Role of Feynman diagrams in energy band structure of materials : A post density functional theory approach

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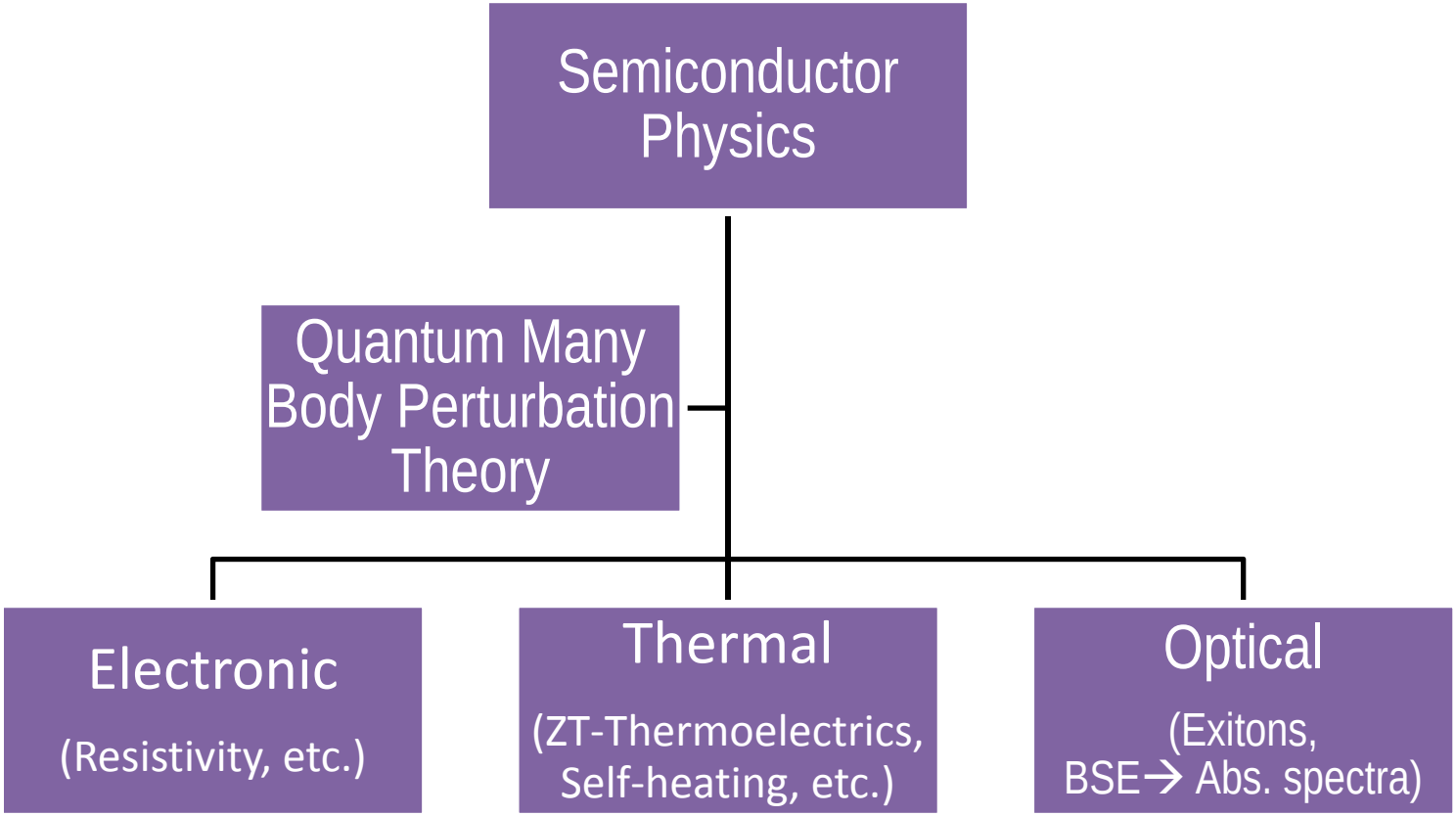
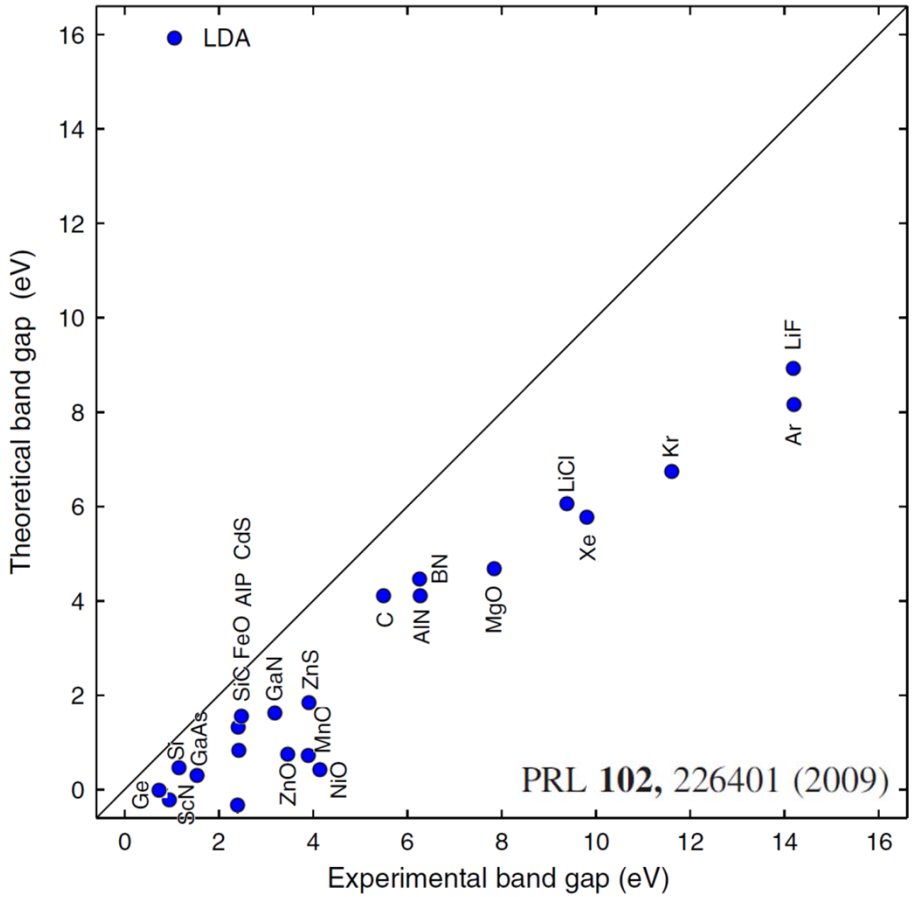
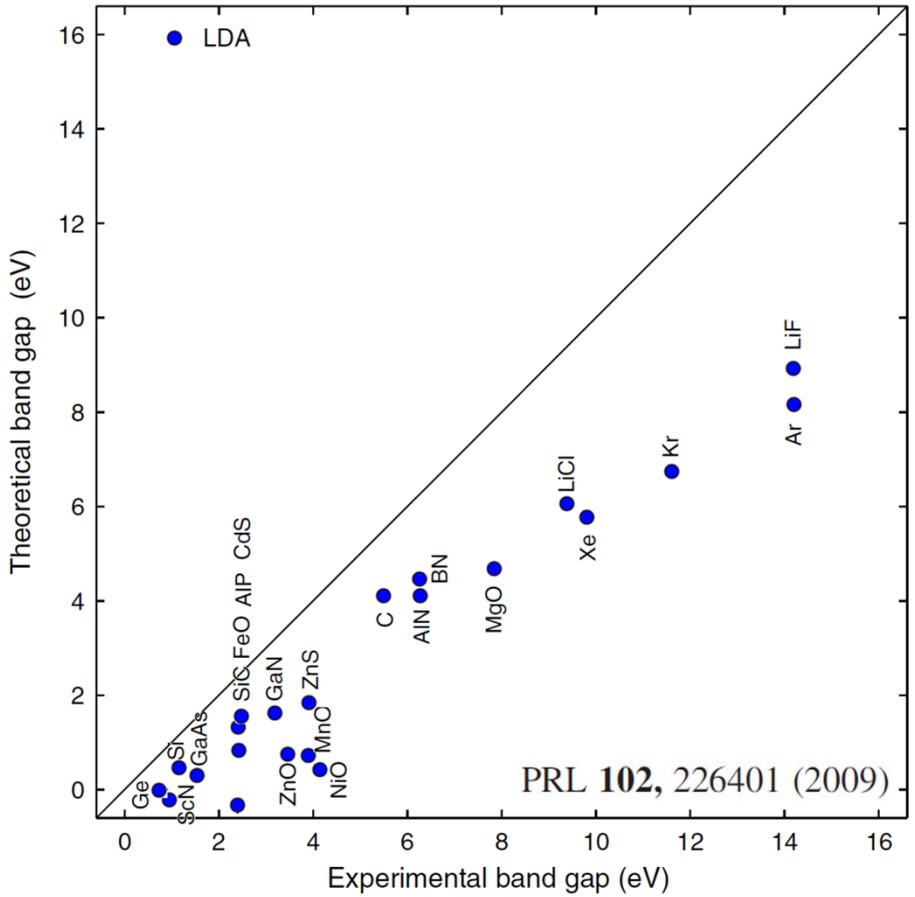
Research Activities : Semiconductor transport phenomena (computational)



