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Large-angle high-energy electron scattering from molecules

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Co-workers — Glyn Cooper, Adam Hitchcock (McMaster, Hamilton, Canada); Aris Chatzidimitriou-Dreismann (Technical University Berlin)

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Atomic and Molecular Physics Laboratories

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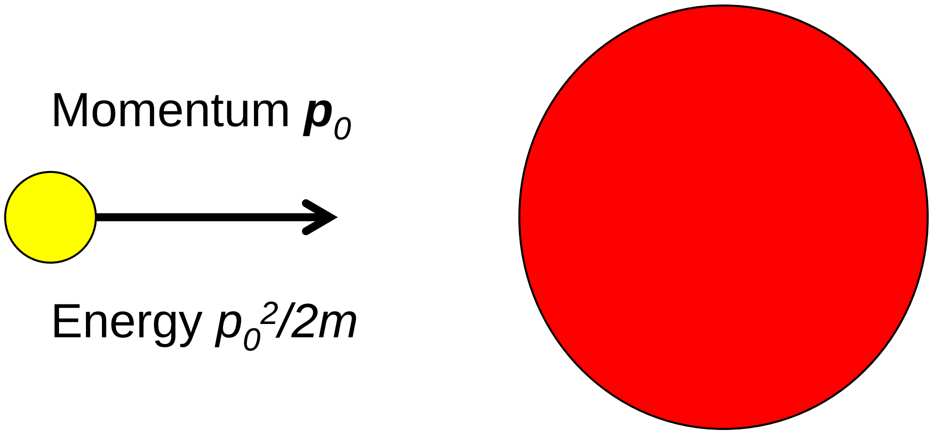
High-school collision physics I: small ball (mass m) hits very large ball (mass M) ($m << M$)

Momentum $\boldsymbol{p}_0$

Energy $p_0^2/2m$

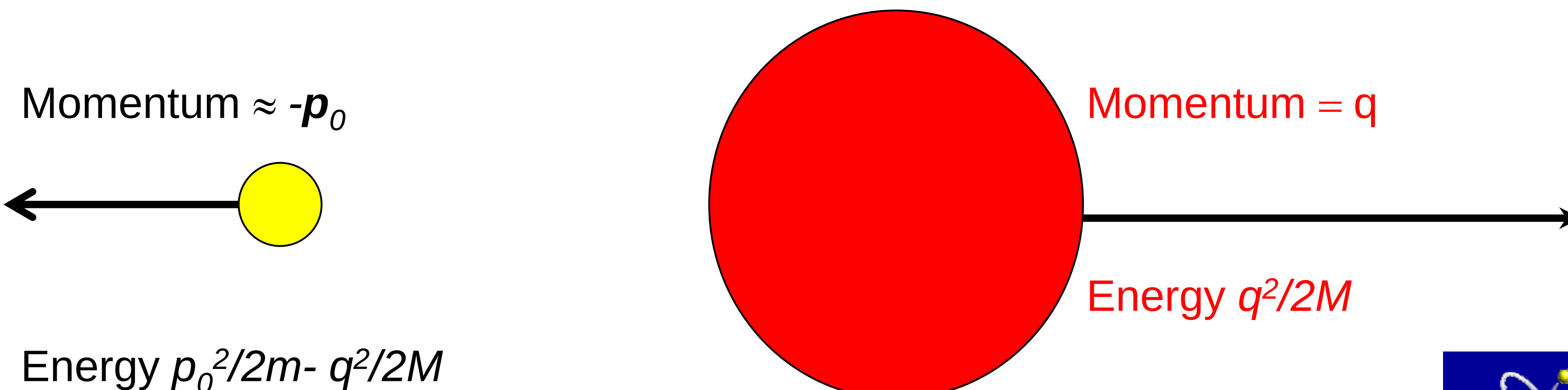


Momentum 0

After collision (for scattering over 180° momentum transfer $q \approx 2p_0$)

Momentum $\approx -\boldsymbol{p}_0$

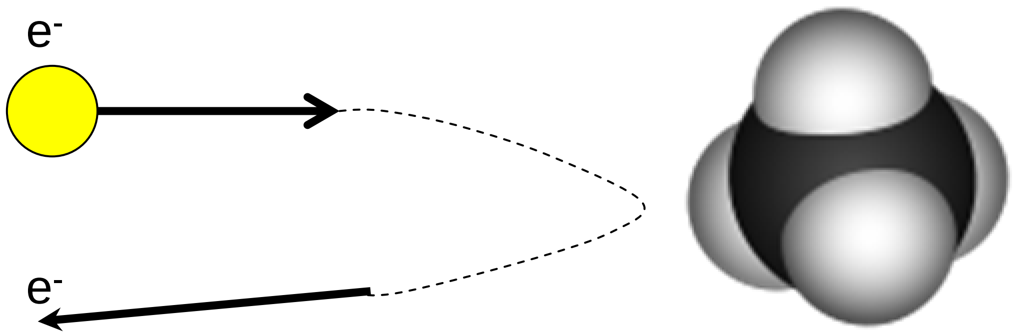
Momentum = q



Energy $q^2/2M$

Energy $p_0^2/2m - q^2/2M$

Electron Scattering from molecule (methane)



What is *M*?

