

phys. stat. sol., (b) 164. 179 (1991)

Subject classification: 71.10

Department of Physics, Ural Polytechnical Institute, Sverdlovsk¹⁾

Interpolation of the One-Electron Energies Using Theoretical-Numerical Nets

By

A. G. KANALIN and L. P. МОКХРАЧЕВА

The method of global Fourier-series approximation of the one-electron energies $\varepsilon(\mathbf{k})$ in the Brillouin zone is considered. To calculate the Fourier series expansions of the $\varepsilon(\mathbf{k})$ -functions optimal for trigonometric polynomials theoretical-numerical nets are used. Convergence and accuracy of the approximation is investigated using one- and two-band models of the $\varepsilon(\mathbf{k})$ -dependence. It is shown that the method described is more accurate than piecewise linear interpolation in the volumes of elementary tetrahedral, generated in regular nets, and is comparable to piecewise quadratic interpolation.

Рассматривается метод глобальной аппроксимации $0,1$ нэлектронных энергий $\varepsilon(\mathbf{k})$ конечной суммой ряда Фурье в 3 о Н е Бриллюэна. Для вычисления Фурье-разложений функций $\varepsilon(\mathbf{k})$ используются теоретико-числовые сетки, оптимальные для тригонометрических полиномов. Сходимость и точность аппроксимации исследуется на примере одно- и двух-зонных модельных зависимостей $\varepsilon(\mathbf{k})$. Показано, что описанный метод обеспечивает более высокую точность, чем кусочно-линейная интерполяция в объемах элементарных тетраэдров, построенных в равномерной сетке, и сопоставим с кусочно-квадратичной интерполяцией.

1. Introduction

Various important characteristics of a crystalline solid (effective electron mass and velocity, electron-phonon coupling constant and others) are defined by means of some integrals or derivatives on the Fermi surface. As a result of a band structure calculation and a subsequent piecewise linear or quadratic interpolation the Fermi surface (FS) can be represented as a set of planes or second-order surfaces, located in elementary volumes formed by Brillouin zone (BZ) dissection. This representation of FS is very inconvenient for studying the features of its topology and calculating the quantities mentioned. To exclude this inconvenience the parametrization based on Fourier series expansion of the matrix elements of the Hamiltonian or the one-electron energies themselves is often preferable [1 to 3]. These expansions are not piecewise (local) but global approximations of the functions in the BZ. Fourier coefficients in both schemes are estimated by least-squares fit and the results obtained are extremely sensitive to the choice of the sample points in the BZ and on its surface [4]. It requires to carry out a detailed analysis of the global approximation of one-electron energies $\varepsilon(\mathbf{k})$ in the Brillouin zone.

In the present work a global Fourier series approximation of the functions $\varepsilon(\mathbf{k})$ is investigated using Korobov's theoretical-numerical nets [5] optimal for trigonometric polynomials. The efficiency of Korobov's method for the calculation of multi-dimensional Fourier expansions [5] allows to regard it as suitable for the interpolation of the one-electron energies $\varepsilon(\mathbf{k})$.

¹⁾ SU-620002 Sverdlovsk, USSR

2. Method

Owing to the symmetry of the $\varepsilon(\mathbf{k})$ function its Fourier series representation in BZ is defined in the following way:

$$\varepsilon(\mathbf{k}) = C' + \sum_{l=1}^m C_l' \sum_{j=1}^{n_l} \cos(\mathbf{k} \cdot \mathbf{R}_{lj}) \tag{1}$$

Here the external sum runs over the coordination spheres of the direct lattice, subscript j numerates lattice sites $\mathbf{R}_{lj}, j = 1, \dots, n_l$ within a fixed sphere, and $C'(l_j) = C_l, j = 1, \dots, n_l$. The Fourier coefficients $C', C(\mathbf{R}_{lj})$ are estimated by

$$CO = \Omega^{-1} \int_{\Omega} d\mathbf{k} \varepsilon(\mathbf{k}), \quad C(\mathbf{R}_{lj}) = \Omega^{-1} \int_{\Omega} d\mathbf{k} c(k) \cos(\mathbf{k} \cdot \mathbf{R}_{lj}), \tag{2}$$

where Ω is the BZ volume.

