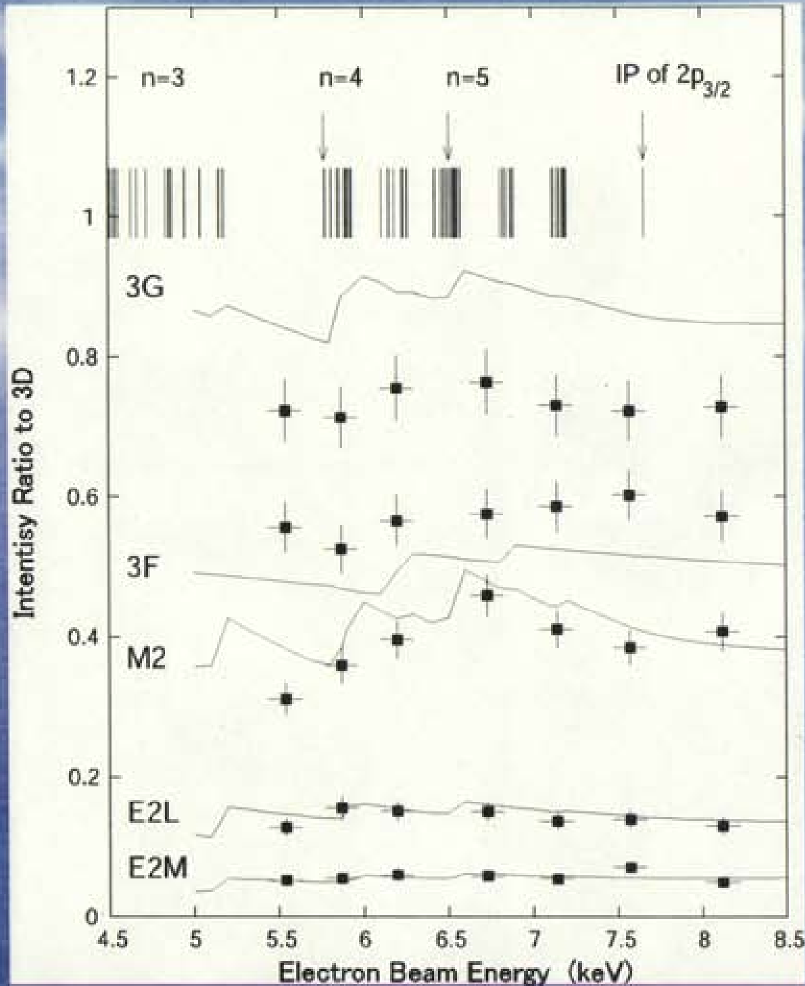
Singlet 1s-2s excitation cross section of H atom



R. Poet, J. Phys. B 11, 3081 (1978).



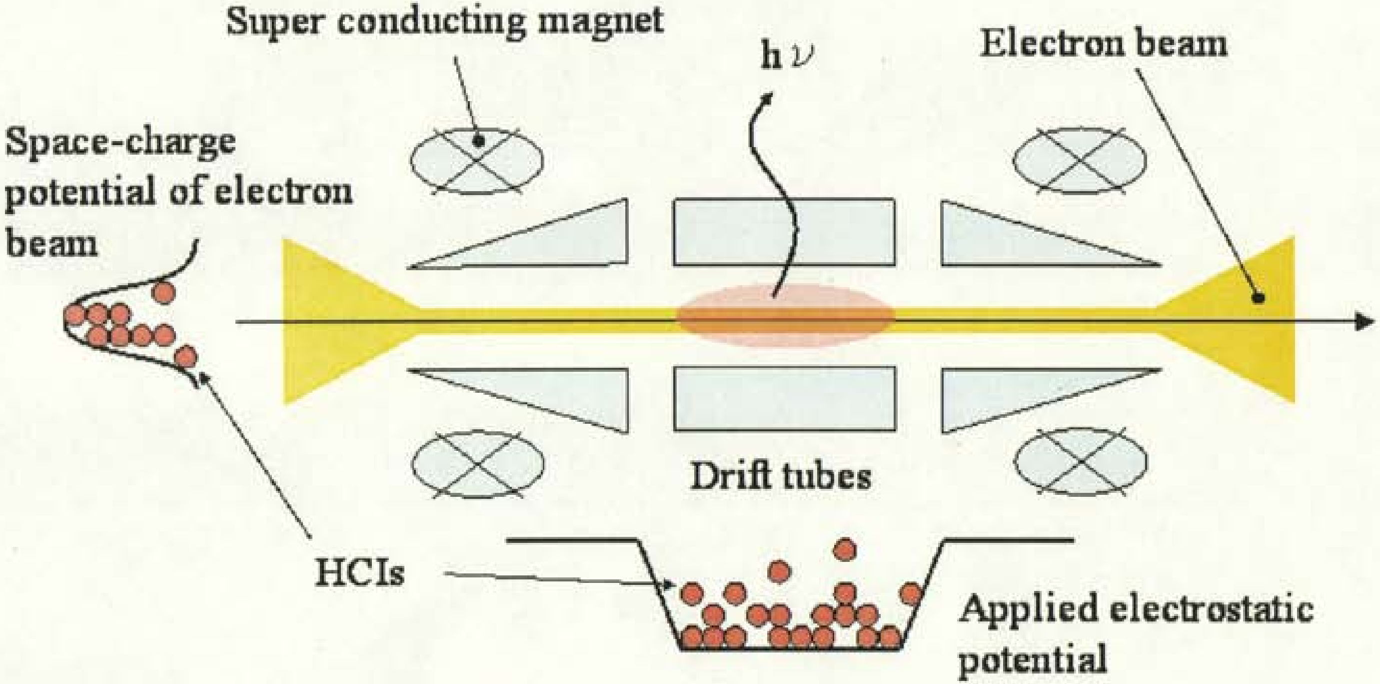
(a) Experimental X-ray spectrum of Xe ions measured at the Tokyo-EBIT. Electron beam energy Ee = 5540 eV (below the ionization energy of the Ne-like Xe ion).
(b) Synthetic spectrum convoluted using the Gaussian distribution function with a full-width-at-half-maximum of 2 eV. 3D, 3E, 3F, 3G, E2M, E2L, and M2 lines are of Ne-like ions.



X-ray Intensity variation as a function of electron energy. $2p_{3/2} \rightarrow nl$ excited level energies and the ionization energy of $2p_{3/2}$ orbital are indicated by vertical lines in the upper part of the figure.

