THE ELECTRONIC SPECTRUM OF COPPER NEAR THE FERMI SURFACE

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Abstract

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THE ELECTRONIC SPECTRUM OF COPPER NEAR THE FERMI SURFACE

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Despite the fact that many works exist on the calculation of electronic spectra of metals, there is still no detailed comparison of the results of an *ab initio* calculation (without any fitting parameters) of the spectrum of any substance with the entire body of available experimental data. This is explained above all by the enormous volume of computations required. As an example we may cite work ([1]), in which an attempt was made to carry out such a comparison for copper.

Many difficulties can be avoided if, on the basis of the results of an accurate calculation, one obtains an analytical description of the electron dispersion law near the Fermi surface. Such a possibility is indicated, in particular, by attempts at an analytical description of the geometry of the Fermi surface of noble metals on the basis of data on the de Haas–van Alphen effect ([2]).

The starting point of our consideration is the possibility of representing the dispersion law near the Fermi surface in the form of a Fourier series

$$\varepsilon(\mathbf{k}) = c_0 + \sum_{n=1}^{\infty} c_n \varphi_n(\mathbf{k}), \tag{1}$$

where c_n are real numerical coefficients,

$$\varphi_n(\mathbf{k}) = \sum_{t=1}^{t_n} \exp[i\mathbf{k}\mathbf{R}_n^{(t)}] \tag{2}$$

and the summation in (2) is over all vectors of the star of the vector $\mathbf{R}_n$. The unknown coefficients of expansion (1) were determined with the aid of the calculated data of work ([3]).

We restricted ourselves in (1) to the first five terms and required that the dispersion law be satisfied as accurately as possible at 11 points $\mathbf{k}_\mu$ of the Brillouin zone with energies ε_μ close to the Fermi energy ε_F. (According to ([3]), $\varepsilon_F = 0.555$

rydberg; ε_μ were taken in the interval 0.500—0.555 rydberg.) The coefficients c_n were determined by the least-squares method and proved to be equal (in rydbergs) to $c_0 = 0.521461$, $c_1 = -0.090437$, $c_2 = -0.000165$, $c_3 = 0.035188$, $c_4 = -0.001469$, while the maximum deviation of $\varepsilon(\mathbf{k}_\mu)$ from ε_μ was less than 0.004 rydberg.

Next, from the formula

$$N(E) = 2\int_{\varepsilon(\mathbf{k})\leq E} d\mathbf{k}/\Omega, \tag{3}$$

where Ω is the volume of the Brillouin zone, the integrated density of states as a function of energy near the Fermi energy was calculated. For a monovalent substance this quantity at $E = \varepsilon_F$ should be equal to unity. The value 1.000 ± 0.001 was obtained at $E = 0.554$ rydberg, which agrees with the value of ε_F indicated in ([3]).

The calculations carried out above allow one to conclude that the analytic expression obtained for the dispersion law has sufficient accuracy.

The next stage of the calculation consisted in determining various characteristics directly related to the dispersion law.

First of all, the characteristic quasimomenta k_F, the areas of the extremal sections S_F, and the cyclotron effective masses m_c were calculated.

Table 1

	Calculation	Work (1)	Experiment	Source
k[100]	1.055 ± 0.005	1.0530	1.06	(7)
k[110]	0.939 ± 0.005	0.9544	0.963	(7)
k_n	0.228 ± 0.005	0.1808	0.195 ± 0.011	(*)
S_b[100]	0.965 ± 0.005	0.9748	0.9810 ± 0.010	(8)
S_b[111]	0.943 ± 0.005		0.9509 ± 0.010	(8)
$S_{d.b}$[110]	0.404 ± 0.005	0.4095	0.4112 ± 0.005	(8)
m_b^*[100]	1.34 ± 0.01	1.22	1.37	(9)
m_b^*[111]	1.44 ± 0.01		1.36	(10)
$m_{d.b}^*$[110]	1.43 ± 0.01	1.12	1.12	(9)
m_{op}	1.47 ± 0.05		1.42 ± 0.05	(11)
m_{th}	1.50 ± 0.05	1.25	1.38	(12)

All the quantities listed are measured in the presence of an external magnetic field, i.e., under conditions in which the electrons move along orbits whose planes are perpendicular to some specified direction $\mathbf{n}$. This makes it possible to use the following system of ordinary differential equations for their calculation:

$$\frac{dk_\perp(\alpha)}{d\alpha} = k_\perp(\alpha) f(\alpha), \qquad \frac{dS(\alpha)}{d\alpha} = \frac{1}{2}\,[k_\perp(\alpha)]^2,$$

$$\frac{dm^*(\alpha)}{d\alpha} = \frac{1}{\pi}\, k_\perp(\alpha) \left[\sqrt{1 + f^2(\alpha)}/V_\perp\right]. \tag{4}$$

