ECE-656: Fall 2009

Lecture 27: Scattering of Bloch electrons

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outline

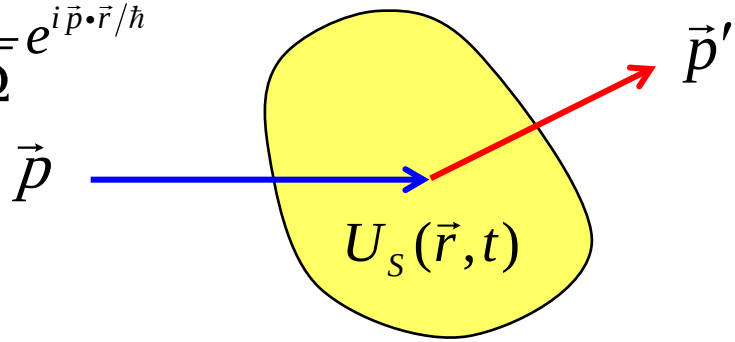
1) **Umklapp processes**

2) Overlap integrals

3) ADP scattering in graphene

scattering of Bloch electrons

$$\psi_i = \frac{1}{\sqrt{N}} u_{\vec{k}}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\bullet\vec{r}/\hbar}$$



$$\psi_f = \frac{1}{\sqrt{N}} u_{\vec{k}'}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\bullet\vec{r}/\hbar}$$

$$S(\vec{p},\vec{p}') = \frac{2\pi}{\hbar}\left|H_{\vec{p}',\vec{p}}\right|^2 \delta(E' - E - \Delta E)$$

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r}) \psi_i d\vec{r}$$

The periodicity of the lattice (Bloch functions) gives rise to additional scattering processes (so-called U-processes) and to overlap integrals for normal processes (N-processes).

1D: periodic functions and Fourier series

$$\psi(x) = \frac{1}{\sqrt{N}} u_{k_x}(x) \frac{1}{\sqrt{L}} e^{ik_x x}$$

$u_{k_x}(x) = u_{k_x}(x + a)$ Periodic with lattice spacing *a*

Any periodic function can be expanded as a Fourier series:

$$u_{k_x}(x) = \sum_{n=-\infty}^{n=+\infty} \tilde{u}_n e^{i2\pi nx/a} = \sum_{n=-\infty}^{n=+\infty} \tilde{u}_n e^{iG_n x} \qquad \tilde{u}_n = \frac{1}{a} \int_{cell} u_{k_x}(x) e^{-iG_n x}$$

$G_n = n(2\pi/a)$ Reciprocal lattice vector in 1D

For a good discussion of Fourier series in 1D and 3D, see Ziman, *Principles of the Theory of Solids*, 2nd Ed., Cambridge, 1972 (pp. 6-9)

3D

$$\psi_i = u_{\vec{k}}(\vec{r})\frac{1}{\sqrt{\Omega}}e^{i\vec{k}\bullet\vec{r}} = \sum_{\vec{G}_n}\tilde{u}_n e^{i\vec{G}_n\bullet\vec{r}}\frac{1}{\sqrt{\Omega}}e^{i\vec{k}\bullet\vec{r}}$$

$$\psi_f = u_{\vec{k}'}(\vec{r})\frac{1}{\sqrt{\Omega}}e^{i\vec{k}'\bullet\vec{r}} = \sum_{\vec{G}_m}\tilde{u}_m e^{i\vec{G}_m\bullet\vec{r}}\frac{1}{\sqrt{\Omega}}e^{i\vec{k}'\bullet\vec{r}}$$

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty}\psi_f^* U_S(\vec{r})\psi_i d\vec{r} \qquad U_S(\vec{r}) = A_\beta e^{\pm i\vec{\beta}\bullet\vec{r}}$$

$$H_{\vec{p}',\vec{p}} = \frac{1}{\Omega}\int_{-\infty}^{+\infty}\sum_{\vec{G}_m}\left(\tilde{u}_m^* e^{-i\vec{G}_m\bullet\vec{r}}e^{-i\vec{k}'\bullet\vec{r}}\right)A_\beta e^{\pm i\vec{\beta}\bullet\vec{r}}\left(\sum_{\vec{G}_n}\tilde{u}_n e^{i\vec{G}_n\bullet\vec{r}}e^{i\vec{k}\bullet\vec{r}}\right)d\vec{r}$$

$$H_{\vec{p}',\vec{p}} = \sum_{\vec{G}_m}\tilde{u}_m^*\sum_{\vec{G}_n}\tilde{u}_n\frac{1}{\Omega}\int_{-\infty}^{+\infty}\left(e^{-i\vec{G}_m\bullet\vec{r}}e^{-i\vec{k}'\bullet\vec{r}}\right)A_\beta e^{\pm i\vec{\beta}\bullet\vec{r}}\left(e^{i\vec{G}_n\bullet\vec{r}}e^{i\vec{k}\bullet\vec{r}}\right)d\vec{r}$$

3D

$$H_{\vec{p}',\vec{p}} = \sum_{m,n} \tilde{u}_m^* \tilde{u}_n \frac{1}{\Omega} \int_{-\infty}^{+\infty} A_\beta \left(e^{-i\left(\vec{k}'-\vec{k}\mp\vec{\beta}-\vec{G}_n+\vec{G}_m\right)\bullet\vec{r}} \right) d\vec{r}$$