16 a.m.u. (scattering from molecule)

12 or 1 a.m.u. (scattering from either H or C atoms)

values: 6 keV electron scattering from $CH4$ over 135^0

Energy transfer to molecule:0.71 eV

Energy transfer to H: 11.3 eV

Energy transfer to C: 0.94 eV

(Energy transfer to Xe: 0.09 eV)

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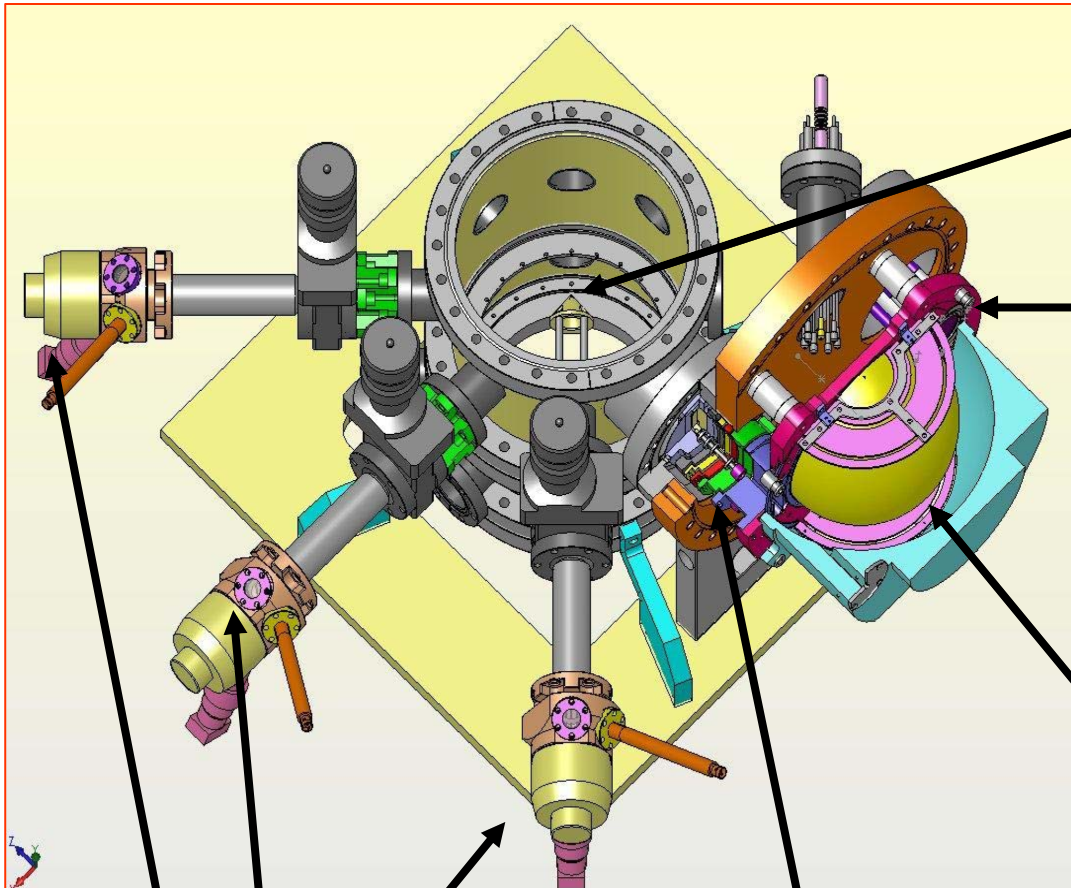
10 keV large angle elastic scattering apparatus at ANU



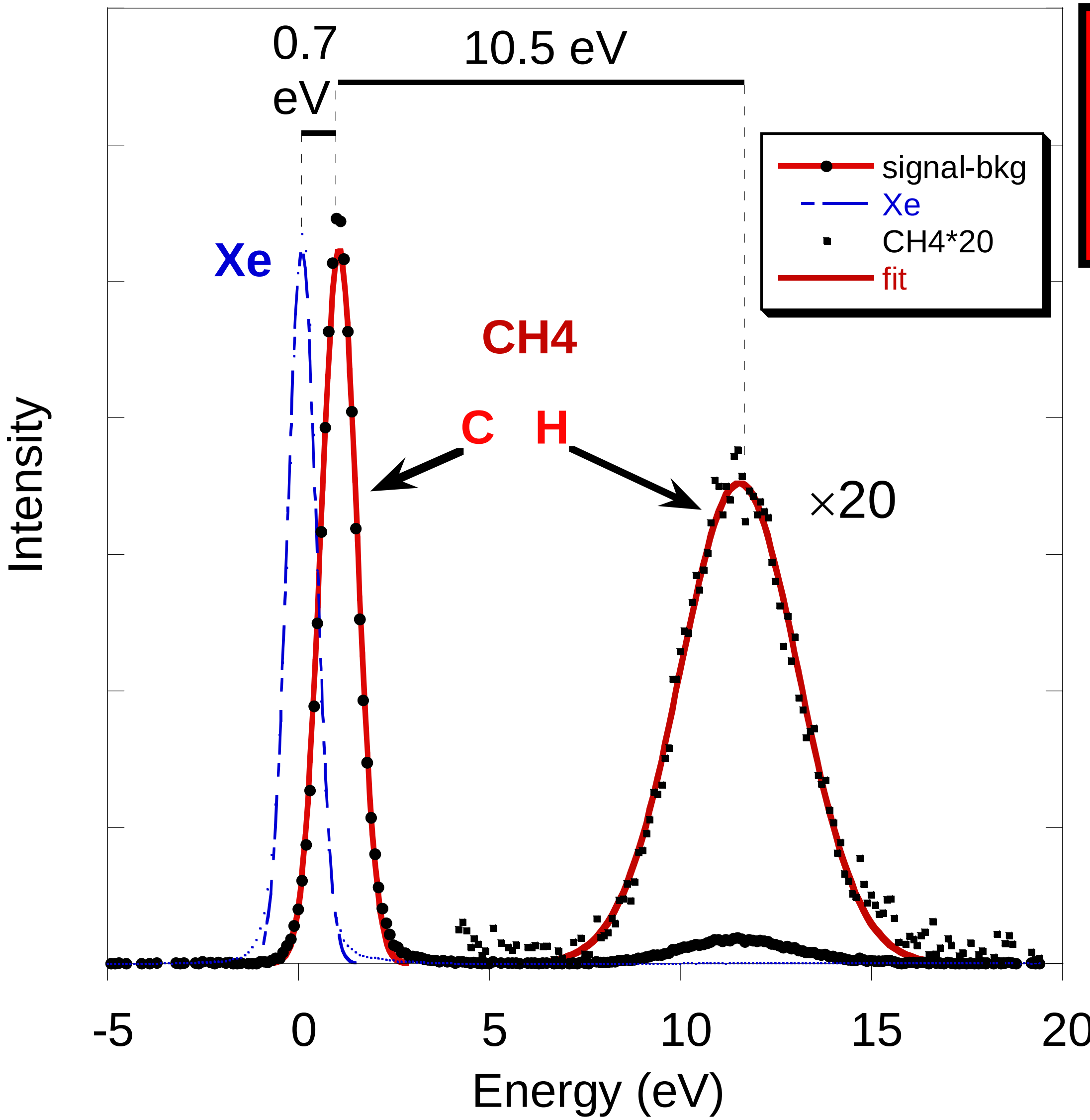
Needle (not shown)

