Introduction to the Effective Mass Model

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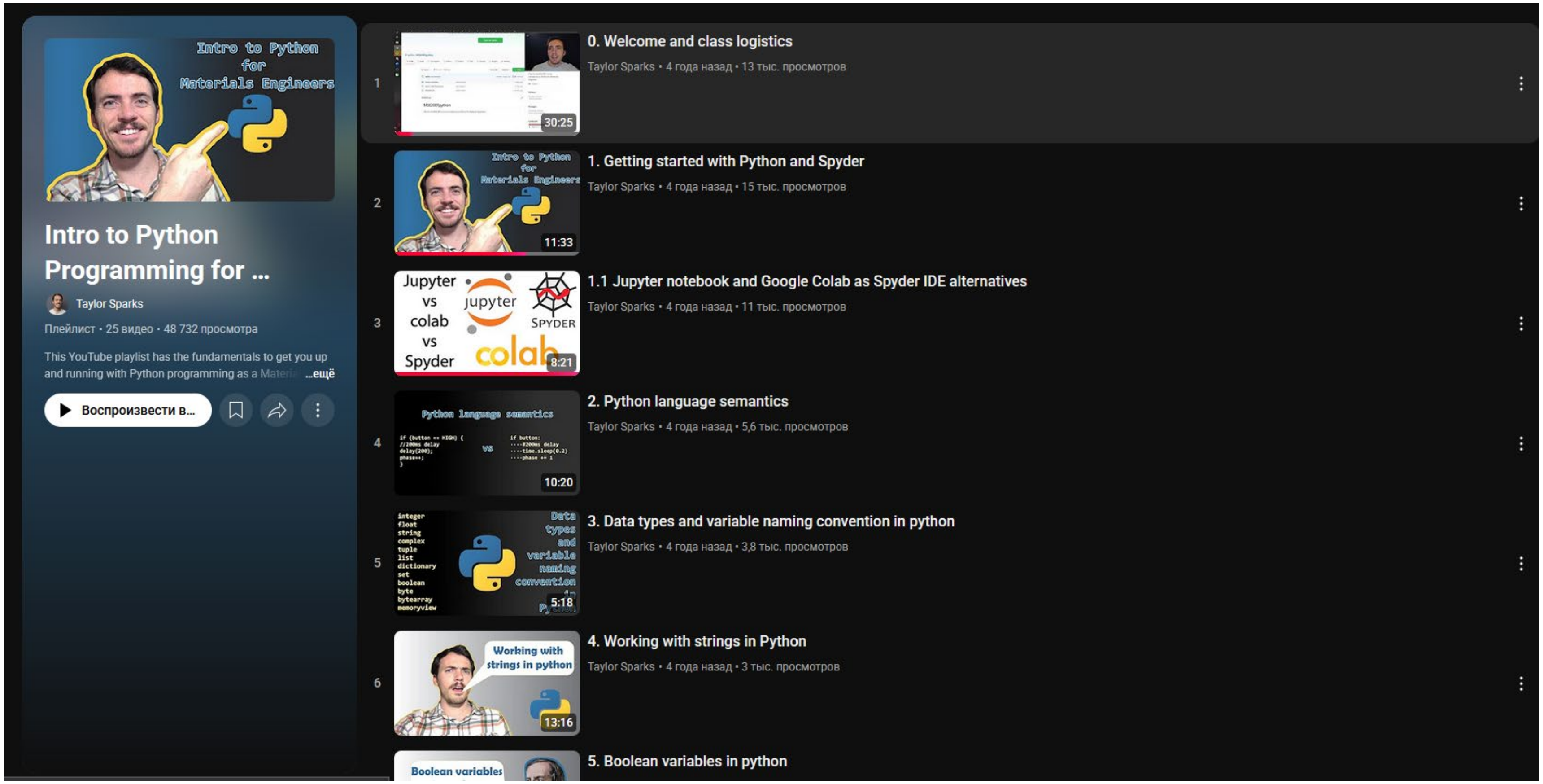
Intro to Python Programming



