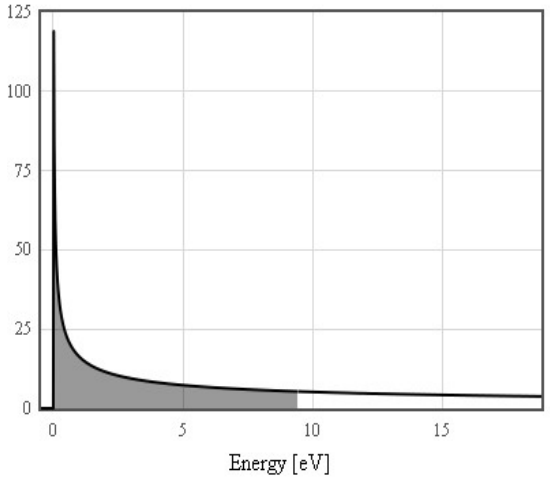
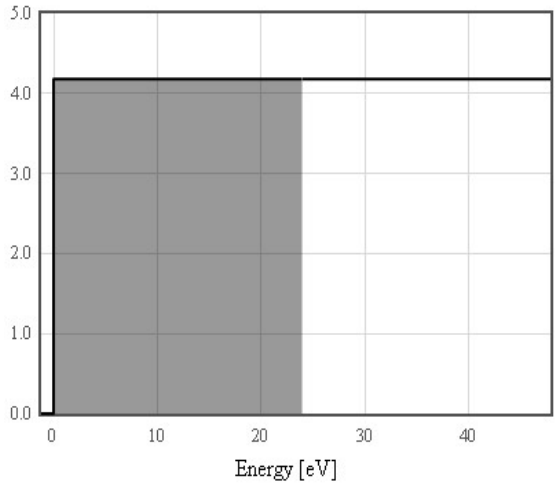
Free electron Fermi gas

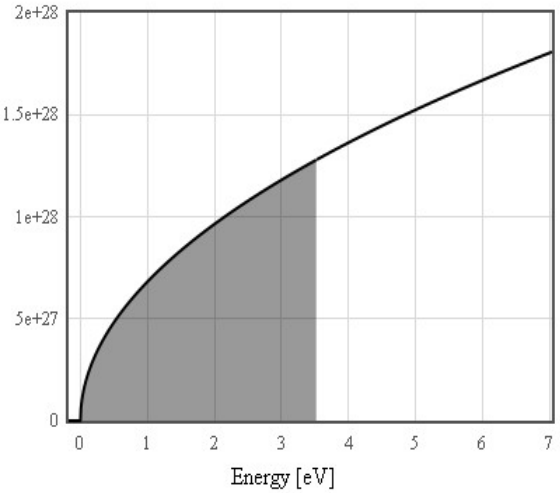
1 - d $$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \quad \mathrm{J^{-1}m^{-1}}$$

2 - d $$D(E) = \frac{m}{\hbar^2 \pi} = \frac{n}{E_F} \quad \mathrm{J^{-1}m^{-2}}$$

3 - d $$D(E) = \frac{\pi}{2}\left(\frac{2m}{\hbar^2 \pi^2}\right)^{3/2} \sqrt{E} = \frac{3n}{2E_F^{3/2}} \sqrt{E} \quad \mathrm{J^{-1}m^{-3}}$$







Results of the quantization of the Schrödinger equation for free fermions in 1, 2, and 3 dimensions.

A simple model for metals is the free electron model where the potential energy of the electrons is zero and the electron-electron interactions are ignored. This is equivalent to any system of noninteracting fermions with zero potential energy. In this model the thermodynamic properties only depend on one parameter, the particle density n. In the table below, n denotes the number of particles per meter in one-dimension, the number of particle per square meter in two-dimensions, and the number of particles per cubic mter in three dimensions.

	1-D Schrödinger equation for a free particle $i\hbar\frac{d\psi}{dx}=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$	**2-D Schrödinger equation for a free particle** $i\hbar\frac{d\psi}{dx}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}\right)$	**3-D Schrödinger equation for a free particle** $i\hbar\frac{d\psi}{dx}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}+\frac{d^2\psi}{dz^2}\right)$
Eigenfunction solutions	$A_k\exp\left(i\left(kx-\omega t\right)\right)$	$A_{\vec{k}}\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$	$A_{\vec{k}}\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$
Dispersion relation	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J
Density of states	$D(k)=\frac{2}{\pi}$	$D(k)=\frac{k}{\pi}$ m^{-1}	$D(k)=\frac{k^2}{\pi^2}$ m^{-2}
Density of states $D(E)=D(k)\frac{dk}{dE}$	$D(E)=\frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}=\frac{n}{2\sqrt{E_FE}}$ $\mathrm{J}^{-1}\mathrm{m}^{-1}$	$D(E)=\frac{m}{\pi\hbar^2}=\frac{n}{E_F}$ $\mathrm{J}^{-1}\mathrm{m}^{-2}$	$D(E)=\frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E}=\frac{3n}{2E_F^{3/2}}\sqrt{E}$ $\mathrm{J}^{-1}\mathrm{m}^{-3}$
Fermi energy E_F $n=\int_{-\infty}^{E_F}D(E)dE$	$E_F=\frac{\pi^2\hbar^2n^2}{8m}$ J	$E_F=\frac{\pi\hbar^2n}{m}$ J	$E_F=\frac{\hbar^2}{2m}\left(3\pi^2n\right)^{\frac{2}{3}}$ J
$D(E_F)$	$D(E_F)=\frac{4m}{\pi^2\hbar^2n}$ $\mathrm{J}^{-1}\mathrm{m}^{-1}$	$D(E_F)=\frac{m}{\pi\hbar^2}$ $\mathrm{J}^{-1}\mathrm{m}^{-2}$	$D(E_F)=\frac{m(3n)^{\frac{1}{3}}}{\pi^{\frac{4}{3}}\hbar^2}$ $\mathrm{J}^{-1}\mathrm{m}^{-3}$
$D'(E_F)=\left.\frac{dD}{dE}\right\|_{E=E_F}$	$D'(E_F)=\frac{-16m^2}{\pi^4\hbar^4n^3}$ $\mathrm{J}^{-2}\mathrm{m}^{-1}$	$D'(E_F)=0$ $\mathrm{J}^{-2}\mathrm{m}^{-2}$	$D'(E_F)=\frac{m^2}{\hbar^4\sqrt[3]{3\pi^8n}}$ $\mathrm{J}^{-2}\mathrm{m}^{-3}$
Chemical potential μ $n=\int_{-\infty}^{\infty}D(E)f(E)dE$	$\mu\approx E_F-\frac{\pi^2}{6}\left(k_BT\right)^2\frac{D'(E_F)}{D(E_F)}$ J $\approx\frac{\pi^2\hbar^2n^2}{8m}+\frac{2m}{3\hbar^2n^2}\left(k_BT\right)^2$ J	$\mu=k_BT\ln\left(\exp\left(\frac{E_F}{k_BT}\right)-1\right)$ J $=k_BT\ln\left(\exp\left(\frac{\pi\hbar^2n}{mk_BT}\right)-1\right)$ J	$\mu\approx E_F-\frac{\pi^2}{6}\left(k_BT\right)^2\frac{D'(E_F)}{D(E_F)}$ J $\approx\frac{\hbar^2}{2m}\left(3\pi^2n\right)^{\frac{2}{3}}-\frac{\pi^{\frac{2}{3}}m}{2\hbar^2\sqrt[3]{3}^{\frac{10}{3}}}\left(k_BT\right)^2$ J

Arnold Sommerfeld

Sommerfeld Expansion

We would like to perform integrals of the form

$$\int_{-\infty}^{\infty} H(E) f(E) dE$$

Examples:

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE \qquad u = \int_{-\infty}^{\infty} E D(E) f(E) dE$$

Integrate by parts (Partielle Integration)