2-dimensional Electron detector

Hemispherical analyser

Slit lenses

Gun at 45°,90° or 135° (relative to analyser)

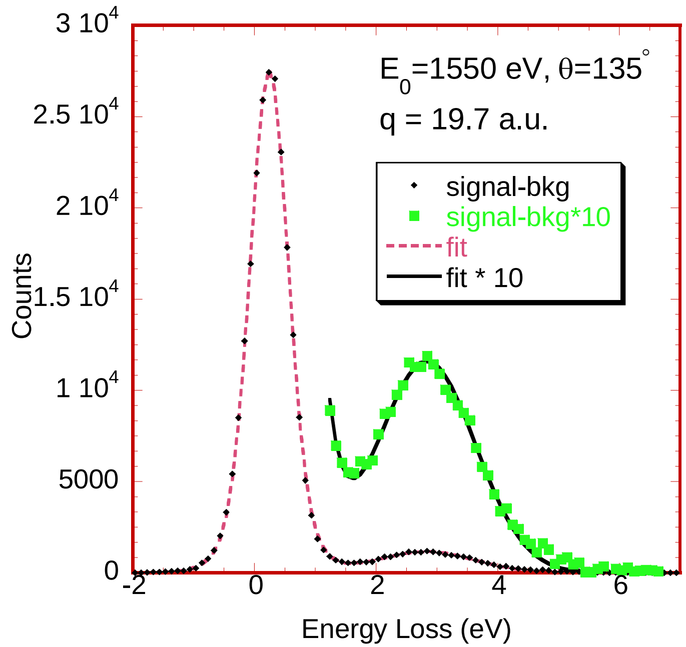


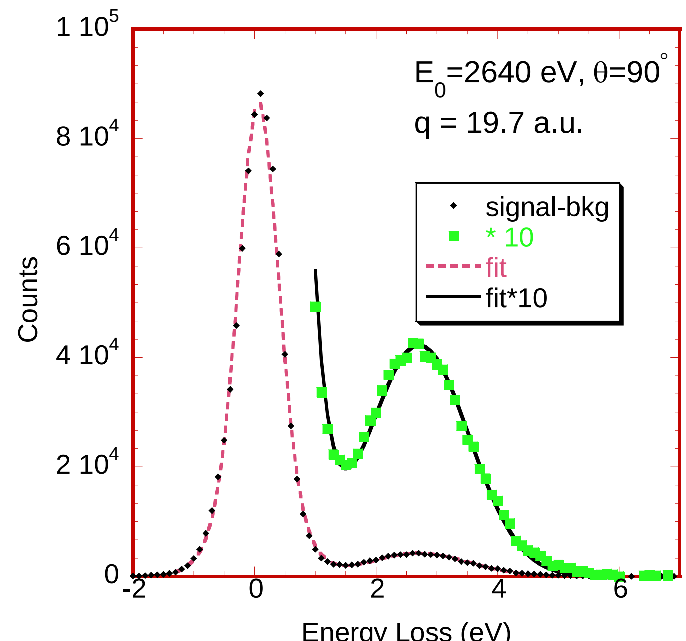
Calc. Xe-C splitting:0.85 eV
Obs. Xe-C splitting:0.71 eV
Calc. H-C splitting: 10.4 eV
Obs. H-C splitting: 10.5 eV

Is peak near 11 eV due to Scattering from H atoms, Maybe some electronic excitation?

Test:
Change incoming energy. This will change the momentum transfer ***q*** and this should affect second peak if it is due to recoil from H atoms

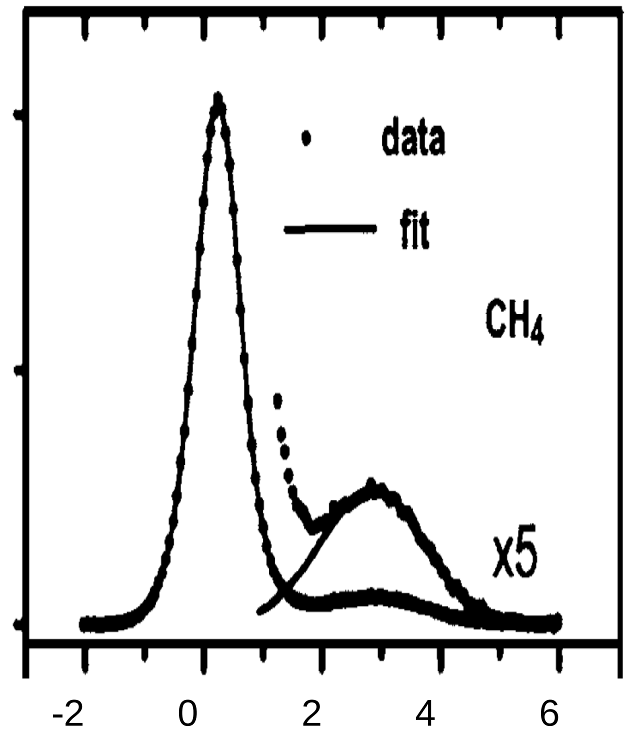
Large-angle high-energy scattering from molecules





Peak separation proportional to incoming energy

Spectra taken at same momentum transfer have same peak separation!



Results from McMaster University, Cooper et al

E_0= 2250 eV
$\theta = 100°$,
q =19.7 a.u.