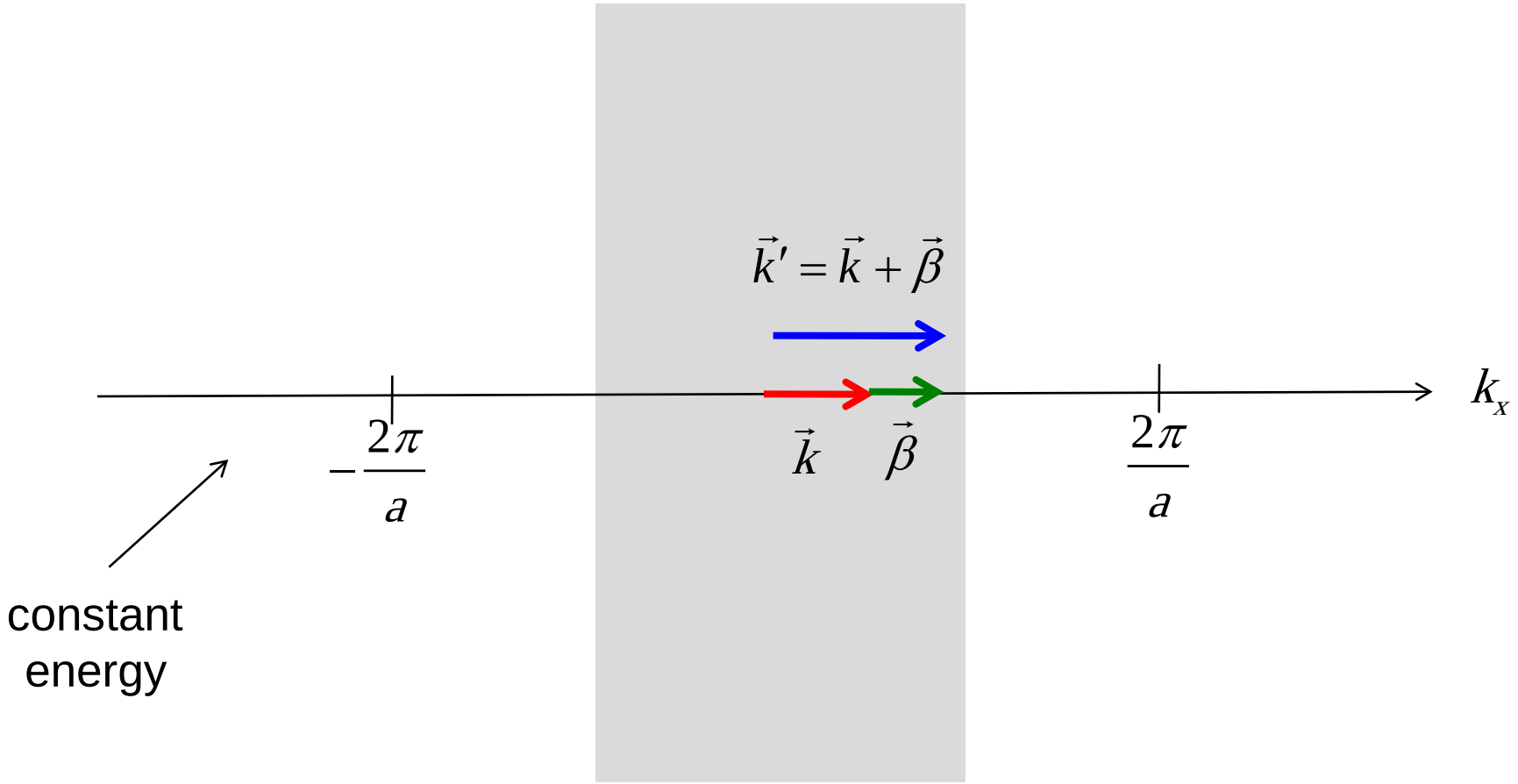
$$H_{\vec{p}',\vec{p}} = \sum_{m,n} \tilde{u}_m^* \tilde{u}_n A_\beta \delta_{\vec{k}',\vec{k}\pm\vec{\beta}+\left(\vec{G}_n-\vec{G}_m\right)}$$

$\vec{k}' = \vec{k} \pm \vec{\beta}$ normal process or N-process (momentum conservation)

$\vec{k}' = \vec{k} \pm \vec{\beta} + \vec{G}$ Umklapp process or "U-process"