D. Kato et al., JPFR Vol. 7, 190 (2006).

Electron Beam Ion Trap (EBIT)

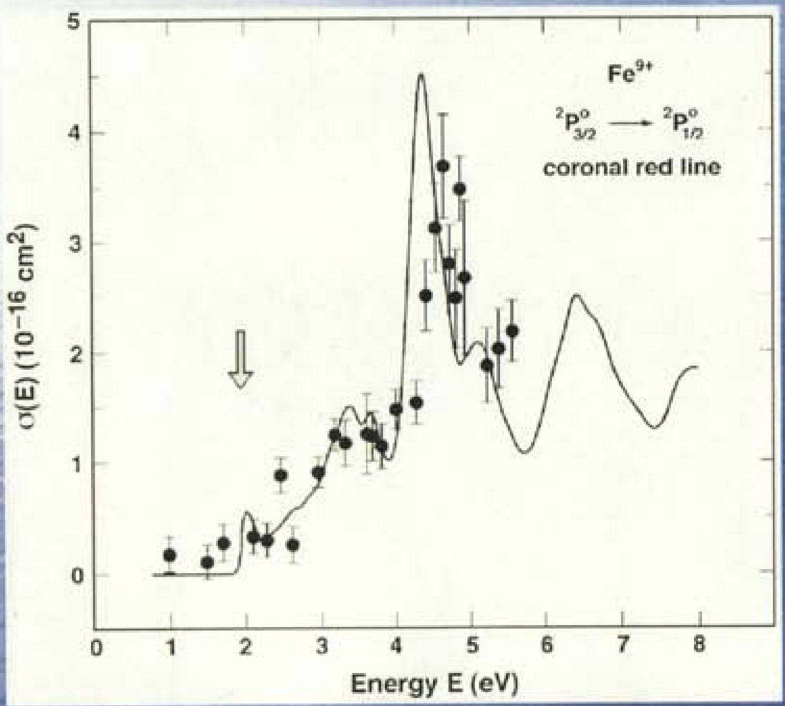


Feshbach resonance of excitation cross section

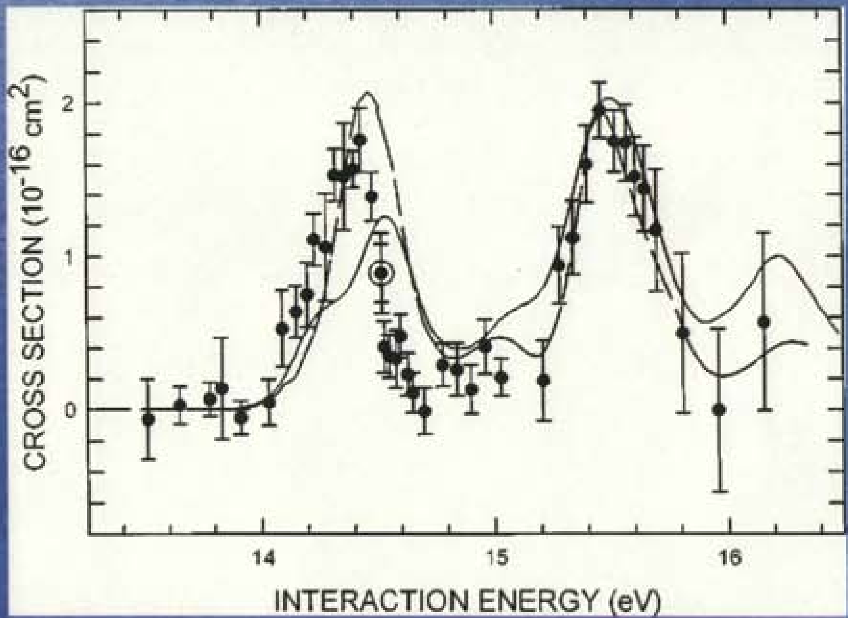
$e + A^{q+} \rightarrow A^{(q-1)+**} \rightarrow e + A^{q+*}$

$e + Fe^{9+}\ (3s^2 3p^5\ {}^2P^o_{3/2}) \rightarrow e + Fe^{9+}\ ({}^2P^o_{1/2})$

$e + Ar^{6+}\ (3s^2\ {}^1S) \rightarrow e + Ar^{6+}\ (3s3p\ {}^3P^o)$



M. Niimura et al., Phys. Rev. Lett. 88, 103201 (2002).



Y.-S. Chung et al., Phys. Rev. A 55, 2044 (1997).

Feshbach resonance of ionization cross section

Excitation Autoionization (EA):

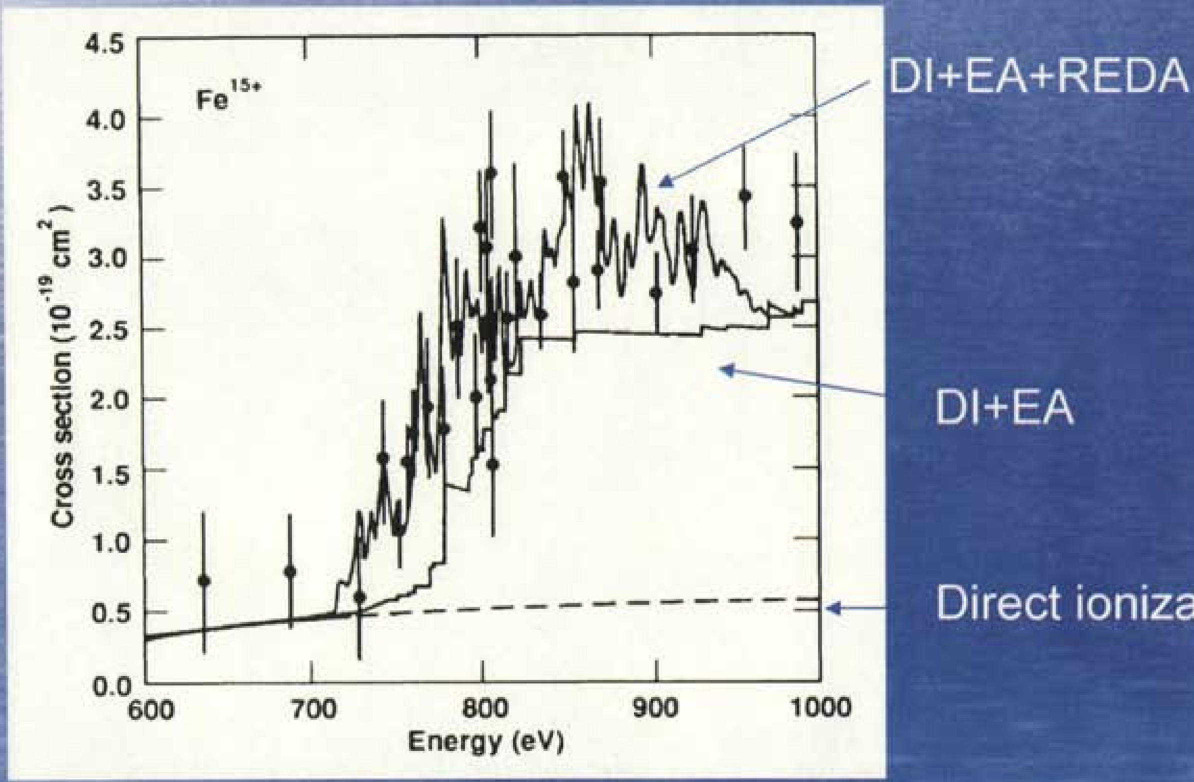
$e + Fe^{15+}(1s^2 2s^2 2p^6 3s) \rightarrow e + Fe^{15+}(1s^2 2l^7 3snl) \rightarrow 2e + Fe^{16+}(1s^2 2s^2 2p^6)$