A visit to the energy band structure in semiconductors



A visit to the energy band structure in semiconductors



Why should this happen? And how to fix this problem ?

Understanding how a band gap is measured first

Electronic Band Gap

Optical Band Gap

Understanding how a band gap is measured first

Electronic Band Gap

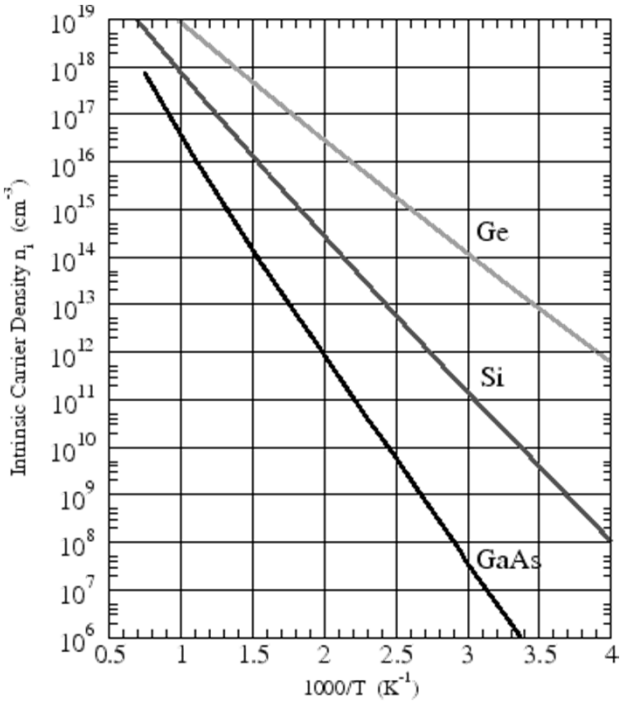
Hall Effect Measurement :

Understanding how a band gap is measured first

Electronic Band Gap

Hall Effect Measurement :

- Find out carrier densities at different temperatures.
- The slope in log scale will give you the band gap.



Understanding how a band gap is measured first

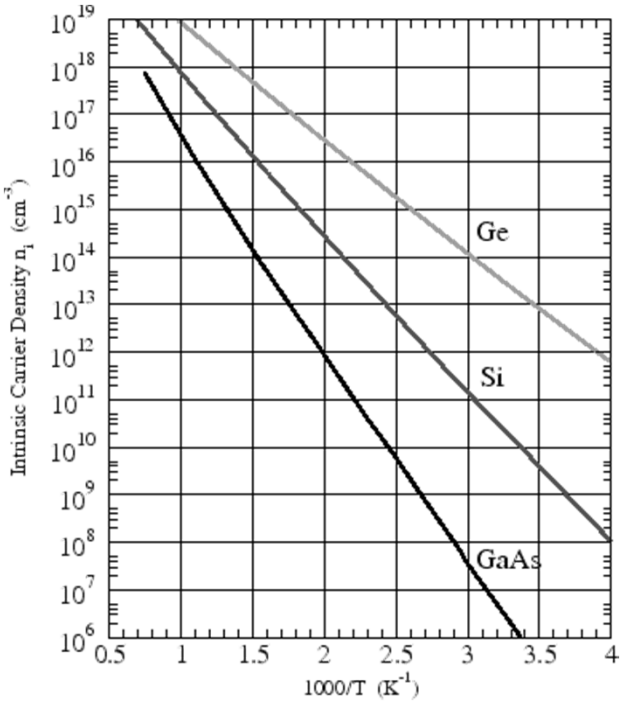
Electronic Band Gap

Hall Effect Measurement :

- Find out carrier densities at different temperatures.
- The slope in log scale will give you the band gap.

However, beware about the Hall-factor coefficient r_H.

$$n_H = \frac{n_S}{r_H}$$



Understanding how a band gap is measured first

Optical Band Gap

Angle Resolved Photo-Emission Spectroscopy Measurement :

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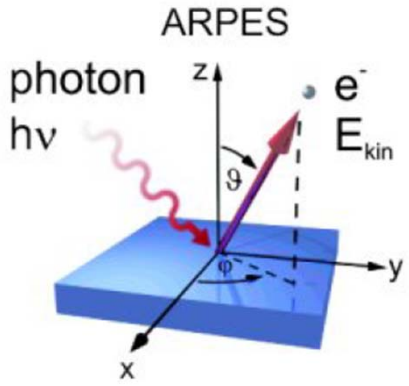
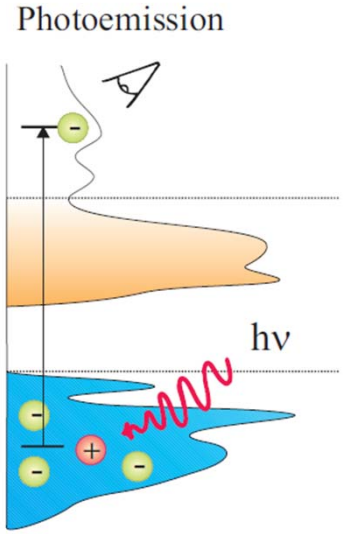