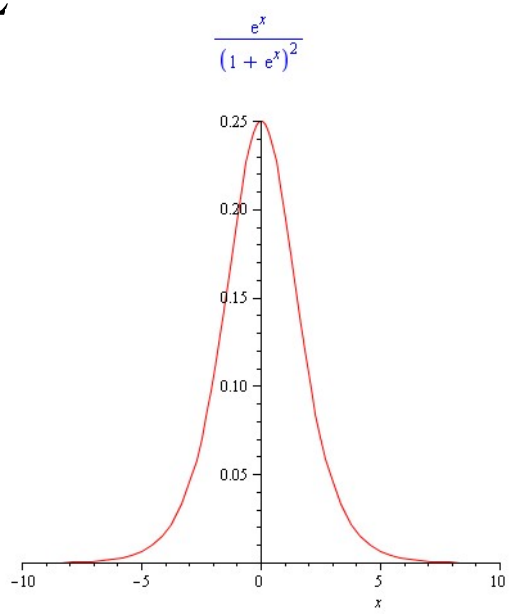
$$\int_{-\infty}^{\infty} \frac{dK(E)}{dE} f(E) dE = K(\infty) f(\infty) - K(-\infty) f(-\infty) - \int_{-\infty}^{\infty} K(E) \frac{df(E)}{dE} dE$$

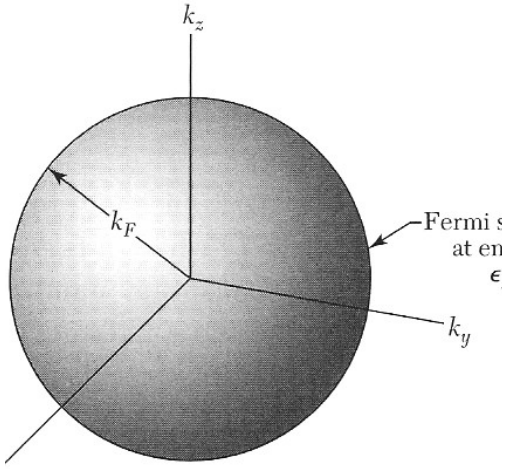
$$K(E) = \int_{-\infty}^{E} H(E') dE' \qquad H(E) = \frac{dK(E)}{dE}$$

Sommerfeld Expansion

$$\int_{-\infty}^{\infty} H(E) f(E) dE = -\int_{-\infty}^{\infty} K(E) \frac{df(E)}{dE} dE$$

$$\frac{-df(E)}{dE} = \frac{\frac{1}{k_B T} \exp\left(\frac{E-\mu}{k_B T}\right)}{\left(1+\exp\left(\frac{E-\mu}{k_B T}\right)\right)^2}$$





Expand $K(E)$ around $E = \mu$

$$K(E) \approx K(\mu) + \left.\frac{dK}{dE}\right|_{E=\mu} (E-\mu) + \tfrac{1}{2} \left.\frac{d^2K}{dE^2}\right|_{E=\mu} (E-\mu)^2 + \cdots$$

Sommerfeld Expansion

$$x = \frac{E - \mu}{k_B T}$$

$$\int_{-\infty}^{\infty} \frac{e^x}{\left(1+e^x\right)^2} dx = 1$$

$$\int_{-\infty}^{\infty} \frac{x e^x}{\left(1+e^x\right)^2} dx = 0$$

$$\int_{-\infty}^{\infty} \frac{x^2 e^x}{\left(1+e^x\right)^2} dx = \frac{\pi^2}{3}$$

$$\int_{-\infty}^{\infty} \frac{x^3 e^x}{\left(1+e^x\right)^2} dx = 0$$

$$\int_{-\infty}^{\infty} \frac{x^4 e^x}{\left(1+e^x\right)^2} dx = \frac{7\pi^4}{15}$$

Sommerfeld Expansion

$$\int_{-\infty}^{\infty} H(E) f(E) dE \approx K(\mu) + \frac{\pi^2}{6} \left(k_B T\right)^2 \left.\frac{dH(E)}{dE}\right|_{E=\mu} + \frac{7\pi^4}{360} \left(k_B T\right)^4 \left.\frac{d^3 H(E)}{dE^3}\right|_{E=\mu} + \cdots$$

$$K(E) = \int_{-\infty}^{E} H(E') dE' \qquad H(E) = \frac{dK(E)}{dE}$$

Sommerfeld Expansion: chemical potential

$$\int_{-\infty}^{\infty} H(E) f(E) dE = K(\mu) + \frac{\pi^2}{6} \left(k_B T\right)^2 \left.\frac{dH(E)}{dE}\right|_{E=\mu} + \frac{7\pi^4}{360} \left(k_B T\right)^4 \left.\frac{d^3 H(E)}{dE^3}\right|_{E=\mu} + \cdots$$

For μ in 3-d:

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE$$

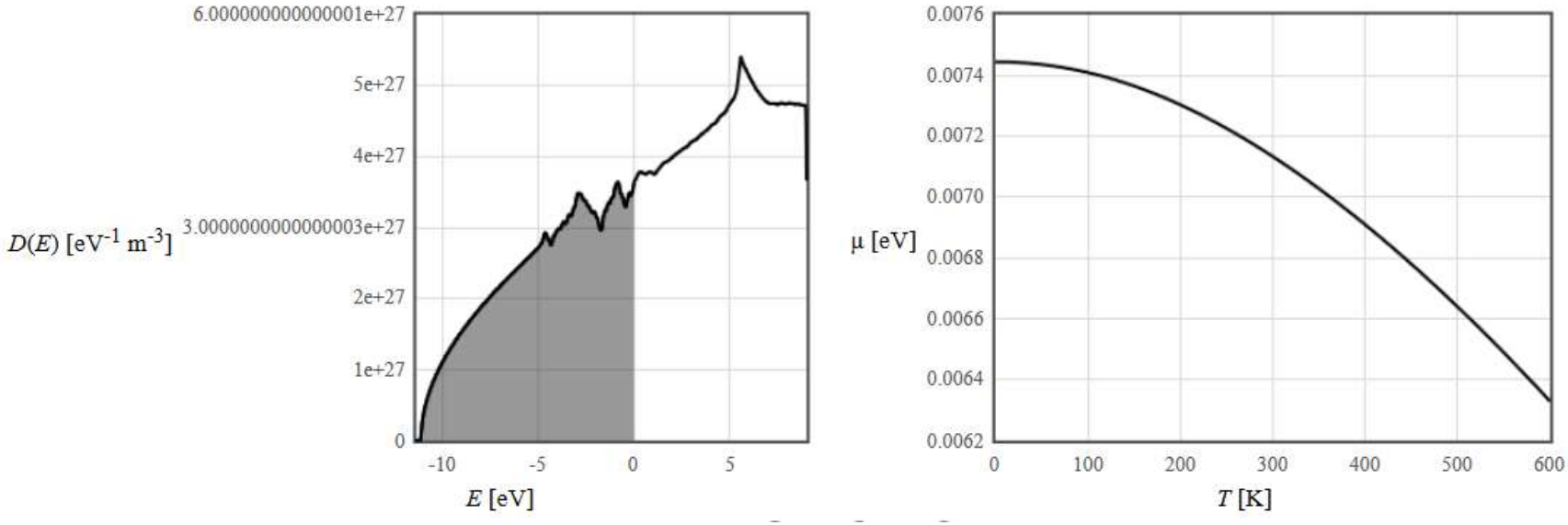
$$n = \int_{-\infty}^{\mu} D(E) dE + \frac{\pi^2}{6} \left(k_B T\right)^2 D'(E_F) + \cdots$$

$$K(\mu) = \int_{-\infty}^{\mu} D(E) dE = \int_{-\infty}^{E_F} D(E) dE + \int_{E_F}^{\mu} D(E) dE \approx n + \left(\mu - E_F\right) D(E_F)$$

Sommerfeld Expansion: chemical potential

$$n = n + \left(\mu - E_F\right) D(E_F) + \frac{\pi^2}{6}\left(k_B T\right)^2 D'(E_F)$$

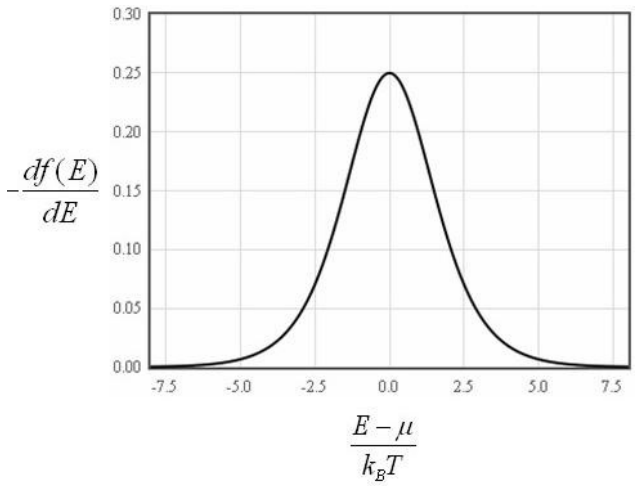
$$\boxed{\mu \approx E_F - \frac{\pi^2}{6}\left(k_B T\right)^2 \frac{D'(E_F)}{D(E_F)}}$$