Resonance Excitation Double Autoionization (REDA):

$e + Fe^{15+}(1s^2 2s^2 2p^6 3s) \rightarrow Fe^{14+}(1s^2 2l^7 3snln'l')$

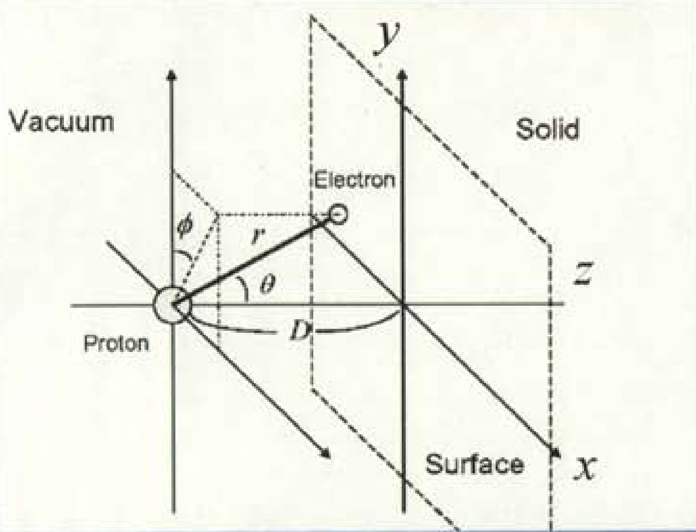
$\rightarrow e + Fe^{15+}(1s^2 2l^7 3snl)$

$\rightarrow 2e + Fe^{16+}(1s^2 2s^2 2p^6)$



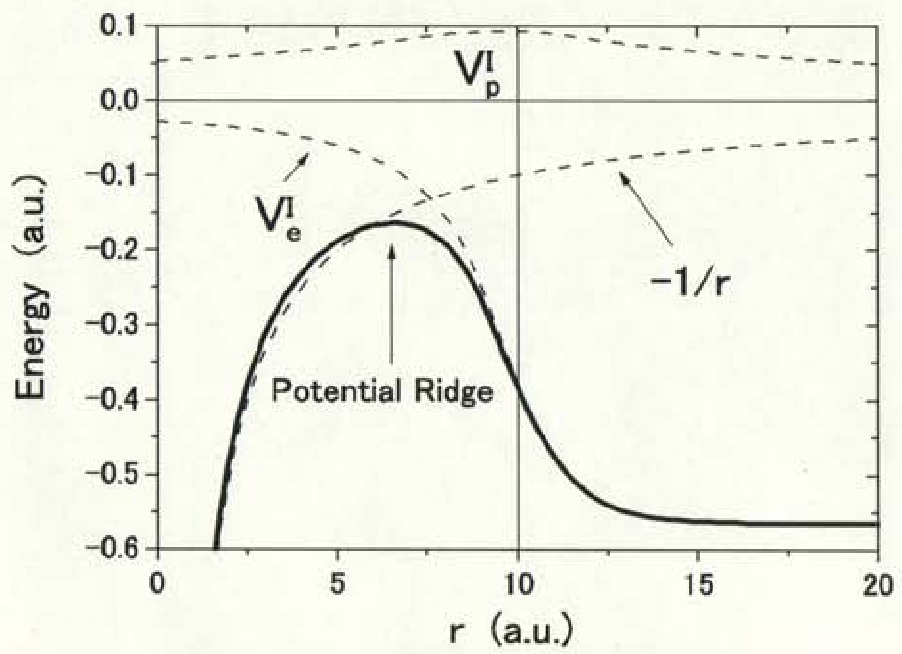
M.H. Chen et al., Phys. Rev. Lett. 64, 1350 (1990)

Shape resonance state of H atom above metal surface



V_e^I : electron self - image potential

V_p^I : proton image potential



Electrons can tunnel under potential barrier between atomic core and conduction band. Atomic-state above metal surface is equivalent to a shape resonance state in scattering of surface conduction electron by atomic core.

D. Kato et al., JPFR Vol. 7, 183 (2006).

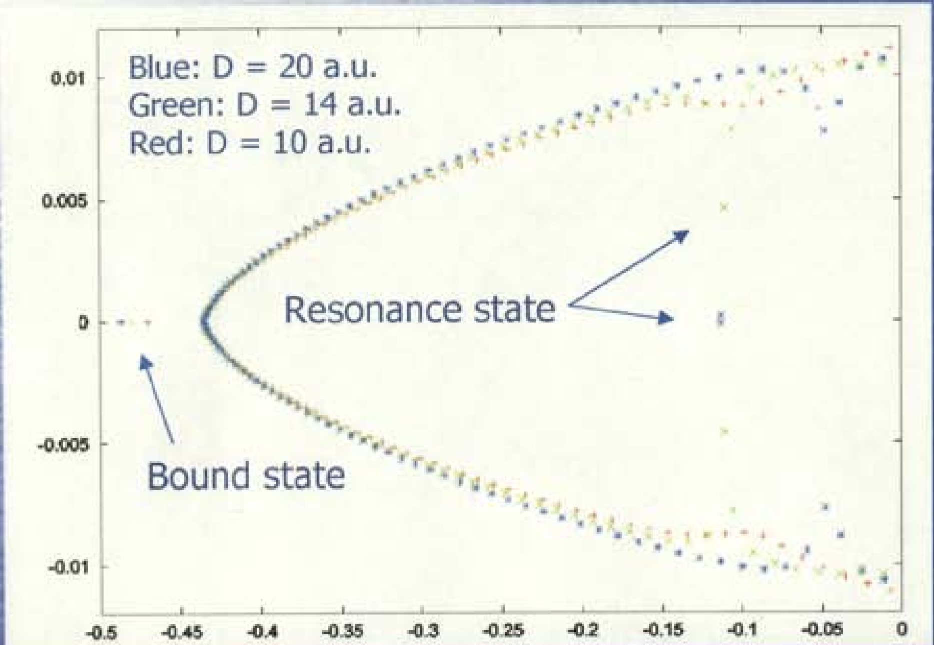
Non-Hermite system (complex eigenvalue problem)
Spherical model

$$\left[-\frac{1}{2}\frac{d^2}{dr^2}-\frac{1}{r}+V_e^I(r;D)+V_p^I(r;D)\right]\Psi=\varepsilon(D)\Psi,$$

with an outgoing wave boundary condition $\left(d/dr-ik\right)\Psi\big|_{r=R}=0$,

