

DENSITY OF STATES IN THIN FILMS

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The density of states and its spatial distribution in thin films are considered as a universal function determined in the same form for phonons, electrons, and magnons. Detailed calculations are given for films with simple cubic crystallographic structure and with (100) orientation of the surfaces.

1. Introduction

In the case of thin films we may distinguish two kinds of thermodynamic mean values:

- 1) the thermodynamic mean values averaged on the whole sample with respect to each position of an atom in the crystallographic lattice, and
- 2) the thermodynamic mean values referring to a lattice point, which corresponds to the spatial distribution of a given property.

Calculations of these values may be carried out using a function of density of states *e. g.* [1] which is determined as follows

$$G(E) = \frac{1}{N^2 n} \sum_{\alpha\lambda\tau h}^{\gamma\Delta n N^2} \delta(E - E_{\tau h}^{\alpha\lambda}) \quad (1)$$

and its spatial distribution is defined by (*cf.* [2])

$$G(E, \nu) = \frac{1}{N^2} \sum_{\alpha\lambda\tau h}^{\gamma\Delta n N^2} (T_{\nu\tau})^2 \delta(E - E_{\tau h}^{\alpha\lambda}) \quad (2)$$

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which leads to the dependence of density of states on the position of layers in a film. Of course, the average value of (2) with respect to ν results (1). In the formulae (1) and (2) E denotes the energy parameter, $E_{\tau h}^{\alpha\lambda}$ are the energy eigenvalues belonging to the state of the wave vector h ($h \in (1, N^2)$) of the mode τ ($\tau \in (1, n)$); α ($\alpha \in (1, \gamma)$) labels the polarization directions and λ ($\lambda \in (1, A)$) refers to the spectrum branches or bands. $T_{\nu\tau}$ (e.g. [3-5]) denote the wave amplitudes of a quasiparticle in the direction perpendicular to the surfaces of the film in the ν -th monoatomic layer ($\nu \in (1, n)$).

The function $G(E, \nu)$ expresses the spatial distribution of a physical quantity P as follows

$$\langle P(\nu) \rangle = \int_0^{\infty} f_P(E) G(E, \nu) dE. \quad (3)$$

The density of states and its spatial distribution are a simple superposition of densities connected with the three directions of polarization and with various bands. The density of states belonging to a given band is calculated here by means of the Fourier representation of the δ -function.

2. Energy eigenvalues and perpendicular wave amplitudes

In our detailed calculations we consider a homogeneous thin film with simple cubic crystallographic structure. We assume that the z -axis is directed along the film thickness and the xy -plane is oriented in the direction of the (100) surface of the film. In general, the energy eigenvalues e.g. [3-5] can be written in the following form

$$E_{\tau h}^{\alpha\lambda} = -E_0^{\alpha\lambda} + E^{\alpha\lambda} \left(\sin^2 \frac{\alpha_\tau}{2} + \sin^2 \frac{h_x a}{2} + \sin^2 \frac{h_y a}{2} \right) \quad (4)$$

where the scaling factors $E_0^{\alpha\lambda}$ and $E^{\alpha\lambda}$ are determined by the physical considerations of the problem in question. The parameter $E_0^{\alpha\lambda}$ corresponds to the constant energy and plays the role of a scaling term in superposition of densities. The parameter $E^{\alpha\lambda}$ is connected with the characteristic features of the problem in question such as the bandwidth, the sound velocity, or the effective mass of magnons.

The parameter α_τ is interpreted as the third component of the propagation vector of the waves in question and it is connected with the perpendicular wave amplitudes $T_{\nu\tau}$. In the case of thin films α_τ runs over a discrete spectrum of values, which is determined by the difference equation [3-5]

$$T_{\nu-1, \tau} + T_{\nu+1, \tau} - 2 \cos \alpha_\tau T_{\nu\tau} = 0 \quad (5)$$

with the boundary conditions

$$(K - 2 \cos \alpha_\tau) T_{1\tau} + T_{2\tau} = 0$$

$$(K - 2 \cos \alpha_\tau) T_{n\tau} + T_{n-1, \tau} = 0 \quad (6)$$

and with the orthogonality relation

$$\sum_{\gamma} T_{\nu\tau} T_{\nu\tau'} = \delta_{\tau\tau'}. \quad (7)$$

The constant K describes the anisotropic properties of the boundary surfaces. From the physical point of view the constant K is determined by various effects such as the inhomogeneity of electron density, the different spacing between atoms in the surface layers and atoms inside the film, the interactions with the substrate, the oxidation of surface layers. The relations between K and parameters having a concrete physical meaning are given in paper *e. g.* [3-5], in which the problems are discussed in detail.

