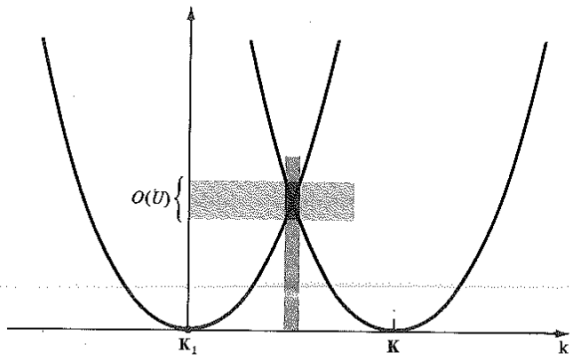


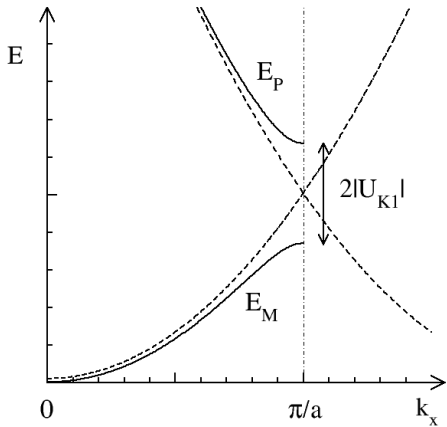
P#6: Elektroni u kristalima s metalnom vezom
Fizika čvrstog stanja 1

predavanja 2021

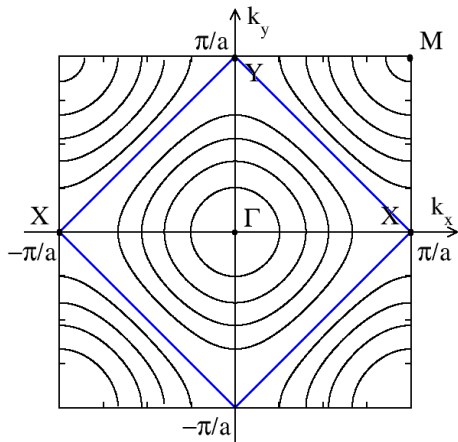
6.3.4 Slučaj degeneriranih nivoa



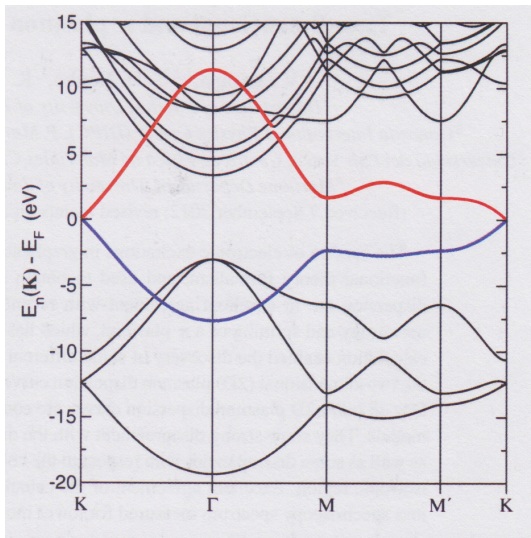
6.3.5 1D primjer za $k_x = \pi/a$



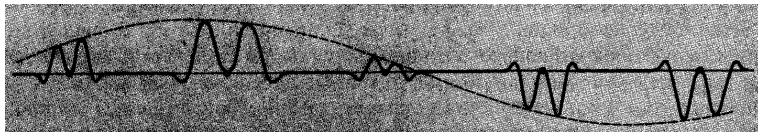
6.4.4 Točke i linije visoke simetrije u IBZ