https://www.youtube.com/playlist?list=PLL0SWcFqypCmkHClksnGlab3wglEVMqNN

Anaconda - Spyder
VS code - Jupyter Notebooks

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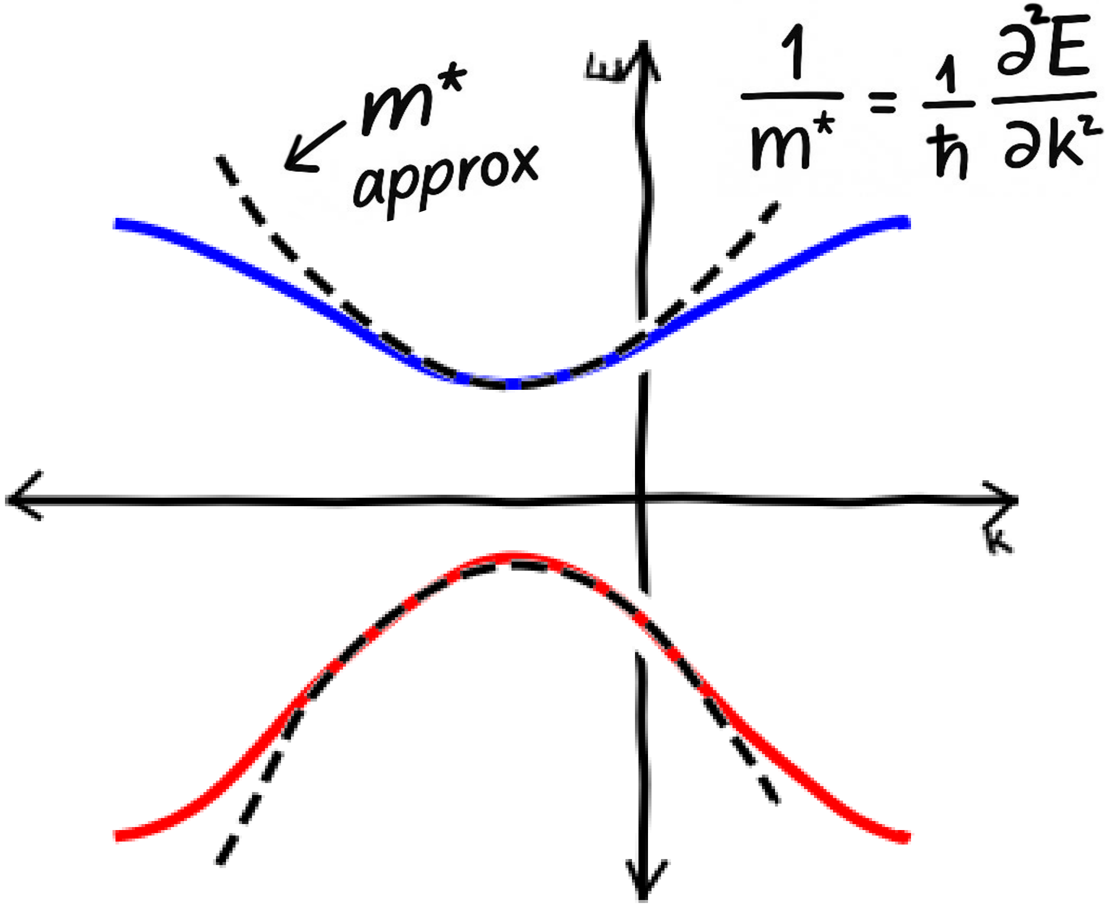
Effective mass model



V.I. Fistul', *Heavily Doped Semiconductors*; Springer: New York, 1969

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Two bands: light and heavy holes (p-PbTe)

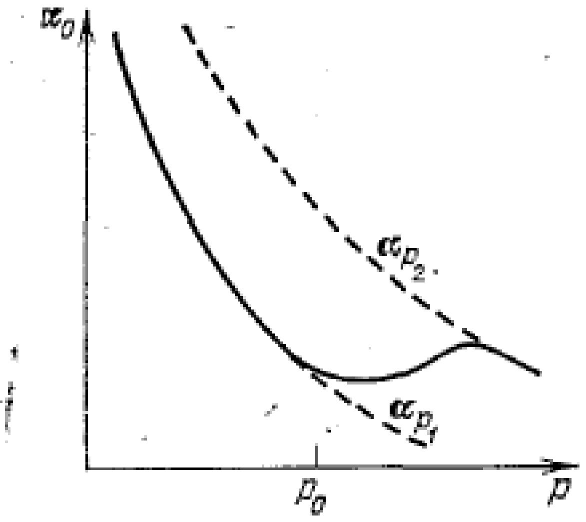

Рис. 19. Зависимость термо-э. д. с. от общей концентрации $p = p_1 + p_2$ в вырожденном p-PbTe (схематически). $p_0 \approx 5 \cdot 10^{19}$ см$^{-3}$. α_{p_1} и $\alpha_{p_2}^{*}$ — парциальные термо-э. д. с. легких и тяжелых дырок

не будет меняться и термо-э. д. с., как функция уровня Ферми ζ_p, почти не будет зависеть от концентрации дырок (см. рис. 19). Пока заполнение зоны тяжелых дырок такое, что $p_2 \ll (u_{p_1}/u_{p_2})\, p_1$, выражение (14.50) можно представить как

$$\alpha_0 \approx \alpha_{p_1}\left(1 + \frac{p_2 u_{p_2}}{p_1 u_{p_1}} \frac{\alpha_{p_2}}{\alpha_{p_1}}\right). \quad (14.51)$$