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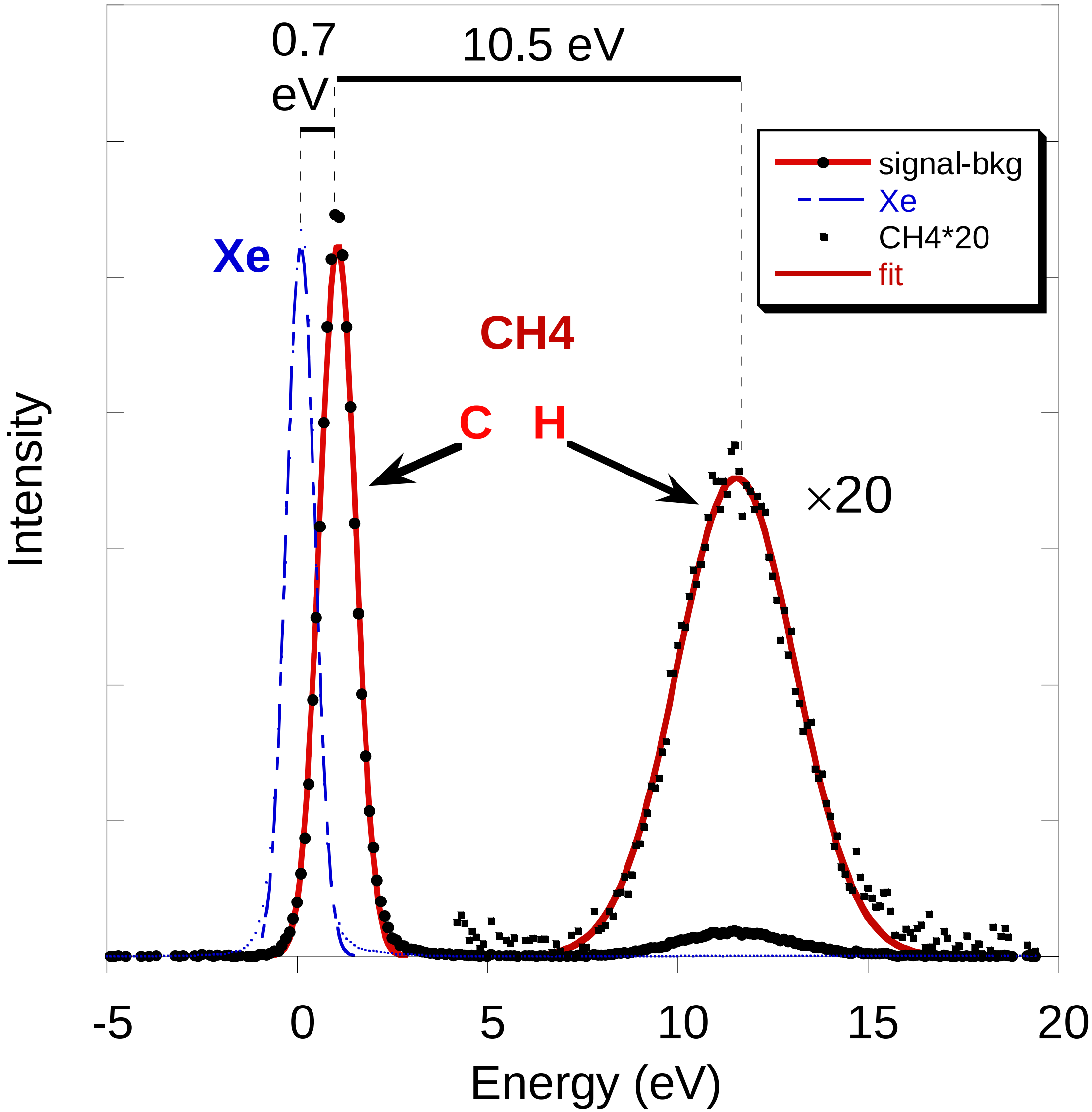
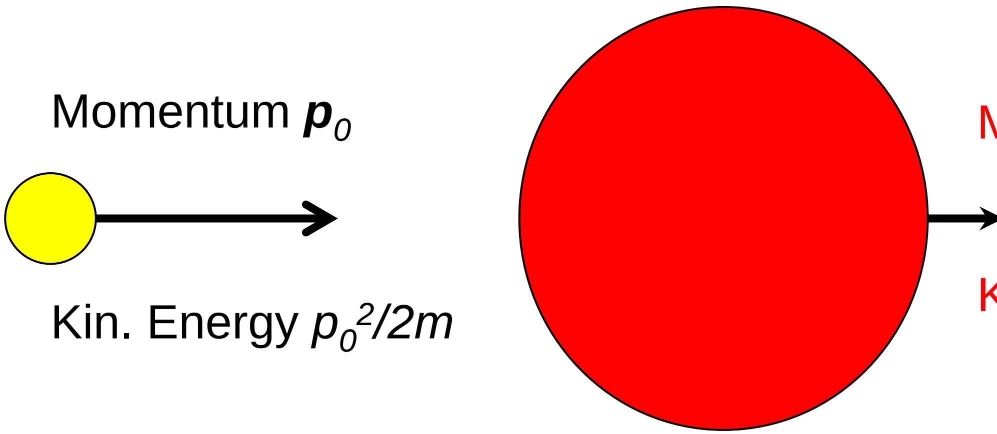


But why have the C and H peak different width?