The solution of (5) can be written in an analytical form *e.g.* [3-5]

$$T_{\nu\tau} = A_{\tau} \cos \left[\alpha_{\tau} \left(\nu - \frac{n+1}{2} \right) + \frac{\pi(\tau-1)}{2} \right] \quad (8)$$

for the volume modes $\tau \in (1, n)$ if $|K| \leq 1$, for the volume modes $\tau \in (2, n)$ if $1 \leq |K| < \frac{n+1}{n-1}$, and for $\tau \in (3, n)$ if $|K| \geq \frac{n+1}{n-1}$;

The surface modes are described by

$$T_{\nu 1} = A_1 \operatorname{ch} \sigma_1 \left[\nu - \frac{n+1}{2} \right], \quad |K| \geq 1 \quad (9)$$

and

$$T_{\nu 2} = A_2 \operatorname{sh} \sigma_2 \left(\nu - \frac{n+1}{2} \right), \quad |K| \geq \frac{n+1}{n-1} \quad (10)$$

where $\sigma_1 = i\alpha_1$ and $\sigma_2 = i\alpha_2$. The normalization constant A_{τ} is expressed by

$$A_{\tau} = \sqrt{2} [n + \sin(n\alpha_{\tau}) \cos \pi(\tau-1) \sin^{-1} \alpha_{\tau}]^{-1/2} \quad (8')$$

for the volume modes, and

$$A_1 = \sqrt{2} [n + \operatorname{sh}(n\sigma_1) \operatorname{sh}^{-1} \sigma_1]^{-1/2} \quad (9')$$

$$A_2 = \sqrt{2} [n + \operatorname{sh}(n\sigma_2) \operatorname{sh}^{-1} \sigma_2]^{-1/2} \quad (10')$$

for the surface modes.

In the case of arbitrary values of K the parameters $\alpha_{\tau}(K)$ can be calculated only numerically. Table I contains the values of α_{τ} for some values of K and for certain film thicknesses. The sign “-” before the numerical values means that this value refers to the surface state. The parameters α_{τ} for negative values of K are given by the following relation

$$\alpha_{\tau}(-K) = \pi - \alpha_{n+1-\tau}(K) \quad (11)$$

which is valid for the both, volume and surface modes.

