Electron density of states and mobility in dilute GaAs:N

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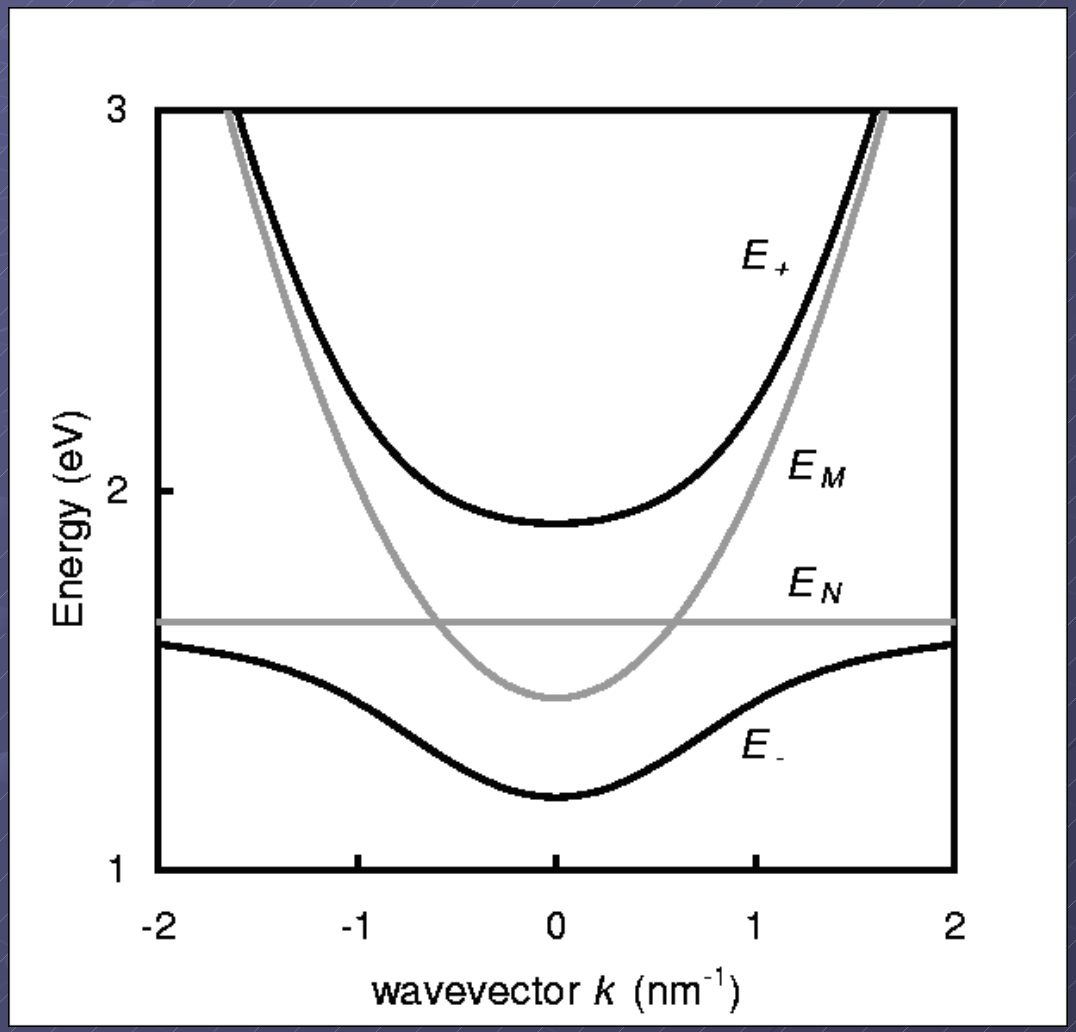
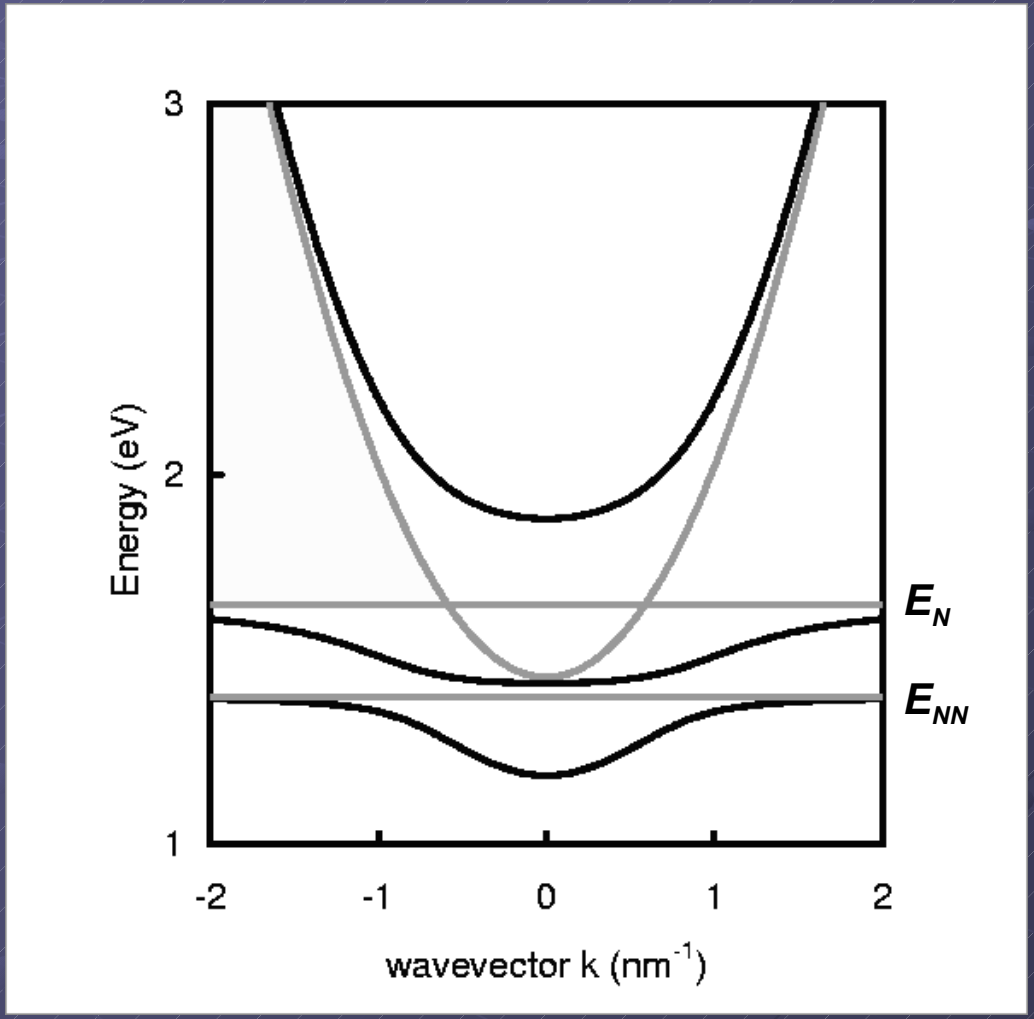
Overview

