

FERMI ENERGY AND RELATED PROPERTIES OF METALS

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In the classical Drude theory of metals, the Maxwell-Boltzmann velocity distribution of electrons is used. It states that the number of electrons per unit volume with velocities in the range of $d\vec{v}$ about any magnitude \vec{v} at temperature T is

$$f_B(\vec{v})d\vec{v} = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{mv^2}{2k_B T}\right) d\vec{v}$$

where n is the total number of conduction electrons in a unit volume of a metal, m is the free electron mass, and k_B is the Boltzmann constant. In an attempt to explain a substantial discrepancy between the experimental data on the specific heat of metals and the values calculated on the basis of the Drude model, Sommerfeld suggested a model of the metal in which the Pauli exclusion principle is applied to free electrons. In this case, the Maxwell-Boltzmann distribution is replaced by the Fermi-Dirac distribution:

$$f(\vec{v})d\vec{v} = \frac{1}{2} \left(\frac{m}{h} \right)^3 d\vec{v} \left\{ \exp\left[\left(\frac{mv^2}{2} - E_F\right)/k_B T_0\right] + 1 \right\}^{-1}$$

Here h is the Planck constant and T_0 is a characteristic temperature which is determined by the normalization condition

$$n = \int d\vec{v} \cdot f(\vec{v})$$

The magnitude of T_0 is quite high; usually, $T_0 > 10^4$ K. So, at common temperatures ($T < 10^3$ K), the free electron density of a metal is much smaller than in the case of the Maxwell-Boltzmann distribution. This allows us to explain why the experimental data on specific heat for metals are close to those for insulators.

The maximum kinetic energy the electrons of a metal may possess at $T = 0$ K is called the Fermi energy, e.g.,

$$E_F = \frac{\hbar^2 k_F^2}{2m} = \left(\frac{e^2}{2k_B} \right) (k_F r_B)^2$$

where k_F is the Fermi momentum or the Fermi wave vector

$$k_F = (3\pi^2 n)^{1/3}$$

e is the electron charge, and r_B is the Bohr radius

$$r_B = \hbar^2/m e^2 = 0.529 \cdot 10^{-10} \text{ m}$$

Another, more common expression for the Fermi energy is

$$E_F = \frac{1}{2} m v_F^2$$

where $v_F = \hbar k_F/m$ is the Fermi velocity which can be expressed using the concept of the electron radius, r_s . It is equal to radius of a sphere occupied by one free electron. If the total volume of a metal sample is V and the number of conduction electrons in this volume is N , then the volume per electron is equal to

$$\frac{V}{N} = \frac{1}{n} = \frac{4}{3} \pi r_s^3$$

and

$$r_s = \left(\frac{3}{4\pi n} \right)^{1/3}$$

The following table contains information pertinent to the Sommerfeld model for some metals. The magnitudes of T_0 are calculated using the expression

$$T_0 = \frac{E_F}{k_B} = \frac{58.2 \cdot 10^4}{(r_s / r_B)^2} \text{ K}$$

Ground State Properties of the Electron Gas in Some Metals

Metal	Valency	$n/10^{28} \text{ m}^{-3}$	r_s/pm	r_s/r_B	E_F/eV	$T_0/10^4 \text{ K}$	$k_F/10^{10} \text{ m}^{-1}$	$v_F/10^6 \text{ m s}^{-1}$
Li ^a	1	4.70	172	3.25	4.74	5.51	1.12	1.29
Na ^b	1	2.65	208	3.93	3.24	3.77	0.92	1.07
K ^b	1	1.40	257	4.86	2.12	2.46	0.75	0.86
Rb ^b	1	1.15	275	5.20	1.85	2.15	0.70	0.81
Cs ^b	1	0.91	298	5.62	1.59	1.84	0.65	0.75
Cu	1	8.47	141	2.67	7.00	8.16	1.36	1.57
Ag	1	5.86	160	3.02	5.49	6.38	1.20	1.39
Au	1	5.90	159	3.01	5.53	6.42	1.21	1.40
Be	2	24.7	99	1.87	14.3	16.6	1.94	2.25
Mg	2	8.61	141	2.66	7.08	8.23	1.36	1.58
Ca	2	4.61	173	3.27	4.69	5.44	1.11	1.28
Sr	2	3.55	189	3.57	3.93	4.57	1.02	1.18
Ba	2	3.15	196	3.71	3.64	4.23	0.98	1.13
Nb	1	5.56	163	3.07	5.32	6.18	1.18	1.37
Fe	2	17.0	112	2.12	11.1	13.0	1.71	1.98
Mn ^c	2	16.5	113	2.14	10.9	12.7	1.70	1.96
Zn	2	13.2	122	2.30	9.47	11.0	1.58	1.83
Cd	2	9.27	137	2.59	7.47	8.68	1.40	1.62

Metal	Valency	$n/10^{28} \text{ m}^{-3}$	r_s/pm	r_s/r_B	E_F/eV	$T_0/10^4 \text{ K}$	$k_F/10^{10} \text{ m}^{-1}$	$\nu_F/10^6 \text{ m s}^{-1}$
Hg ^a	2	8.65	140	2.65	7.13	8.29	1.37	1.58
Al	3	18.1	110	2.07	11.7	13.6	1.75	2.03
Ga	3	15.4	116	2.19	10.4	12.1	1.66	1.92
In	3	11.5	127	2.41	8.63	10.0	1.51	1.74
Tl	3	10.5	131	2.48	8.15	9.46	1.46	1.69
Sn	4	14.8	117	2.22	10.2	11.8	1.64	1.90
Pb	4	13.2	122	2.30	9.47	11.0	1.58	1.83
Bi	5	14.1	119	2.25	9.90	11.5	1.61	1.87
Sb	5	16.5	113	2.14	10.9	12.7	1.70	1.96

^a At 78 K.^b At 5 K.^c α -phase.

The data in the table are for atmospheric pressure and room temperature unless otherwise noted.

References

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