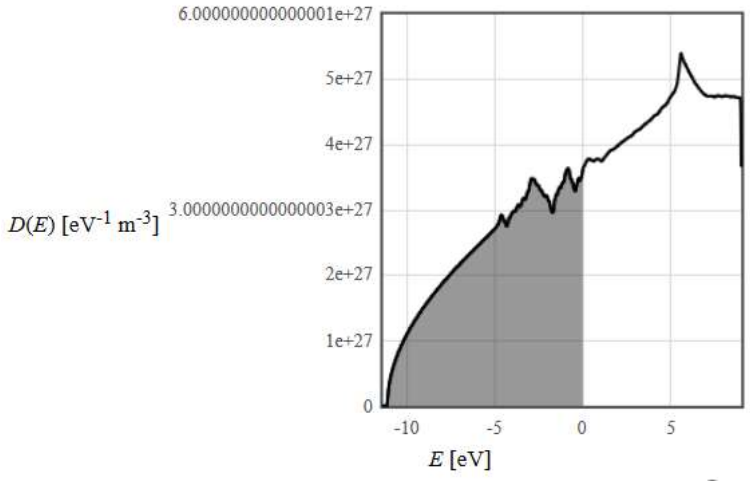


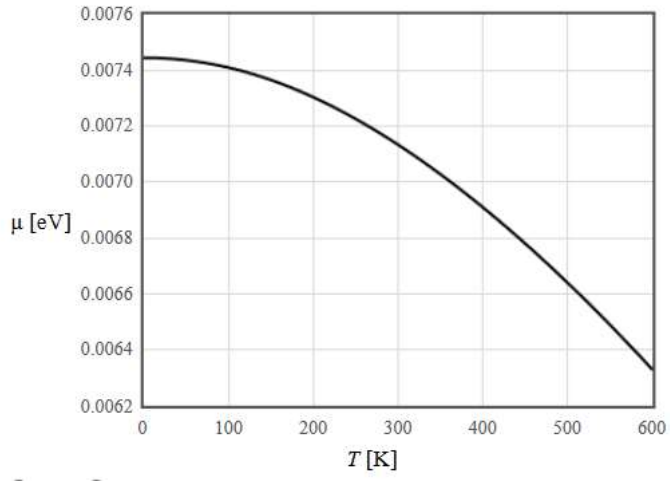
Aluminum

Sommerfeld Expansion: chemical potential

$$n = -\int_{-\infty}^{\infty} K(E)\frac{df(E)}{dE}dE = \int_{-\infty}^{\infty} \frac{K(E)\exp\left(\frac{E-\mu}{k_BT}\right)dE}{k_BT\left(\exp\left(\frac{E-\mu}{k_BT}\right)+1\right)^2}.$$







http://lampx.tugraz.at/~hadley/ss1/materials/thermo/dos2mu.html

Sommerfeld Expansion: internal energy

$$\int_{-\infty}^{\infty} H(E) f(E) dE = K(\mu) + \frac{\pi^2}{6} \left(k_B T\right)^2 \left.\frac{dH(E)}{dE}\right|_{E=\mu} + \frac{7\pi^4}{360} \left(k_B T\right)^4 \left.\frac{d^3 H(E)}{dE^3}\right|_{E=\mu} + \cdots$$

$$u = \int_{-\infty}^{\infty} ED(E) f(E) dE$$

$$H(E) = ED(E)$$

$$K(\mu) = \int_{-\infty}^{\mu} ED(E) dE$$

$$\left.\frac{dH}{dE}\right|_{E=\mu} = D(\mu) + \mu \frac{dD(\mu)}{dE} \approx D(E_F) + E_F \frac{dD(E_F)}{dE}$$

$$u = \int_{-\infty}^{\mu} ED(E) dE + \frac{\pi^2}{6} \left(k_B T\right)^2 \left(D(E_F) + E_F D'(E_F)\right)$$

Sommerfeld Expansion: internal energy

$$u = \int_{-\infty}^{\mu} ED(E)dE + \frac{\pi^2}{6}\left(k_B T\right)^2 \left(D(E_F) + E_F D'(E_F)\right)$$

$$u = \int_{-\infty}^{E_F} ED(E)dE + (\mu - E_F)E_F D(E_F) + \frac{\pi^2}{6}\left(k_B T\right)^2 \left(D(E_F) + E_F D'(E_F)\right)$$

$$\mu \approx E_F - \frac{\pi^2}{6}\left(k_B T\right)^2 \frac{D'(E_F)}{D(E_F)}$$

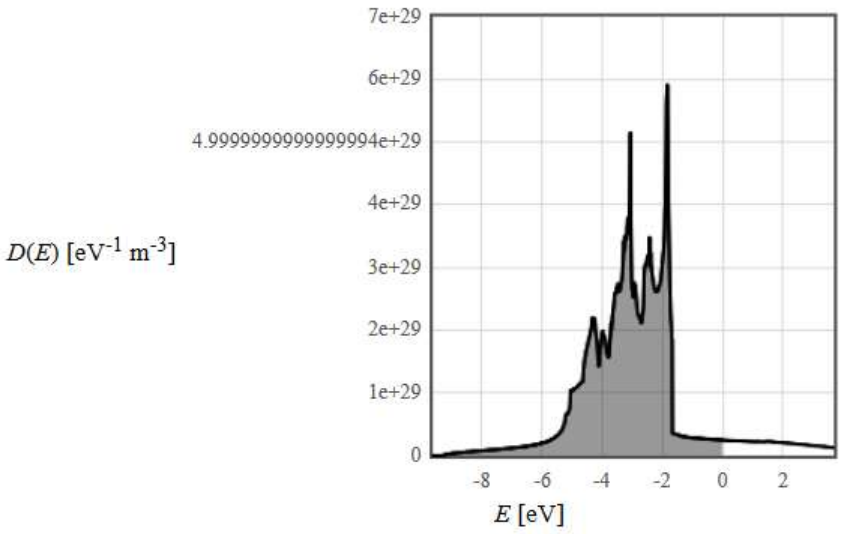
$$u = \int_{-\infty}^{E_F} ED(E)dE + (E_F - \frac{\pi^2}{6}\left(k_B T\right)^2 \frac{D'(E_F)}{D(E_F)} - E_F)E_F D(E_F) + \frac{\pi^2}{6}\left(k_B T\right)^2 \left(D(E_F) + E_F D'(E_F)\right)$$

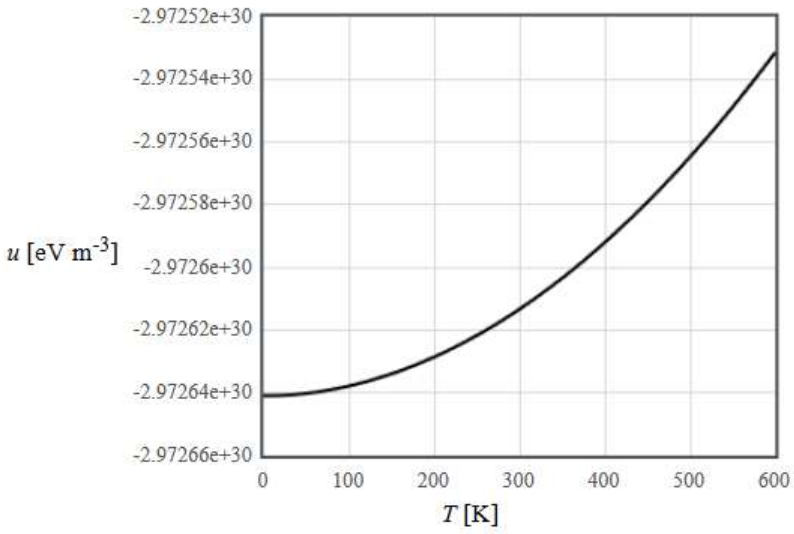
$$\boxed{u \approx \int_{-\infty}^{E_F} ED(E)dE + \frac{\pi^2}{6}\left(k_B T\right)^2 D(E_F)}$$

Free electrons: $u \approx \frac{3}{5} n E_F + \frac{\pi^2 D(E_F)}{6}\left(k_B T\right)^2 = \frac{\hbar^2}{10m}\left(\pi^4 3^5 n^5\right)^{\frac{1}{3}} + \frac{m\left(3\pi^2 n\right)^{\frac{1}{3}}}{6\hbar^2}\left(k_B T\right)^2$ J m^{-3}