- The interaction picture – *n*-band model
- Problem with the density of states
- The Anderson Hamiltonian
- The density of states
- Nitrogen scattering
- Mobility calculations

Dispersion relations in the BAC model



3 band model [1]



[1] A. Lindsay, PhD Thesis, University of Surrey, (unpublished) (2002); S.B. Healy, A. Lindsay and E.P. O'Reilly, *IEE Proc.-Optoelectron.*, **151**, 397 (2004)

Generalisation of the BAC model

'*n*-band' model

$$H = \begin{bmatrix} E_M(\mathbf{k}) & V_1 x_1^{1/2} & V_2 x_2^{1/2} & \cdots & V_{n-1} x_{n-1}^{1/2} \\ V_1 x_1^{1/2} & E_1 & 0 & \cdots & 0 \\ V_2 x_2^{1/2} & 0 & E_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ V_{n-1} x_{n-1}^{1/2} & 0 & 0 & 0 & E_{n-1} \end{bmatrix}$$

Example: the 3-band model due to Lindsay [1] in terms of isolated nitrogen centres and N-N pairs

A more general model is given by the **LCINS** (linear combination of isolated nitrogen states) model, in which the nitrogen states are note assumed to be orthogonal. See, for instance, Lindsay and O'Reilly [2].

[1] A. Lindsay, PhD Thesis, University of Surrey, (unpublished) (2002); S.B. Healy, A. Lindsay and E.P. O'Reilly, *IEE Proc.-Optoelectron.*, **151**, 397 (2004)
[2] A. Lindsay and E. P. O'Reilly, *Phys. Rev. Lett.*, **93**, 196402 (2004)

Non-parabolicity

From the characteristic equation of the *n* – band Hamiltonian

$$E_M(\mathbf{k}) = \sum_i \frac{V_i^2 x_i}{E_i - E} + E \equiv \gamma(E)$$

Note: for any nitrogen energy E_i

$$\text{As} \quad E \to E_i, \quad \gamma(E) \to \infty$$

Assuming $E_M(\mathbf{k})$ is parabolic greatly simplifies the mathematics. (Note that m_0^* is the *matrix semiconductor effective mass*).

$$\frac{\hbar^2 k^2}{2m_0^*} = \gamma(E)$$

Problem with the density of states (DOS)

From the dispersion relations, the densities of states are

$$N_{3D}(E) = \frac{(2m_0^*)^{3/2}}{4\pi^2\hbar^3}\gamma^{1/2}(E)\frac{d\gamma(E)}{dE}$$

and

$$N_{2D}(E) = \frac{m_0^*}{2\pi\hbar^2}\frac{d\gamma(E)}{dE}$$

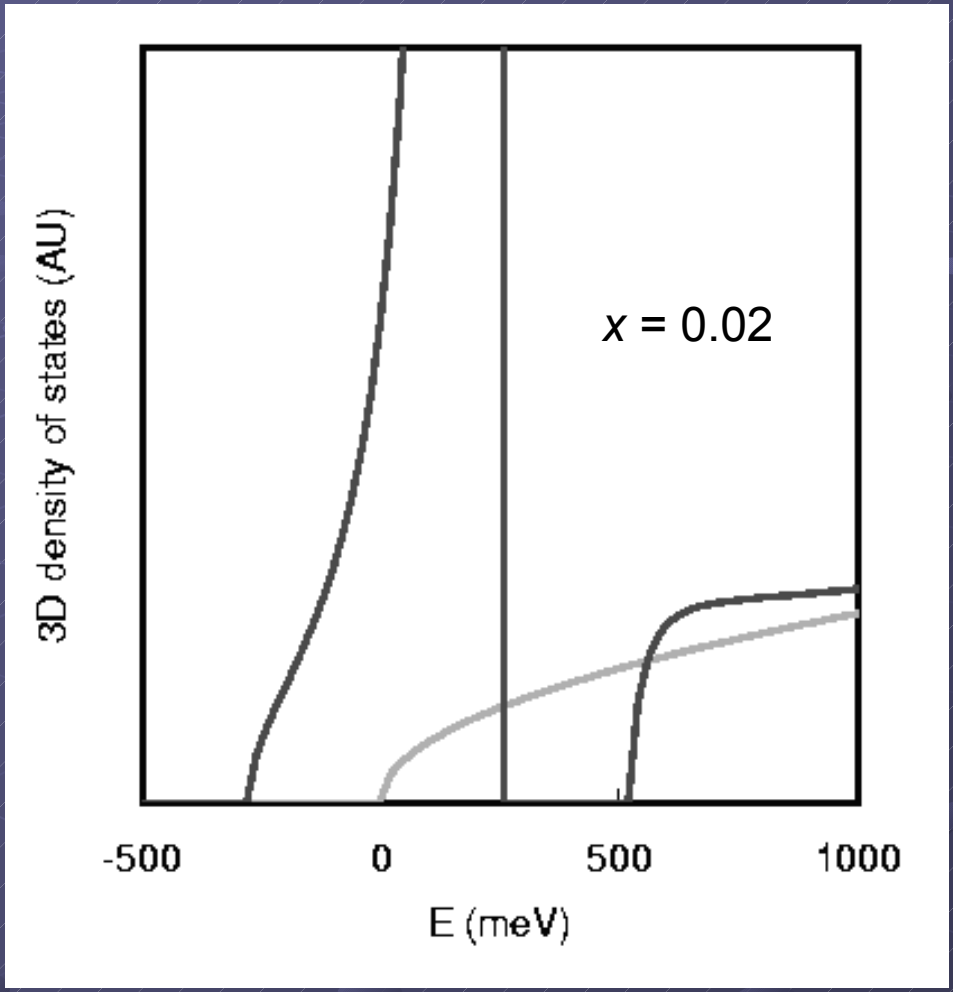
But

$$\text{number of states} < E_i = \int_0^{E_i}\frac{(2m_0^*)^{3/2}}{4\pi^2\hbar^3}\gamma^{1/2}(E)\frac{d\gamma(E)}{dE}dE$$

$$= \frac{2}{3}\frac{(2m_0^*)^{3/2}}{4\pi^2\hbar^3}\gamma^{3/2}(E_i) = \infty(!)$$

with a similar problem in 2D.