Parameters α_r for certain values K and n

| $\tau \backslash K$ | 0.2 | 0.3 | 0.5 | 0.7 | 0.8 | 0.9 | 0.95 | 0.98 | 0.99 | 1.01 |
|---------------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|---------|
| $n = 2$ | | | | | | | | | | |
| 1 | 0.9273 | 0.8633 | 0.7228 | 0.5548 | 0.4510 | 0.3176 | 0.2241 | 0.1415 | 0.1000 | -0.1000 |
| 2 | 1.9823 | 1.9283 | 1.8234 | 1.7213 | 1.6710 | 1.6207 | 1.5957 | 1.5809 | 1.5757 | 1.5656 |
| $n = 3$ | | | | | | | | | | |
| 1 | 0.7093 | 0.6664 | 0.5678 | 0.4430 | 0.3630 | 0.2574 | 0.1823 | 0.1154 | 0.0816 | -0.0817 |
| 2 | 1.4707 | 1.4203 | 1.3180 | 1.2132 | 1.1592 | 1.1040 | 1.0759 | 1.0587 | 1.0530 | 1.0415 |
| 3 | 2.2901 | 2.2603 | 2.2057 | 2.1572 | 2.1352 | 2.1141 | 2.1041 | 2.0982 | 2.0962 | 2.0925 |
| $n = 5$ | | | | | | | | | | |
| 1 | 0.4859 | 0.4632 | 0.4067 | 0.3274 | 0.2725 | 0.1963 | 0.1401 | 0.0891 | 0.0631 | -0.0634 |
| 2 | 0.9855 | 0.9513 | 0.8758 | 0.7887 | 0.7379 | 0.6868 | 0.6583 | 0.6406 | 0.6344 | 0.6221 |
| 3 | 1.5042 | 1.4712 | 1.4066 | 1.3440 | 1.3139 | 1.2848 | 1.2705 | 1.2621 | 1.2595 | 1.2538 |
| 4 | 2.0404 | 2.0160 | 1.9719 | 1.9335 | 1.9161 | 1.9000 | 1.8924 | 1.8879 | 1.8864 | 1.8835 |
| 5 | 2.5880 | 2.5753 | 2.5534 | 2.5355 | 2.5275 | 2.5202 | 2.5165 | 2.5145 | 2.5140 | 2.5125 |
| $n = 10$ | | | | | | | | | | |
| 1 | 0.2735 | 0.2655 | 0.2437 | 0.2075 | 0.1785 | 0.1334 | 0.0971 | 0.0625 | 0.0445 | -0.0450 |
| 2 | 0.5484 | 0.5343 | 0.4980 | 0.4463 | 0.4119 | 0.3691 | 0.3435 | 0.3264 | 0.3204 | 0.3077 |
| 3 | 0.8262 | 0.8082 | 0.7665 | 0.7165 | 0.6885 | 0.6588 | 0.6437 | 0.6345 | 0.6314 | 0.6252 |
| 4 | 1.1072 | 1.0880 | 1.0471 | 1.0047 | 0.9834 | 0.9626 | 0.9524 | 0.9464 | 0.9445 | 0.9405 |
| 5 | 1.3913 | 1.3728 | 1.3366 | 1.3023 | 1.2862 | 1.2710 | 1.2638 | 1.2595 | 1.2581 | 1.2553 |
| 6 | 1.6786 | 1.6621 | 1.6315 | 1.6045 | 1.5924 | 1.5811 | 1.5758 | 1.5728 | 1.5718 | 1.5698 |
| 7 | 1.9683 | 1.9547 | 1.9303 | 1.9097 | 1.9007 | 1.8925 | 1.8886 | 1.8863 | 1.8856 | 1.8843 |
| 8 | 2.2600 | 2.2496 | 2.2314 | 2.2167 | 2.2104 | 2.2045 | 2.2017 | 2.2001 | 2.1997 | 2.1986 |
| 9 | 2.5533 | 2.5459 | 2.5340 | 2.5247 | 2.5203 | 2.5165 | 2.5151 | 2.5140 | 2.5136 | 2.5130 |
| 10 | 2.8471 | 2.8436 | 2.8376 | 2.8327 | 2.8308 | 2.8289 | 2.8281 | 2.8279 | 2.8275 | 2.8274 |
| $n = 20$ | | | | | | | | | | |
| 1 | 0.1462 | 0.1438 | 0.1368 | 0.1368 | 0.1234 | 0.1108 | 0.0876 | 0.0660 | 0.0312 | -0.0321 |
| 2 | 0.2924 | 0.2879 | 0.2748 | 0.2519 | 0.2330 | 0.2045 | 0.1842 | 0.1689 | 0.1632 | 0.1561 |
| 3 | 0.4390 | 0.4325 | 0.4149 | 0.3874 | 0.3680 | 0.3436 | 0.3295 | 0.3204 | 0.3173 | 0.3110 |
| 4 | 0.5858 | 0.5779 | 0.5574 | 0.5290 | 0.5114 | 0.4919 | 0.4816 | 0.4754 | 0.4733 | 0.4692 |
| 5 | 0.7332 | 0.7241 | 0.7021 | 0.6750 | 0.6597 | 0.6440 | 0.6361 | 0.6314 | 0.6298 | 0.6268 |
| 6 | 0.8810 | 0.8712 | 0.8490 | 0.8238 | 0.8107 | 0.7978 | 0.7915 | 0.7878 | 0.7866 | 0.7842 |
| 7 | 1.0292 | 1.0192 | 0.9974 | 0.9747 | 0.9635 | 0.9526 | 0.9475 | 0.9445 | 0.9435 | 0.9416 |
| 8 | 1.1780 | 1.1679 | 1.1472 | 1.1268 | 1.1171 | 1.1081 | 1.1037 | 1.1012 | 1.1004 | 1.0987 |
| 9 | 1.3273 | 1.3175 | 1.2970 | 1.2798 | 1.2717 | 1.2638 | 1.2601 | 1.2580 | 1.2574 | 1.2559 |
| 10 | 1.4769 | 1.4676 | 1.4498 | 1.4338 | 1.4264 | 1.4198 | 1.4149 | 1.4166 | 1.4143 | 1.4131 |
| 11 | 1.6270 | 1.6181 | 1.6021 | 1.5881 | 1.5817 | 1.5760 | 1.5733 | 1.5719 | 1.5713 | 1.5703 |
| 12 | 1.7776 | 1.7695 | 1.7549 | 1.7426 | 1.7371 | 1.7324 | 1.7300 | 1.7288 | 1.7282 | 1.7275 |
| 13 | 1.9284 | 1.9210 | 1.9081 | 1.8976 | 1.8929 | 1.8887 | 1.8867 | 1.8858 | 1.8854 | 1.8847 |
| 14 | 2.0794 | 2.0728 | 2.0616 | 2.0528 | 2.0488 | 2.0451 | 2.0437 | 2.0427 | 2.0424 | 2.0417 |
| 15 | 2.2308 | 2.2251 | 2.2157 | 2.2080 | 2.2048 | 2.2018 | 2.2004 | 2.1997 | 2.1994 | 2.1989 |
| 16 | 2.3823 | 2.3774 | 2.3697 | 2.3635 | 2.3608 | 2.3583 | 2.3574 | 2.3567 | 2.3563 | 2.3561 |
| 17 | 2.5337 | 2.5303 | 2.5241 | 2.5119 | 2.5166 | 2.5151 | 2.5142 | 2.5135 | 2.5136 | 2.5129 |
| 18 | 2.6857 | 2.6827 | 2.6784 | 2.6747 | 2.6730 | 2.6715 | 2.6710 | 2.6708 | 2.6705 | 2.6702 |
| 19 | 2.8376 | 2.8356 | 2.8328 | 2.8301 | 2.8293 | 2.8283 | 2.8279 | 2.8276 | 2.8273 | 2.8276 |
| 20 | 2.9895 | 2.9885 | 2.9872 | 2.9860 | 2.9852 | 2.9852 | 2.9847 | 2.9845 | 2.9846 | 2.9844 |