Поскольку парциальная термо-э. д. с. $\alpha_{p_2} \gg \alpha_{p_1}$ из-за большой разности эффективных масс плотности состояний для тяжелых и легких дырок, то может выполняться равенство $p_2 u_{p_2} \alpha_{p_2} \approx p_1 u_{p_1} \alpha_{p_1}$. Тогда $\alpha_0 > \alpha_{p_1}$ и термо-э.д.с. может расти с ростом

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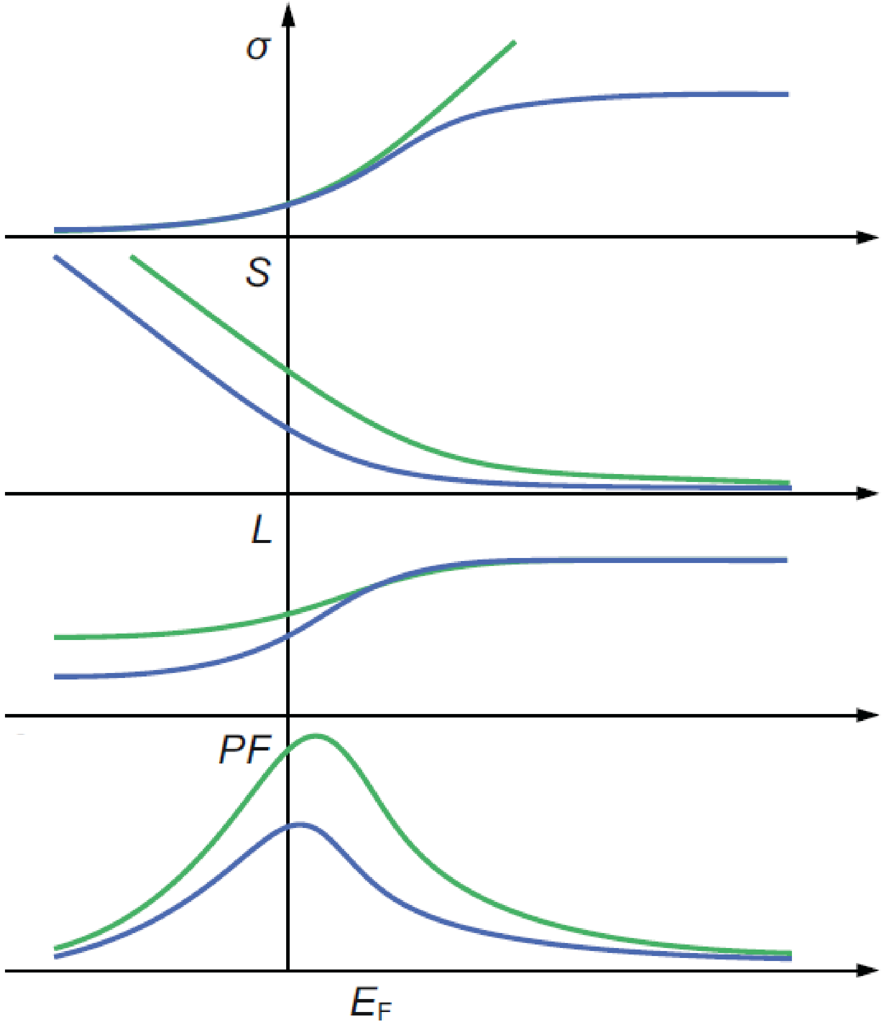
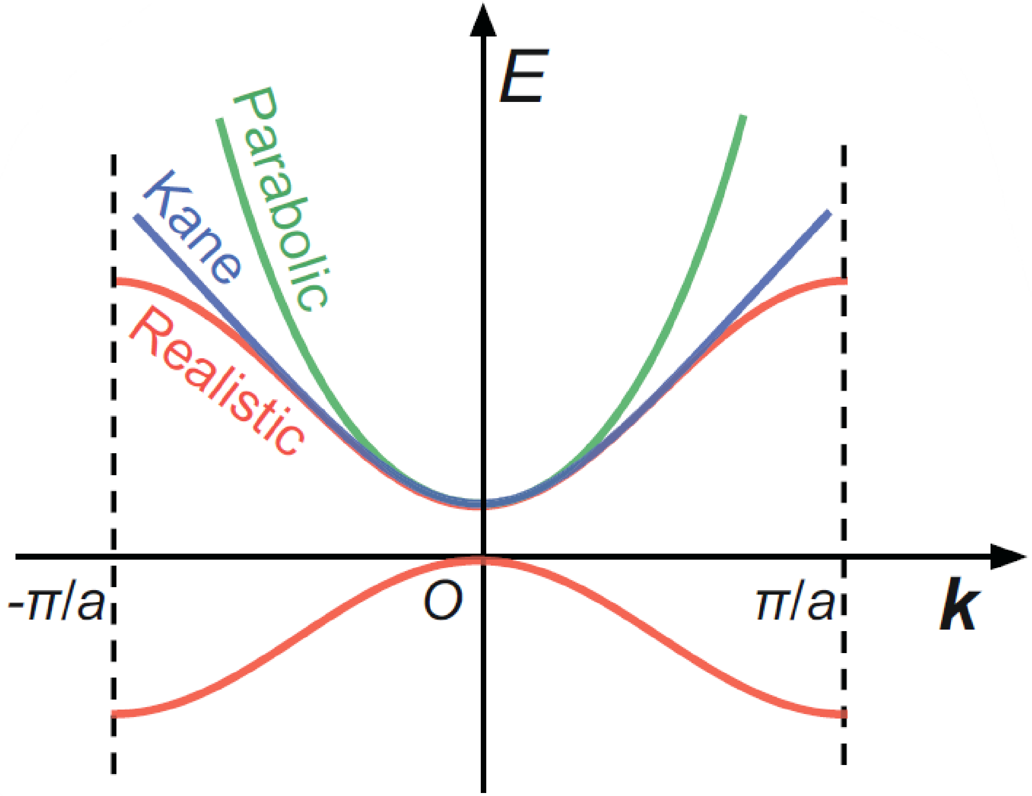
Parabolic dispersion vs Kane dispersion