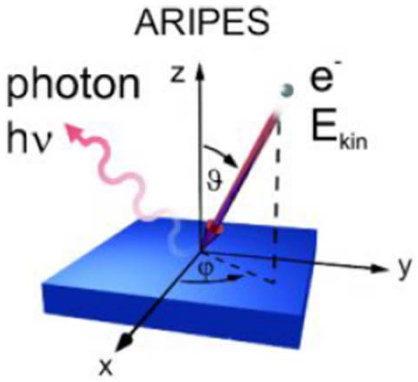
Removal of Electron:

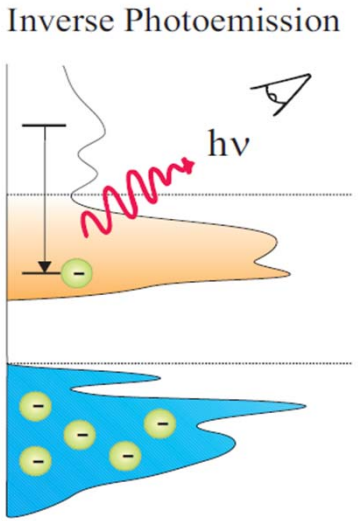
$\varepsilon_r = E(N,s) - E(N-1,s)$

Understanding how a band gap is measured first

Optical Band Gap

Angle Resolved Photo-Emission Spectroscopy Measurement :





Addition of Electron:

$\varepsilon_a = E\,(N+1,s) - E\,(N,s)$

Understanding how a band gap is measured first

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Angle Resolved Photo-Emission Spectroscopy Measurement :

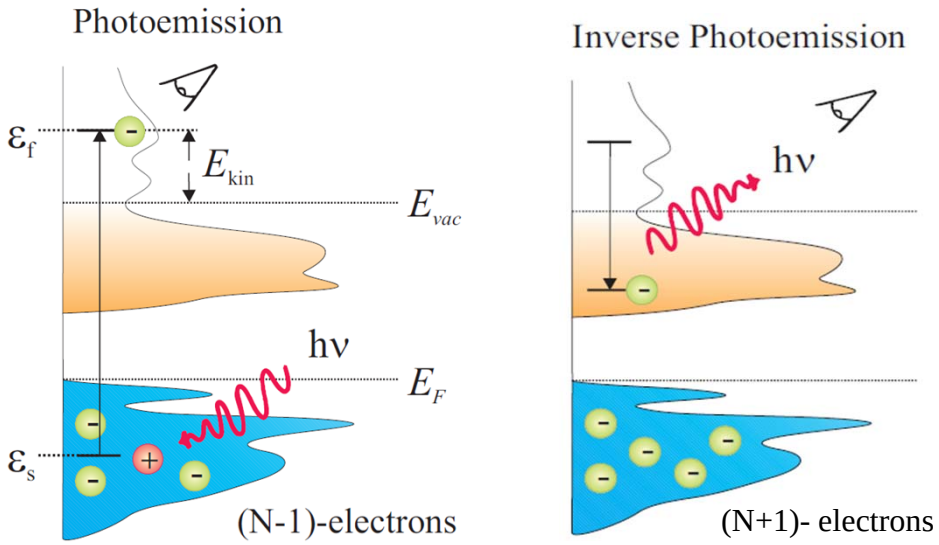
Fundamental Band Gap:

$$\varepsilon_G = \varepsilon_a - \varepsilon_r$$

Understanding how a band gap is measured first

Optical Band Gap

Angle Resolved Photo-Emission Spectroscopy Measurement :



The states E(N+1,s) and E(N-1,s) are called as the excited states and contains all the information that you need for the correction of the underestimated band gap.

Understanding how DFT calculate the band-gap

DFT underlying principles: Hohenberg-Kohn Theorem

- For any interacting particle system in an external potential, the density is uniquely determined.

For eg, see: Walter Harrison: Elementary Electronic Structure

Understanding how DFT calculate the band-gap

DFT underlying principles: Hohenberg-Kohn Theorem

- For any interacting particle system in an external potential, the density is uniquely determined.
- A universal *functional* for the energy E[n] can be defined in terms of the density. The exact ground state is the global minimum value of this functional.

DFT is a ground state story

For eg, see: Walter Harrison: Elementary Electronic Structure

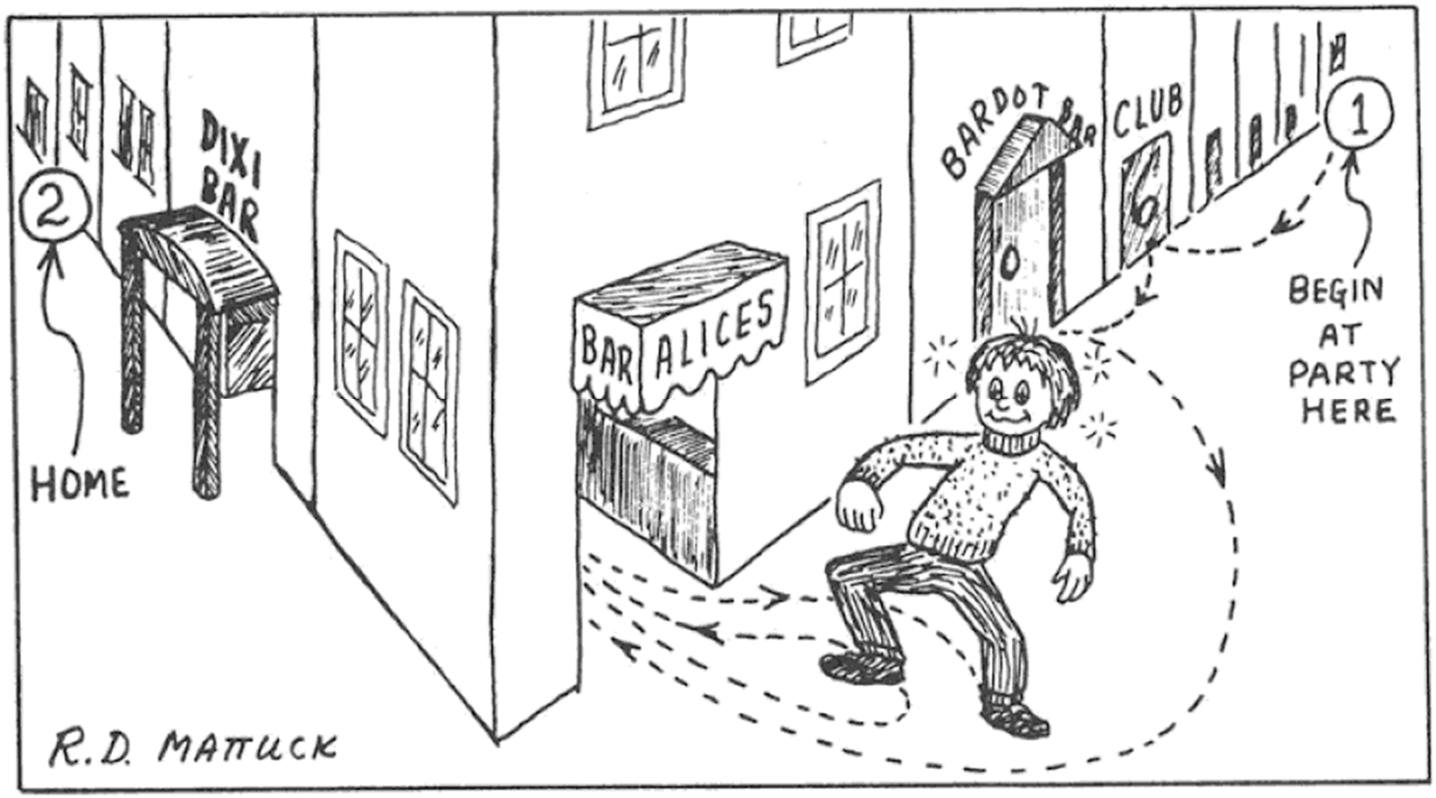
Include dynamic screening!