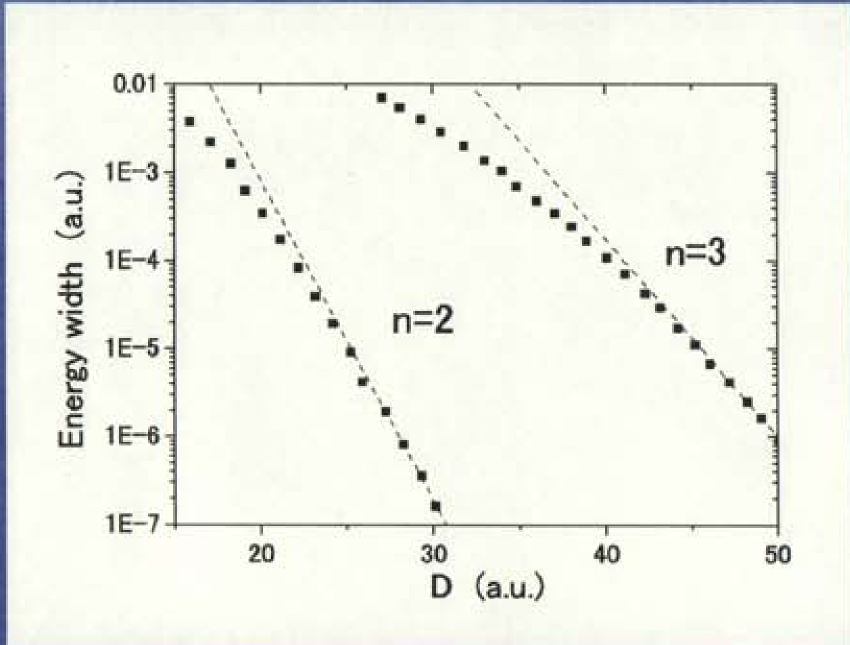
where $k=\sqrt{2\varepsilon}$ measured from the bottom of conduction band.

Complex eigenvalues
Horizontal axis: real part of k^2,
Vertical axis imaginary part of $-k^2$

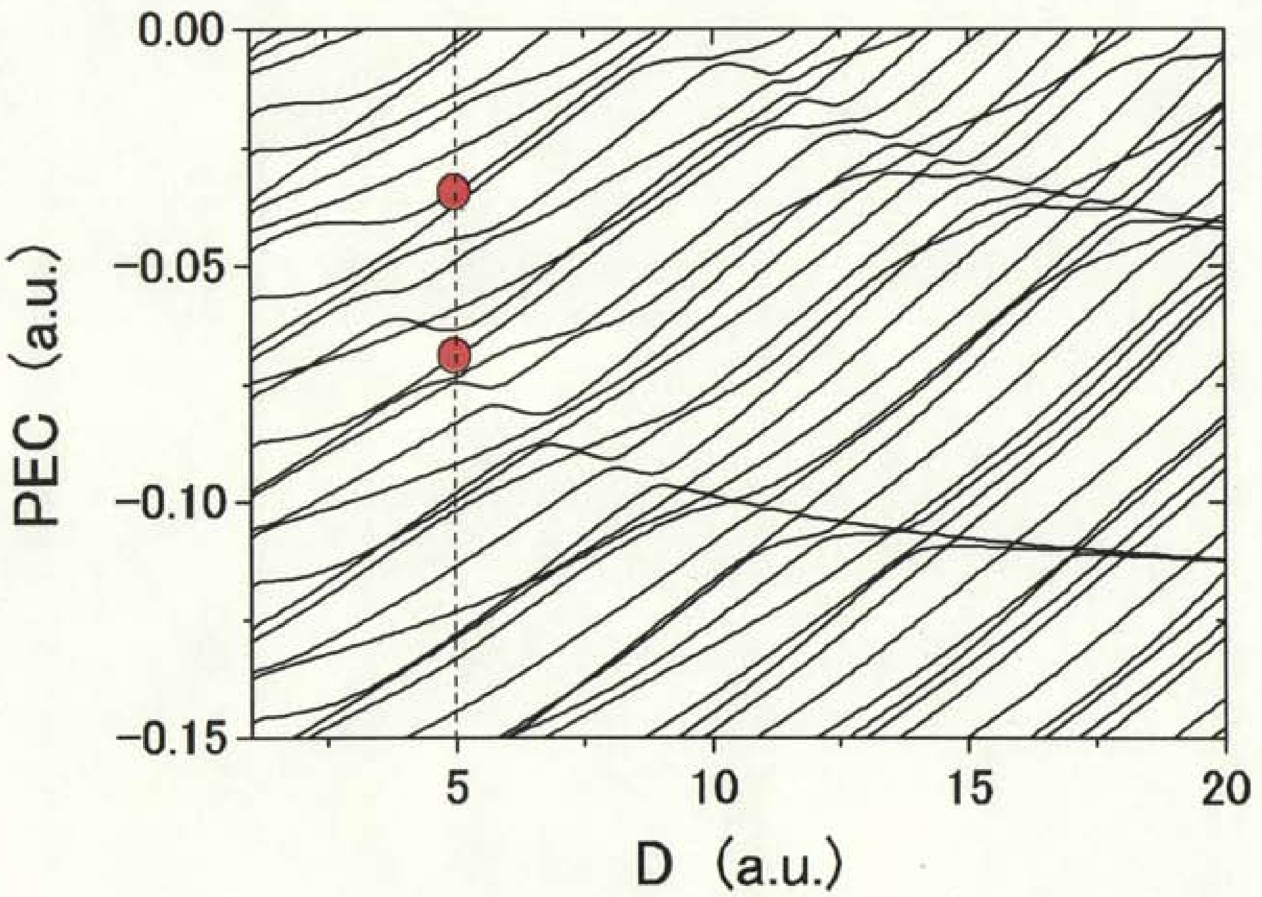


$$\exp\left[-i\varepsilon t/\hbar\right]=\exp\left[-i\varepsilon_R t/\hbar-\varepsilon_I t/\hbar\right]$$