N-process

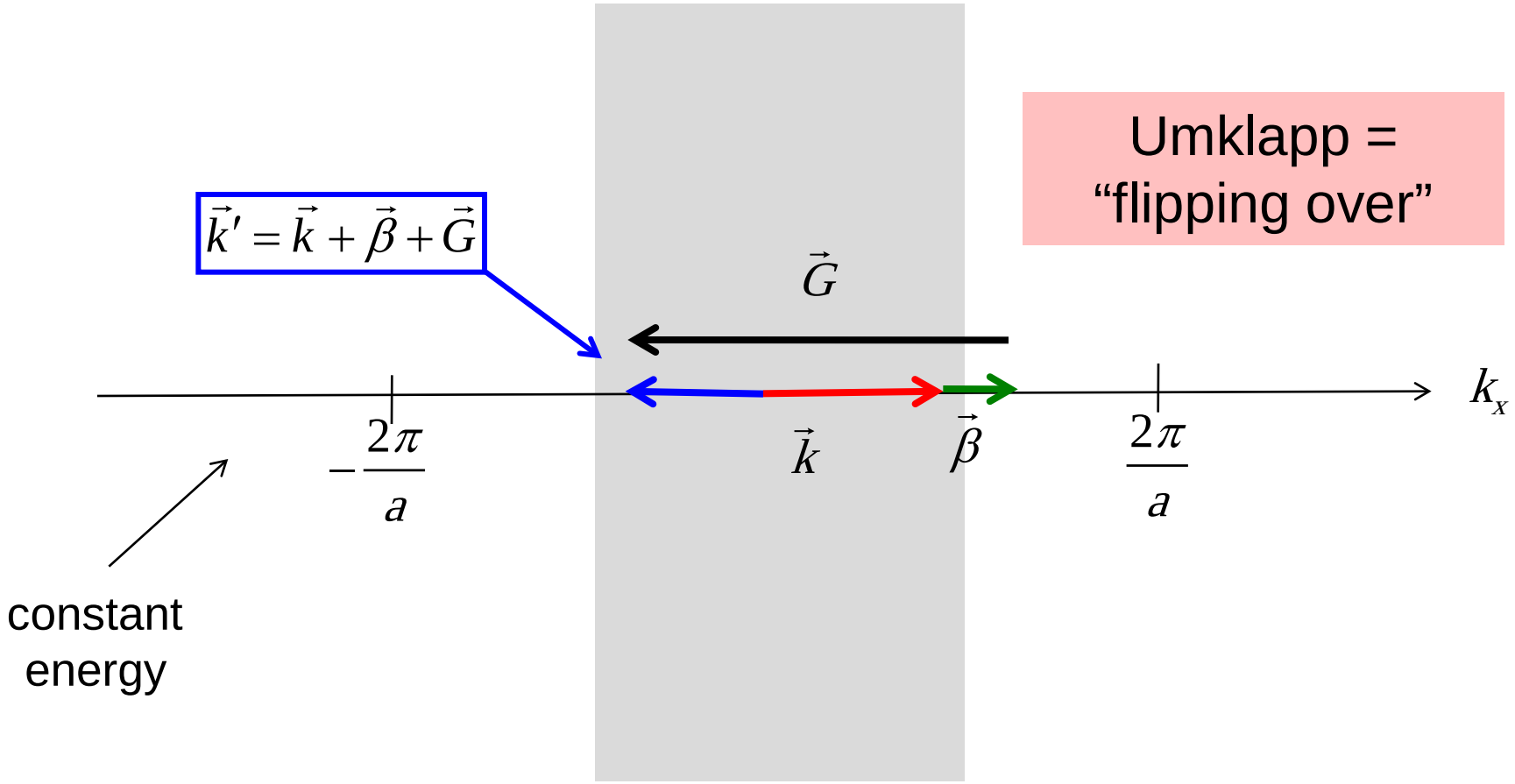
phonon absorption



(after Kittel, *Intro to Solid State Phys*.,4th Ed., Fig. 23, p. 229)

U-process

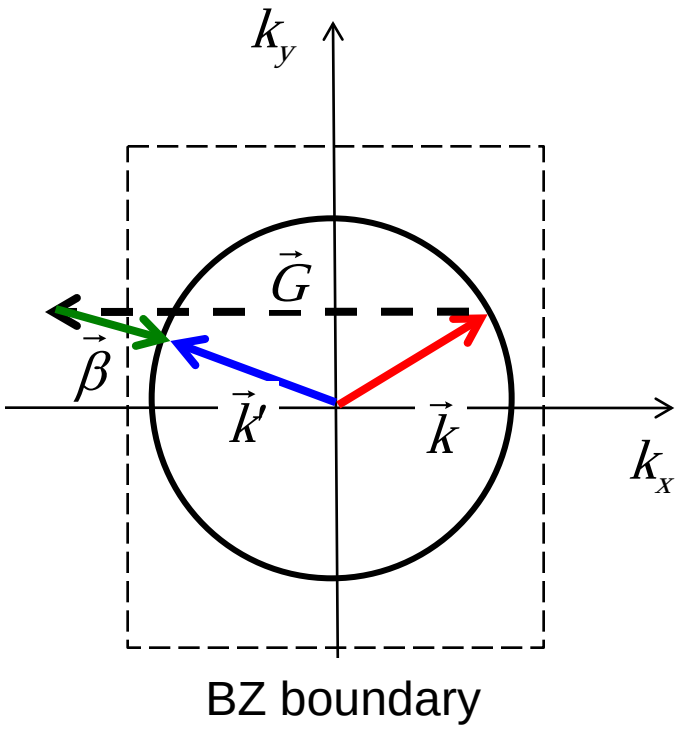
phonon absorption

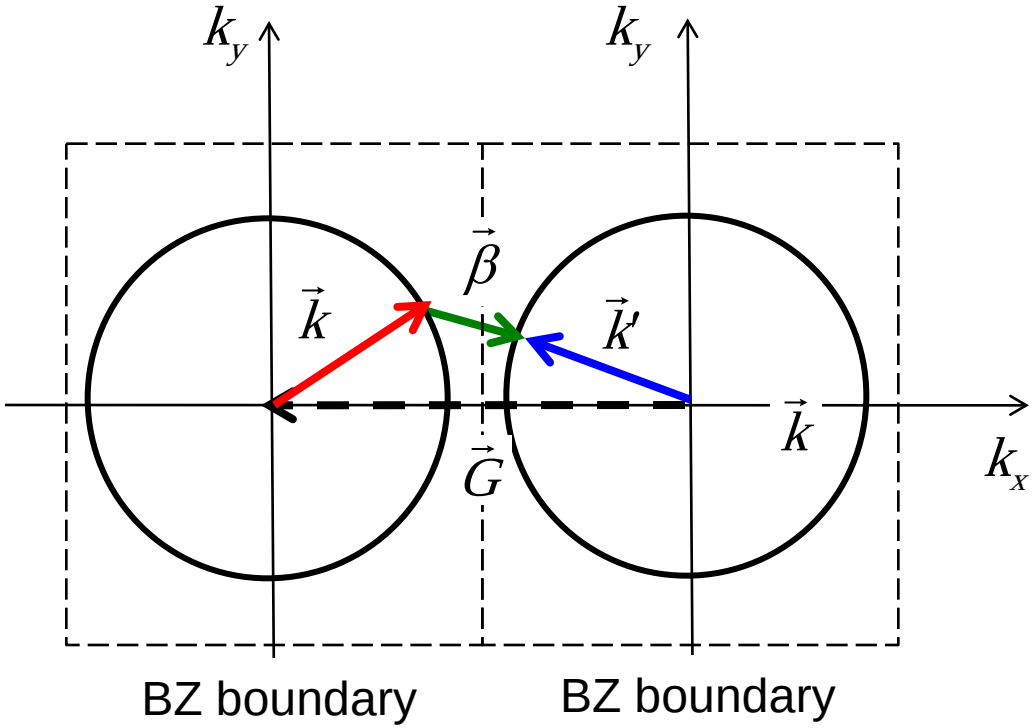


Umklapp = "flipping over"

(after Kittel, *Intro to Solid State Phys*.,4th Ed., Fig. 23, p. 229)