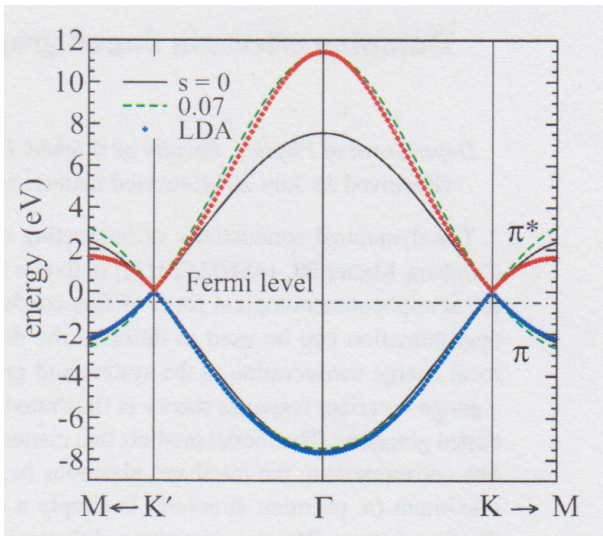
Primjer: grafen



6.4.5 Reprezentacija delokaliziranih orbitala



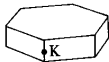
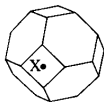
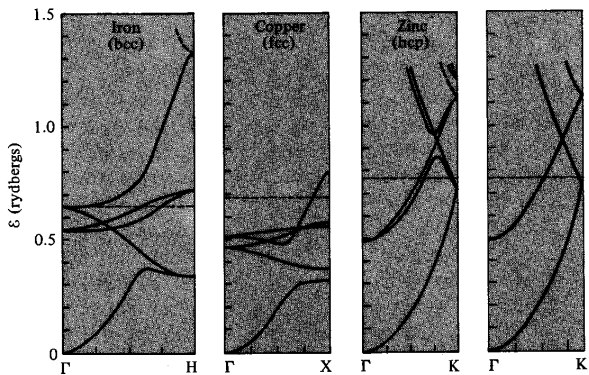
6.4.6 Wannierove funkcije



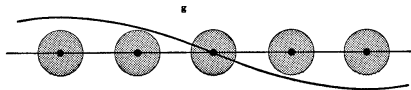
6.5 Doprinos kohezivnoj energiji od čvrsto vezanih elektrona

Ca²⁰	Sc²¹	Ti²²	V²³	Cr²⁴	Mn²⁵	Fe²⁶	Co²⁷	Ni²⁸	Cu²⁹
$4s^2$	$3d$ $4s^2$	$3d^2$ $4s^2$	$3d^3$ $4s^2$	$3d^5$ $4s$	$3d^5$ $4s^2$	$3d^6$ $4s^2$	$3d^7$ $4s^2$	$3d^8$ $4s^2$	$3d^{10}$ $4s$
Sr³⁸	Y³⁹	Zr⁴⁰	Nb⁴¹	Mo⁴²	Tc⁴³	Ru⁴⁴	Rh⁴⁵	Pd⁴⁶	Ag⁴⁷
$5s^2$	$4d$ $5s^2$	$4d^2$ $5s^2$	$4d^4$ $5s$	$4d^5$ $5s$	$4d^6$ $5s$	$4d^7$ $5s$	$4d^8$ $5s$	$4d^{10}$ -	$4d^{10}$ $5s$
Ba⁵⁶	La⁵⁷	Hf⁷²	Ta⁷³	W⁷⁴	Re⁷⁵	Os⁷⁶	Ir⁷⁷	Pt⁷⁸	Au⁷⁹
$6s^2$	$5d$ $6s^2$	$4f^{14}$ $5d^2$ $6s^2$	$5d^3$ $6s^2$	$5d^4$ $6s^2$	$5d^5$ $6s^2$	$5d^6$ $6s^2$	$5d^9$ -	$5d^9$ $6s$	$5d^{10}$ $6s$

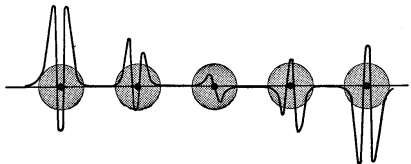
Prijelazni metali



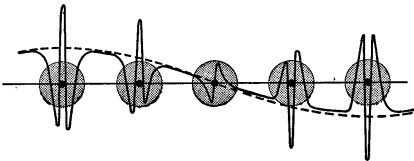
6.6.2 Reprezentacija ortogonaliziranih ravnih valova (OPW)



(a) Plane wave



(b) Core function



(c) O.P.W. = plane wave - core function

Literatura

- 1) Ashcroft & Mermin, *Solid State Physics*, §§ 9.U - 9.5, 10.U - 10.4, 11.5 - 11.6
- 1) Despoja et al., *Phy. Rev. B* 87, 075447 (2013)
- 1) bilješke