Energy width of atomic levels



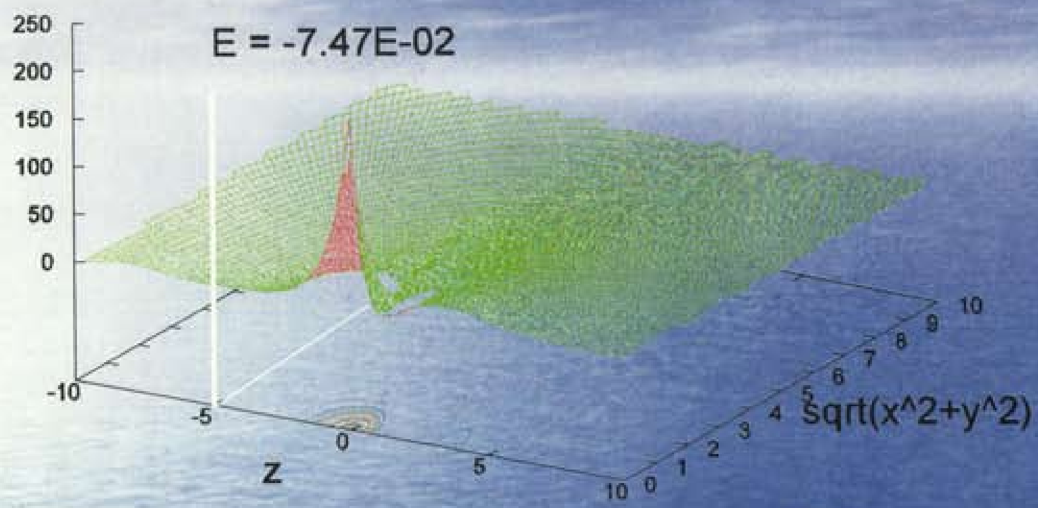
Energy level structure of H + Al surface



n=3

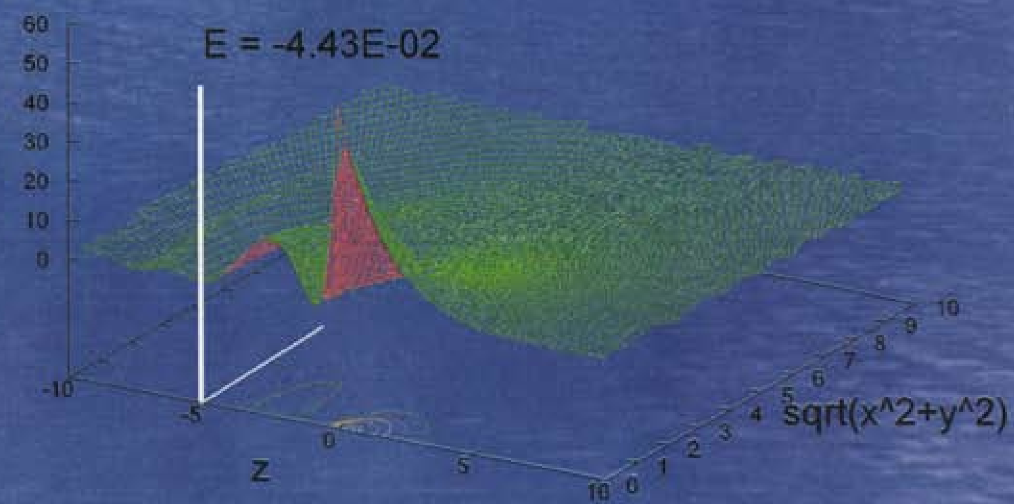
n=2

Squared of wavefunction for resonance state of H(n=2) sp-hybridization

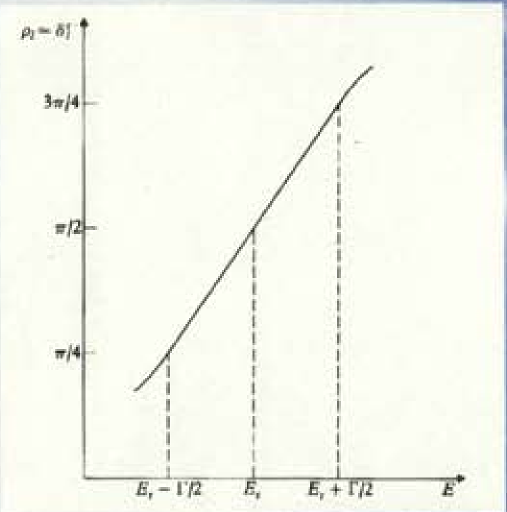


Electron stays far side.
Lower energy.

Stronger coupling with conduction band. Larger energy width.

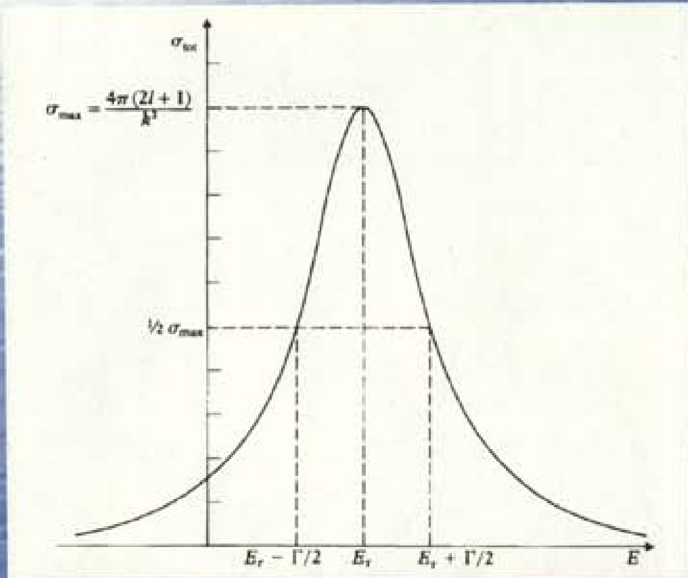


Resonance profile (Breit-Wigner formula)



Resonance component of phase shift with width Γ:

$$\delta_l^r = \tan^{-1}\frac{\Gamma}{2(E_r - E)}$$



Resonance component of scattering amplitude:

$$f \approx \frac{2l+1}{k}\frac{\Gamma/2}{E_r - E - i\Gamma/2}P_l(\cos\theta)$$

Resonance profile of cross section (Lorentzian):

$$\sigma \approx \frac{4\pi(2l+1)}{k^2}\frac{\Gamma^2/4}{(E-E_r)^2+\Gamma^2/4}$$

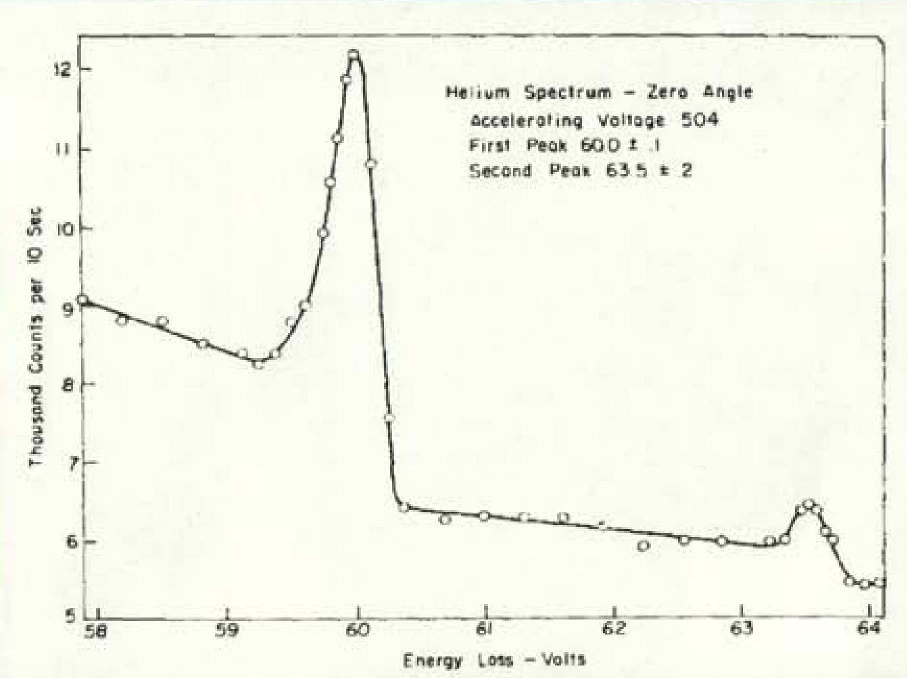
Lifetime of intermediate state:

$$\tau \approx \frac{\hbar}{\Gamma}$$

Fano's formula (asymmetric profile)