3D DOS from dispersion relations



Summary of problem

- The densities of states derived from the dispersion relations are non-integrable, implying an infinite number of states
- The singularities re-appear even when we relax the assumption of spherical energy bands
- Van Hove singularities *do not* make the DOS non-integrable

The Anderson model [1]

$$H = H_0 + V$$

H_0 is a sum of two terms describing the energies of extended and localised states,

$$H_0 = \sum_{\mathbf{k}} E_{\mathbf{k}} b_{\mathbf{k}}^{+} b_{\mathbf{k}} + \sum_{\mathbf{j}} E_{\mathbf{j}} b_{\mathbf{j}}^{+} b_{\mathbf{j}} \qquad V = \frac{1}{\sqrt{N_C}} \sum_{\mathbf{j},\mathbf{k}} \left\{ e^{i\mathbf{k}\cdot\mathbf{j}} V_{\mathbf{kj}} b_{\mathbf{k}}^{+} b_{\mathbf{j}} + e^{-i\mathbf{k}\cdot\mathbf{j}} V_{\mathbf{kj}}^{*} b_{\mathbf{j}}^{+} b_{\mathbf{k}} \right\}$$

N_C is the number of primitive cells in the crystal and the $V_{\mathbf{kj}}$ characterise the hybridisation strength.

For a single impurity, the Green's function of the system has been found by Wu *et al* [2]

[1] P.W. Anderson, *Phys. Rev.*, **124**, 41 (1961);
[2] J. Wu, K.M. Yu and W. Walukiewicz, *IEE Proc.-Optoelectron.*, **151**, 460 (2004)

The generalised Hamiltonian

We find the Green's function for many impurities to be

$$G_{\mathbf{kk}} = \left\{ E - E_{\mathbf{k}} - \frac{1}{N_C} \sum_{\mathbf{j}} \frac{V_{\mathbf{j}}^2}{E - E_{\mathbf{j}} + i\Delta_{\mathbf{j}}} \right\}^{-1}$$

where the Δ_j are interpreted as energy broadenings on the **j**th impurity. From the poles of $G_{\mathbf{kk}}$, we can construct the generalised Hamiltonian

$$H = \begin{bmatrix} E_M(\mathbf{k}) & V_1/\sqrt{N_C} & V_2/\sqrt{N_C} & \cdots & V_{n-1}/\sqrt{N_C} \\ V_1/\sqrt{N_C} & E_1 - i\Delta_1 & 0 & \cdots & 0 \\ V_2/\sqrt{N_C} & 0 & E_2 - i\Delta_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ V_{n-1}/\sqrt{N_C} & 0 & 0 & 0 & E_{n-1} - i\Delta_{n-1} \end{bmatrix}$$

This can be rendered in terms of concentrations by putting $x_i = N_i/N_C$

The DOS from the Green's function

Because of the relation between Im G_{kk} and the density matrix, the density of states can be found from

$$N(E) = -\frac{1}{\pi}\,\mathrm{Im}\int G_{\mathbf{kk}} N_0(E_{\mathbf{k}})\,dE_{\mathbf{k}}$$

This gives

$$N_{3D}(E) = -\frac{(2m_0^*)^{3/2}}{4\pi^2\hbar^3}\,\Omega(E)\left\{2\left[\left(\Gamma^2(E)+\Omega^2(E)\right)^{1/2}-\Gamma(E)\right]\right\}^{-1/2}$$

and

$$N_{2D}(E) = \frac{m_0^*}{2\pi\hbar^2}\sum_n\left\{\frac{1}{2}-\frac{1}{\pi}\arctan\left(\frac{\Gamma(E)-E_n}{\Omega(E)}\right)\right\}$$

where

$$\Omega(E) = -\sum_j \frac{V_j^2 x_j \Delta_j}{\left(E-E_j\right)^2+\Delta_j^2} \qquad \text{and} \qquad \Gamma(E) = E - \sum_j \frac{V_j^2 x_j \left(E-E_j\right)}{\left(E-E_j\right)^2+\Delta_j^2}$$

Limits as $\Delta \to 0$

As the broadenings $\Delta_i \to 0$, $\Omega(E) \to 0$ and $\Gamma(E) \to \gamma(E)$, so

$$-\frac{1}{\pi}\lim_{\Delta_j \to 0} \mathrm{Im}\, G_{\mathbf{kk}} = \frac{1}{\pi}\lim_{\Omega \to 0} \frac{\Omega(E)}{\left(\gamma(E) - E_M\right)^2 + \Omega^2(E)} = \delta\left(\gamma(E) - E_M\right)$$

giving the general result

$$N(E) = \int N_0(E_M)\,\delta\left(\gamma(E) - E_M\right) dE_M = N_0\{\gamma(E)\}$$

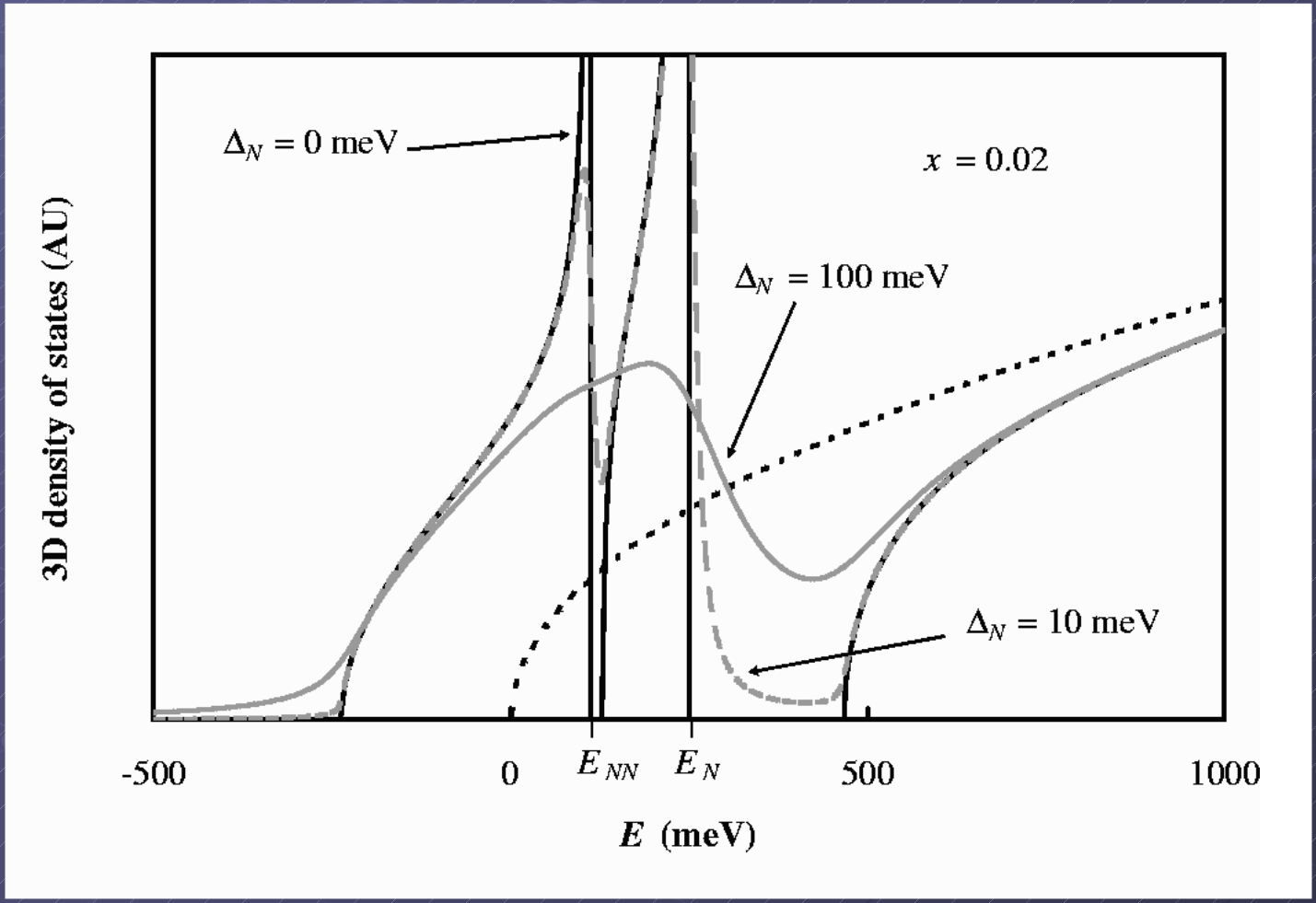
For the simplified model in which E_M is parabolic