Table I — continued

| $\tau \backslash K$ | 1.1 | 1.4 | 1.6 | 1.8 | 4 | 6 | 10 |
|---------------------|---------|---------|---------|---------|---------|---------|---------|
| 1 | -0.3149 | -0.6224 | -0.7565 | -0.8671 | -1.5667 | -1.9251 | -2.3894 |
| 2 | 1.5210 | 1.3693 | 1.2662 | 1.1593 | -0.9625 | -1.5667 | -2.1848 |
| $n = 3$ | | | | | | | |
| 1 | -0.2589 | -0.5213 | -0.6407 | -0.7421 | -1.4377 | -1.8171 | -2.3123 |
| 2 | 0.9885 | 0.7953 | 0.6434 | 0.4511 | -1.3171 | -1.7629 | -2.2922 |
| 3 | 2.0758 | 2.0252 | 1.9958 | 1.9695 | 1.7975 | 1.7297 | 1.6691 |
| $n = 5$ | | | | | | | |
| 1 | -0.2036 | -0.4284 | -0.5406 | -0.6407 | -1.7927 | -2.3025 | -2.3025 |
| 2 | 0.5631 | 0.2826 | -0.2830 | -0.4904 | -1.7908 | -2.3025 | -2.3025 |
| 3 | 1.2298 | 1.1567 | 1.1148 | 1.0784 | 0.8992 | 0.8555 | +0.8247 |
| 4 | 1.8710 | 1.8342 | 1.8135 | 1.7954 | 1.6892 | 1.6521 | 1.6203 |
| 5 | 2.5069 | 2.4907 | 2.4818 | 2.4736 | 2.4249 | 2.4057 | 2.3879 |
| $n = 10$ | | | | | | | |
| 1 | -0.1501 | -0.3565 | -0.4782 | -0.5911 | -1.3865 | -1.7918 | -2.3025 |
| 2 | 0.2385 | -0.3057 | -0.4604 | -0.5842 | -1.3865 | -1.7918 | -2.3025 |
| 3 | 0.5977 | 0.5156 | 0.4763 | 0.4490 | 0.3755 | 0.3647 | 0.3576 |
| 4 | 0.9234 | 0.8740 | 0.8480 | 0.8270 | 0.7138 | 0.7260 | 0.7138 |
| 5 | 1.2433 | 1.2093 | 1.1910 | 1.1756 | 1.1020 | 1.0824 | 1.0676 |
| 6 | 1.5611 | 1.5366 | 1.5232 | 1.5120 | 1.4519 | 1.4334 | 1.4184 |
| 7 | 1.8781 | 1.8602 | 1.8505 | 1.8422 | 1.7958 | 1.7801 | 1.7666 |
| 8 | 2.1943 | 2.1818 | 2.1751 | 2.1690 | 2.1354 | 2.1231 | 2.1125 |
| 9 | 2.5102 | 2.5021 | 2.4978 | 2.4942 | 2.4719 | 2.4640 | 2.4564 |
| 10 | 2.8261 | 2.8243 | 2.8219 | 2.8201 | 2.8074 | 2.8030 | 2.7992 |
| $n = 20$ | | | | | | | |
| 1 | -0.1161 | -0.3372 | -0.4700 | -0.5878 | -1.3865 | -1.7918 | -2.2025 |
| 2 | 0.03766 | -0.3356 | -0.4699 | -0.5878 | -1.3865 | -1.7918 | -2.3025 |
| 3 | 0.2818 | 0.2144 | 0.1977 | 0.1891 | +0.1713 | +0.1689 | 0.1673 |
| 4 | 0.3508 | 0.4027 | 0.3842 | 0.3724 | 0.3422 | 0.3376 | 0.3345 |
| 5 | 0.6134 | 0.5772 | 0.5608 | 0.5491 | 0.5124 | 0.5060 | 0.5016 |
| 6 | 0.7738 | 0.7451 | 0.7312 | 0.7206 | 0.6817 | 0.6739 | 0.6684 |
| 7 | 0.9331 | 0.9096 | 0.8978 | 0.8884 | 0.8500 | 0.8414 | 0.8351 |
| 8 | 1.0917 | 1.0723 | 1.0621 | 1.0539 | 1.0173 | 1.0083 | 1.0015 |
| 9 | 1.2502 | 1.2336 | 1.2249 | 1.2178 | 1.1838 | 1.1746 | 1.1674 |
| 10 | 1.4081 | 1.3940 | 1.3866 | 1.3804 | 1.3493 | 1.3404 | 1.3332 |
| 11 | 1.5660 | 1.5539 | 1.5477 | 1.5422 | 1.5142 | 1.5057 | 1.4988 |
| 12 | 1.7237 | 1.7136 | 1.7081 | 1.7034 | 1.6785 | 1.6705 | 1.6638 |
| 13 | 1.8814 | 1.8728 | 1.8680 | 1.8640 | 1.8423 | 1.8350 | 1.8286 |
| 14 | 2.0391 | 2.0317 | 2.0279 | 2.0244 | 2.0054 | 1.9991 | 1.9935 |
| 15 | 2.1968 | 2.1906 | 2.1873 | 2.1843 | 2.1685 | 2.1627 | 2.1578 |
| 16 | 2.3542 | 2.3493 | 2.3465 | 2.3442 | 2.3311 | 2.3263 | 2.3221 |
| 17 | 2.5116 | 2.5076 | 2.5057 | 2.5040 | 2.4933 | 2.4895 | 2.4863 |
| 18 | 2.6694 | 2.6664 | 2.6645 | 2.6633 | 2.6556 | 2.6527 | 2.6500 |
| 19 | 2.8267 | 2.8247 | 2.8238 | 2.8230 | 2.8178 | 2.8159 | 2.8142 |
| 20 | 2.9840 | 2.9830 | 2.9826 | 2.9823 | 2.9795 | 2.9786 | 2.9779 |