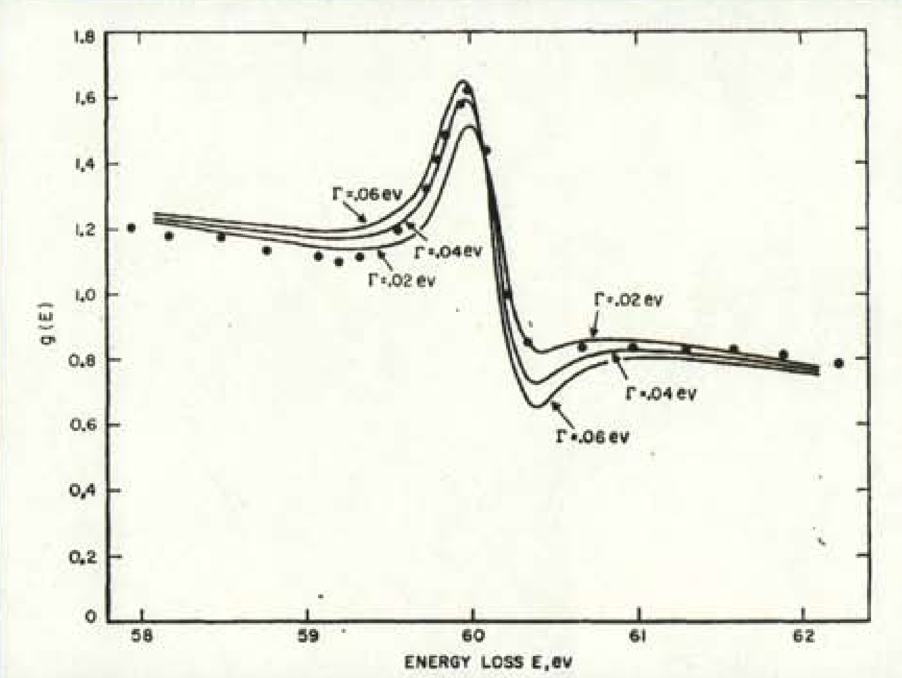
$e + He(1s^2\ {}^1S) \rightarrow e + He(2s2p\ {}^1P) \rightarrow 2e + He^+(1s)$

Energy-loss spectrum of forward scattering



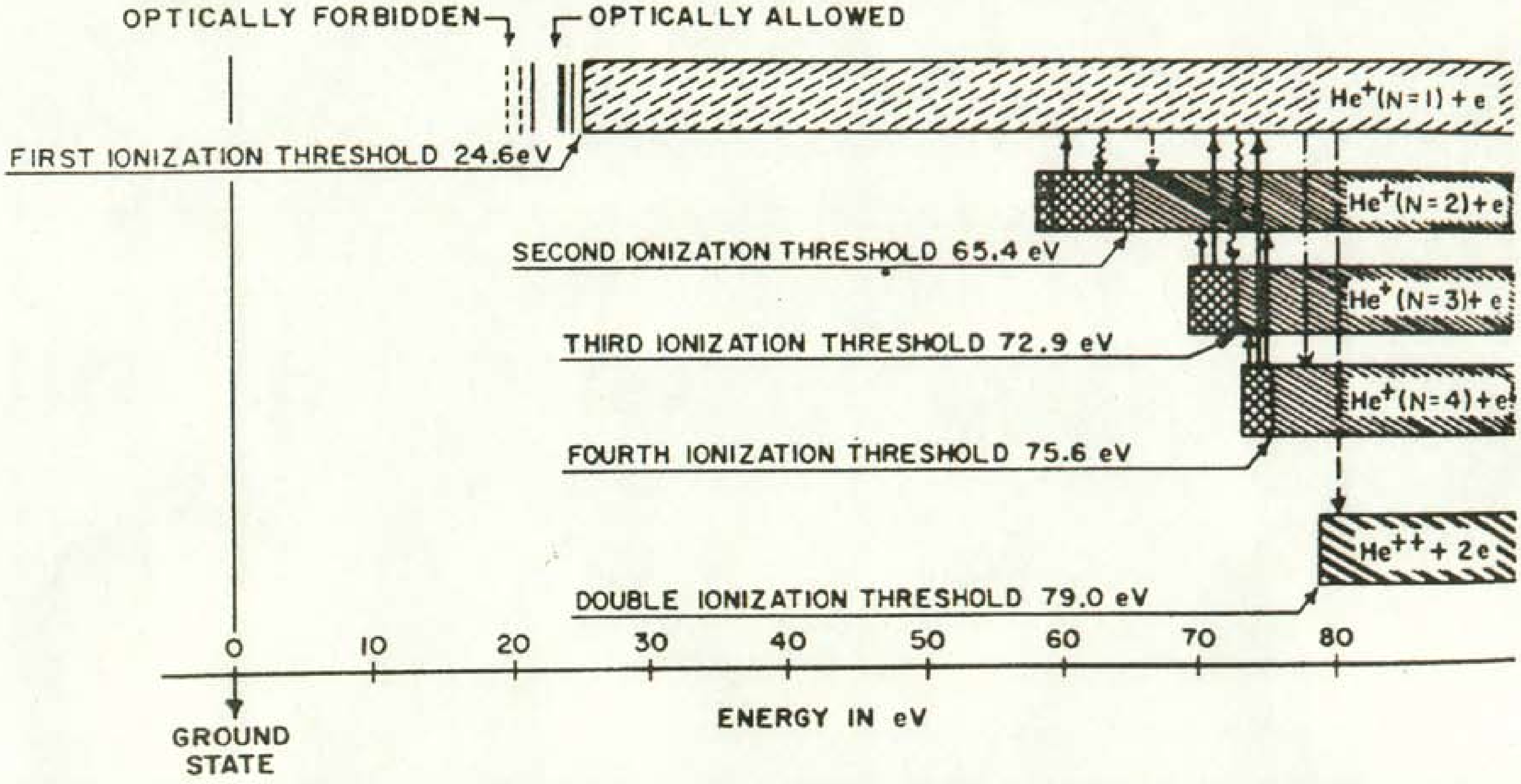
S.M. Silverman and E.N. Lassettre, J. Chem. Phys. 40, 1265 (1964)