U-processes: extended zone



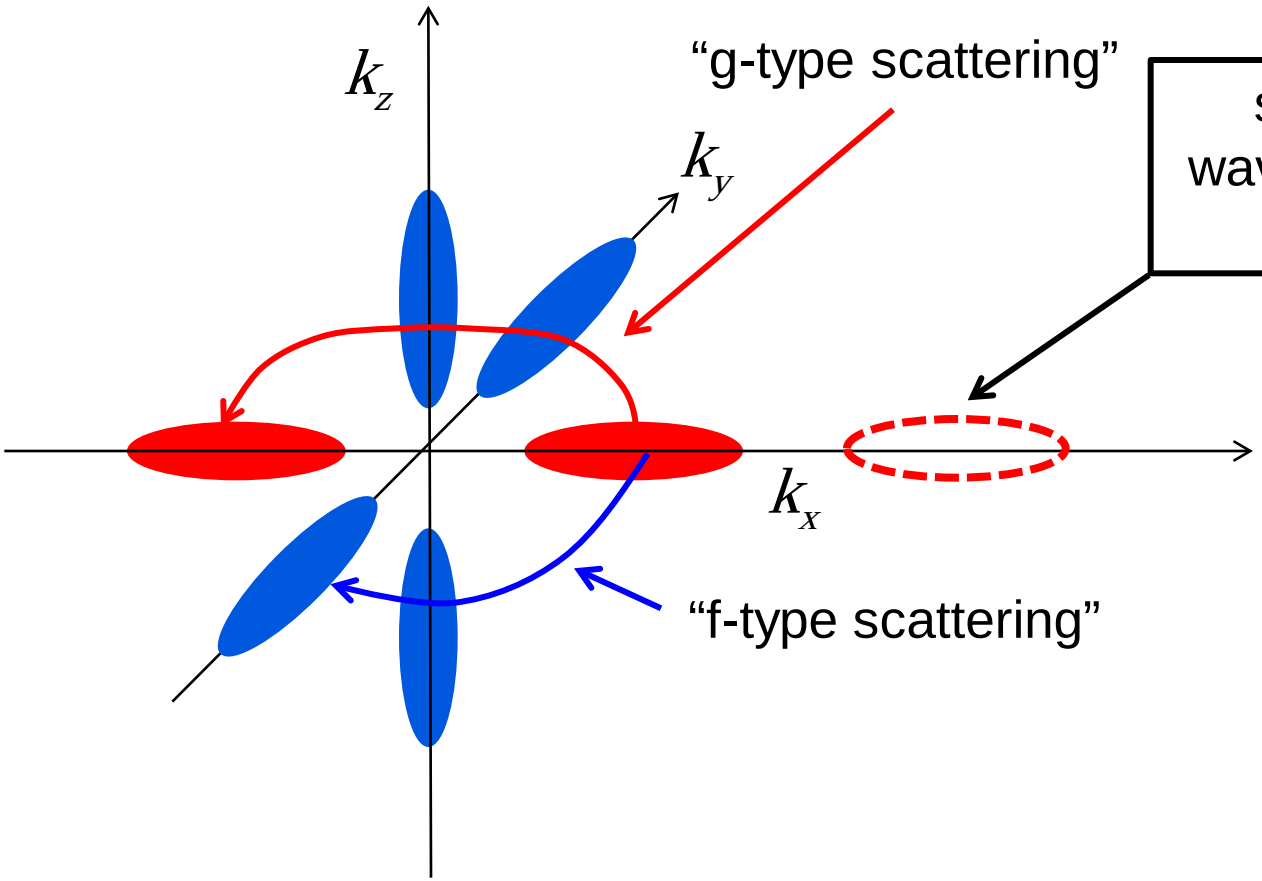


$$\vec{k}' = \vec{k} + \vec{\beta} + \vec{G}$$

(after Ziman, Fig. 124, p. 226

intervalley scattering in Si

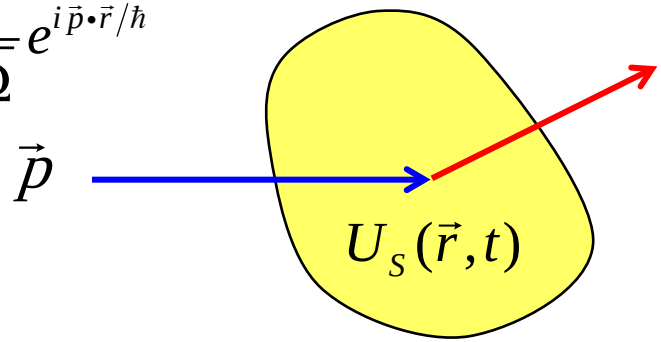
Si conduction band



smallest phonon wavevector occurs for a U-process

scattering of Bloch electrons

$$\psi_i = \frac{1}{\sqrt{N}} u_{\vec{k}}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\bullet\vec{r}/\hbar}$$



$$\psi_f = \frac{1}{\sqrt{N}} u_{\vec{k}'}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\bullet\vec{r}/\hbar}$$

The periodicity of the lattice (Bloch functions) gives rise to:

1) additional scattering processes (so-called U-processes) and

2) to overlap integrals for normal processes (N-processes).

outline

1) Umklapp processes

2) Overlap integrals

3) ADP scattering in graphene

matrix elements for Bloch functions

$$\psi_f = \frac{1}{\sqrt{N}} u_{\vec{k}'}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}'\cdot\vec{r}/\hbar}$$

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \psi_f^* U_S(\vec{r}) \psi_i d\vec{r}$$

$$\psi_i = \frac{1}{\sqrt{N}} u_{\vec{k}}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\cdot\vec{r}/\hbar}$$

$$H_{\vec{p}',\vec{p}} = \int_{-\infty}^{+\infty} \left(\frac{1}{\sqrt{N}} u^*_{\vec{k}'}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{-i\vec{p}'\cdot\vec{r}/\hbar} \right) U_S(\vec{r}) \left(\frac{1}{\sqrt{N}} u_{\vec{k}}(\vec{r}) \frac{1}{\sqrt{\Omega}} e^{i\vec{p}\cdot\vec{r}/\hbar} \right) d\vec{r}$$

$$H_{p',p} \approx \int \text{rapidly varying part} \times \int \text{slowly varying part}$$

$$H_{\vec{p}',\vec{p}} = N \int_{cell} \left(\frac{1}{\sqrt{N}} u^*_{\vec{k}'}(\vec{R}) \frac{1}{\sqrt{N}} u_{\vec{k}}(\vec{R}) d\vec{R} \right) \times \frac{1}{\Omega} \int_{\Omega} e^{-i\vec{p}'\cdot\vec{r}/\hbar} U_S(\vec{r}) e^{i\vec{p}\cdot\vec{r}/\hbar} d\vec{r}$$