Sommerfeld Expansion: internal energy

$$u \approx \int_{-\infty}^{E_F} ED(E)dE + \frac{\pi^2}{6}\left(k_B T\right)^2 D(E_F)$$



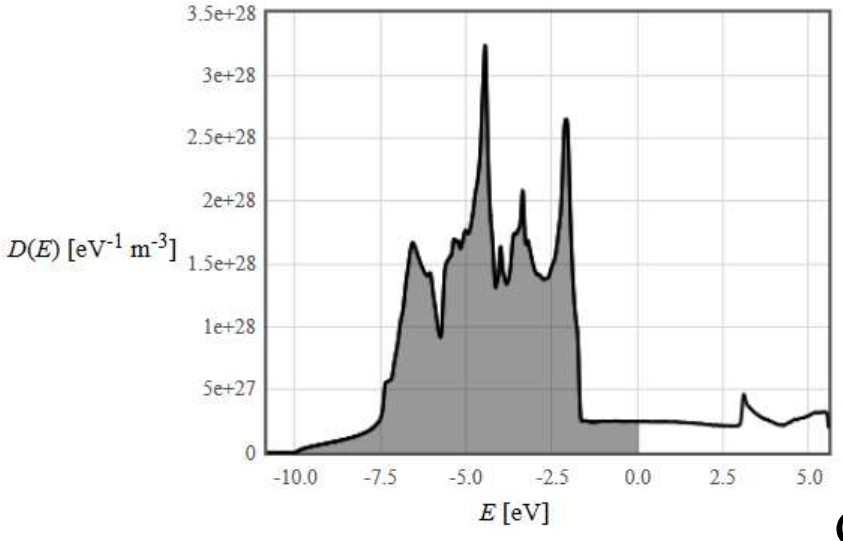


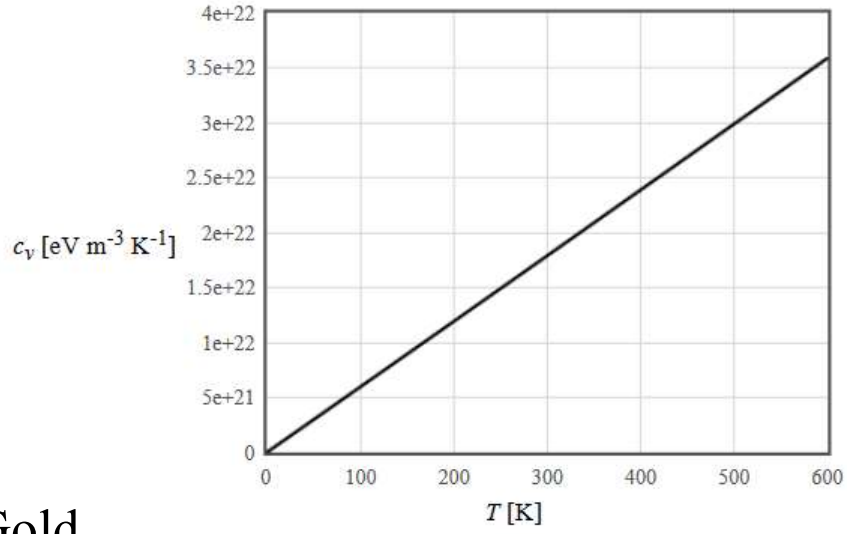
Copper

Sommerfeld Expansion: specific heat

$$c_v = \frac{du}{dT} \approx \frac{d}{dT}\left(u(T=0) + \frac{\pi^2}{6}\left(k_B T\right)^2 D(E_F) \right) = \frac{\pi^2 D(E_F)}{3} k_B^2 T \quad \text{J K}^{-1}\text{m}^{-3}$$

free electrons: $\approx \left(\frac{\pi}{3}\right)^{\frac{2}{3}} \frac{m n^{\frac{1}{3}}}{\hbar^2} k_B^2 T \quad \text{J K}^{-1}\text{m}^{-3}$





Gold

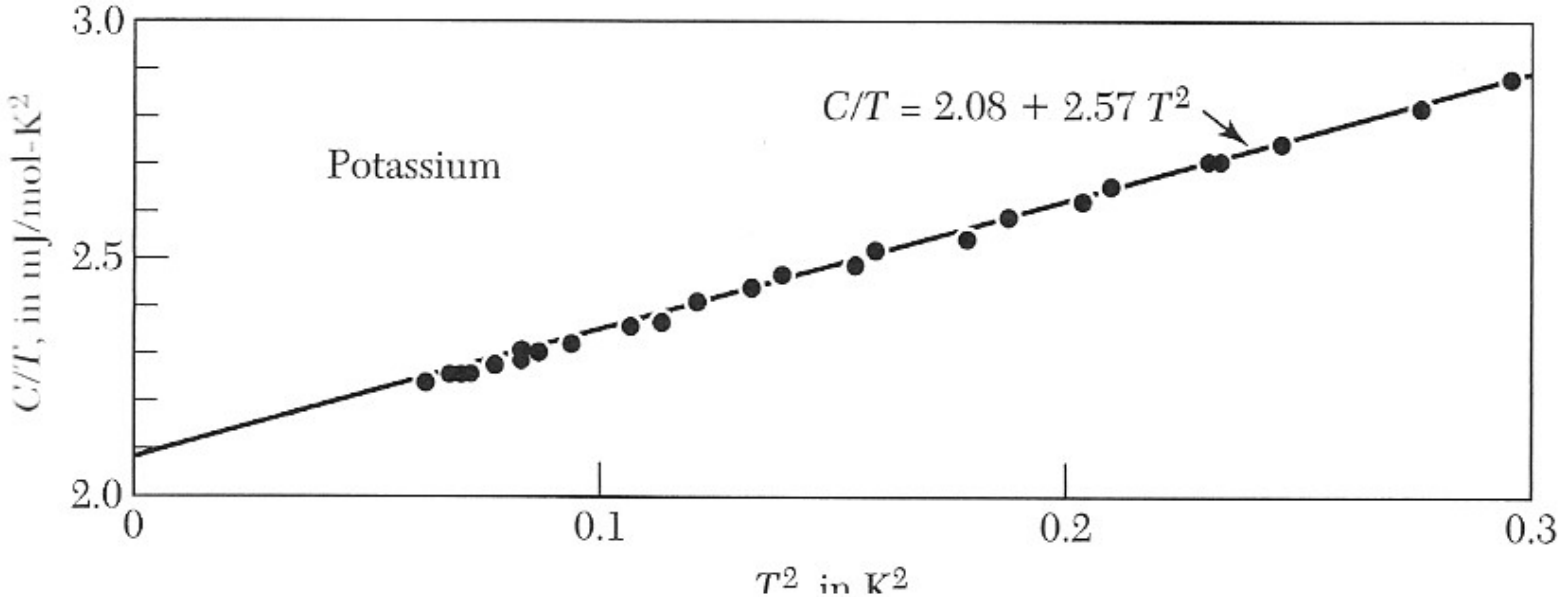
The electronic specific heat is linear in temperature

Electronic specific heat

$$c_{v,electrons} = \frac{du}{dT} \approx \left(\frac{\pi}{3}\right)^{\frac{2}{3}} \frac{mn^{\frac{1}{3}}}{\hbar^2} k_B^2 T \quad \text{J K}^{-1}\text{m}^{-3}$$

$$c_{v,total} = \gamma T + AT^3$$

electrons phonons



Effective mass

$$c_{v,electrons} = \frac{du}{dT} \approx \left(\frac{\pi}{3}\right)^{\frac{2}{3}} \frac{mn^{\frac{1}{3}}}{\hbar^2} k_B^2 T \quad \mathrm{J\,K^{-1}m^{-3}}$$

$$C_v = \gamma T + AT^3$$

$$\frac{m^*}{m} = \frac{\gamma_{observed}}{\gamma} = \frac{D(E_F)_{observed}}{D(E_F)_{free\ electron}}$$