Fitting by Fano's formula

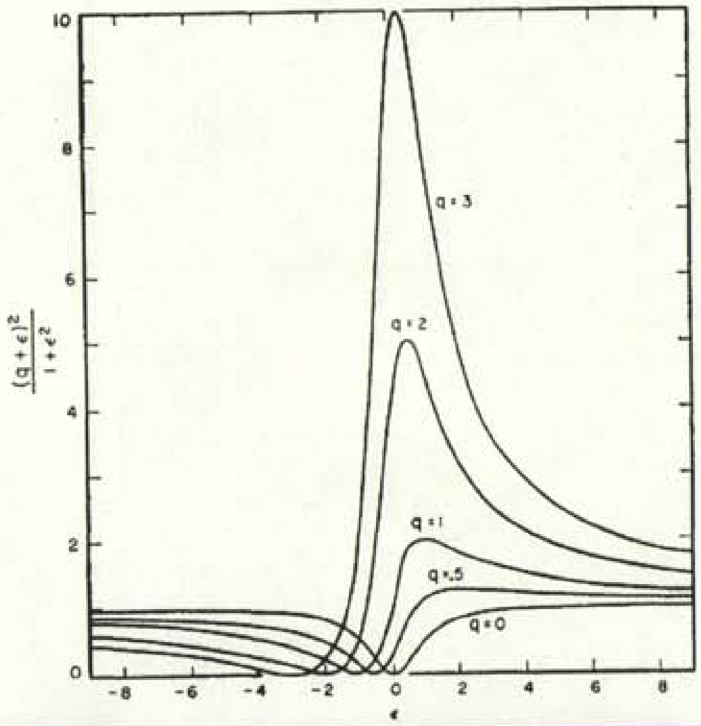


U. Fano, Phys. Rev. 124, 1866 (1961)

Autoionizing state of He atoms



Configuration interaction with continuum
Non-perturbative treatment and q-parameter



U. Fano, Phys. Rev. 124, 1866 (1961)

Linear combination of a discrete autoionizing state (φ) and a continuum state ($\psi_{E'}$) :

$$\Psi_E = a\varphi + \int dE' b_{E'} \psi_{E'}$$

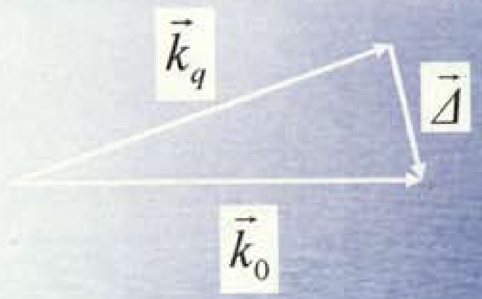
Fano profile of transition probability :

$$\frac{\left|\langle \Psi_E | T | \Psi_i \rangle\right|^2}{\left|\langle \psi_E | T | \Psi_i \rangle\right|^2} = \frac{(q+\varepsilon)^2}{1+\varepsilon^2}, \quad \text{where} \quad \varepsilon = (E - E_r)/(\Gamma/2)$$

q parameter :

$$\frac{1}{2}\pi q^2 \approx \frac{\left|\langle \varphi | T | \Psi_i \rangle\right|^2}{\left|\langle \psi_E | T | \Psi_i \rangle\right|^2 \Gamma}$$

Excitation cross section by fast electrons
(Generalized oscillator strength)



Differential cross section :

$$\frac{d\sigma_{q0}}{d\Omega} = \frac{k_q}{k_0}\left|f_q\right|^2$$

First Born approximation of scattering amplitude :

$$f_q = -\frac{1}{4\pi}\int e^{i\vec{\Delta}\cdot\vec{r}'}\int \Phi_q(\vec{r})\frac{2}{|\vec{r}'-\vec{r}|}\Phi_0(\vec{r})d\vec{r}d\vec{r}',$$

where $\vec{\Delta} = \vec{k}_0 - \vec{k}_q$.

Bethe integral of the amplitude :

$$f_q = -\frac{2}{\Delta^2}\int \Phi_q(\vec{r})e^{i\vec{\Delta}\cdot\vec{r}}\Phi_0(\vec{r})d\vec{r}$$

Generalized oscillator strength :

$$F_{q0}(\vec{\Delta}) = \left(E_q - E_0\right)\frac{2}{\Delta^2}\left|\int \Phi_q(\vec{r})e^{i\vec{\Delta}\cdot\vec{r}}\Phi_0(\vec{r})d\vec{r}\right|^2$$

$$\sigma_{\bar{q}}(k_0) = \frac{4\pi}{k_0^2}\left(E_q - E_0\right)^{-1}\int_{(E_q-E_0)/k_0}^{2k_0}\sum_m F_{q0}(\vec{\Delta})\frac{d\Delta}{\Delta}$$

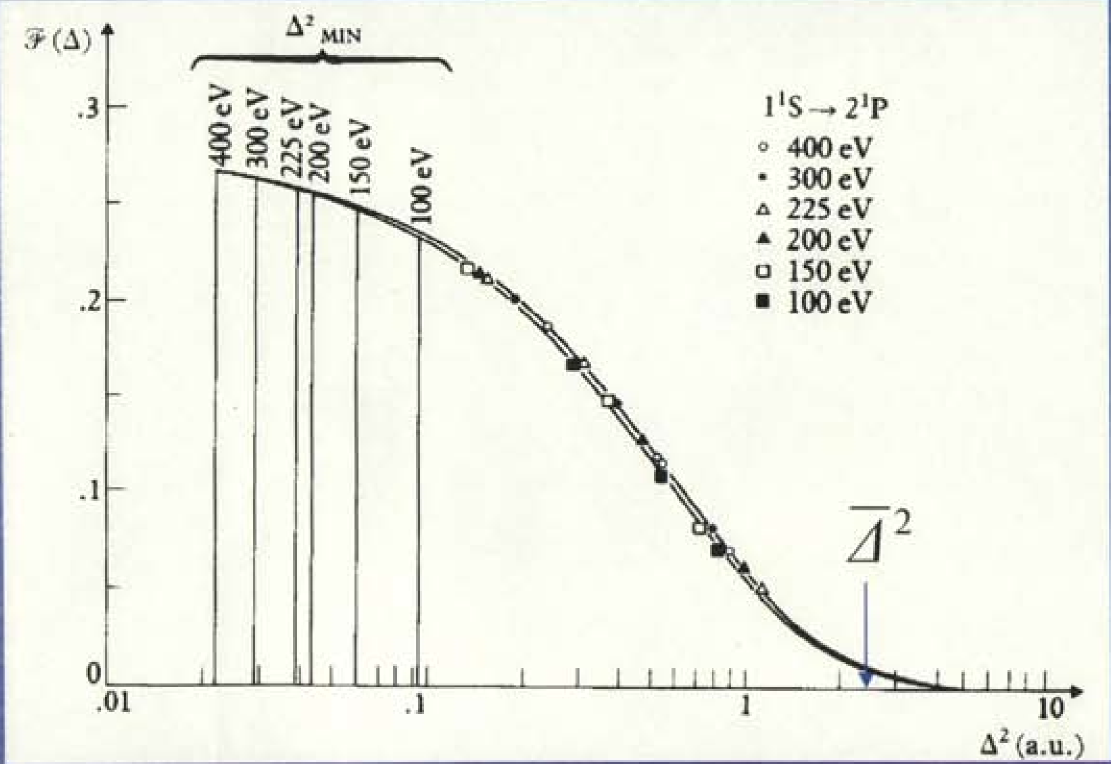
Optical oscillator strength :

$$F_{q0} \underset{\Delta\to 0}{\approx} 2\left(E_q - E_0\right)\left|\langle \Phi_q|z|\Phi_0\rangle\right|^2 \equiv f_{q0}$$