As a supplement of Table I we give the analytical solutions for certain film thicknesses in the case of arbitrary K :

| $ K $ | $n = 2$ | $n = 3$ |
|-----------------------------|---|--|
| $ K \leq 1$ | $\sigma_1 = \arccos \frac{K+1}{2}$ $\alpha_2 = \arccos \frac{K-1}{2}$ | $\alpha_1 = \arccos \frac{K + \sqrt{K^2 + 8}}{4}$ $\alpha_2 = \arccos (K/2)$ $\alpha_3 = \arccos \frac{-K + \sqrt{K^2 + 8}}{4}$ |
| $1 < K < \frac{h+1}{n-1}$ | $\sigma_1 = \ln \left(\frac{K+1}{2} + \sqrt{\left(\frac{K+1}{2}\right)^2 - 1} \right)$ $\alpha_2 = \arccos \frac{K-1}{2}$ | $\sigma_1 = \ln \left(\frac{K}{4} + \frac{\sqrt{K^2 + 8}}{4} + \sqrt{\frac{1}{2} \left(\left(\frac{K}{2}\right)^2 - 1 + \frac{K}{2} \sqrt{2 + \left(\frac{K}{2}\right)^2} \right)} \right)$ $\alpha_2 = \arccos (K/2)$ $\alpha_3 = \arccos \frac{-K + \sqrt{K^2 + 8}}{4}$ |
| $ K > \frac{n+1}{n-1}$ | $\sigma_1 = \ln \left(\frac{K+1}{2} + \sqrt{\left(\frac{K+1}{2}\right)^2 - 1} \right)$ $\sigma_2 = \ln \left(\frac{K-1}{2} + \sqrt{\left(\frac{K-1}{2}\right)^2 - 1} \right)$ | $\sigma_1 = \ln \left(\frac{K}{4} + \frac{\sqrt{K^2 + 8}}{4} + \sqrt{\frac{1}{2} \left(\left(\frac{K}{2}\right)^2 - 1 + \frac{K}{2} \sqrt{2 + \left(\frac{K}{2}\right)^2} \right)} \right)$ $\sigma_2 = \ln \left(\frac{K}{2} + \sqrt{\left(\frac{K}{2}\right)^2 - 1} \right)$ $\alpha_3 = \arccos \frac{-K + \sqrt{K^2 + 8}}{4}$ |

The values of $\alpha_r(K)$ can be approximated by the formula

$$\alpha_r(K) = \frac{\pi(\tau-1-\varepsilon)}{n-\varepsilon}; \quad \varepsilon = \frac{K-1}{K+1} \quad (12)$$

$$\sigma_1(K) \approx \ln K \quad (13')$$

$$\sigma_2(K) \approx \ln \left(K - \frac{n+1}{n-1} \right). \quad (13'')$$

The simple approximation proposed above reproduces the exact analytical solutions which are well known for some values of K : $-\infty, -1, 0, 1, \infty$.

3. Formula for the density of states

Starting from (4) the density of states and its spatial distribution given by (1) and (2) rewritten by means of Fourier transformation take the forms:

$$G_{\alpha\lambda}(E) = \frac{1}{2\pi n} \sum_{\tau} \int_{-\infty}^{+\infty} \exp\left(-ix\left(E - E_0^{\alpha\lambda} - E^{\alpha\lambda} \sin^2 \frac{\alpha_{\tau}}{2}\right)\right) f(x) dx \quad (14)$$

$$G_{\alpha\lambda}(E, \nu) = \frac{1}{2\pi} \sum_{\tau} \int_{-\infty}^{+\infty} (T_{\nu\tau})^2 \exp\left(-ix\left(E - E_0^{\alpha\lambda} - E^{\alpha\lambda} \sin^2 \frac{\alpha_{\tau}}{2}\right)\right) f(x) dx \quad (15)$$

where

$$f(x) = \frac{1}{N^2} \sum_h \exp\left(ixE^{\alpha\lambda} \left(\sin^2 \frac{h_x a}{2} + \sin^2 \frac{h_y a}{2}\right)\right) \quad (16)$$

Integration over h_x, h_y leads to the result

$$f(x) = e^{ixE^{\alpha\lambda}} J_0^2(xE^{\alpha\lambda}/2) \quad (17)$$

where $J_0(z)$ denotes the Bessel function. Next, we replace the variable x by $z = xE^{\alpha\lambda}/2$. This allows us to discuss the function $G(E)$ and $G(E, \nu)$ as the universal density of states which is independent of the specification of the physical problem in question. Namely, we get

$$G_{\alpha\lambda}(\varepsilon) = \frac{1}{\pi E^{\alpha\lambda}} \frac{1}{n} \sum_{\tau} \int_{-\infty}^{+\infty} \exp(2iz\delta_{\tau}) J_0^2(z) dz \quad (18)$$