Electrons are screened.

This is known as GW formalism.

Lets understand this...

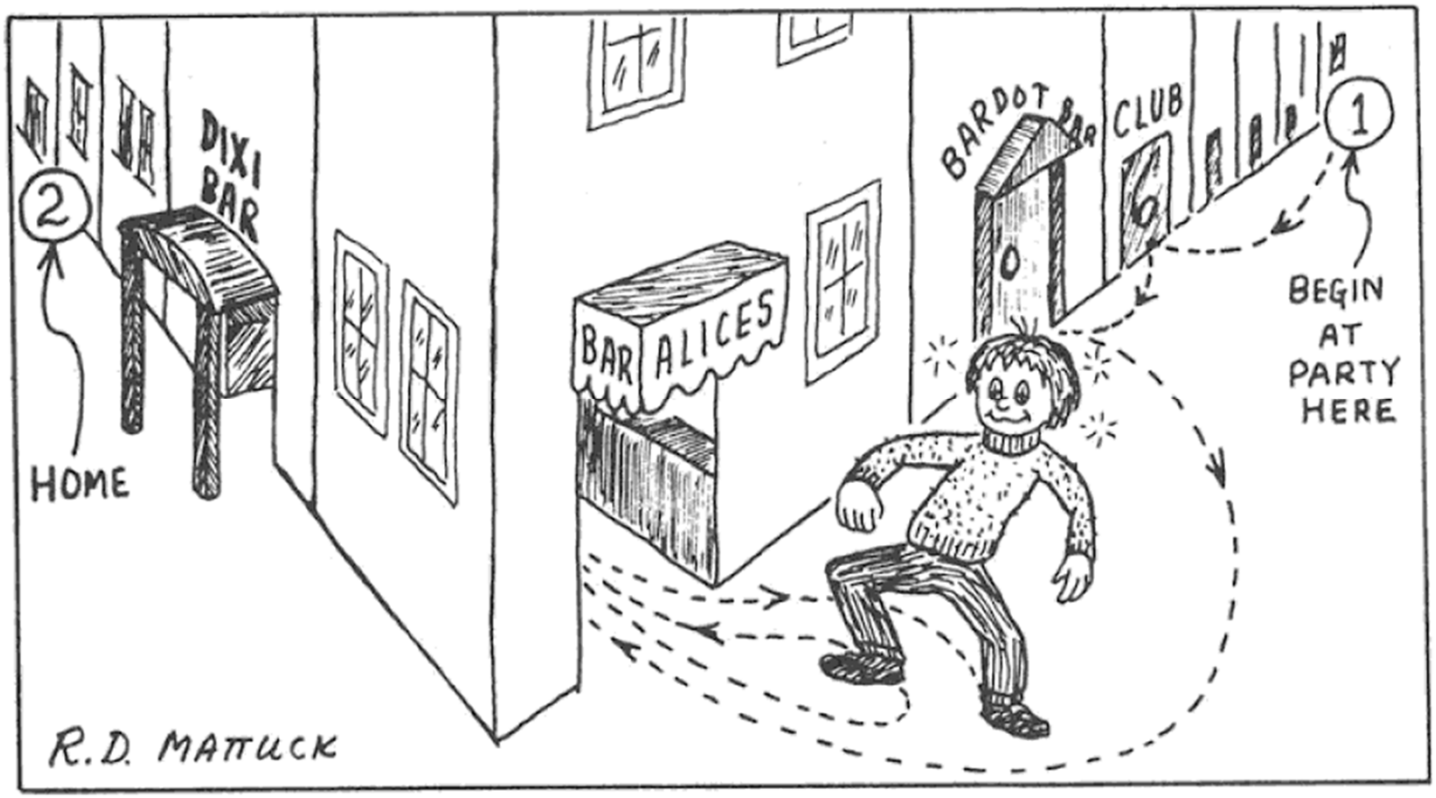
A strict drunker case: Random Walk Problem



What is the probability the drunker can end up in his home?

See: Encyclopedia of Physics, page 442

A strict drunker case: Random Walk Problem

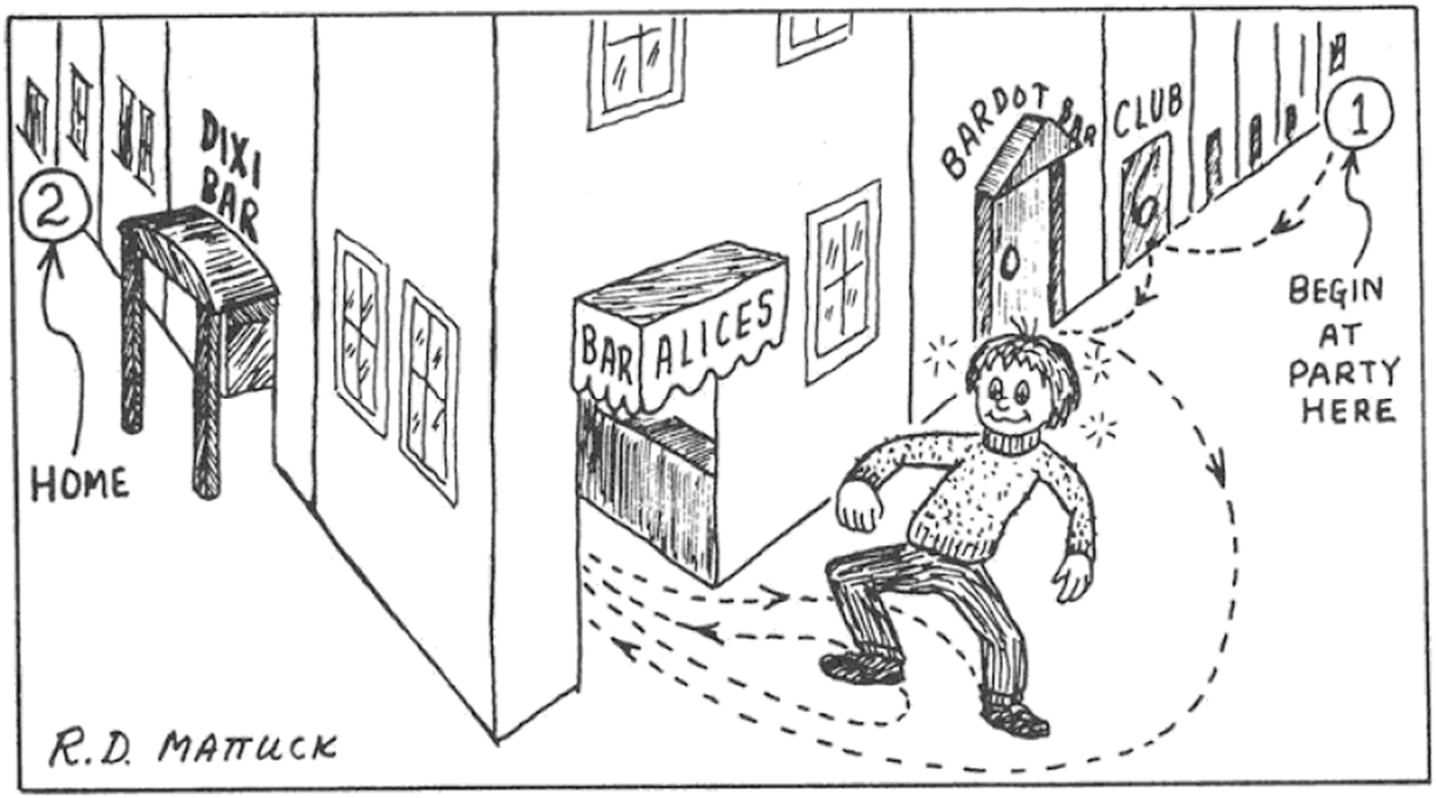


1st way:

Go free from 1 to 2 without stopping = $P_0(2,1)$

See: Encyclopedia of Physics, page 442

A strict drunker case: Random Walk Problem

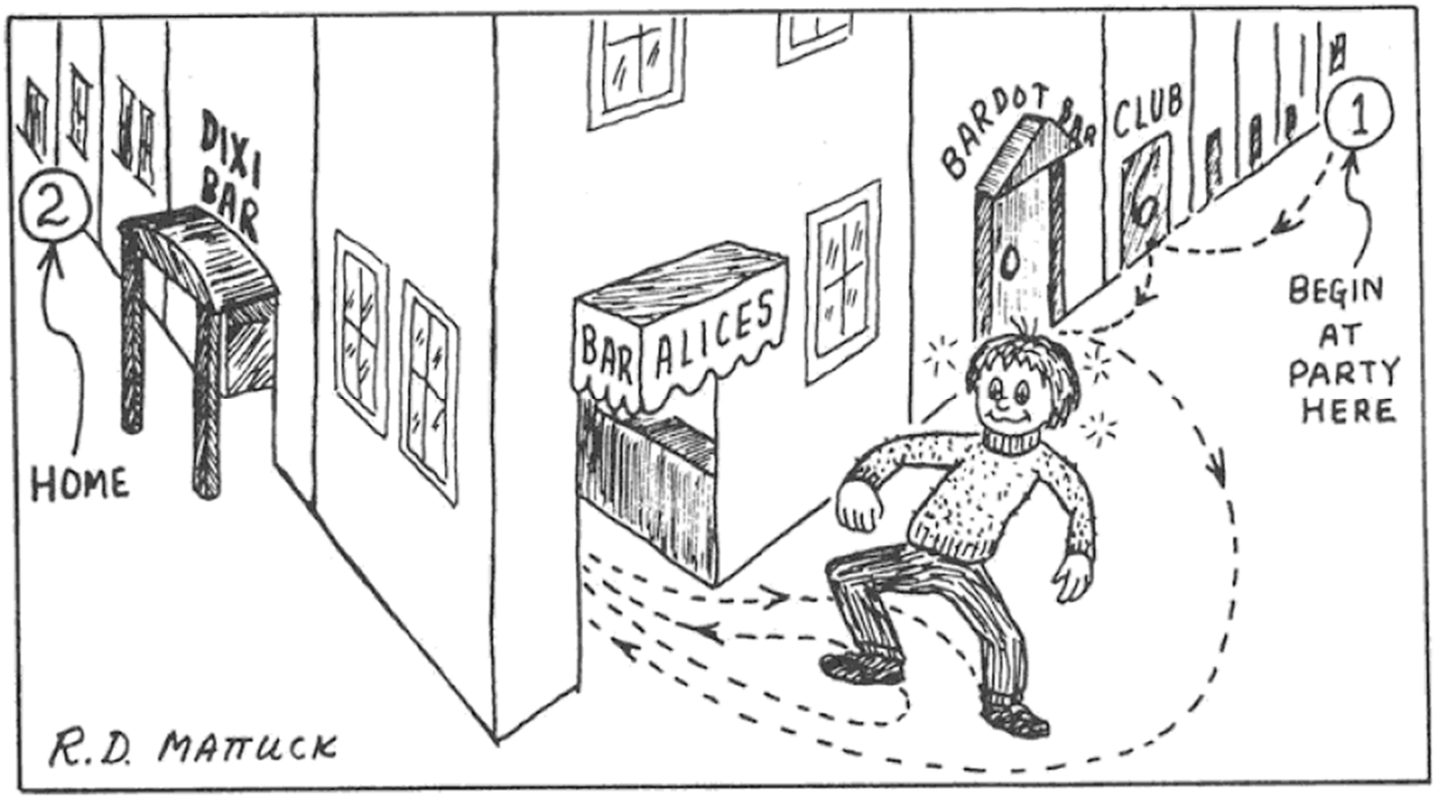


2nd way:

Go freely from 1 to bar A ($P_0(A,1)$) and then stop for a drink ($P(A)$) and then go freely from A to 2 ($P_0(2,A)$).