$$\lim_{\Delta_j \to 0} N_{3D}(E) = \frac{\left(2m_0^*\right)^{3/2}}{4\pi^2 \square^3}\,\gamma^{1/2}(E)$$

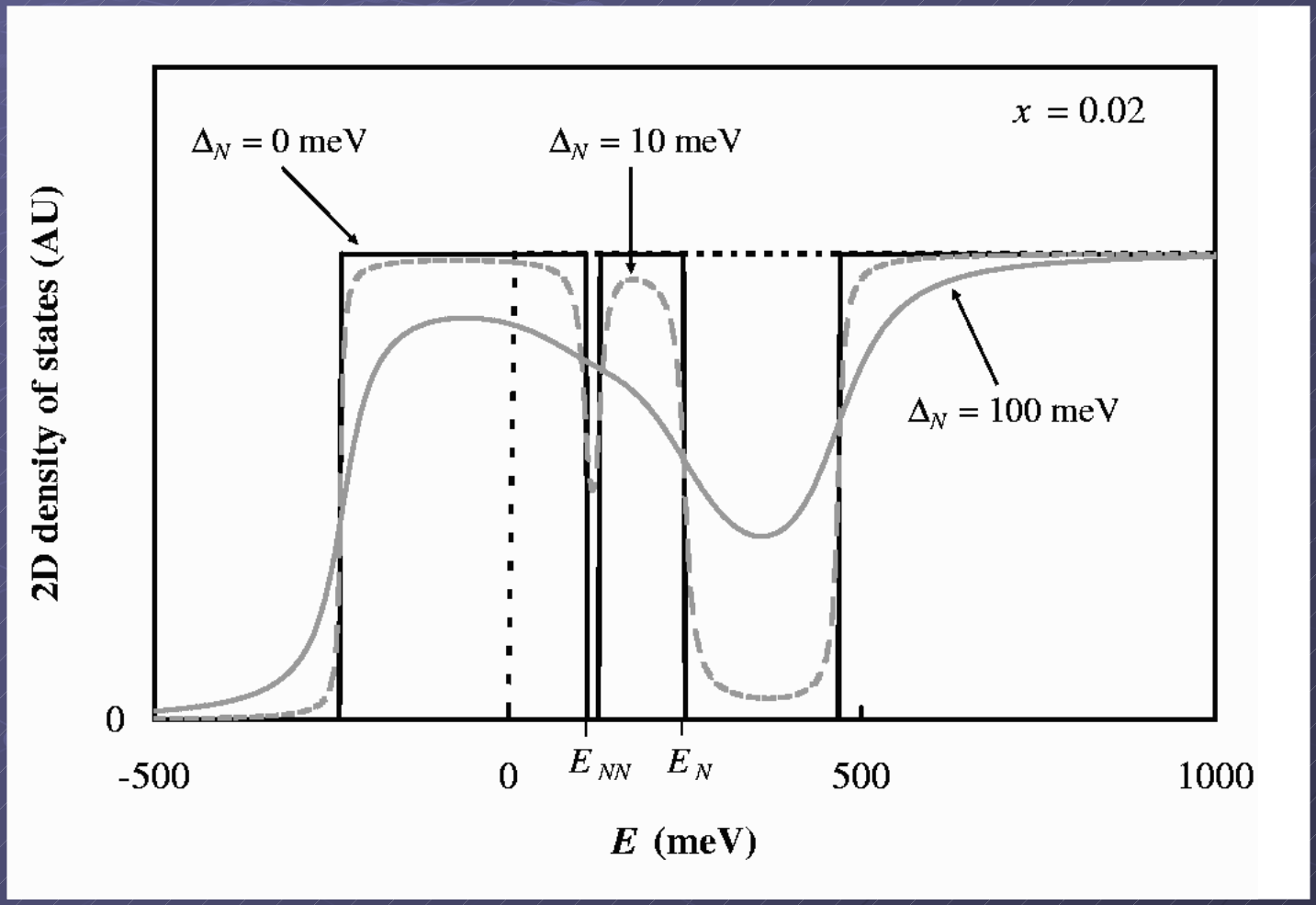
and

$$\lim_{\Delta_j \to 0} N_{2D}(E) = \frac{m_0^*}{2\pi \square^2} \sum_n \theta\left[\gamma(E) - E_n\right]$$