Assumes that the scattering potential does not change rapidly on the scale of the unit cell.

matrix elements for Bloch functions

$$H_{\vec{p}',\vec{p}} = N \int_{cell} \left(\frac{1}{\sqrt{N}} u^*_{\vec{k}'}\left(\vec{R}\right) \frac{1}{\sqrt{N}} u_{\vec{k}}\left(\vec{R}\right) d\vec{R} \right) \times \frac{1}{\Omega} \int_{\Omega} e^{-i\vec{p}'\bullet\vec{r}/\hbar} U_S(\vec{r})\, e^{i\vec{p}\bullet\vec{r}/\hbar} d\vec{r}$$

$$H_{\vec{p}',\vec{p}} = I\left(\vec{k},\vec{k}'\right) \times \frac{1}{\Omega} \int_{\Omega} e^{-i\vec{p}'\bullet\vec{r}/\hbar} U_S(\vec{r})\, e^{i\vec{p}\bullet\vec{r}/\hbar} d\vec{r}$$

$$I\left(\vec{k},\vec{k}'\right) = \int_{cell} u^*_{\vec{k}'}\left(\vec{R}\right) u_{\vec{k}}\left(\vec{R}\right) d\vec{R}$$

some facts about overlap factors

For N-processes (e.g. intra-valley):

$I(k,k')$ = 1 for parabolic energy bands

for nonparabolic energy bands:

$$E\left(1+\alpha E\right)=\frac{\hbar^2 k^2}{2m^*}$$

$$I\left(\vec{k},\vec{k}'\right)=\frac{\left[\left(1+\alpha E\right)^{1/2}\left(1+\alpha E'\right)^{1/2}+\alpha\left(EE'\right)^{1/2}\cos\theta\right]^2}{\left(1+2\alpha E\right)\left(1+2\alpha E'\right)}$$

some more facts about overlap factors

For U-processes (e.g. intervalley:

The angle theta, between k and k' is mainly fixed by the initial and final valley, so we can assume that $I(k,k')$ = 1 and include the effect in the deformation potential.

some final facts about overlap factors

For holes:

For intra-band scattering (hh → hh or lh → lh)

$$I\left(\vec{k},\vec{k}'\right)=\frac{1}{4}\left(1+3\cos^2\theta\right)$$

For inter-band scattering (hh → lh or lh → hh)

$$I\left(\vec{k},\vec{k}'\right)=\frac{3}{4}\sin^2\theta$$

overlap integrals

B.K. Ridley, *Quantum Processes in Semiconductors, 4th Ed.*, pp. 82-86, Cambridge, 1997

B.K. Ridley, *Electrons and Phonons in Semiconductor Multilayers*, pp. 60-63, Cambridge, 1997

D.K. Ferry, *Semiconductors,* pp. 214, 461-464, Macmillan, 1991

C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation,* pp. 27-30, Springer-Verlag, 1989.

J.H. Davies, *The Physics of Low-Dimensional Semiconductors,* pp. 307-308, Cambridge Univ. Press, 1998.

J. Singh, *The Physics of Semiconductors and Their Heterostructures, ,* pp. 397-403, McGraw-Hill, 1993.

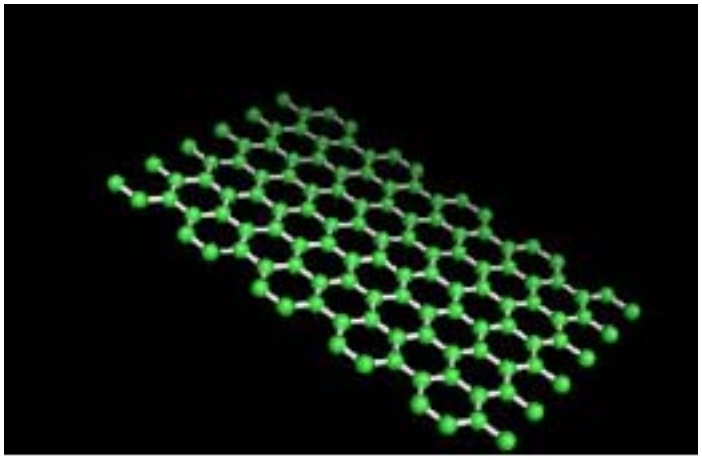
outline

1) Umklapp processes

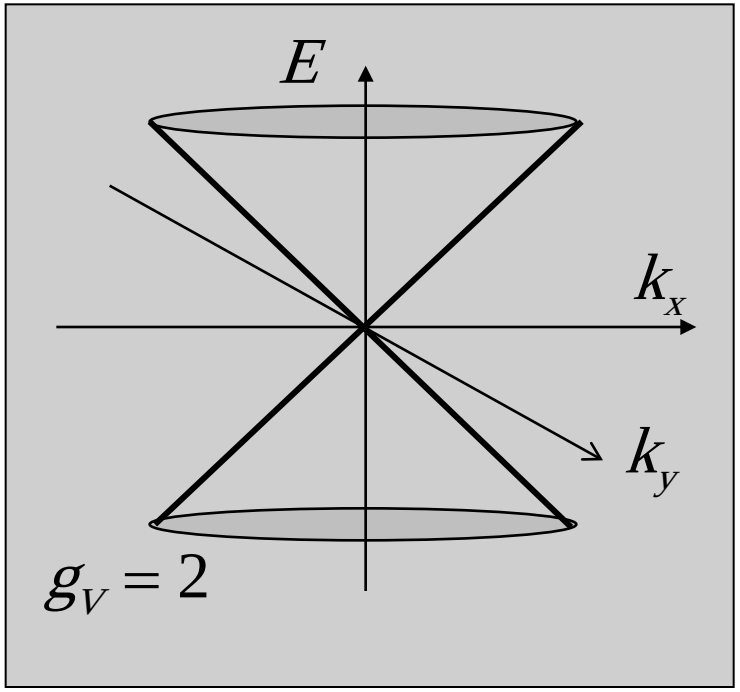
2) Overlap integrals

3) ADP scattering in graphene

graphene



(CNTBands on www.nanoHUB.org)