High-school collision physics II: small ball (mass m) hits moving large ball (mass M) ($m << M$)

Momentum $\boldsymbol{p}_0$

Momentum $\boldsymbol{k}_0$



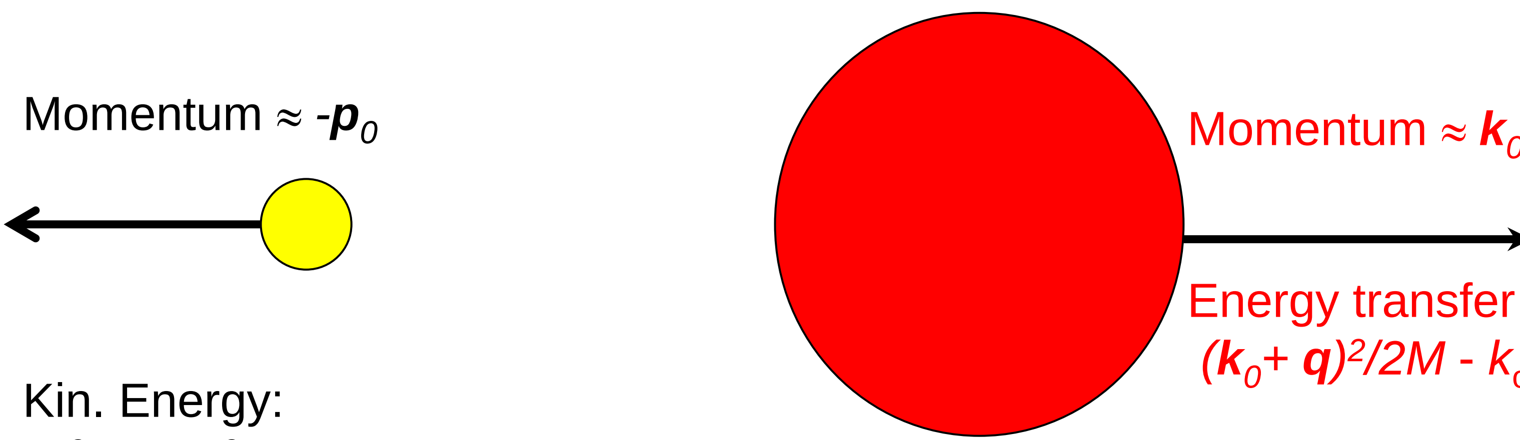
Kin. Energy $p_0^2/2m$

Kin. Energy $k_0^2/2M$

After collision (for scattering over 180° momentum transfer q ≈ $2p_0$)

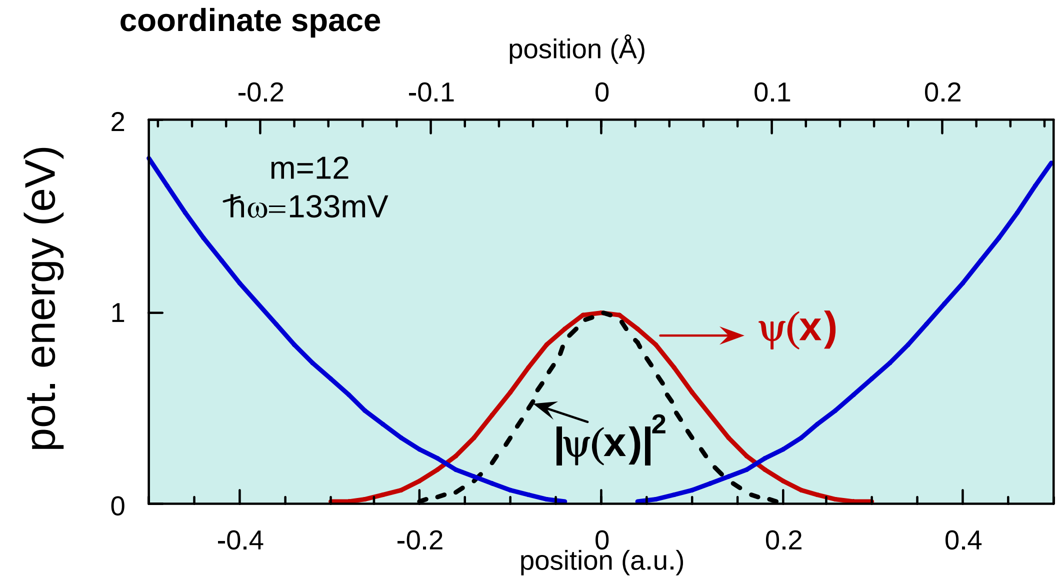
Momentum ≈ $-\boldsymbol{p}_0$

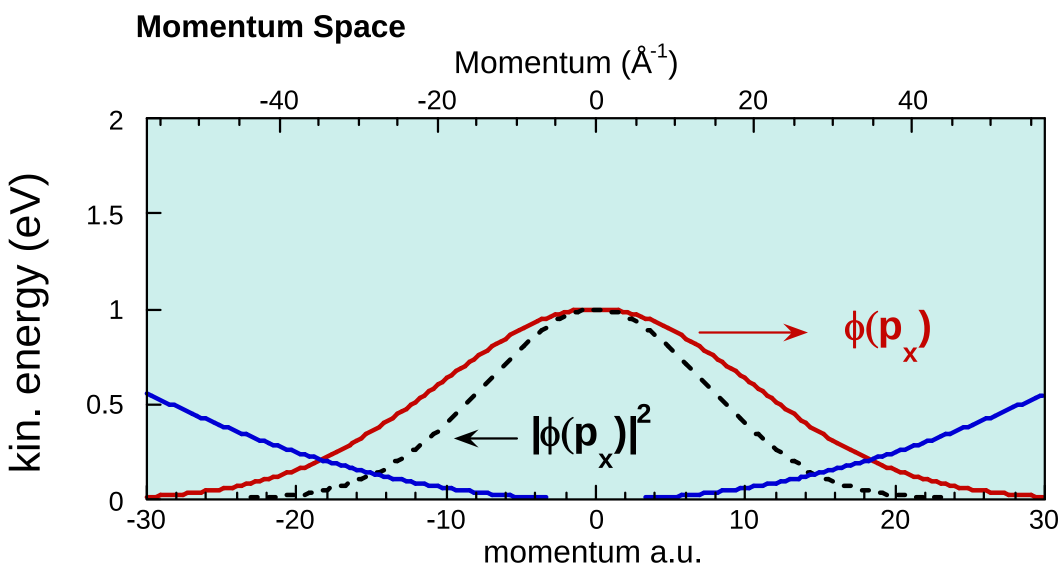
Momentum ≈ $\boldsymbol{k}_0 + \boldsymbol{q}$



Energy transfer
$(\boldsymbol{k}_0 + \boldsymbol{q})^2/2M - k_0^2/2M$

Kin. Energy:
$p_0^2/2m - q^2/2M - \boldsymbol{k}_o \cdot \boldsymbol{q}/M$





Why are the protons moving?