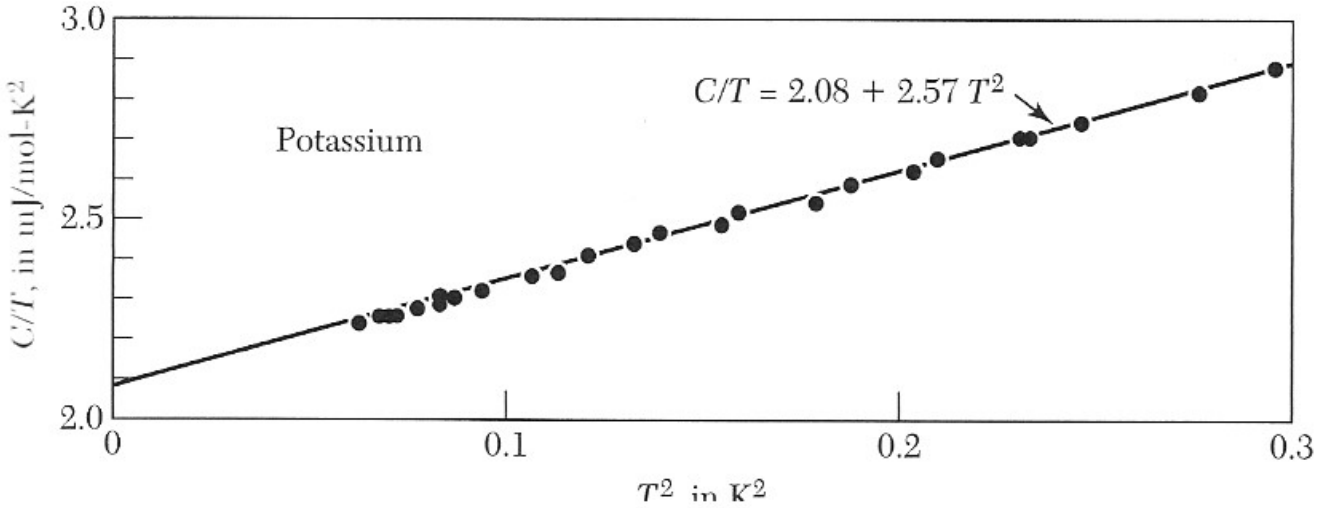


Table 2 Experimental and free electron values of electronic heat capacity constant γ of metals

(From compilations kindly furnished by N. Phillips and N. Pearlman. The thermal effective mass is defined by Eq. (38).)

Observed γ in mJ mol^{-1} K^{-2}.
Calculated free electron γ in mJ mol^{-1} K^{-2}
m_{th}/m = (observed γ)/(free electron γ).

Li	Be											B	C	N
1.63	0.17													
0.749	0.500													
2.18	0.34													
Na	Mg											Al	Si	P
1.38	1.3											1.35		
1.094	0.992											0.912		
1.26	1.3											1.48		
K	Ca	Sc	Ti	V	Cr	Mn(γ)	Fe	Co	Ni	Cu	Zn	Ga	Ge	As
2.08	2.9	10.7	3.35	9.26	1.40	9.20	4.98	4.73	7.02	0.695	0.64	0.596		0.19
1.668	1.511									0.505	0.753	1.025		
1.25	1.9									1.38	0.85	0.58		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn (w)	Sb
2.41	3.6	10.2	2.80	7.79	2.0	—	3.3	4.9	9.42	0.646	0.688	1.69	1.78	0.11
1.911	1.790									0.645	0.948	1.233	1.410	
1.26	2.0									1.00	0.73	1.37	1.26	
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg(α)	Tl	Pb	Bi
3.20	2.7	10.	2.16	5.9	1.3	2.3	2.4	3.1	6.8	0.729	1.79	1.47	2.98	0.008
2.238	1.937									0.642	0.952	1.29	1.509	
1.43	1.4									1.14	1.88	1.14	1.97	

from Kittel

Heavy Fermions

$$\frac{m^*}{m} = \frac{\gamma_{observed}}{\gamma}$$

Heavy fermions are materials that have effective masses 100 - 1000 times larger than the value expected from the free-electron theory. Examples are $CeCu_6$, the UBe_{13}, and $CeAl_3$. The last two are superconductors.

Something goes seriously wrong with the free electron model in these materials.

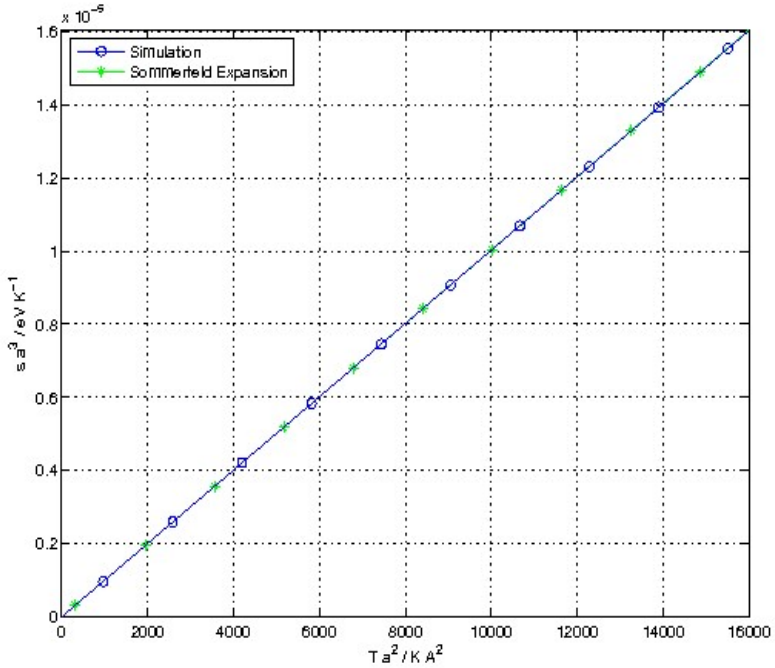
Entropy

$$c_v = \frac{du}{dT} \approx \frac{\pi^2 D(E_F)}{3} k_B^2 T \quad \text{J K}^{-1}\text{m}^{-3}$$

$$\frac{c_v}{T} = \frac{\partial s}{\partial T}\bigg|_{N,V} \approx \frac{\pi^2 D(E_F)}{3} k_B^2 \quad \text{J K}^{-1}\text{m}^{-3}$$

free electrons: $s \approx \left(\frac{\pi}{3}\right)^{\frac{2}{3}} \frac{m n^{\frac{1}{3}}}{\hbar^2} k_B^2 T \quad \text{J K}^{-1}\text{m}^{-3}$

Entropy density



Helmholtz free energy

$$s \approx \frac{\pi^2 D(E_F)}{3} k_B^2 \mathrm{T} \quad \mathrm{J\,K^{-1}m^{-3}}$$

free electrons: $$\approx \left(\frac{\pi}{3}\right)^{\frac{2}{3}} \frac{m n^{\frac{1}{3}}}{\hbar^2} k_B^2 T \quad \mathrm{J\,K^{-1}m^{-3}}$$

Helmholtz free energy density

$$f = u - Ts \approx \int_{-\infty}^{E_F} E D(E) dE - \frac{\pi^2 D(E_F)}{6} \left(k_B T\right)^2 \quad \mathrm{J\,m^{-3}}$$

free electrons: $$f \approx \frac{\hbar^2}{10m} \left(\pi^4 3^5 n^5\right)^{\frac{1}{3}} - \frac{m\left(3\pi^2 n\right)^{\frac{1}{3}}}{6\hbar^2} \left(k_B T\right)^2 \quad \mathrm{J\,m^{-3}}$$