$$G_{\alpha\lambda}(\varepsilon, \nu) = \frac{1}{\pi E^{\alpha\lambda}} \sum_{\tau} (T_{\nu\tau})^2 \int_{-\infty}^{+\infty} \exp(2iz\delta_{\tau}) J_0^2(z) dz \quad (19)$$

where

$$\delta_{\tau} = 1 + \sin^2 \frac{\alpha_{\tau}}{2} + \varepsilon_0^{\alpha\lambda} - \varepsilon \quad (20)$$

and $\varepsilon_0^{\alpha\lambda} = E_0^{\alpha\lambda}/E^{\alpha\lambda}$. ε denotes the variable of energy in relative units $E^{\alpha\lambda}$. After integrating we obtain the following:

$$G_{\alpha\lambda}(\varepsilon) = \frac{1}{\pi E^{\alpha\lambda}} \frac{1}{n} \sum_{\tau} \Gamma(\varepsilon, \tau) \quad (21)$$

$$G_{\alpha\lambda}(\varepsilon, \nu) = \frac{1}{\pi E^{\alpha\lambda}} \sum_{\tau} (T_{\nu\tau})^2 \Gamma(\varepsilon, \tau) \quad (22)$$

and $\Gamma(\varepsilon, \tau)$ is expressed by the hypergeometric series

$$\Gamma(\varepsilon, \tau) = {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; 1 - \delta_\tau^2\right) \quad (23)$$

for $0 \leq \delta_\tau^2 \leq 1$ or $\Gamma(\varepsilon, \tau) = 0$ otherwise.

In the same interval (0,1) for δ_τ^2 the function $\Gamma(\varepsilon, \tau)$ can be written in a form more convenient for practical calculations by the complete elliptical integral $K(k)$ in the following way

$$\Gamma(\varepsilon, \tau) = \frac{2}{\pi} K(\sqrt{1 - \delta_\tau^2}). \quad (24)$$

Finally, the summation in (21) and (22) over τ with respect to (23) or (24) must be carried out numerically even if analytical solutions for α_τ are known, as for example if $K = 1$, and the more when numerical solutions for α_τ are obtained. The numerical character of the calculations in question is caused by the fact, that $\Gamma(\varepsilon, \tau)$ is a discontinuous function of ε and it is determined only in certain intervals of ε , which depend on τ . This shall be shown below.

However, we can derive from (21), (22) and (20) some general properties of the universal functions $G(E)$ and $G(E, \nu)$. Namely: 1) the functions in question differ from zero if ε belongs to the interval $(\varepsilon_{\min}, \varepsilon_{\max})$ where

$$\begin{aligned} \varepsilon_{\min} &= \min \left(\varepsilon_0^{\alpha_\lambda} + \sin^2 \frac{\alpha_\tau}{2} \right) \\ \varepsilon_{\max} &= \max \left(\varepsilon_0^{\alpha_\lambda} + 2 + \sin^2 \frac{\alpha_\tau}{2} \right). \end{aligned} \quad (25)$$

For example, ε belongs to $(0, 2 + \cos^2 \pi/2n)$ when $\varepsilon_0^{\alpha_\lambda} = 0$, $K = 1$; 2) the total density functions are simple compositions of the density functions for every τ , which are determined in the intervals $(\varepsilon_{\min}, \varepsilon_{\max})$ of ε given directly by the expressions in the brackets in (25); 3) the functions $\Gamma(\varepsilon, \tau)$ at the points

$$\varepsilon = \varepsilon_0^{\alpha_\lambda} + 1 + \sin^2 \frac{\alpha_\tau}{2} \quad (26)$$

have points of singularity. The normalization integral of $\Gamma(\varepsilon, \tau)$ over ε is convergent and it is equal to π . Thus the integration of $G(\varepsilon)$ and $G(\varepsilon, \nu)$ over ε show that the density functions in question are normalized to unity.

From our remarks it is evident that the parameters α_τ play the role of numerical coefficients which are necessary to construct the total density of states. In the present paper we give by graphs 1-3 representative curves for the universal function of the density of states for one-band spectrum of energy, so we have put $\varepsilon_0^{\alpha_\lambda} = 0$, $\lambda = 1$, $\gamma = 1$. The curves related to $\pi E^{\alpha_\lambda}/2$ are traced in arbitrary units.