Here $k_\perp(\alpha)$ is the modulus of the component, perpendicular to $\mathbf{n}$, of the radius vector of the electron orbit relative to its center; α is the angle measured from some direction $\mathbf{m}$ (perpendicular to $\mathbf{n}$) and determining the position of a point on the orbit. The function $f(\alpha)$ is given by the equality

$$f(\alpha) = \frac{(\mathbf{V}\cdot\mathbf{m})\sin\alpha + (\mathbf{V}[\mathbf{m}\times\mathbf{n}])\cos\alpha}{(\mathbf{V}\cdot\mathbf{m})\cos\alpha - (\mathbf{V}[\mathbf{m}\times\mathbf{n}])\sin\alpha}, \tag{5}$$

where $\mathbf{V}$ is the electron velocity on the Fermi surface. Finally,

$$V_\perp = \sqrt{(\mathbf{V}\cdot\mathbf{V}) - (\mathbf{V}\cdot\mathbf{n})}. \tag{6}$$

The quantities $S(\alpha)$ and $m^*(\alpha)$ at $\alpha = 2\pi$ are equal to the area of the extremal section corresponding to the orbit under consideration and to the cyclotron mass of the electron on this orbit.

The initial conditions for system (4) have the form

$$k_\perp(0) = k_0, \qquad S(0) = 0, \qquad m^*(0) = 0, \tag{7}$$

where k_0 itself is determined from the transcendental equation

$$\varepsilon(\mathbf{k}) = \varepsilon_F \tag{8}$$

by the bisection method.

Calculations were carried out for a number of orbits with different directions of the magnetic field. Table 1 gives the Fermi momenta in the directions [100] and [110], the areas of the extremal sections and cyclotron masses for magnetic-field directions [100] and [111] for the "belly," the radius of the "neck," the area of the extremal section and the cyclotron mass for the field direction [110] for the "dog' s bone." All data are expressed relative to the corresponding quantities for free electrons.

In addition, the inverse optical effective mass and the thermal effective mass associated with the density of states on the Fermi surface were calculated. The optical effective mass was calculated by two formulas

$$m_{\text{op}}^{-1} = \frac{1}{3\Omega}\int_{\varepsilon(\mathbf{k})<\varepsilon_F} \Delta\varepsilon(\mathbf{k})\,d\mathbf{k} = \frac{1}{3\Omega}\left[\frac{d}{dE}\int_{\varepsilon(\mathbf{k})<E} |\nabla\varepsilon(\mathbf{k})|^2\,d\mathbf{k}\right]_{E=\varepsilon_F}, \quad (9)$$

which made it possible to estimate the total error of the calculations more reliably. The thermal effective mass was calculated from the formula

$$m_{th} = \frac{2}{3}\left(\frac{3}{8\pi}\Omega\right)^{2/3}\left[\frac{dN(E)}{dE}\right]_{E=\varepsilon_F}. \quad (10)$$

The quantities obtained are also given in Table 1. The same table gives the most recent experimental data and the calculated data of Ref. (1), where, in order to achieve better agreement with experiment, the contribution of the exchange energy to the crystal potential was varied.

Integration of the system of differential equations (4) was carried out by the Adams method (4). The volume integrals (3) and (9) were evaluated by the Monte Carlo method (5) using 800,000 points in the Brillouin zone.

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REFERENCES

[1] H. L. Davis, J. S. Faulkner, H. W. Joy, Phys. Rev., **167**, 601 (1968).
[2] D. J. Roaf, Phil. Trans. Roy. Soc., **A255**, 135 (1962).
[3] G. A. Burdick, Phys. Rev., **129**, 138 (1963).
[4] I. S. Berezin, N. P. Zhidkov, *Methods of Computation*, **2**, Moscow, 1962.
[5] N. P. Buslenko et al., *Method of Statistical Trials (Monte Carlo)*, Moscow, 1961.
[6] H. V. Bohm, V. J. Easterling, Phys. Rev., **128**, 1021 (1962).
[7] G. N. Kamm, Bull. Am. Phys. Soc., **11**, 446 (1966).
[8] W. J. O' Sullivan, W. J. E. Schirber, Phys. Rev., **181**, 1367 (1969).
[9] J. F. Koch, R. A. Stradling, A. F. Kip, Phys. Rev., **133**, 1240 (1964).
[10] D. A. Smith, Proc. Roy. Soc., **A296**, 476 (1967).
[11] H. Ehrenreich, H. R. Philipp, Phys. Rev., **128**, 1622 (1962).
[12] D. L. Martin, Phys. Rev., **170**, 650 (1968).

Note: Figure translations are in progress. See original paper for figures.