$$E(k) = \pm\hbar\upsilon_F\sqrt{k_x^2 + k_y^2} = \pm\hbar\upsilon_F k$$

$$\upsilon_g(\vec{k}) = \frac{1}{\hbar}\frac{dE(k)}{dk} = \upsilon_F$$

3D to graphene

3D result

$$S\left(\vec{p},\vec{p}'\right)=\frac{2\pi}{\hbar}\left|H_{p',p}\right|^2\delta\left(E'-E\mp\hbar\omega\right)$$

$$H_{p',p}=\frac{1}{\Omega}\int_{-\infty}^{+\infty}e^{-i\vec{p}'\bullet\vec{r}/\hbar}U_S\left(\vec{r}\right)e^{i\vec{p}\bullet\vec{r}/\hbar}d\vec{r}$$

$$U_S=\sum_\beta K_\beta\, u_\beta$$

$$\left|K_\beta\right|^2=\beta^2 D_A^2$$

graphene

p and *p'* are 2D vectors

$$H_{p',p}=\frac{1}{A}\int_{-\infty}^{+\infty}e^{-i\vec{p}_\parallel'\bullet\vec{\rho}/\hbar}U_S\left(\vec{r}\right)e^{i\vec{p}_\parallel\bullet\vec{\rho}/\hbar}d\vec{\rho}$$

β is a 2D vector

same

3D to graphene (ii)

3D result

$$u_\beta(\vec{r}) = A_\beta e^{\pm i\vec{\beta}\cdot\vec{r}}$$

$$\left|A_\beta\right|^2 = \frac{\hbar}{2\rho\Omega\,\omega}\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)$$

$$N_\omega = \frac{1}{e^{\hbar\omega/k_BT} - 1} \approx \frac{k_BT}{\hbar\omega}$$

$$N_\omega \approx N_\omega + 1$$

graphene

β is a 2D vector

$$\left|A_\beta\right|^2 = \frac{\hbar}{2\rho_m A\,\omega}\left(N_\omega + \frac{1}{2} \mp \frac{1}{2}\right)$$

ρ_m: $\mathrm{Kg/m^2}$

same

same

3D to graphene (iii)

3D result

$$H_{p',p} = \frac{1}{\Omega}\int_{-\infty}^{+\infty} e^{-i\vec{p}'_{\|}\bullet\vec{r}/\hbar}\left(\sum_{\beta} K_\beta u_\beta\right)e^{i\vec{p}\bullet\vec{r}/\hbar}d\vec{r} \rightarrow$$

$$\left|H_{p',p}\right|^2 = U_{ac}\frac{1}{\Omega}\left|\int_{-\infty}^{+\infty} e^{-i\vec{p}'\bullet\vec{r}/\hbar}\left(e^{\pm i\vec{\beta}\bullet\vec{r}}\right)e^{i\vec{p}\bullet\vec{r}/\hbar}d\vec{r}\right|^2$$

$$U_{ac} = \left|K_\beta\right|^2\left|A_\beta\right|^2 = \frac{D_A^2 k_B T}{2c_l}$$

$$\left|H_{p',p}\right|^2 = \frac{1}{\Omega}U_{ac}\delta_{\vec{p}',\vec{p}\pm\hbar\vec{\beta}}$$

graphene

$$\frac{1}{A}\int_{-\infty}^{+\infty} e^{-i\vec{p}'_{\|}\bullet\vec{\rho}/\hbar}\left(\sum_{\beta} K_\beta u_\beta\right)e^{i\vec{p}_{\|}\bullet\vec{\rho}/\hbar}d\vec{\rho}$$

$$\rightarrow U_{ac}\frac{1}{A}\left|\int_{-\infty}^{+\infty} e^{-i\vec{p}'_{\|}\bullet\vec{\rho}/\hbar}\left(e^{\pm i\vec{\beta}_{\|}\bullet\vec{\rho}}\right)e^{i\vec{p}_{\|}\bullet\vec{\rho}/\hbar}d\vec{r}\right|^2$$

$$U_{ac} = \frac{D_A^2 k_B T}{2\rho_m \upsilon_s^2} \qquad \upsilon_s = \sqrt{c_l/\rho_m}$$

$$\left|H_{p',p}\right|^2 = \frac{1}{\Omega}U_{ac}\delta_{\vec{p}'_{\|},\vec{p}_{\|}\pm\hbar\vec{\beta}_{\|}}$$

3D to graphene (iv)

3D result

$$S\left(\vec{p},\vec{p}'\right)=\frac{2\pi}{\hbar}\frac{U_{ac}}{\Omega}\delta_{\vec{p}',\vec{p}\pm\hbar\vec{\beta}}\delta\left(E'-E\right)$$

$$U_{ac}=\frac{D_A^2 k_B T}{2c_l}$$

$$\frac{1}{\tau}=\frac{1}{\tau_m}=\sum_{\vec{p}'}S\left(\vec{p},\vec{p}'\right)$$

$$\frac{1}{\tau}=\frac{2\pi}{\hbar}U_{ac}\frac{D_{3D}\left(E\right)}{2}$$

graphene

$$S\left(\vec{p}_{\|},\vec{p}_{\|}\right)=\frac{2\pi}{\hbar}\frac{U_{ac}}{A}\delta_{\vec{p}_{\|}',\vec{p}_{\|}\pm\hbar\vec{\beta}_{\|}}\delta\left(E'-E\right)$$

$$U_{ac}=\frac{D_A^2 k_B T}{2\rho_m \upsilon_s^2}$$

$$\frac{1}{\tau}=\frac{1}{\tau_m}=\sum_{\vec{p}_{\|}'}S\left(\vec{p}_{\|},\vec{p}_{\|}'\right)$$

$$\frac{1}{\tau}=\frac{2\pi}{\hbar}U_{ac}\frac{D\left(E\right)}{4}\qquad D\left(E\right)=\frac{2E}{\pi\hbar^2\upsilon_F^2}$$

intravalley

finally

$$\frac{1}{\tau}=\frac{1}{\tau_{abs}}+\frac{1}{\tau_{ems}}=\frac{2\pi}{\hbar}U_{ac}\frac{D(E)}{2} \qquad U_{ac}=\frac{D_A^2 k_B T}{2\rho_m \upsilon_s^2} \qquad D(E)=\frac{2E}{\pi\hbar^2\upsilon_F^2} \qquad (E>0)$$