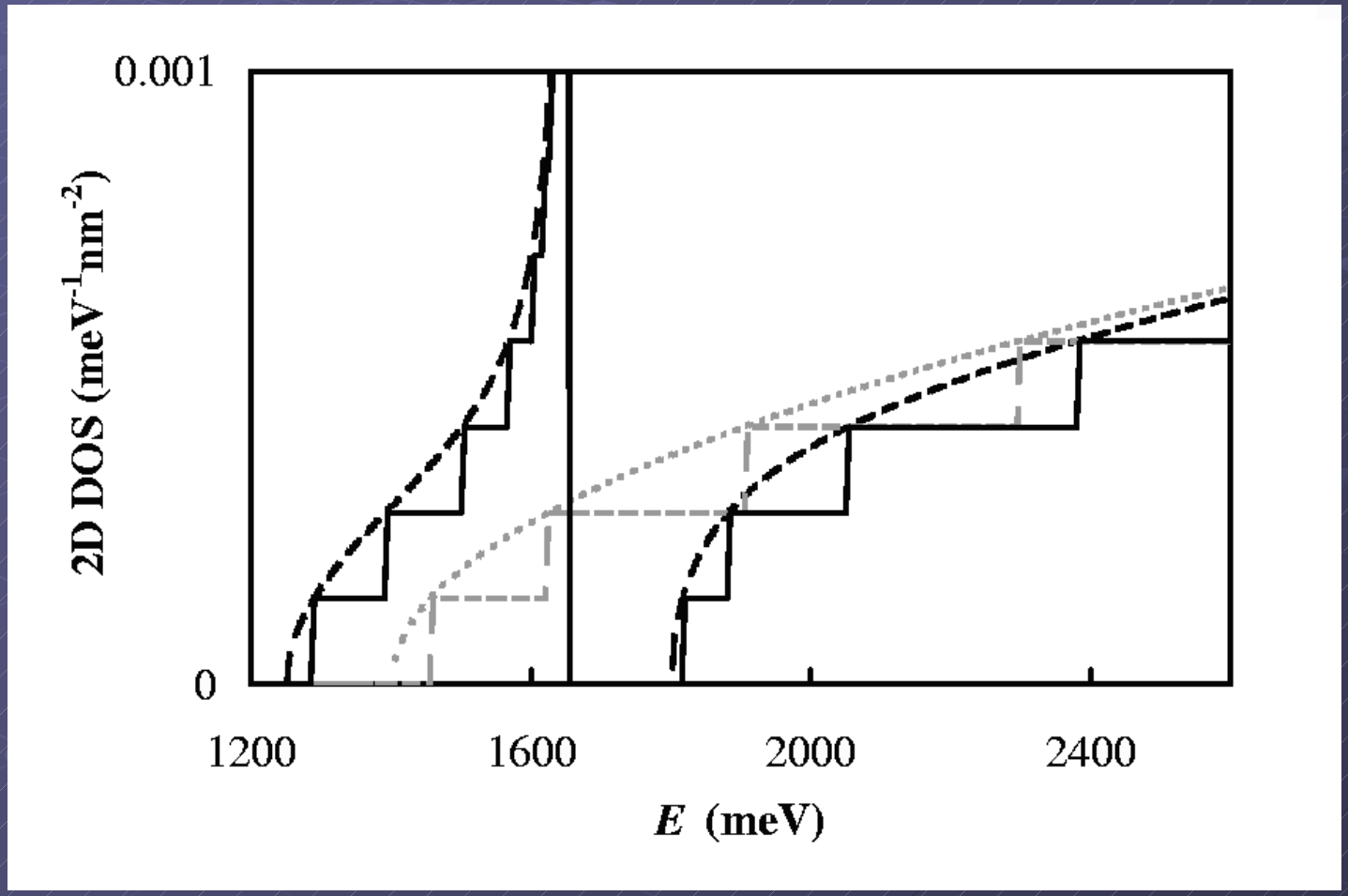
The 3D density of states (3-band model)



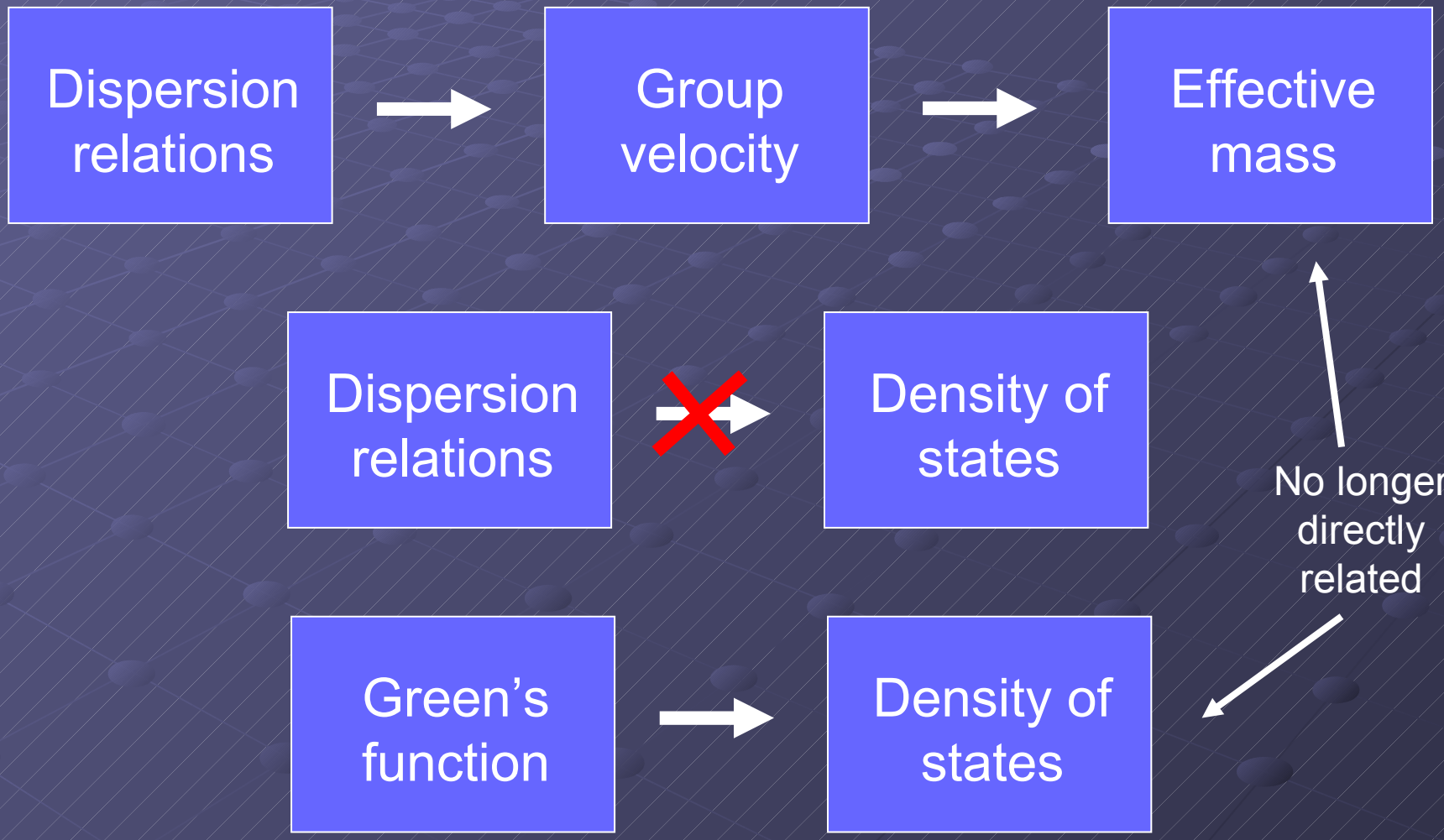
The 2D density of states in a single sub-band (3 – band model)