See: Encyclopedia of Physics, page 442

A strict drunker case: Random Walk Problem

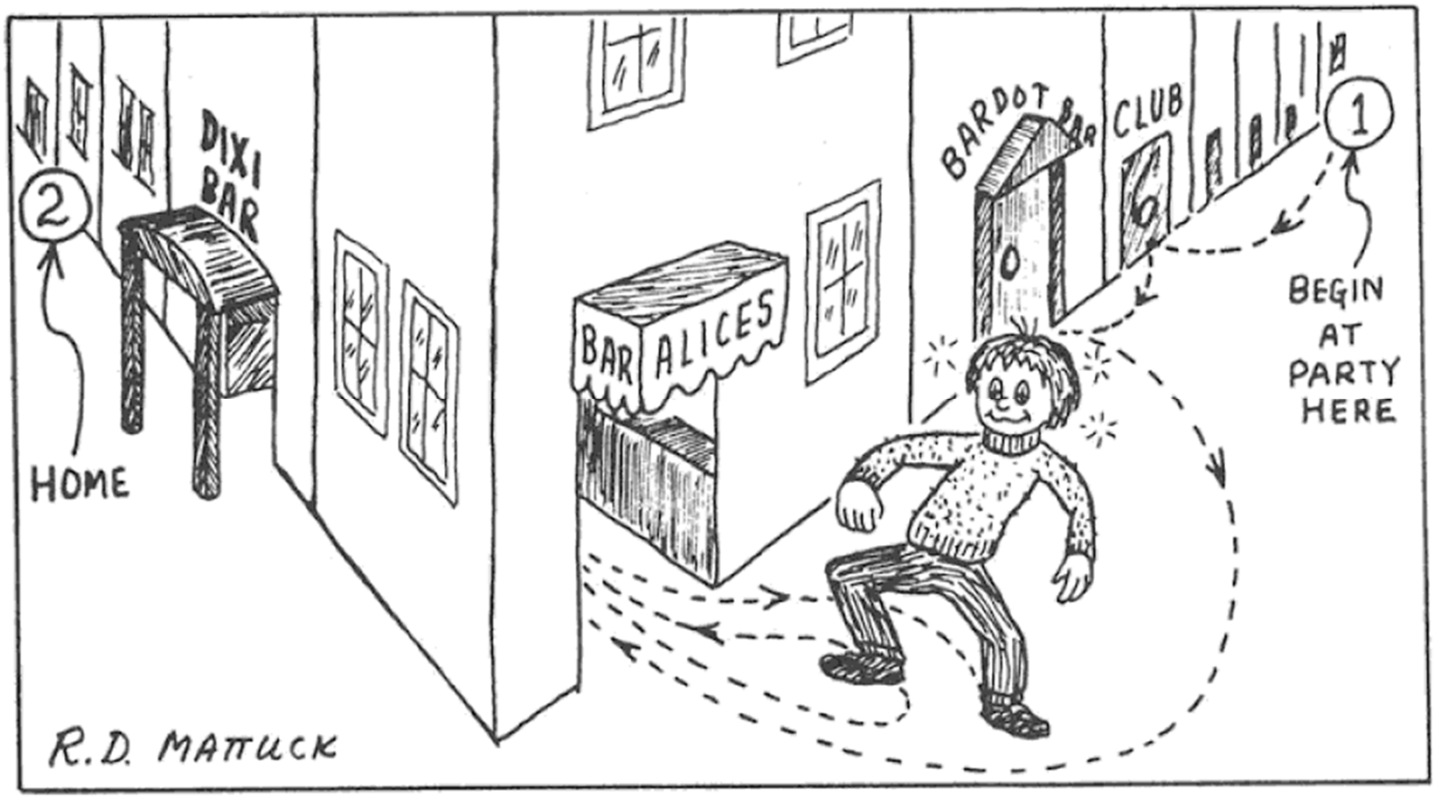


2nd way:

$P_0(A,1) \times P(A) \times P_0(2,A)$

See: Encyclopedia of Physics, page 442

A strict drunker case: Random Walk Problem

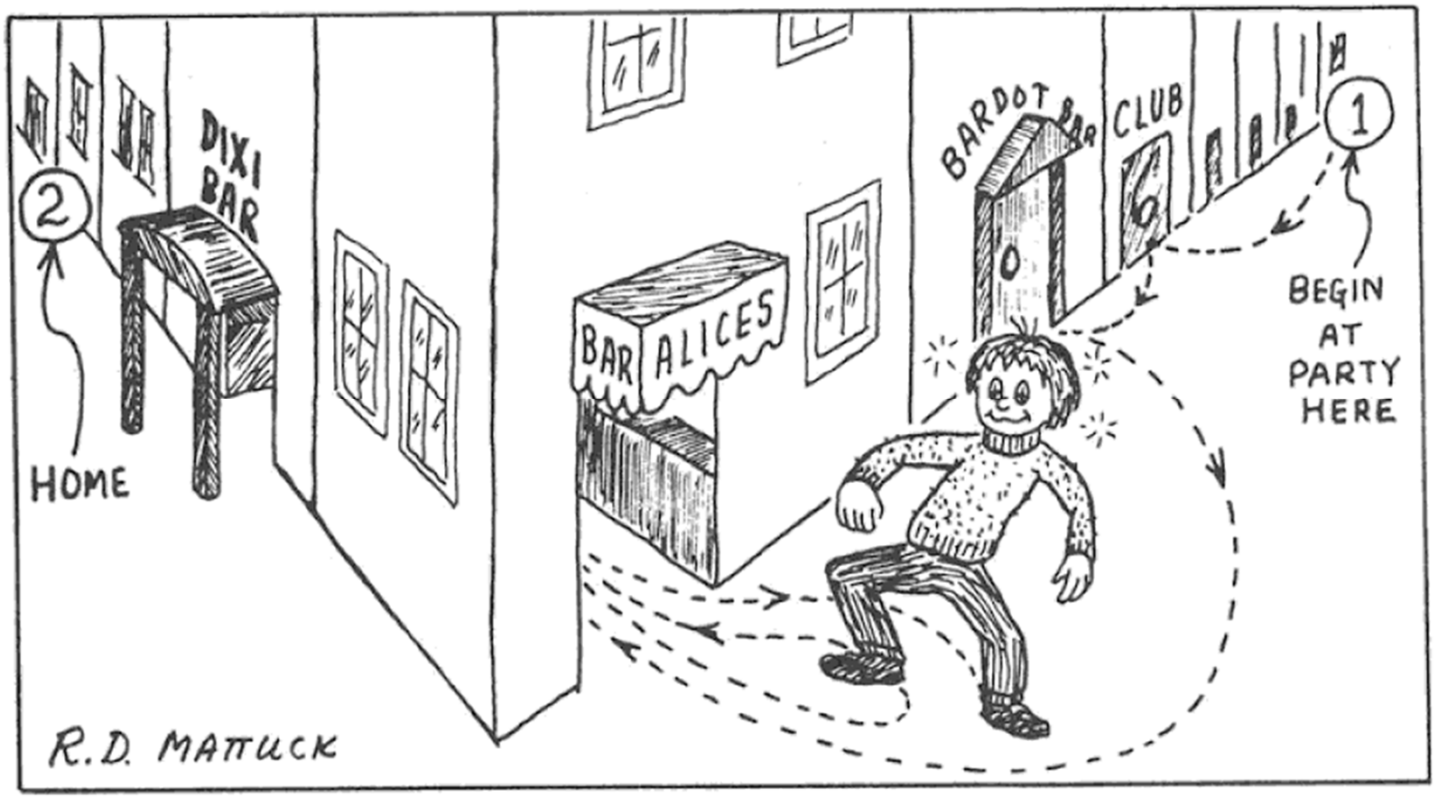


3rd way:

$P_0(B,1) \times P(B) \times P_0(2,B)$ … and so on

See: Encyclopedia of Physics, page 442

A strict drunker case: Random Walk Problem



Total probability:

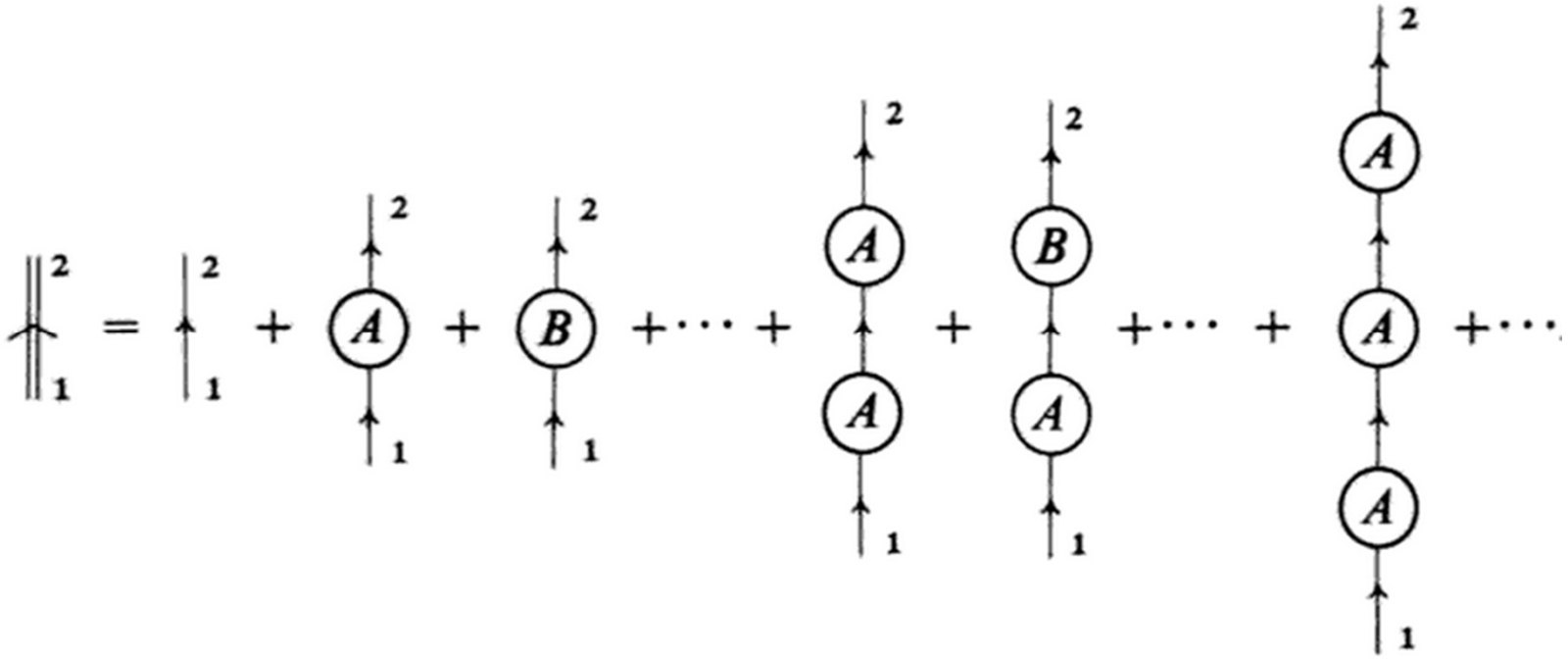
$$P(2,1) = P_0(2,1) + P_0(A,1)\,P(A)\,P_0(2,A) + P_0(B,1)\,P(B)\,P_0(2,B) + P_0(A,1)\,P(A)\,P_0(B,A)\,P(B)\,P_0(2,B) + \ldots$$

See: Encyclopedia of Physics, page 442

Feynman's view

Total probability:

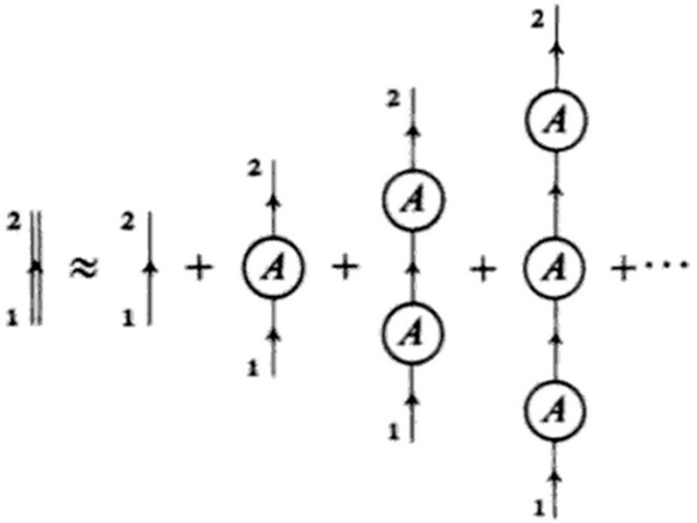
$$P(2,1) = P_0(2,1) + P_0(A,1)\,P(A)\,P_0(2,A) + P_0(B,1)\,P(B)\,P_0(2,B) + P_0(A,1)\,P(A)\,P_0(B,A)\,P(B)\,P_0(2,B) + \ldots$$

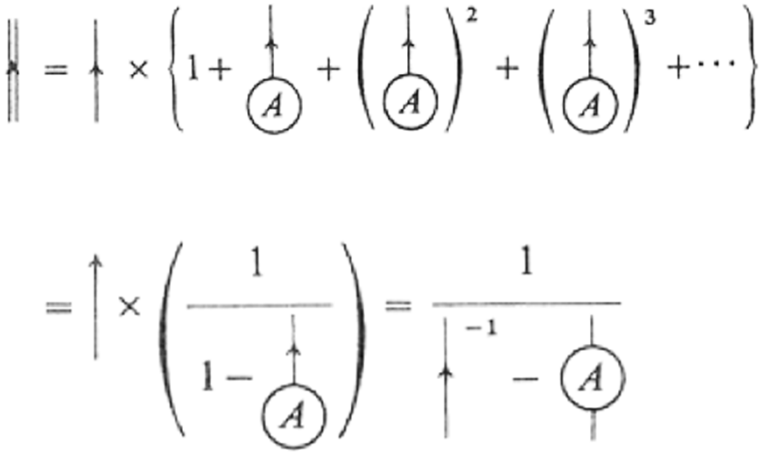


Feynman's view

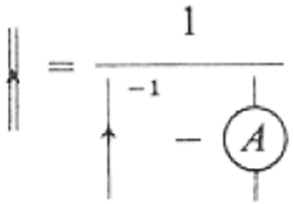
Diagrammatically:

$$P(2,1) = \frac{1}{a^{-1} - P(A)}$$





Quasi-particle GW Formalism



This is my Green's function propagator formalism.

Mathematically (in FT-plane):

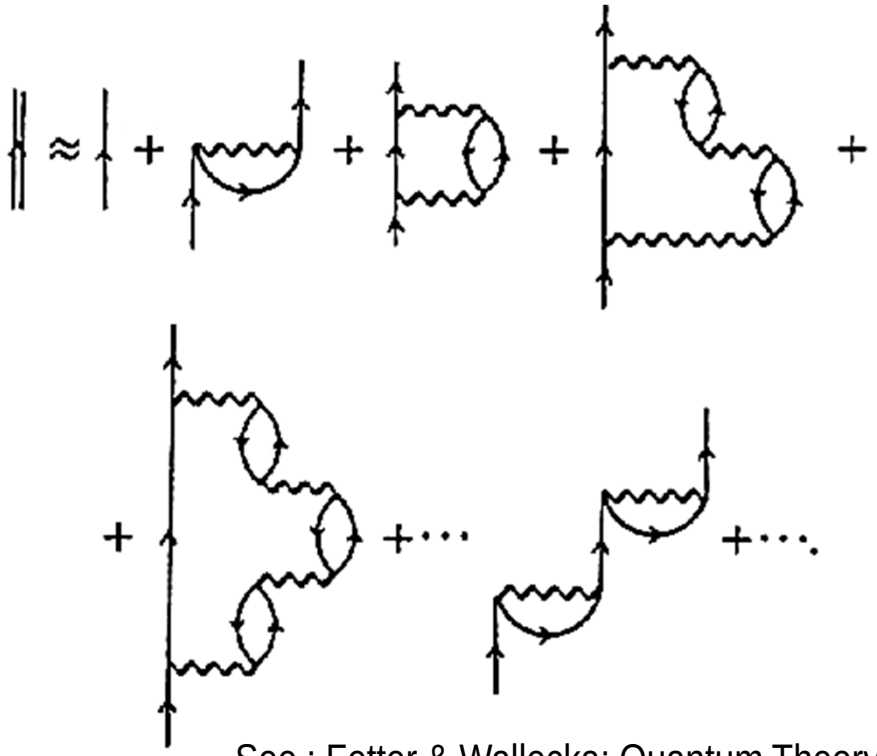
$$G^{+}(k,\omega)=\frac{1}{\left[G_{0}^{+}(k,\omega)\right]^{-1}-V_{m_{kk}}}$$