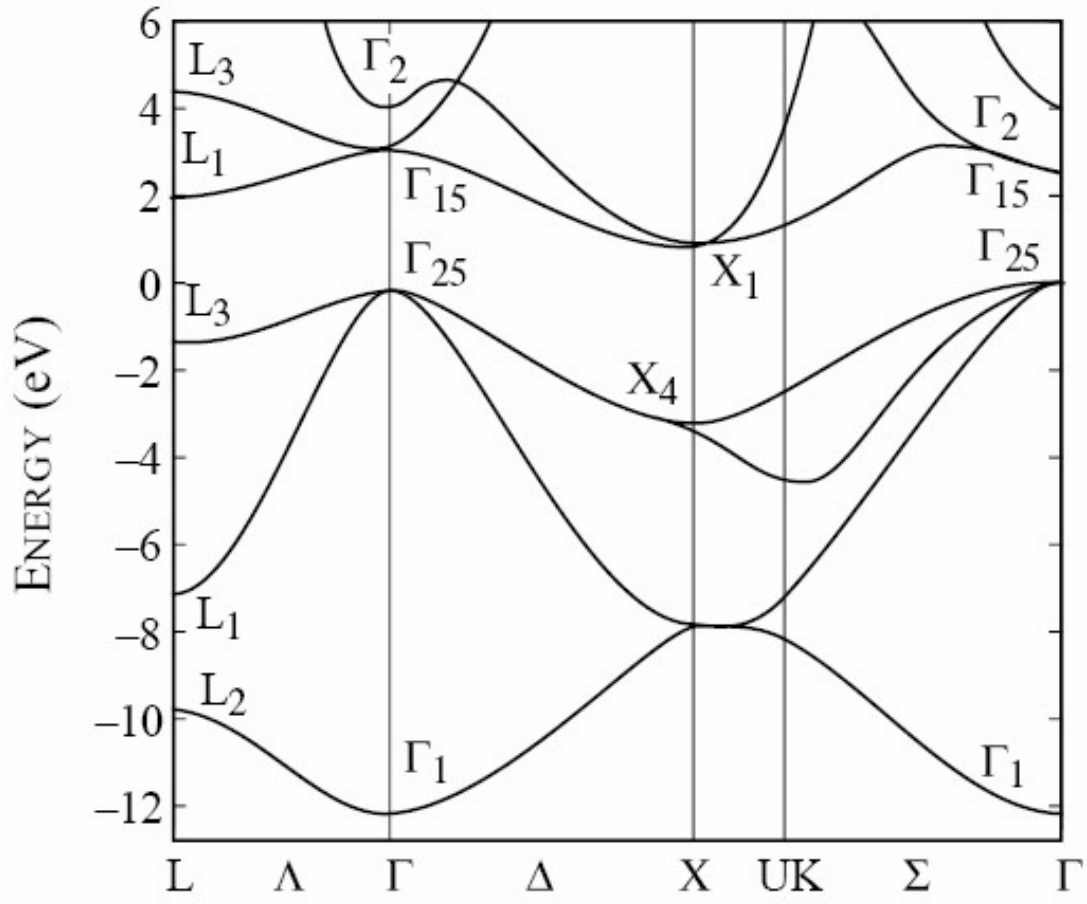
Results of the quantization of the Schrödinger equation for free fermions in 1, 2, and 3 dimensions.

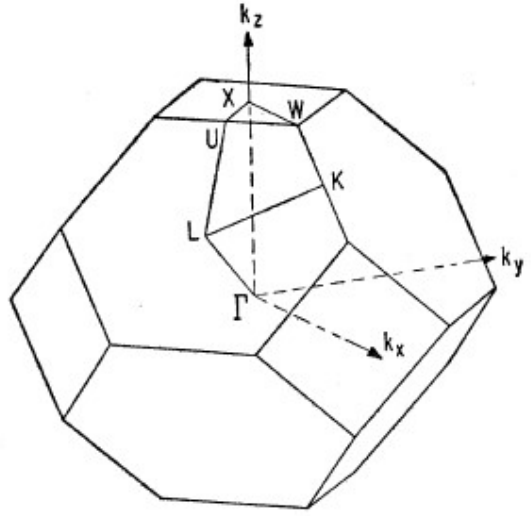
A simple model for metals is the free electron model where the potential energy of the electrons is zero and the electron-electron interactions are ignored. This is equivalent to any system of noninteracting fermions with zero potential energy. In this model the thermodynamic properties only depend on one parameter, the particle density n. In the table below, n denotes the number of particles per meter in one-dimension, the number of particle per square meter in two-dimensions, and the number of particles per cubic mter in three dimensions.

	1-D Schrödinger equation for a free particle $i\hbar\frac{d\psi}{dx}=-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}$	**2-D Schrödinger equation for a free particle** $i\hbar\frac{d\psi}{dx}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}\right)$	**3-D Schrödinger equation for a free particle** $i\hbar\frac{d\psi}{dx}=-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{dx^2}+\frac{d^2\psi}{dy^2}+\frac{d^2\psi}{dz^2}\right)$
Eigenfunction solutions	$A_k\exp\left(i\left(kx-\omega t\right)\right)$	$A_{\vec{k}}\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$	$A_{\vec{k}}\exp\left(i\left(\vec{k}\cdot\vec{r}-\omega t\right)\right)$
Dispersion relation	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J	$E=\hbar\omega=\frac{\hbar^2k^2}{2m}$ J
Density of states	$D(k)=\frac{2}{\pi}$	$D(k)=\frac{k}{\pi}$ m^{-1}	$D(k)=\frac{k^2}{\pi^2}$ m^{-2}
Density of states $D(E)=D(k)\frac{dk}{dE}$	$D(E)=\frac{1}{\pi\hbar}\sqrt{\frac{2m}{E}}=\frac{n}{2\sqrt{E_FE}}$ $\mathrm{J}^{-1}\mathrm{m}^{-1}$	$D(E)=\frac{m}{\pi\hbar^2}=\frac{n}{E_F}$ $\mathrm{J}^{-1}\mathrm{m}^{-2}$	$D(E)=\frac{(2m)^{\frac{3}{2}}}{2\pi^2\hbar^3}\sqrt{E}=\frac{3n}{2E_F^{3/2}}\sqrt{E}$ $\mathrm{J}^{-1}\mathrm{m}^{-3}$
Fermi energy E_F $n=\int_{-\infty}^{E_F}D(E)dE$	$E_F=\frac{\pi^2\hbar^2n^2}{8m}$ J	$E_F=\frac{\pi\hbar^2n}{m}$ J	$E_F=\frac{\hbar^2}{2m}\left(3\pi^2n\right)^{\frac{2}{3}}$ J
$D(E_F)$	$D(E_F)=\frac{4m}{\pi^2\hbar^2n}$ $\mathrm{J}^{-1}\mathrm{m}^{-1}$	$D(E_F)=\frac{m}{\pi\hbar^2}$ $\mathrm{J}^{-1}\mathrm{m}^{-2}$	$D(E_F)=\frac{m(3n)^{\frac{1}{3}}}{\pi^{\frac{4}{3}}\hbar^2}$ $\mathrm{J}^{-1}\mathrm{m}^{-3}$
$D'(E_F)=\left.\frac{dD}{dE}\right\|_{E=E_F}$	$D'(E_F)=\frac{-16m^2}{\pi^4\hbar^4n^3}$ $\mathrm{J}^{-2}\mathrm{m}^{-1}$	$D'(E_F)=0$ $\mathrm{J}^{-2}\mathrm{m}^{-2}$	$D'(E_F)=\frac{m^2}{\hbar^4\sqrt[3]{3\pi^8n}}$ $\mathrm{J}^{-2}\mathrm{m}^{-3}$
Chemical potential μ $n=\int_{-\infty}^{\infty}D(E)f(E)dE$	$\mu\approx E_F-\frac{\pi^2}{6}\left(k_BT\right)^2\frac{D'(E_F)}{D(E_F)}$ J $\approx\frac{\pi^2\hbar^2n^2}{8m}+\frac{2m}{3\hbar^2n^2}\left(k_BT\right)^2$ J	$\mu=k_BT\ln\left(\exp\left(\frac{E_F}{k_BT}\right)-1\right)$ J $=k_BT\ln\left(\exp\left(\frac{\pi\hbar^2n}{mk_BT}\right)-1\right)$ J	$\mu\approx E_F-\frac{\pi^2}{6}\left(k_BT\right)^2\frac{D'(E_F)}{D(E_F)}$ J $\approx\frac{\hbar^2}{2m}\left(3\pi^2n\right)^{\frac{2}{3}}-\frac{\pi^{\frac{2}{3}}m}{2\hbar^2\sqrt[3]{3}^{\frac{10}{3}}}\left(k_BT\right)^2$ J