$$\frac{1}{\tau}=\frac{D_A^2 k_B T}{\hbar^3\rho_m\left(\upsilon_F\upsilon_s\right)^2}E \qquad (E>0)$$

$$\tau=\tau_0\left(E/k_BT\right)^{-1}$$

$$\tau_0=\frac{\hbar^3\rho_m\left(\upsilon_F\upsilon_s\right)^2}{D_A^2\left(k_BT\right)^2}$$

$$\mu_{ADP}=\frac{q\tau\left(E_F\right)}{E_F/\upsilon_F^2}=\frac{q\hbar^3\rho_m\upsilon_F^4\upsilon_s^2}{D_A^2k_BT}\frac{1}{E_F^2}$$

$$n_S=E_F^2/\pi\hbar^2\upsilon_F^2$$

$$\mu_{ADP}=\left(\frac{q\hbar\rho_m\upsilon_F^2\upsilon_s^2}{\pi D_A^2k_BT}\right)\frac{1}{n_S}$$

$$\mu_{ADP}\neq\frac{q\langle\langle\tau\rangle\rangle}{m^*} \qquad m^*=E_F/\upsilon_F^2$$

$$\sigma_S=n_Sq\mu_{ADP}=\left(\frac{q^2\hbar\rho_m\upsilon_F^2\upsilon_s^2}{\pi D_A^2k_BT}\right)$$

independent of carrier density!

but….

We have missed something important for graphene!

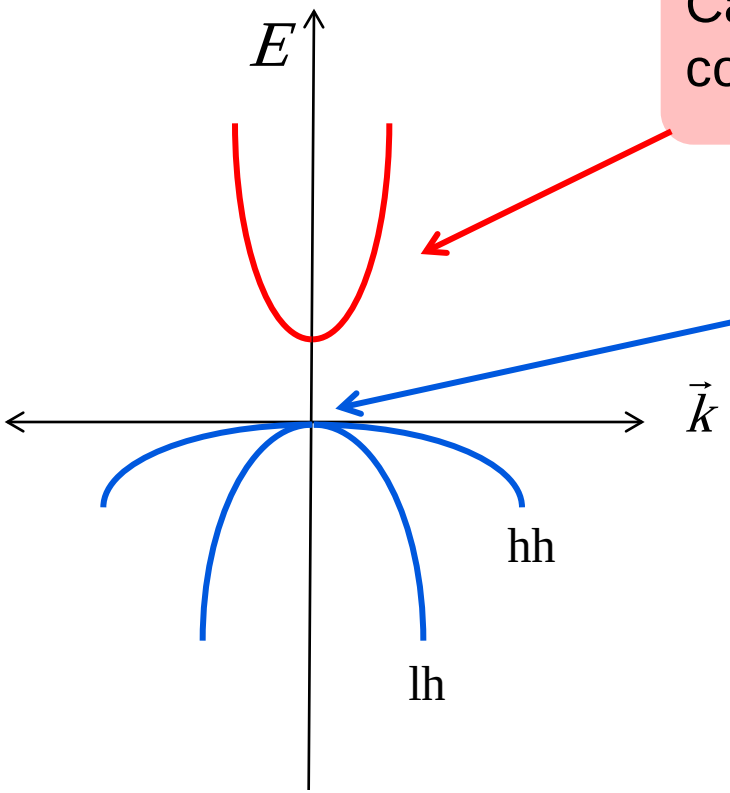
The remainder of the lecture closely follows:

"Lecture Notes on Low Bias Transport in Graphene: An Introduction,"
Dionisis Berdebes, Tony Low, and Mark Lundstrom, July 13, 2009

These notes are available at: http://nanohub.org/resources/7180

multi-component wavefunctions

semiconductors



Can often use a single component wavefunction $\psi_c(\vec{r})$

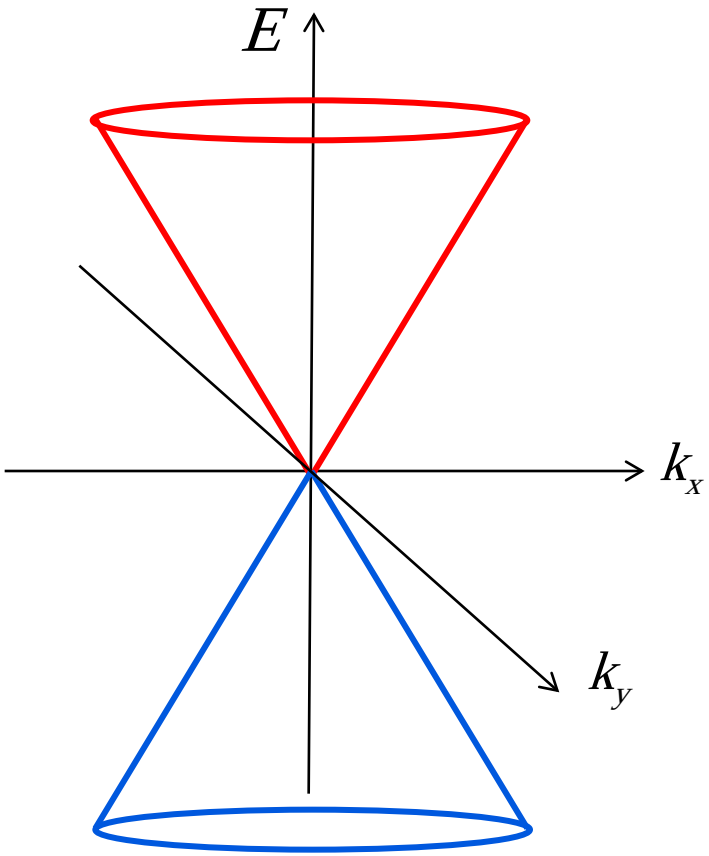
Should use a two component wavefunction (or 3 if we include SO coupling).