<u>Quantum Mechanics!</u>

Due to the chemical Bond the proton is in a potential well. Its wave-function is localised in coordinate space, hence delocalised in momentum space. In a one-dimensional world the measured H peak would be a direct measure of $|\phi(p)|^2$.

Relative intensity of C and H peak

History

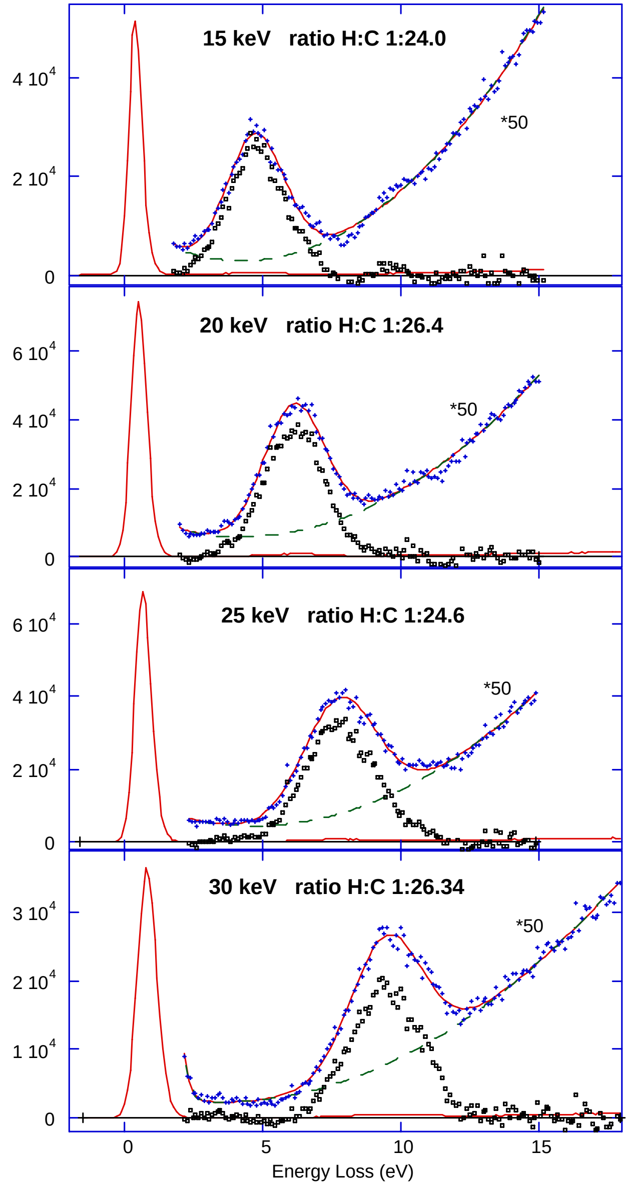
Collisions with the same momentum transfer were studied in solids (in particular polyethylene: $(\text{-CH2-})_n$) using either neutrons (at ISIS, UK) or electrons (at ANU) as the probing particle. Peak width and peak separation were in good agreement with theory, but the relative intensity of the hydrogen peak was smaller than expected in both the neutron and electron experiment. This was interpreted by Chatzidimitriou-Dreismann as a sign of 'quantum entanglement' of the protons.

This prompted these gas-phase measurements, as they are, in many ways simpler.

-no background

-no radiation damage

-smaller system, easier to describe theoretically (decoherence of the proton wave function)



results for polyethylene (PE): $(\text{-CH}_2\text{-})_n$

These films were obtained by dissolving polyethylene in xylene at 100 ^{0}C and removing a glass slide slowly out this solution. The PE films were subsequently floated off on distilled water and mounted on the sample holder.

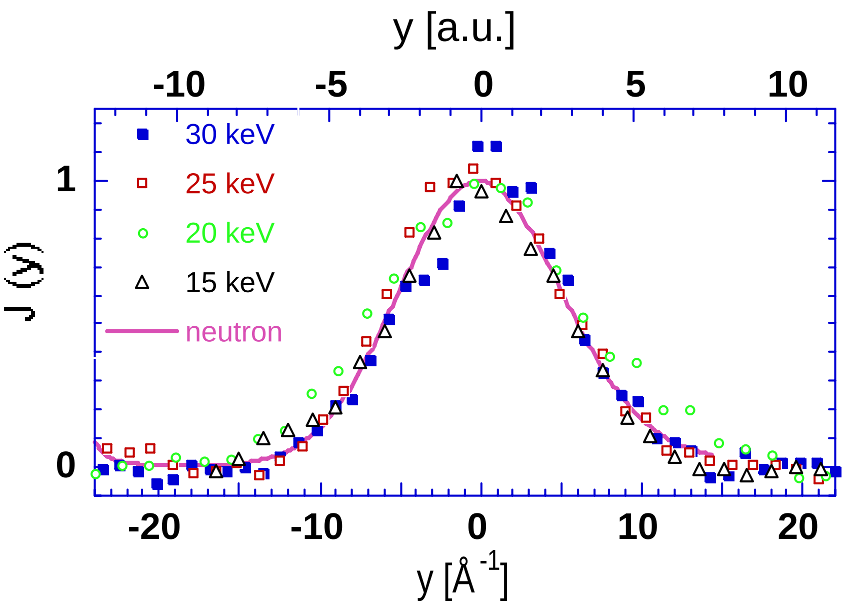
Hydrogen peak even broader then C peak!