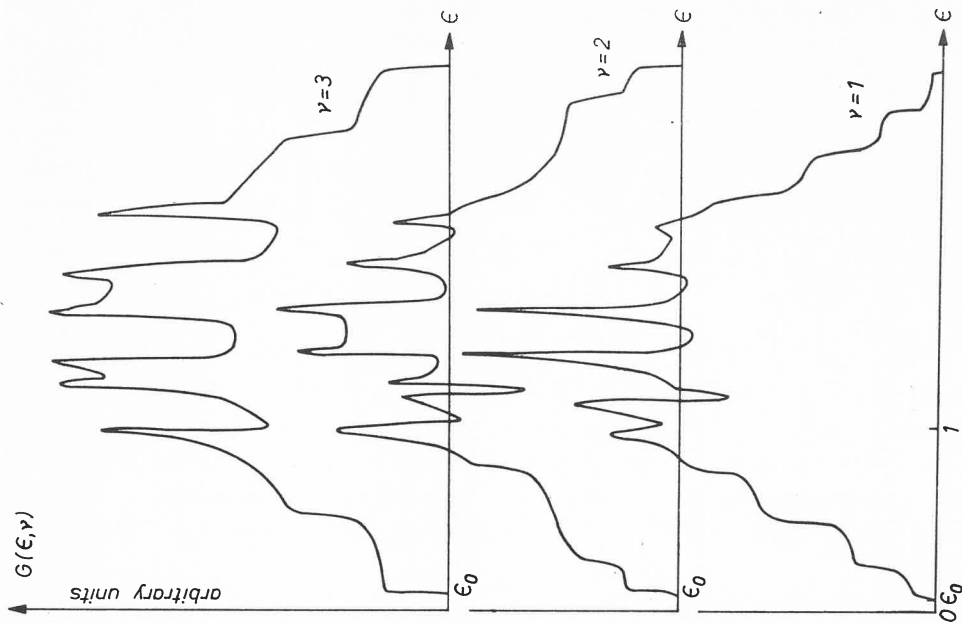


Fig. 2. Spatial distribution $G(\epsilon, \nu)$ of the density of states for $n = 5$ and $K = 0.2$

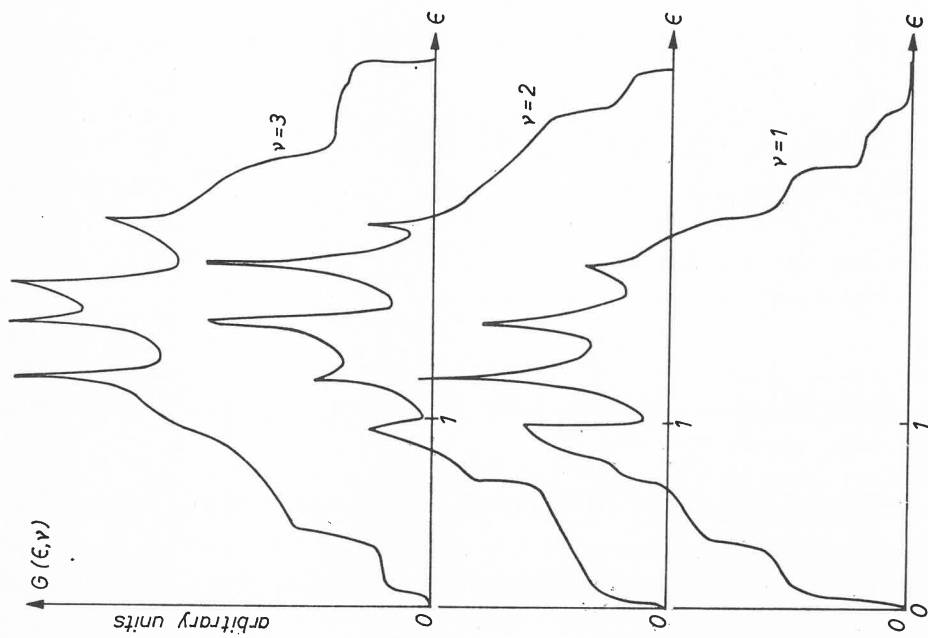


Fig. 1. Spatial distribution $G(\epsilon, \nu)$ of the density of states for $n = 5$ and $K = 1$

