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 \[^{[1]}\]

Generalisation of the BAC model

‘n-band’ model

\[
H = \begin{bmatrix}
E_M(k) & V_1x_1^{1/2} & V_2x_2^{1/2} & \ldots & V_{n-1}x_{n-1}^{1/2} \\
V_1x_1^{1/2} & E_1 & 0 & \ldots & 0 \\
V_2x_2^{1/2} & 0 & E_2 & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
V_{n-1}x_{n-1}^{1/2} & 0 & 0 & 0 & E_{n-1}
\end{bmatrix}
\]

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 not assumed to be orthogonal. See, for instance, Lindsay and O'Reilly \[2\].

Non-parabolicity

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

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

**Note:** for any nitrogen energy $E_i$

As $E \rightarrow E_i$, $\gamma(E) \rightarrow \infty$

Assuming $E_M(k)$ is parabolic greatly simplifies the mathematics. (Note that $m_0^*$ is the *matrix semiconductor effective mass*).
Problem with the density of states (DOS)

From the dispersion relations, the densities of states are

\[ N_{3D}(E) = \frac{(2m_0 \gamma_0)^{3/2}}{4\pi^2 \gamma_0^3} \gamma^{1/2}(E) \frac{d\gamma(E)}{dE} \]

and

\[ N_{2D}(E) = \frac{m_0 \gamma_0}{2\pi \gamma_0^2} \frac{d\gamma(E)}{dE} \]

But

number of states \(< E_i = \int_0^{E_i} \frac{(2m_0 \gamma_0)^{3/2}}{4\pi^2 \gamma_0^3} \gamma^{1/2}(E) \frac{d\gamma(E)}{dE} dE \]

\[ = \frac{2}{3} \frac{(2m_0 \gamma_0)^{3/2}}{4\pi^2 \gamma_0^3} \gamma^{3/2}(E_i) = \infty \]

with a similar problem in 2D.
3D DOS from dispersion relations

\[ x = 0.02 \]
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,

\[ H_0 = \sum_k E_k b_k^+ b_k + \sum_j E_j b_j^+ b_j \]

\[ V = \frac{1}{\sqrt{N_C}} \sum_{j,k} \left\{ e^{i k_j} V_{kj} b_k^+ b_j + e^{-i k_j} V_{kj}^* b_j^+ b_k \right\} \]

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

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

The generalised Hamiltonian

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

\[ G_{kk} = \left\{ E - E_k - \frac{1}{N_c} \sum_j \frac{V_j^2}{E - E_j + i\Delta_j} \right\}^{-1} \]

where the \( \Delta_j \) are interpreted as energy broadenings on the \( j \)th impurity. From the poles of \( G_{kk} \), we can construct the generalised Hamiltonian

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

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 $\text{Im } G_{kk}$ and the density matrix, the density of states can be found from

$$N(E) = -\frac{1}{\pi} \text{Im} \int G_{kk} N_0(E_k) dE_k$$

This gives

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

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

$$\Omega(E) = -\sum_j \frac{V_j^2 x_j \Delta_j}{(E - E_j)^2 + \Delta_j^2}$$

and

$$\Gamma(E) = E - \sum_j \frac{V_j^2 x_j (E - E_j)}{(E - E_j)^2 + \Delta_j^2}$$
Limits as $\Delta \to 0$

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

$$-\frac{1}{\pi} \lim_{\Delta_i \to 0} \text{Im} G_{kk} = \frac{1}{\pi} \lim_{\Omega \to 0} \frac{\Omega(E)}{(\gamma(E) - E_M)^2 + \Omega^2(E)} = \delta(\gamma(E) - E_M)$$

giving the general result

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

For the simplified model in which $E_M$ is parabolic

$$\lim_{\Delta_i \to 0} N_{3D}(E) = \frac{(2m_0^*)^{3/2}}{4\pi^2 \Box^3} \gamma^{1/2}(E)$$

and

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

Dispersion relations → Group velocity → Effective mass

Dispersion relations → Density of states

Green’s function → Density of states

No longer directly related
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

$$|\psi_k\rangle = \alpha_M|\phi_k\rangle + \sum_j \alpha_j|j\rangle$$

The fractional $\Gamma$ character is

$$|\alpha_M|^2 = \left(\frac{1}{N_C} \sum_j \frac{V_j^2}{(E_j - E)^2 + (\Delta_j - \Delta(E))^2} + 1\right)^{-1}$$

Note that

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

The projection of the $j$th impurity is

$$|\alpha_j|^2 = \frac{|\alpha_M|^2}{N_C} \frac{V_j^2}{(E - E_j)^2 + (\Delta(E) - \Delta_j)^2}$$
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 \( \gamma(E) \) the \( i \)th component of \( \mathbf{v} \) 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.

The S-matrix element

The S-matrix is

\[ S(k, k) = \langle k | V | \psi(k) \rangle \]

so, in this model

\[ |S(k, k)|^2 = \sum_j \frac{V_j^2}{N_C} |\alpha_j|^2 + \text{interference terms} \]

We argue that the interference terms are due to random phases on the \( V_j \) and \( \alpha_j \) which tend to cancel out.

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

\[ w(E) = \frac{\pi}{20} a_0^3 |\alpha_M|^2 \sum_j \frac{V_j^4 x_j}{(E - E_j)^2 + (\Delta(E) - \Delta_j)^2} N(E) \]
The relaxation time

![Graph showing the relaxation time as a function of energy (meV) at different temperatures (meV): T = 300 K, x = 0.01. The graph plots Tau (ps) on the y-axis against Energy (meV) on the x-axis.}]
Drop in mobility at high carrier concentrations due to Fermi energy coming close to nitrogen impurity energies where the fractional $\Gamma$ character is greatly reduced.
Mobility v nitrogen concentration

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.
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