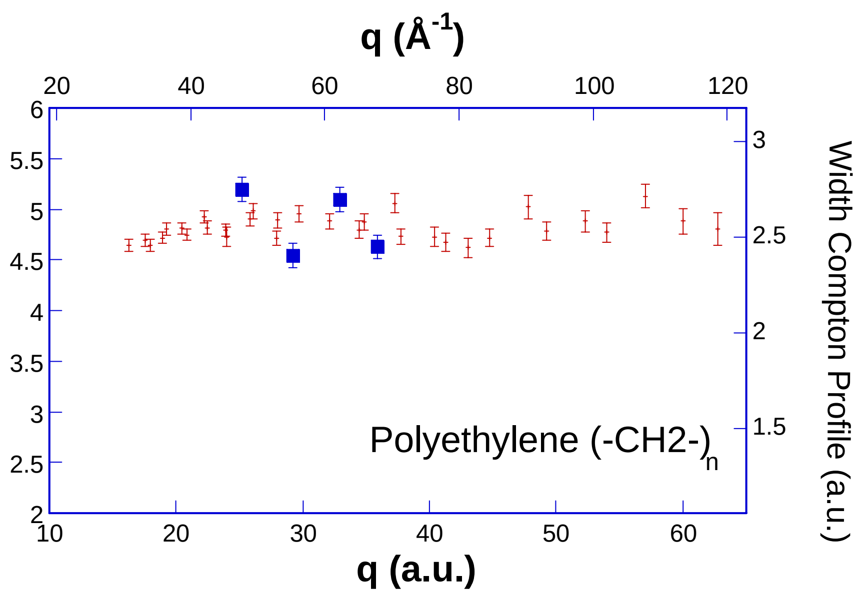
Compare areas C and H peak

Rutherford cross section ∞ Z^2

H:C peak area $(2´1^2) : 6^2$=1:18

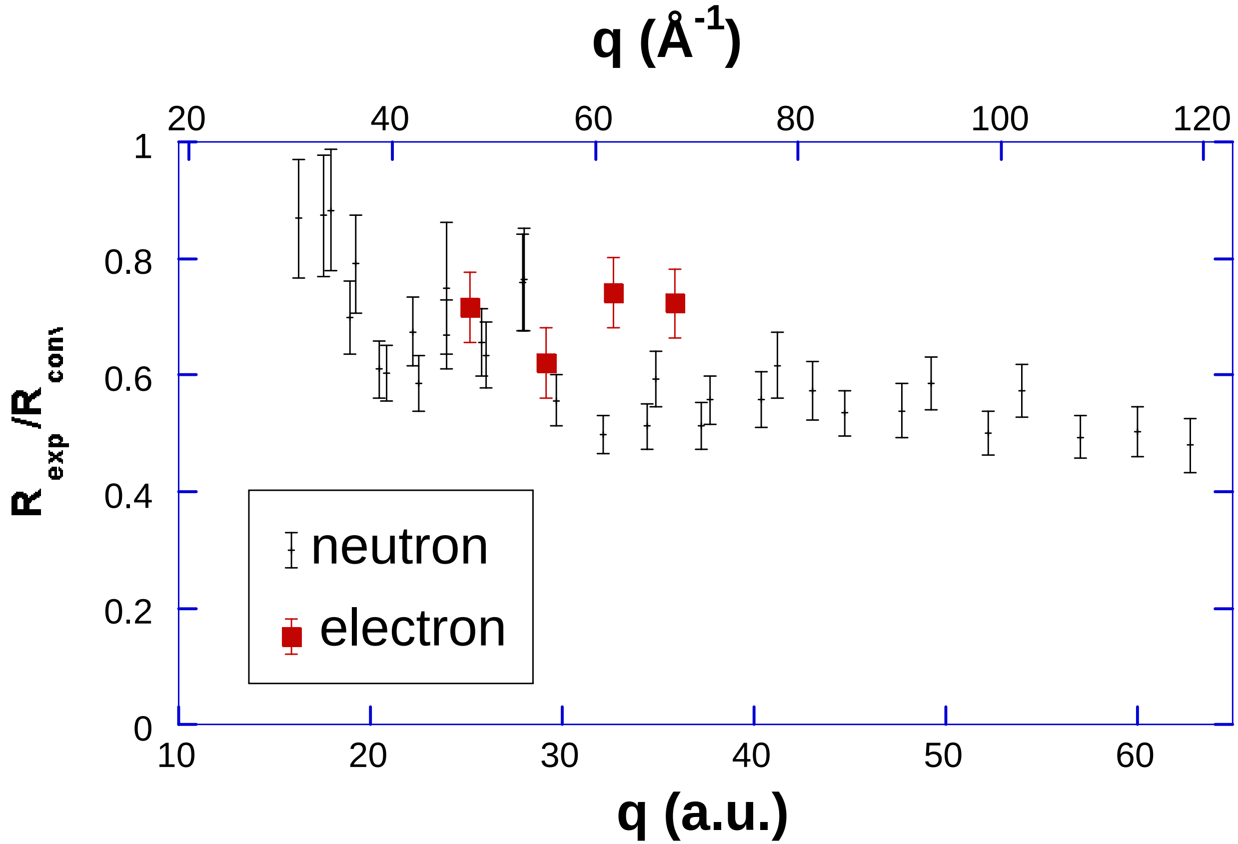
Again the measured Hydrogen peak area is a smaller than expected.





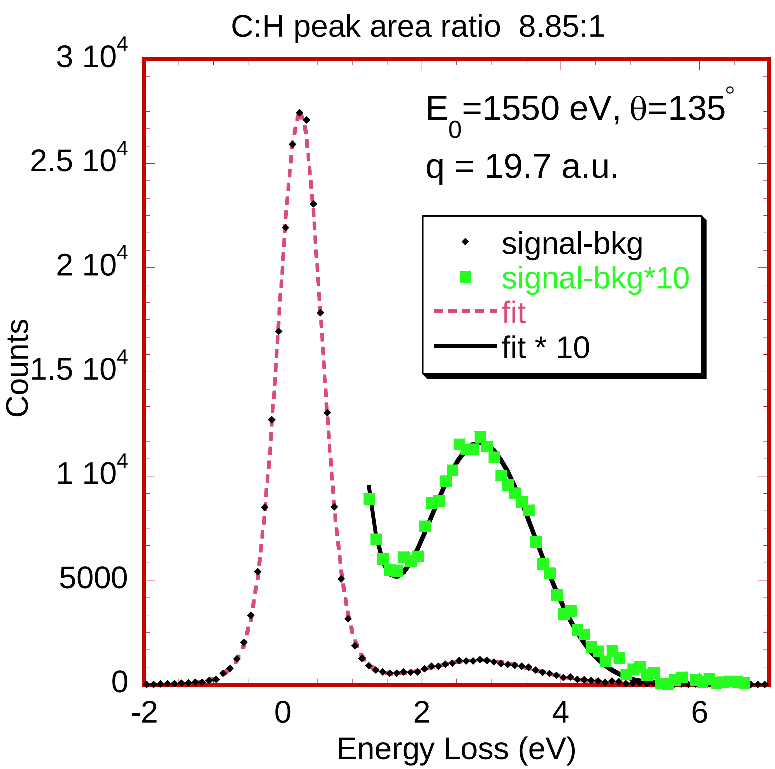
The Compton profile of hydrogen as obtained for electron measurements as energies as indicated and from a fit of a representative neutron detector. Thus, although the width of the energy loss distribution increases with energy, the width of the derived Compton profiles is constant.