Jianbo Zhu et al., Natl. Sci. Rev. 12 (2025)
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Parabolic dispersion vs Kane dispersion

Table 1. Single Band Expressions for Charge Carrier Concentration (n), Seebeck Coefficient (S), Hall Prefactor (r_H), Lorenz Number (L), Hall Mobility (μ_H), and Power Factor ($S^2\sigma$) for the SPB and SKB Models[a]

property	SPB	SKB
n	$\frac{(2m_D^* k_B T)^{3/2}}{3\pi^2\hbar^3}F_{1/2}(\eta)$	$\frac{(2m_{D0}^* k_B T)^{3/2}}{3\pi^3\hbar^3}({}^0F_0^{3/2}(\eta))$
S	$\frac{k_B}{e}\left(\frac{2F_1(\eta)}{F_0(\eta)}-\eta\right)$	$\frac{k_B}{e}\left[\frac{{}^1F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)}-\eta\right]$
r_H	$\frac{3}{4}F_{1/2}(\eta)\frac{F_{-1/2}(\eta)}{F_0^2(\eta)}$	$\frac{3K(K+2)({}^0F_0^{3/2})({}^0F_{-4}^{1/2})}{(2K+1)^2({}^0F_{-2}^1)^2}$
L	$\left(\frac{k_B}{e}\right)^2\frac{3F_0(\eta)F_2(\eta)-4F_1^2(\eta)}{F_0^2(\eta)}$	$\left(\frac{k_B}{e}\right)^2\left[\frac{{}^2F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)}-\left(\frac{{}^1F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)}\right)^2\right]$
μ_H	$\mu_0\frac{F_{-1/2}(\eta)}{2F_0(\eta)}$	$r_H\mu_0\frac{{}^0F_{-2}^1(\eta)}{{}^0F_0^{3/2}(\eta)}$
$S^2\sigma$	$\left(\frac{8\pi}{3e}\right)\mu_0 k_B^2\left(\frac{2m_D^* k_B T}{h^2}\right)^{3/2}F_0(\eta)\left(\frac{2F_1(\eta)}{F_0(\eta)}-\eta\right)^2$	$\left(\frac{8\pi}{3e}\right)\mu_0 k_B^2\left(\frac{2m_{D0}^* k_B T}{h^2}\right)^{3/2}{}^0F_{-2}^1(\eta)\left(\frac{{}^1F_{-2}^1(\eta)}{{}^0F_{-2}^1(\eta)}-\eta\right)^2$

[a] m_D^* represents the density of states effective mass of a parabolic band, while m_{D0}^* is the density of states effective mass at the band extremum ($E = 0$) of a nonparabolic band. μ_0 represents the mobility free parameter, and K is the ratio of the longitudinal to transverse effective mass.[3,4].

H. Naithani and T. Dasgupta, ACS Appl. Energy Mater. 3 (2020) 2200–2213; https://doi.org/10.1021/acsaem.9b02015

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