Quasi-particle GW Formalism

Picture example of a particle Green's function:

Ring Diagram

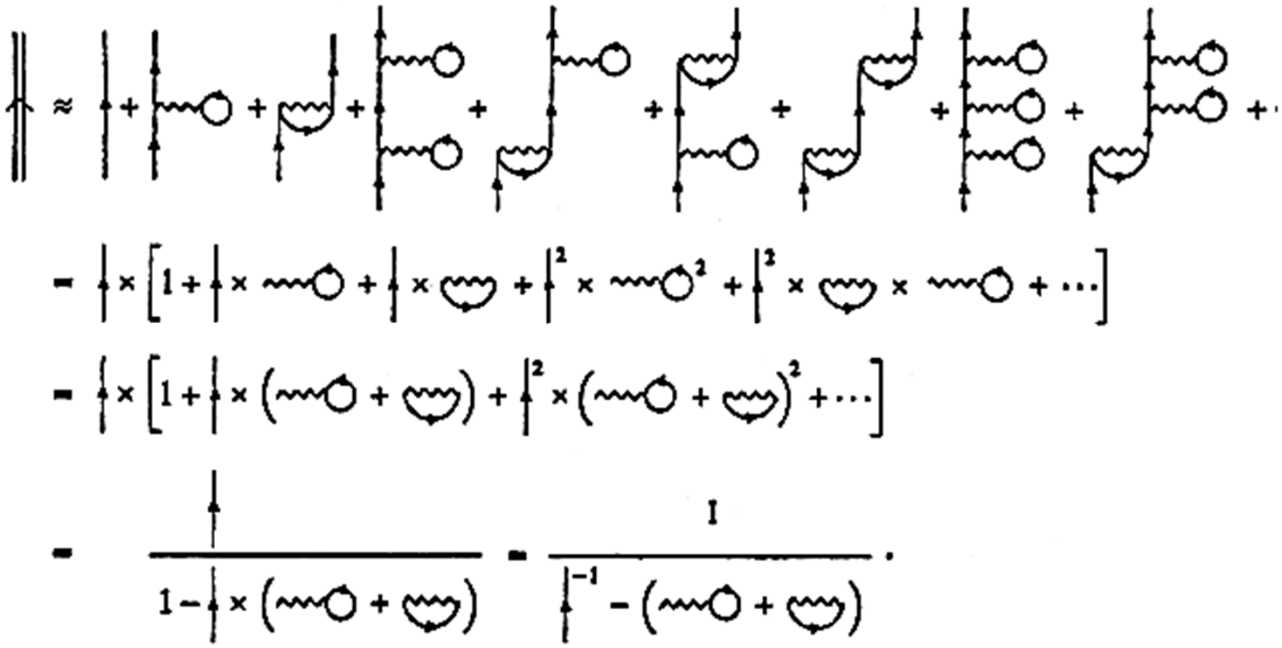
"Random-Phase Approximation in post- DFT"



See : Fetter & Wallecka: Quantum Theory of Many Particle Systems

Quasi-particle GW Formalism

Hartree-Fock Term:



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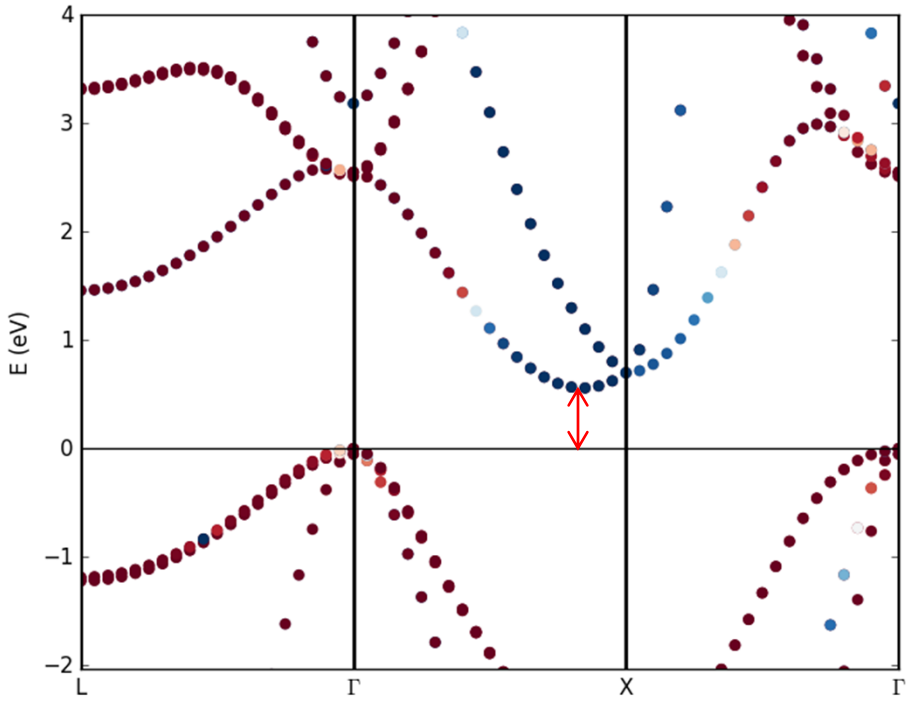
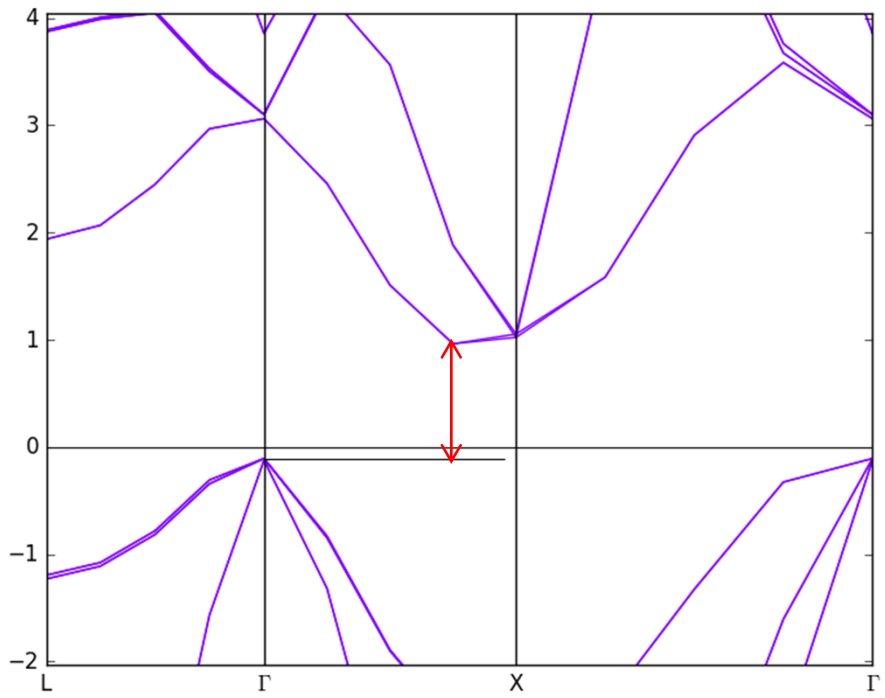
Quasi-particle GW Formalism (Relativistic Correction)



Si band gap DFT ~ 0.55eV



Si band gap GW_0 ~ 1.07 eV
GW Approximation

Thank You all.