The width of the proton Compton profile as measured with electrons and with neutrons.

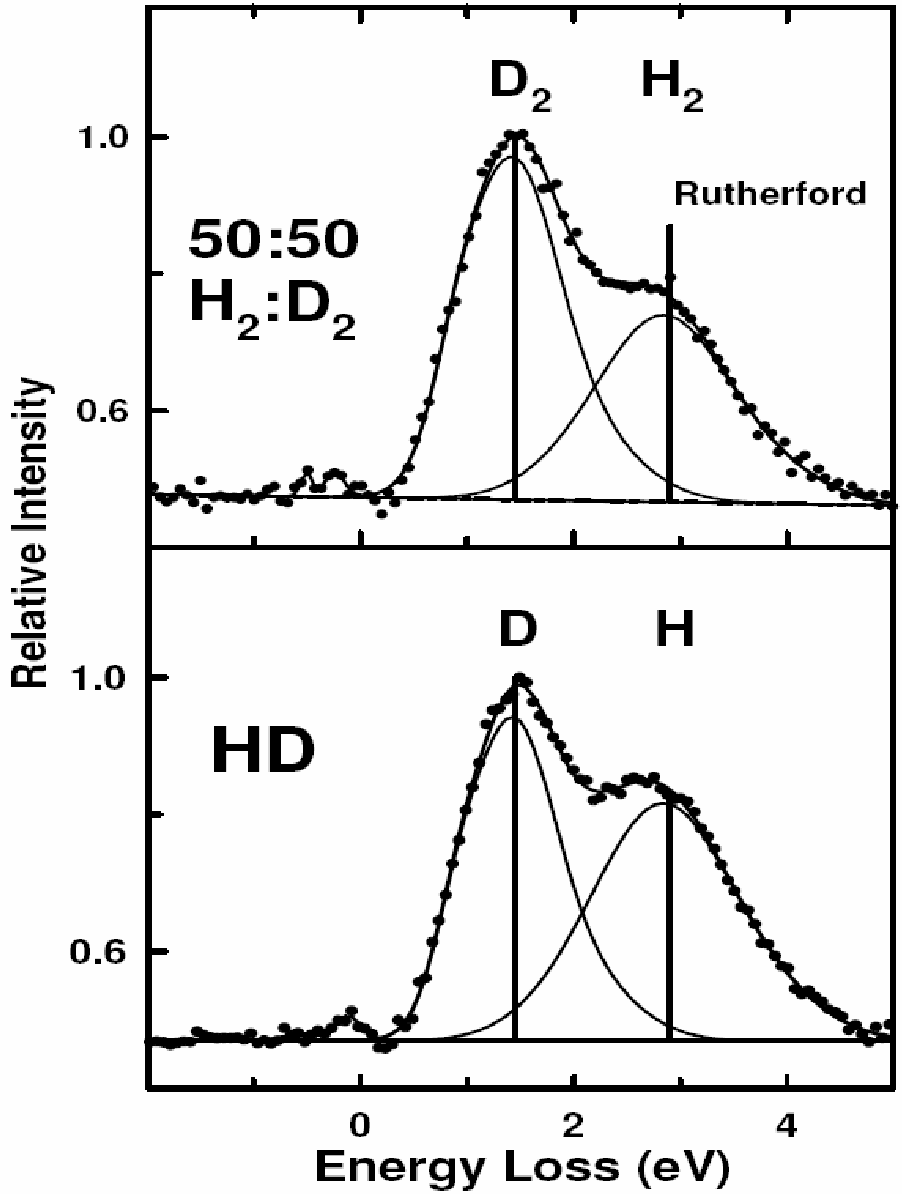


The experimentally observed hydrogen intensity R_{exp} divided by the value that is conventionally expected R_{conv}, based on cross section and material composition of PEr, for both the neutron experiment and the electron scattering experiment. This ratio is always smaller than 1 and decreases with increasing momentum transfer.

At these high energies the differential elastic cross section is reasonably-well approximated by the Rutherford formula. It is thus proportional to Z^2. The intensity ratio C : H in CH_4 should thus be 36:4*1=9:1. The observed values are very close to this ratio. (deviations less than 10%, probably less than 5%). No unexplained quantum effects in the gas-phase?



However new unexplained effects are reported for electron scattering from 50%-H_2, 50% D_2 mixtures compared to electron scattering from HD (Cooper, Hitchcock, Chatzidimitriou-Dreismann, Phys. Rev. Lett. In press)



From Cooper, Hitchcock, Chatzidimitriou-Dreismann, Phys. Rev. Lett. In press.

Hydrogen intensity to low in H_2:D_2 mixture??

This measurement can be done with much better H-D separation (up to 5 eV) using the ANU spectrometer

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Conclusion

-Elastic scattering does not mean that projectile energy is unchanged
-Scattering at high momentum transfer is from atoms, not molecules
-Peak width and peak separation are well understood.
-For methane the relative peak intensity seems in agreement with simple theory

High energy electron scattering can give new, clear unambiguous information
Other example see poster:
Electron Scattering from Xe at extremely high momentum transfer

Thanks for your attention!