The 2D density of states summed over sub-bands (2 – band model)



A note on the effective mass



The Green's function DOS

- The densities of states remain integrable
- The number of states in the system is conserved
- In the limit of zero energy broadening, we have a general procedure for finding the density of states from the density of states of the matrix semiconductor

States of the system

The states of the system are a superposition of the host states and impurity states

$$|\psi_{\mathbf{k}}\rangle = \alpha_M |\phi_{\mathbf{k}}\rangle + \sum_{\mathbf{j}} \alpha_{\mathbf{j}} |\mathbf{j}\rangle$$

The **fractional Γ character** is

$$|\alpha_M|^2 = \left(\frac{1}{N_C} \sum_{\mathbf{j}} \frac{V_{\mathbf{j}}^2}{(E_{\mathbf{j}} - E)^2 + (\Delta_{\mathbf{j}} - \Delta(E))^2} + 1 \right)^{-1}$$

Note that

$$\lim_{\Delta_j \to 0} |\alpha_M|^2 = \left(\frac{d\gamma(E)}{dE} \right)^{-1}$$

The projection of the **j**th impurity is

$$|\alpha_{\mathbf{j}}|^2 = \frac{|\alpha_M|^2}{N_C} \frac{V_{\mathbf{j}}^2}{(E - E_{\mathbf{j}})^2 + (\Delta(E) - \Delta_{\mathbf{j}})^2}$$

Group velocity

The group velocity is given by

$$\mathbf{v}(\mathbf{k}) = \nabla_{\mathbf{k}}\omega = \frac{1}{\hbar}\nabla_{\mathbf{k}}E = \frac{1}{\hbar}\left(\frac{dE_M}{dE}\right)^{-1}\nabla_{\mathbf{k}}E_M$$

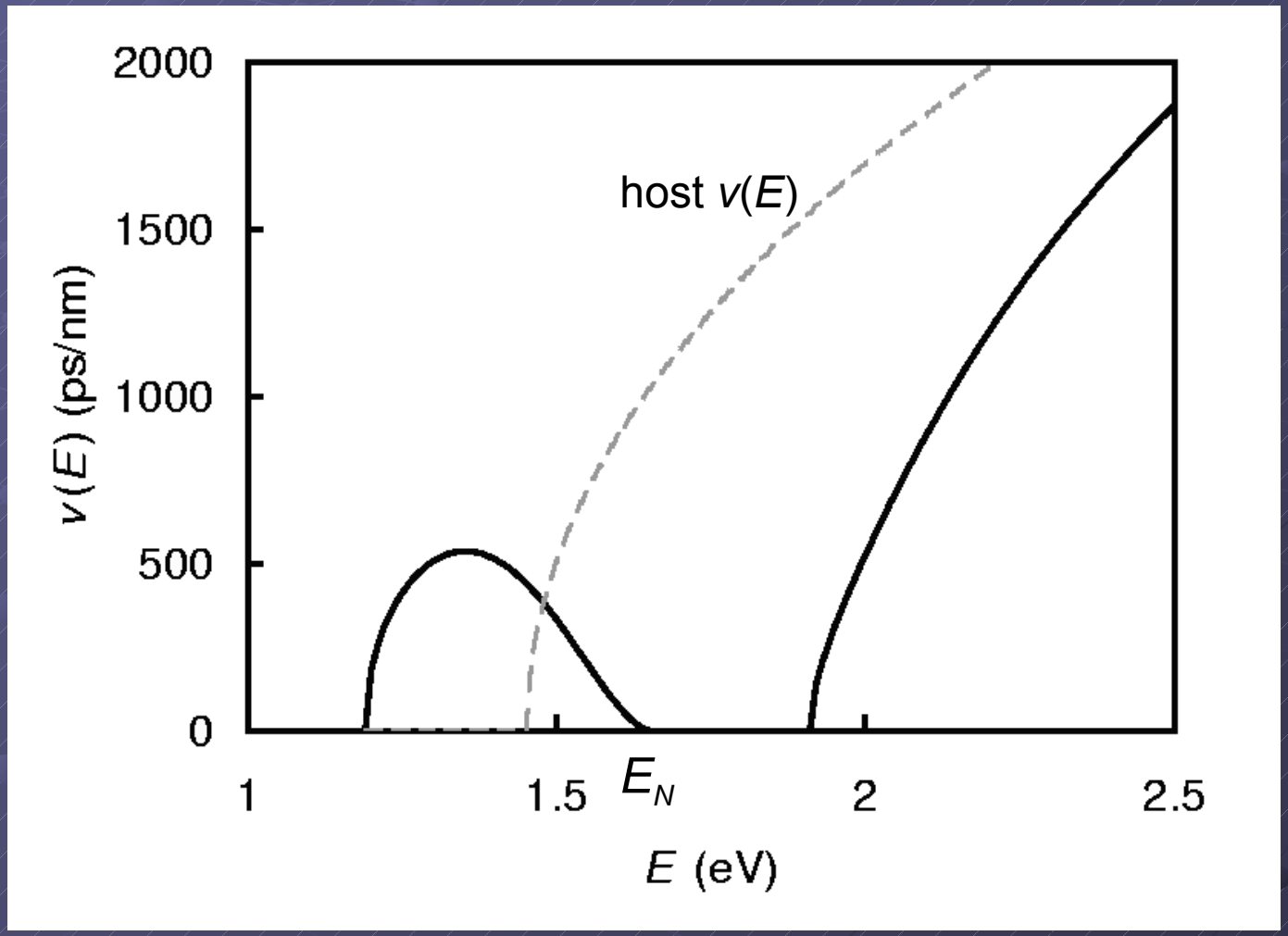
In terms of γ (E) the ith component of **v** is

$$v_i(E) = \left(\frac{d\gamma(E)}{dE}\right)^{-1} v_i^0(\gamma(E)) = |\alpha_M|^2 v_i^0(\gamma(E))$$

Note that the effective mass in the dilute nitride is

$$m^* = \frac{d\gamma(E)}{dE} m_0^*$$

Example: 2-band model with parabolic E_M



S-matrix theory

S-matrix theory gives higher order results for scattering than Fermi's golden rule for scattering.

S-matrix theory was used by Fahy and O'Reilly [1] to develop a model of a scattering from a single isolated nitrogen impurity.

Later used by Fahy *et al* [2] to develop a model of resonant scattering in conjunction with the LCINS model.