Asymptotic formula of inelastic cross section for optically allowed transition

$$\sigma(k_0) \approx \frac{2\pi}{k_0^2}\left(E_q - E_0\right)^{-1} \sum_m f_{q0} \log\left(\frac{\overline{\Delta}^2 k_0^2}{\left(E_q - E_0\right)^2}\right)$$

Generalized oscillator strength for He(1s^2 ^{1}S) → He(1s2p ^{1}P)

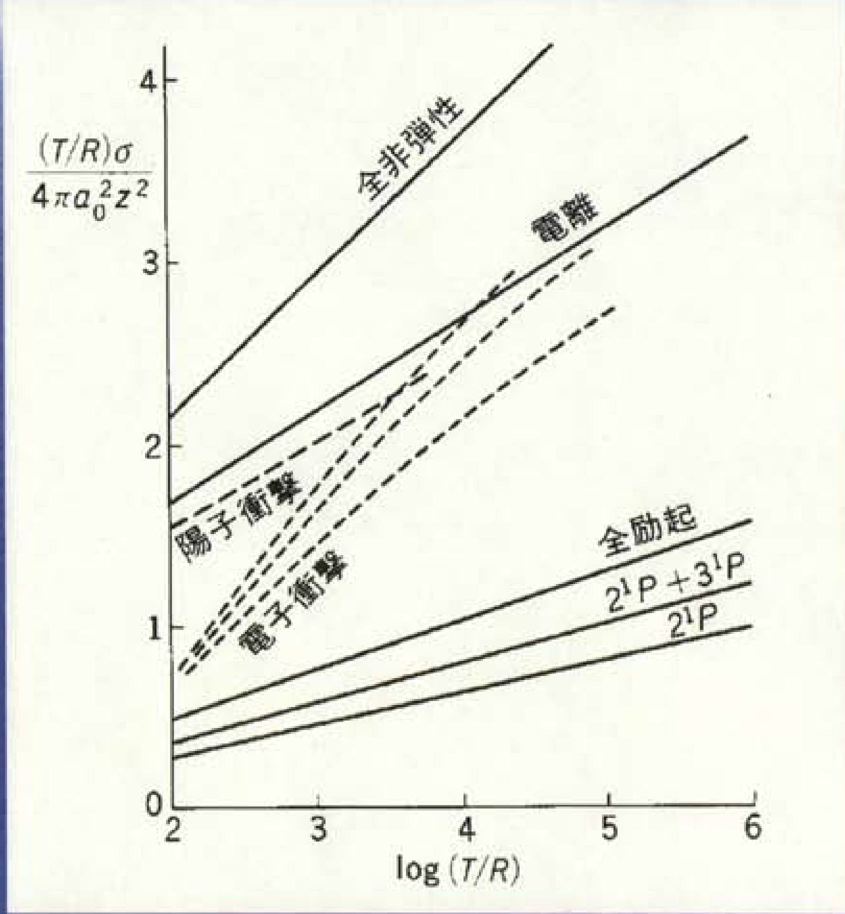


Scaling of inelastic cross section

Reduced kinetic energy : $T = \frac{m_e}{\mu} \frac{k_0^2}{2\mu}$

Scaling of mass and charge number of projectile particle is valid at high energies. Cross section curves of proton and electron are merged into an asymptote.

Excitation of He atom
Solid: asymptotic formula
Dashed: experiments.

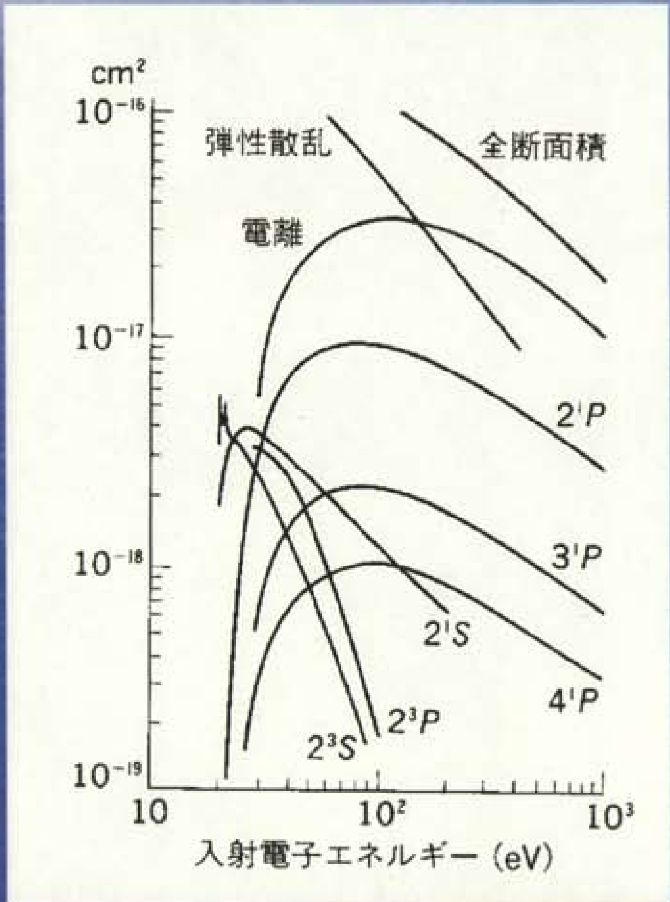


Asymptotic formula for forbidden transition

$$\sigma_{\bar{q}0}(k_0) \approx \frac{\pi}{k_0^2} \sum_m \left| \left\langle \Phi_q \left| z^2 \right| \Phi_0 \right\rangle \right|^2 \overline{\Delta}^2$$

Inelastic cross section of He atom

2,3,4 ^1P are optically allowed. Forbidden 2 ^1S cross section declines steeply as E^{-1}. Cross sections of 2 ^3P and 2 ^3S decrease more rapidly as energy increases. They are due to exchange scattering: exchange between projectile electron and one of target electrons (Born-Oppenheimer approx. or Ochkur-Rudge approx.).



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