$$\begin{pmatrix} \psi_{hh}(\vec{r}) \\ \psi_{lh}(\vec{r}) \end{pmatrix}$$

For small bandgap semiconductors, it may be necessary to use a 4-component wavefunction (or 8 if we include SO coupling)

multi-component wavefunctions

graphene



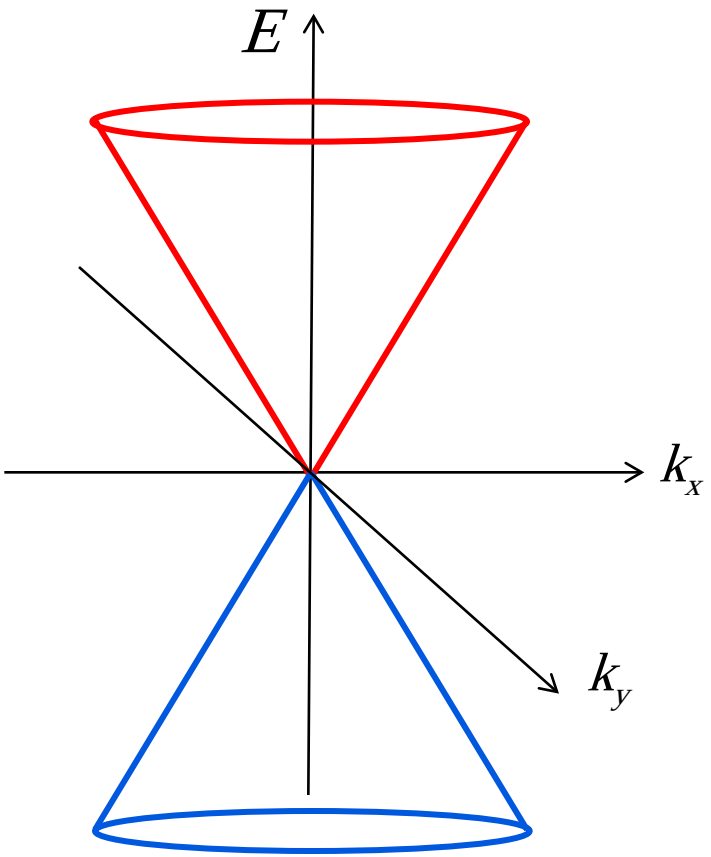
For graphene, we should expect that we will always need to use a 2-component wavefunction.

$$\begin{pmatrix} \psi_a(\vec{\rho}) \\ \psi_b(\vec{\rho}) \end{pmatrix}$$

The "a" and "b" refer to the "a" and "b" carbon atoms in the graphene unit cell.

graphene wavefunction

graphene



$$\Psi(x,y) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ se^{i\theta} \end{pmatrix}\frac{1}{\sqrt{A}}e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}$$

$$s = \text{sgn}(E) \quad \theta = \arctan\left(k_y/k_x\right) \quad e^{i\theta} = \left(k_x + ik_y\right)/k$$

$$\int \Psi^{\dagger}\Psi d\vec{\rho} = \int \begin{pmatrix} \Psi_a \\ \Psi_b \end{pmatrix}^{\dagger}\begin{pmatrix} \Psi_a & \Psi_b \end{pmatrix} d\vec{\rho} =$$

$$= \int \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & se^{-i\theta} \end{pmatrix}\frac{e^{-i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ se^{i\theta} \end{pmatrix}\frac{e^{i\vec{k}_{\parallel}\cdot\vec{\rho}}}{\sqrt{A}} d\vec{\rho}$$

$$= \frac{1}{2}\left(1+s^2\right)\frac{1}{A}\int e^{-i\vec{k}_{\parallel}\cdot\vec{\rho}}e^{i\vec{k}_{\parallel}\cdot\vec{\rho}} d\vec{\rho}$$

$$= 1$$

matrix element

$$H_{p',p} = \frac{1}{A}\int_{-\infty}^{+\infty} e^{-i\vec{p}'_{\|}\cdot\vec{\rho}/\hbar}\, U_S\left(\vec{\rho}\right) e^{i\vec{p}_{\|}\cdot\vec{\rho}/\hbar} d\vec{\rho} \rightarrow \int_{-\infty}^{+\infty} \Psi'^{\dagger}\left[U_S\left(\vec{\rho}\right)\right]\Psi d\vec{\rho}$$

$$\left[U_S\left(\vec{\rho}\right)\right] = \begin{bmatrix} U_S^{aa} & U_S^{ab} \\ U_S^{ba} & U_S^{bb} \end{bmatrix} \approx U_{ac}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad U_{ac} = \frac{D_A^2 k_B T}{2\rho_m \upsilon_s^2}$$

$$S\left(p_{\|}, p'_{\|}\right) = \frac{2\pi}{\hbar}\left[\frac{1}{2}\left(1+\cos\theta\right)\right] U_{ac}\,\delta_{\vec{p}'_{\|},\,\vec{p}_{\|}\pm\hbar\vec{\beta}_{\|}}\,\delta\left(E'-E\right)$$

The angle θ is now the angle between the incident and scattered electron. Note that direct backscattering ($\theta = \pi$) is forbidden. The extra term in the transition rate looks something like an overlap integral or form factor.

momentum relaxation rate

$$S\left(p_{\|},p'_{\|}\right)=\frac{2\pi}{\hbar}\left[\frac{1}{2}\left(1+\cos\theta\right)\right]U_{ac}\delta_{\vec{p}'_{\|},\vec{p}_{\|}\pm\hbar\vec{\beta}_{\|}}\delta\left(E'-E\right) \qquad U_{ac}=\frac{D_A^2 k_B T}{2\rho_m \upsilon_s^2}$$

$$\frac{1}{\tau_m\left(E\right)}=\sum_{p'_{\|}}\left(1-\cos\theta\right)S\left(p_{\|},p'_{\|}\right)$$

$$\frac{1}{\tau_m\left(E\right)}=\frac{D_A^2 k_B T}{4\hbar^3\rho_m\left(\upsilon_F\upsilon_S\right)^2}E$$

The scattering rate is 1/4 of what we computed earlier when we ignored the 2-component wavefunction, so the correct approach gives a mobility that is 4 times higher than the simpler approach!

questions

1) Umklapp processes

2) Overlap integrals

3) ADP scattering in graphene

Wavefunctions can be important (including the phonons too)!