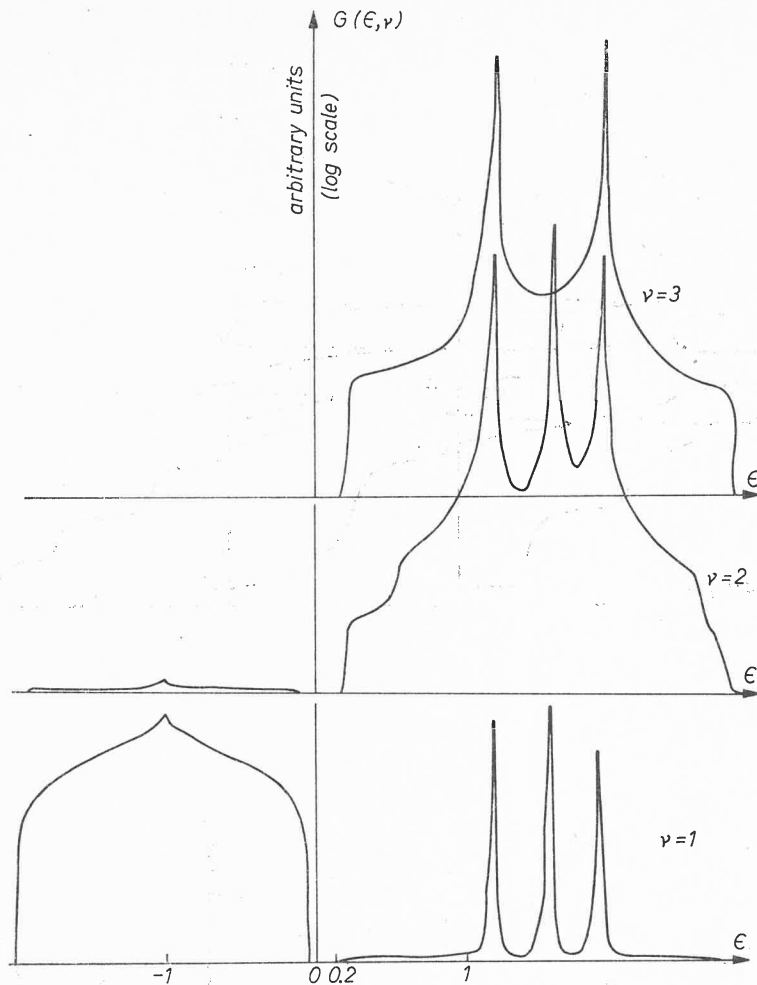


Fig. 3. Spatial distribution $G(\epsilon, \nu)$ of the density of states for $n = 5$ and $K = 10$

We would like to remind here again that 4) the spatial distribution of the density of states satisfies the relation

$$G(\epsilon, \nu) = G(\epsilon, n + 1 - \nu), \quad (27)$$

if symmetric boundary conditions for $T_{\nu r}$ [6] are taken into account.

4. Certain application of the spatial distribution of density of states

We shall apply the obtained spatial distribution of the density of states in the sense of formulae (2) and (22) to a certain problem connected with the electron density distribution at the surfaces of thin films. Our results are purely qualitative since we would like

to stress that the properties of the density of states distribution obtained here are sufficient to allow us to interpret some experimental facts from the physical point of view.

We consider a two-band model with the relative energy gap $\varepsilon_0^2 - \varepsilon_0^1 = \varepsilon_0 > 0$ where $\varepsilon_0^1 = 0$ is the reference level of the energy scale. The surface parameters are $K^1 \approx 1$, $K^2 \gg 1$. A total spatial distribution of the density of states is given by the formula $G(E, \nu) = G_1(E, \nu) + G_2(E, \nu)$. We are now interested in obtaining the form of the distribution of electrons in surface layers and within a film. Thus, at the basis of (25) we can see that the energy intervals in which the electron energies are localized are of the following forms:

a) within a film

$$\left(0, 2 + \cos^2 \frac{\pi}{2n}\right) \quad \text{and} \quad \left(\varepsilon_0, \varepsilon_0 + 2 + \cos^2 \frac{\pi}{2(n-1)}\right) \quad (28)$$

b) in surface layers

$$\left(0, 2 + \cos^2 \frac{\pi}{2n}\right) \quad \text{and} \quad \left(\varepsilon_0 - \frac{1}{4}K + \frac{1}{2} - \frac{1}{4K}, \varepsilon_0 - \frac{1}{4}K + \frac{5}{2} - \frac{1}{4K}\right). \quad (29)$$

Thus we see, according to (28) and (29) that for properly chosen ε_0 and K it may occur that within a film the bands are separated while in surface films they are situated within one interval of energy. Hence the electrons in surface states are subject to quantum rules valid for two bands simultaneously since, filling the levels of these bands they cannot have arbitrary oriented spins. It may thus occur, the conditions being properly chosen, that electrons in surface states mainly localized in surface layers have spins fully compensated while electrons in volume states, the probability of whose existence at the surfaces is very small, may have spins of parallel directions.

The discussed case explains in a simple way the existence of magnetization inside a film and its absence in surface layers. This phenomenon has been explained by means of the same physical principle but along a different procedure [7]. The fact of ascertaining this well known conclusion only shows the effectiveness of the presented method, which, in a similar way, may be used in many problems of thin films. The possibility of effective application of properties of the spatial distribution of density of states proves the usefulness of introducing this distribution.

5. Final physical conclusions

The density of states is a function of the film thickness, of the position of a layer in the film and, of the surface anisotropy. At the same time the shape of this function determines the dependence of physical properties on the factors mentioned above.

The spatial distribution of density of states indicates the different character of oscillations for different layers.

The surface anisotropy $K \leq 1$ causes the shift to the beginning of the density curve from $\varepsilon = 0$ to $\varepsilon = \varepsilon_{\min} \neq 0$. This shift removes the divergence in formulae describing

physical properties of thin films. Sufficiently strong surface anisotropy $K > 1$ leads to the appearance of two separate subbands; one of them is called the surface subband.

If the film thickness increases the function $G(\varepsilon)$ behaves in the following way: $G(\varepsilon)$ for $\varepsilon = \varepsilon_{\min}$ and $\varepsilon = \varepsilon_{\max}$ decreases from $(\pi E^{\alpha\lambda})^{-1}$ to 0; $G(\varepsilon)$ in the whole interval of ε becomes more and more oscillating. The interval of ε , in which $G(\varepsilon)$ differs from zero, increases from $\varepsilon = 2$ to $\varepsilon = 3$.

The shape of the function $G(\varepsilon)$ depends on the approximation method used for obtaining the energy spectrum. In this sense, the different approximation methods, even if the physical assumptions are the same, will lead to different results being the basis of the physical interpretation of phenomena. For this reason, not only assumptions due to the physical mechanism and experimental data but also the formal procedure must be taken into account to verify possible conclusions.

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