[1] S. Fahy and E.P. O'Reilly, *Appl. Phys. Lett*, **83**, 3731 (2003); S. Fahy and E.P. O'Reilly, *Physica E*, **21**, 881 (2004)
[2] S. Fahy, A. Lindsay, H. Ouerdane and E. P. O'Reilly, *Phys. Rev. B*, **74**, 035203 (2006)

The *S*-matrix element

The *S*-matrix is

$$S(k,k) = \langle \mathbf{k} | V | \psi(\mathbf{k}) \rangle$$

so, in this model

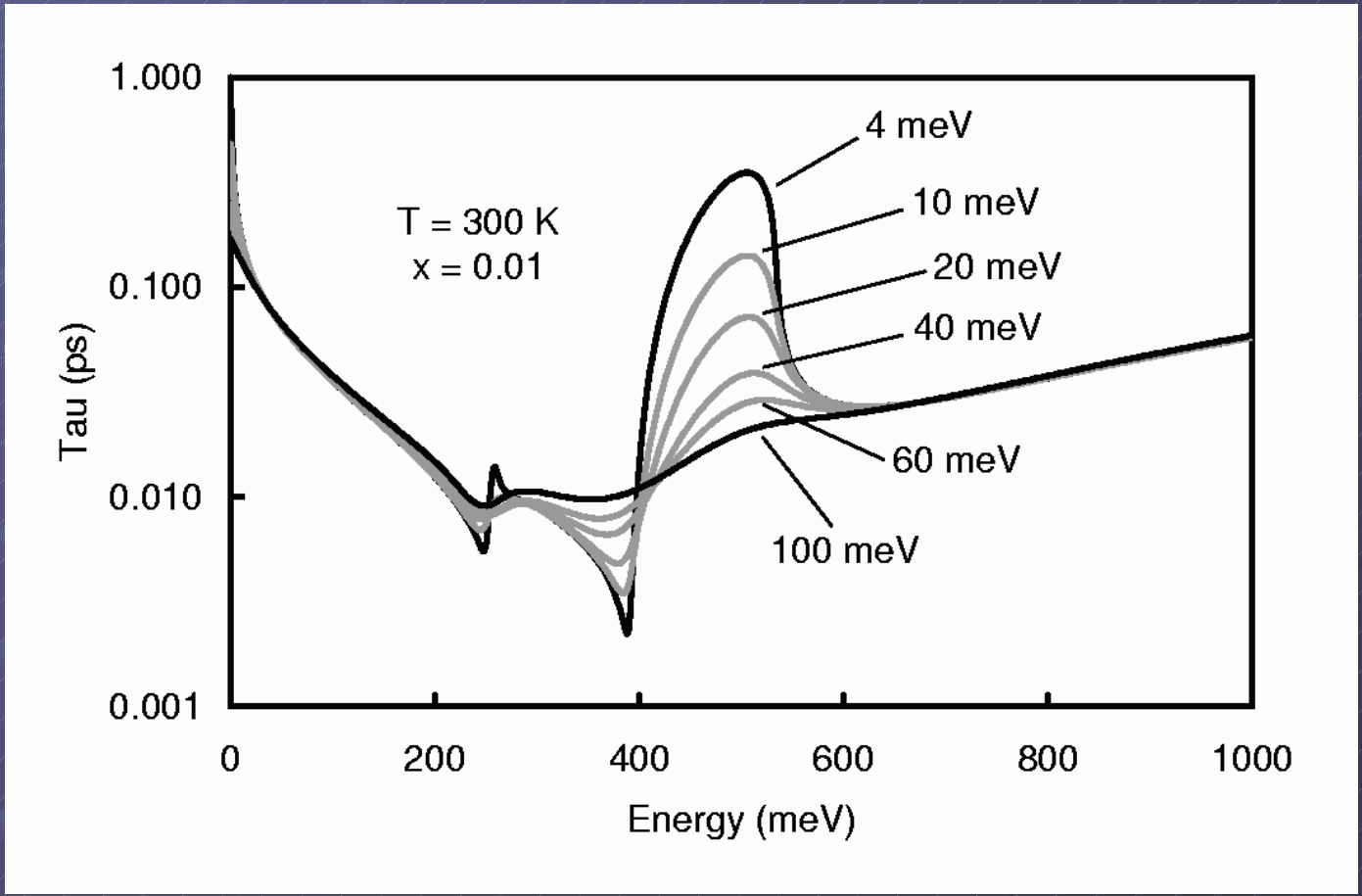
$$|S(k,k)|^2 = \sum_{\mathbf{j}} \frac{V_{\mathbf{j}}^2}{N_C} |\alpha_{\mathbf{j}}|^2 + \text{ interference terms}$$

We argue that the interference terms are due to random phases on the V_j and α_j which tend to cancel out.

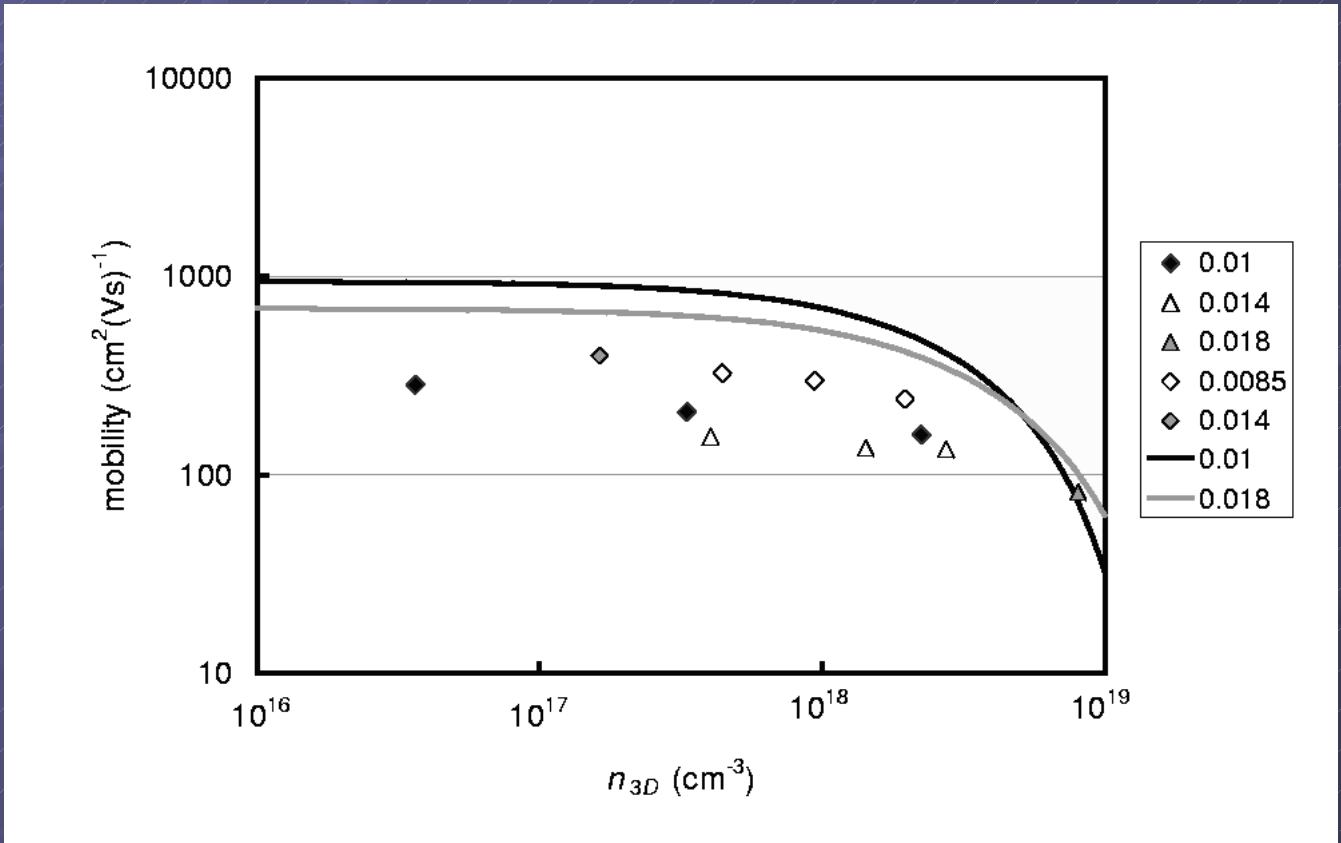
The scattering rate is then the result for independent scattering centres:

$$w(E) = \frac{\pi}{2\hbar} a_0^3 |\alpha_M|^2 \sum_j \frac{V_j^4 x_j}{(E - E_j)^2 + (\Delta(E) - \Delta_j)^2} N(E)$$

The relaxation time



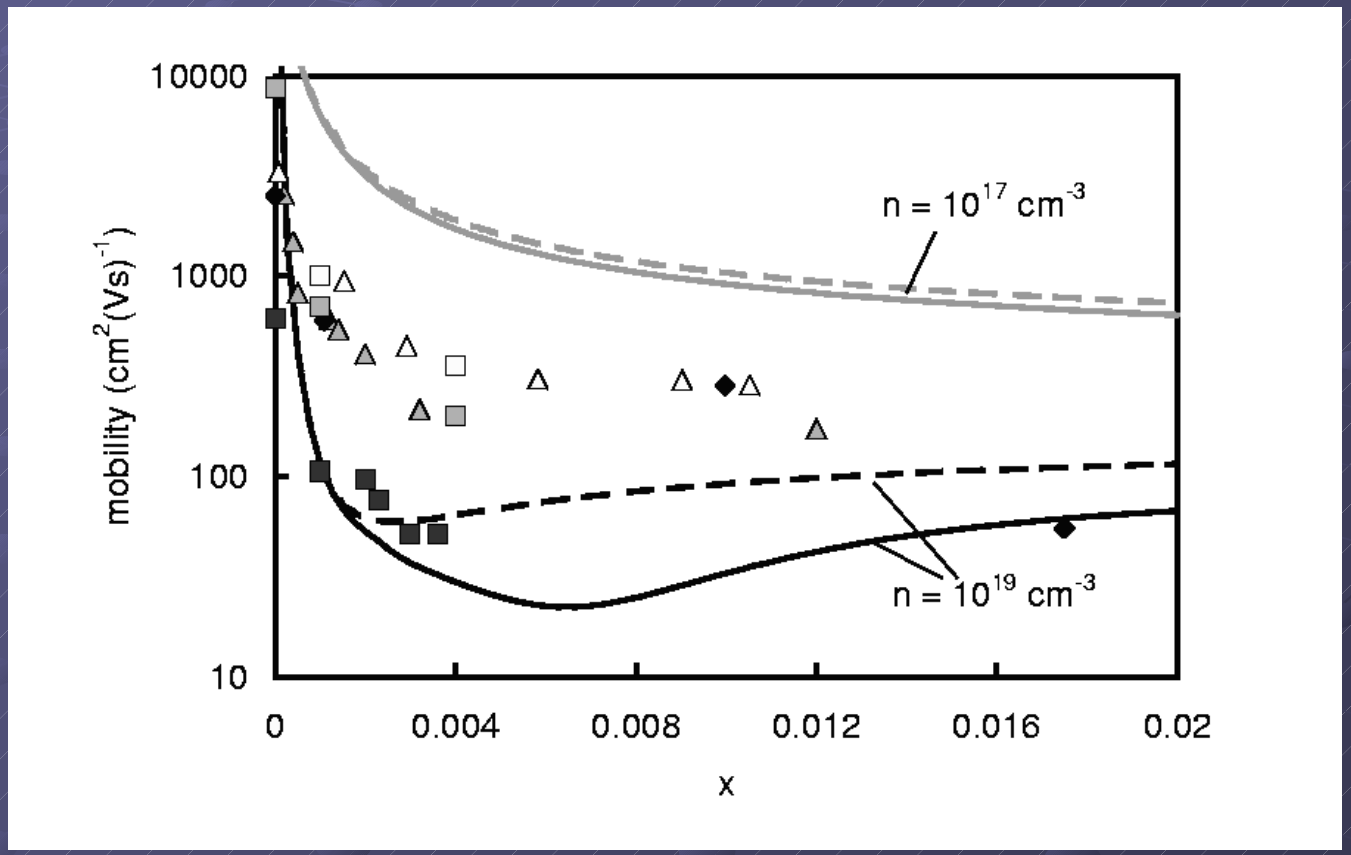
Mobility v carrier density



Data points: R. Mouillet, PhD thesis, *l'Université Paris V1* (2004)

Drop in mobility at high carrier concentrations due to Fermi energy coming close to nitrogen impurity energies where the fractional Γ character is greatly reduced.

Mobility v nitrogen concentration



D. Fowler *et al*, *AIP Conference Proceedings*, **772**, 497 (2005)

R. Mouillet, PhD thesis, *l'Université Paris V1* (2004)

E. Strohm , MSc thesis, *University of British Columbia* (2002)

Summary

- An *n*-band model can be derived from the Green's function of the Anderson Hamiltonian
- A well-behaved density of states can be found from the imaginary part of the Green's function
- The scattering rate can be found from *S*-matrix theory
- Model calculations for the highly degenerate case show reasonable agreement with experiment

Acknowledgements

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Thanks also to

Dr Amelia Patanè for providing mobility measurements by Fowler *et al* [1]

Prof Eoin O'Reilly for providing a proof copy of Fahy *et al* [2]

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[1] D. Fowler *et al*, *AIP Conference Proceedings*, **772**, 497 (2005)
[2] S. Fahy, A. Lindsay, H. Ouerdane and E. P. O'Reilly, *Phys. Rev. B*, **74**, 035203 (2006)