Band Theory, Kittel chapter 7

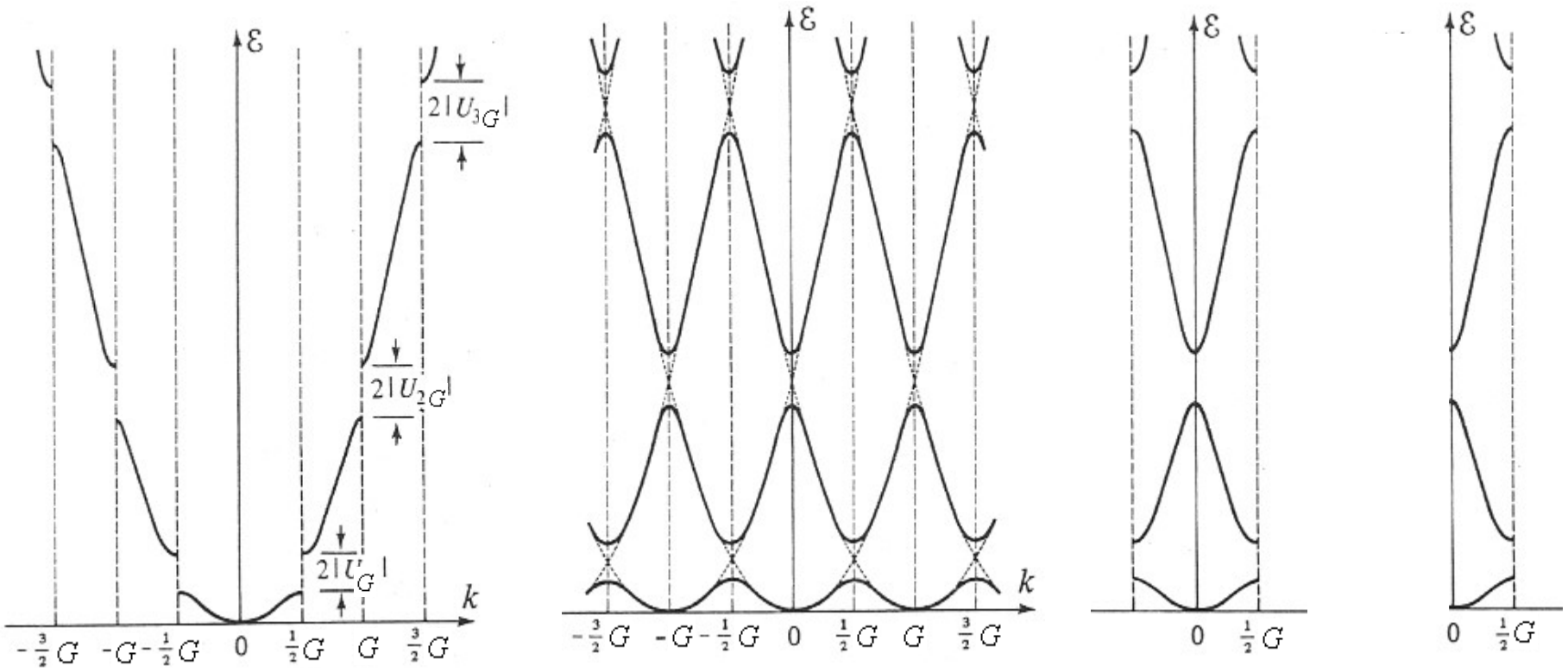
Calculate the dispersion relation for electrons in a crystal





silicon

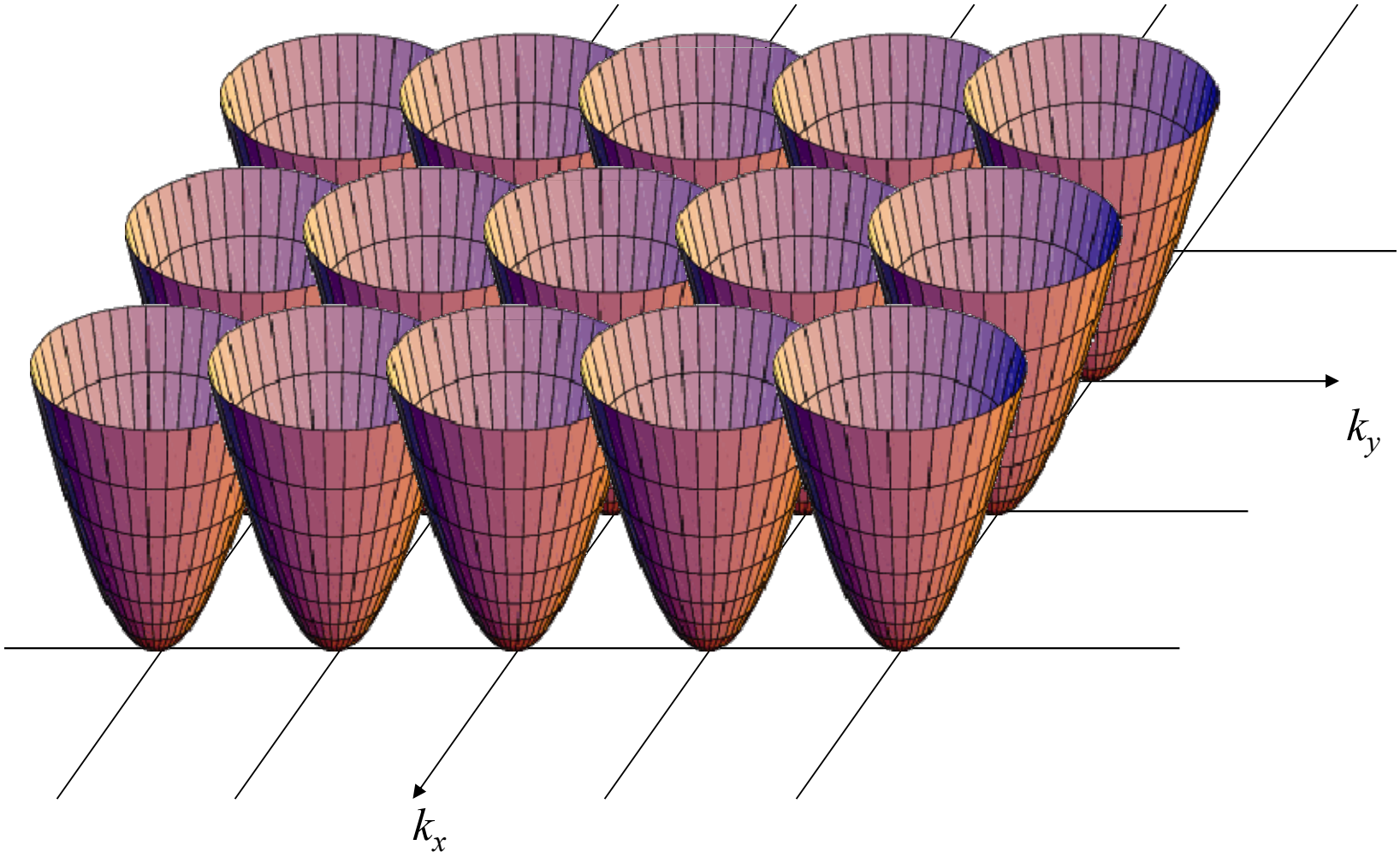
Empty lattice approximation



Extended Repeated Reduced

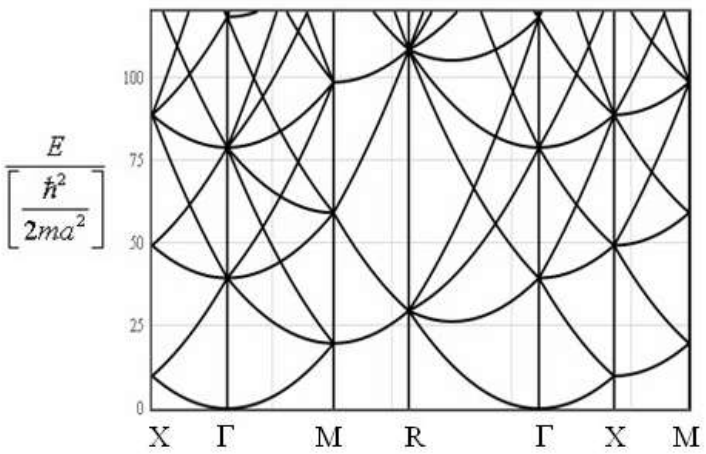
$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \underbrace{e^{i\vec{G}_0\cdot\vec{r}} e^{-i\vec{G}_0\cdot\vec{r}}}_{1} \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\left(\vec{k}+\vec{G}_0\right)\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{G}} e^{i\left(\vec{G}-\vec{G}_0\right)\cdot\vec{r}}$$

Empty lattice approximation



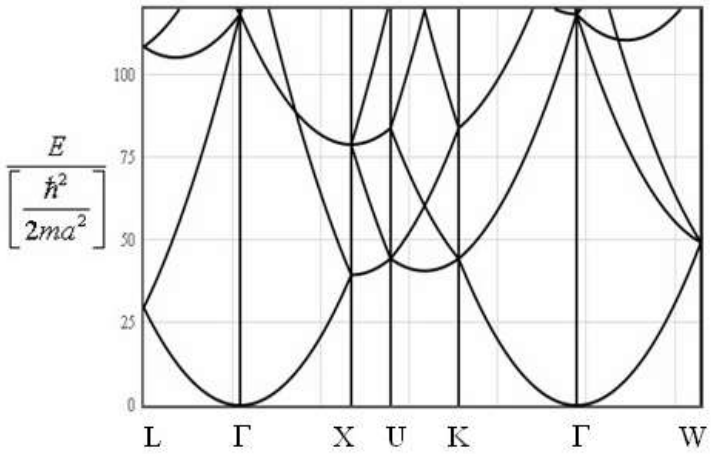
Empty lattice approximation

Simple cubic



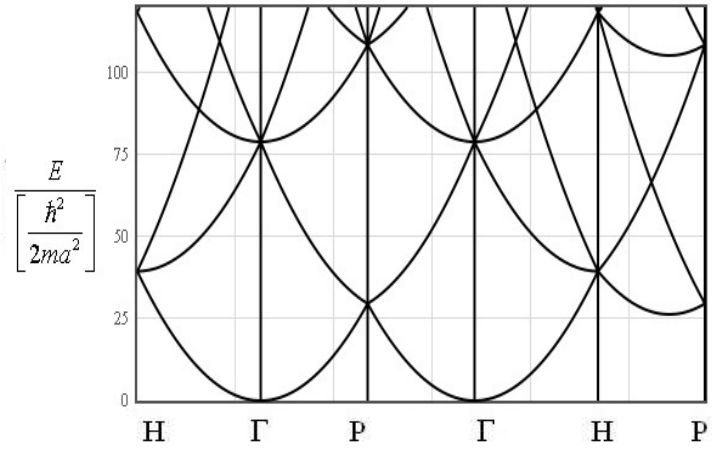
Choose a different order for the symmetry points

Face centered cubic

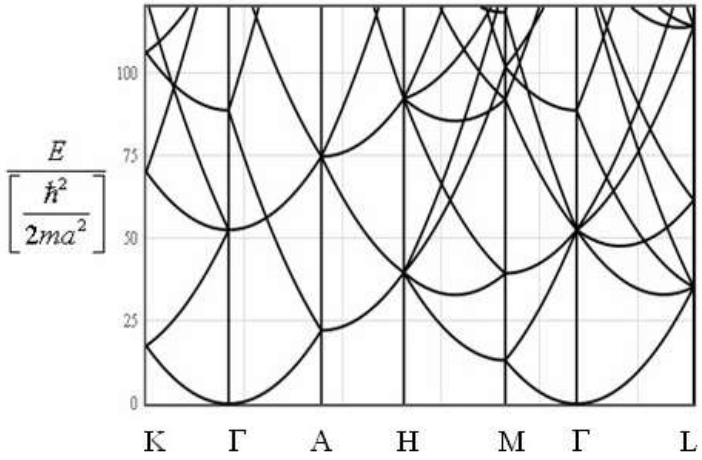


Choose a different order for the symmetry points

Body centered cubic



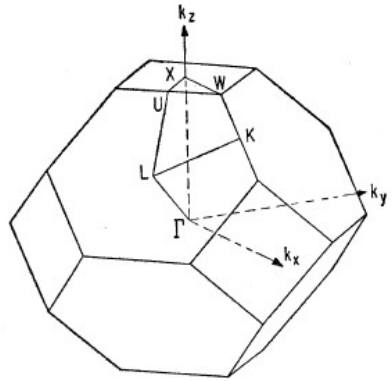
Hexagonal



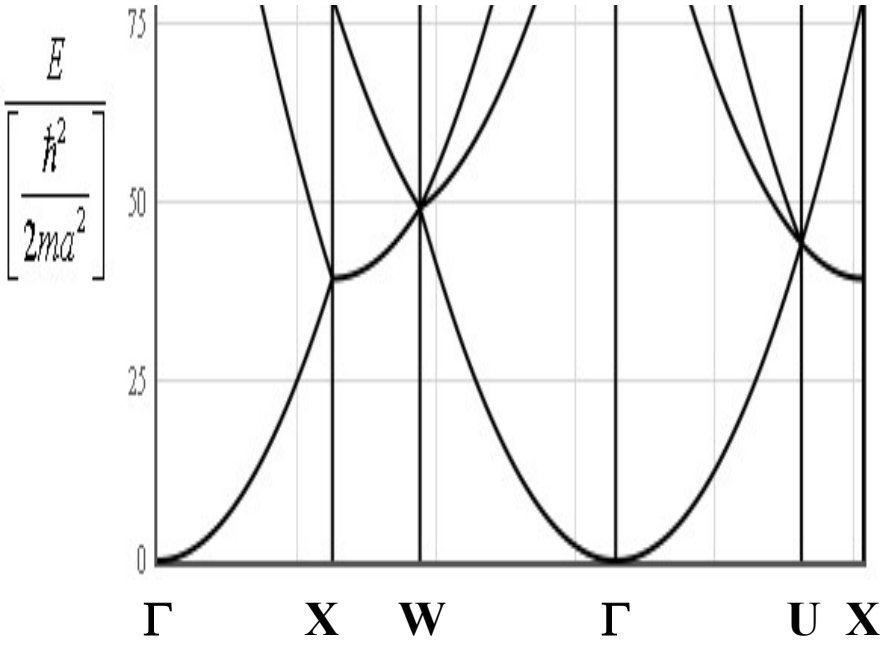
PHYSICAL REVIEW VOLUME 118, NUMBER 5 JUNE 1, 1960

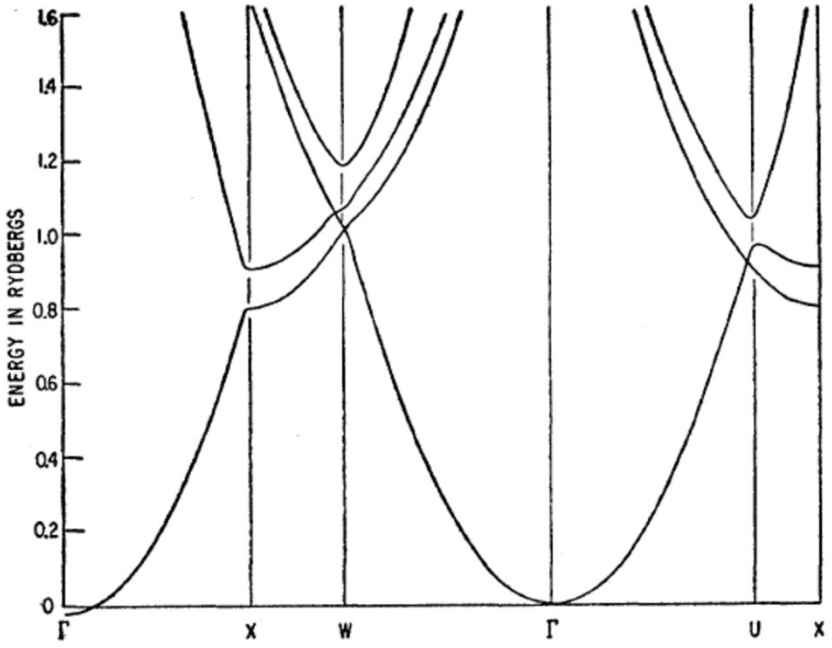
Band Structure of Aluminum

WALTER A. HARRISON
General Electric Research Laboratory, Schenectady, New York

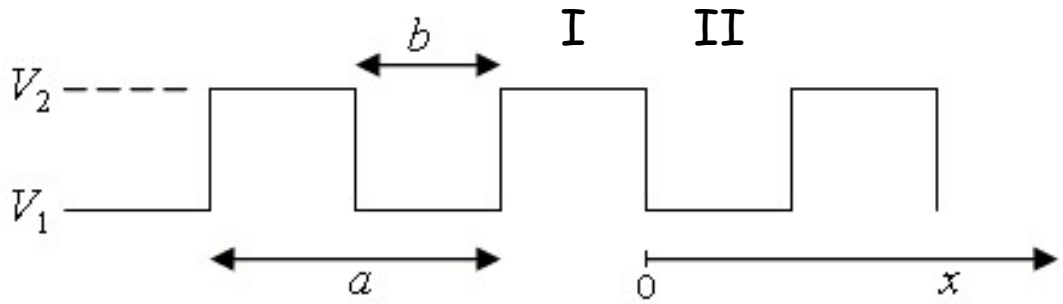


empty lattice approximation





Kronig-Penney model



$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V(x)\psi=E\psi$$

Solutions can be found in region I and region II
Match boundary conditions