In terms of Korobov's method a triple integral is calculated by the numerical integration formula

$$\int_0^1 dx \int_0^1 dy \int_0^1 dz f(x, y, z) = \frac{1}{2P} \sum_{k=1}^P [f(x_k, y_k, z_k) + f(x'_k, y'_k, z'_k)], \tag{3}$$

where $f(x, y, z)$ is periodic in the unit cube. Here

$$M_k = (x_k, y_k, z_k) = \left(\left\{ \frac{\alpha_1 k}{P} \right\}, \left\{ \frac{\alpha_2 k}{P} \right\}, \left\{ \frac{\alpha_3 k}{P} \right\} \right), \tag{4}$$

$$M'_k = (x'_k, y'_k, z'_k) = \left(\left\{ \frac{(2k-1)\alpha_1}{2P} \right\}, \left\{ \frac{(2k-1)\alpha_2}{2P} \right\}, \left\{ \frac{(2k-1)\alpha_3}{2P} \right\} \right)$$

are the sites of parallelepipedal nets, P is a prime number, $\{t\}$ is the fractional part of t , and $\alpha_1, \alpha_2, \alpha_3$ are optimal coefficients (integer numbers) to be determined for any P .

If the function $f(x, y, z)$ is a harmonic polynomial of finite order, then the cubature formula (3) becomes exact for an appropriate number of sites. This fact is confirmed by the data of Table 1, where the number of Fourier coefficients of functions

$$f_m^\alpha(\mathbf{k}) = 1 + \sum_{l=1}^m C_l^\alpha \sum_{j=1}^{n_l} \cos(\mathbf{k} \cdot \mathbf{R}_{lj})$$

exactly calculated by this method is given. Here $C_l^\alpha = \exp(-\alpha|\mathbf{R}_{lj}|), \alpha = 1, \dots, 6$ and \mathbf{R}_{lj}, n_l correspond to the simple cubic lattice ($a = 1$).

Table 1
Number of Fourier coefficients of functions $H(\sim), \dots, f_{12}^\alpha(\mathbf{k})$ exactly calculated by Korobov's method

number of sites	function												
	f_1^α	f_2^α	f_3^α	f_4^α	f_5^α	f_6^α	f_7^α	f_8^α	f_9^α	f_{10}^α	f_{11}^α	f_{12}^α	
24	25			15		11	11	1	0	0	0	0	0
54	33	12		12		3	3	3	3	3	2	2	1
102	31	24	22	22	16	16	16	11	11	9	8	8	6
152	37*)	37*)	37*)	37*)	37*)	37*)	37*)	18	18	14	14	7	7
308	37*)	37*)	37*)	37*)	37*)	37*)	37*)	37*)	25	14	14	14	12
524	37*)	37*)	37*)	37*)	37*)	37*)	37*)	37*)	37*)	25	25	25	14

*) Coefficients C_l^α were calculated only for 36 coordination spheres.

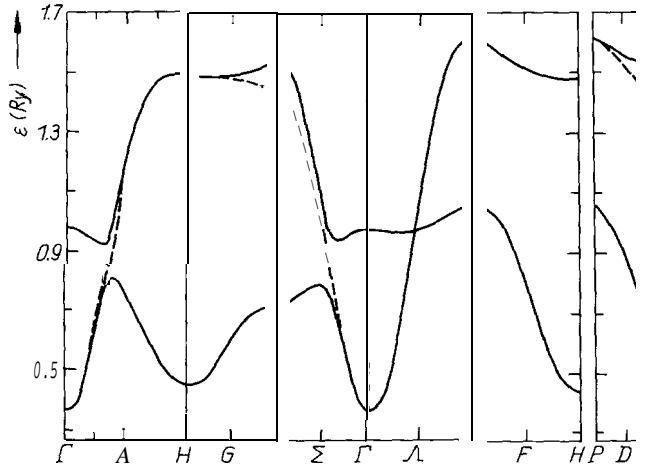


Fig. 1. Structure of the model bands in symmetry directions of BZ. - - - One-band spectrum, — two-band spectrum

To demonstrate the possibilities of the method described, one-band (s-type) and two-band (s-, d-types) models of a transition metal spectrum were considered. The energy bands were calculated in terms of the Slater-Koster scheme [6] with the parameters taken from [7] for three coordination spheres of b.c.c. niobium. The structure of the bands in symmetry directions of the BZ is presented in Fig. 1. In the case of a two-band spectrum there is a hybridization of bands in A- and Z-directions and a band crossing in A-direction. The latter leads to arising of zigzags in the $s(k)$ -dependence since the bands were separated in an ordinary way, i.e. according to energy increase.

Fourier coefficients of the model functions $\varepsilon(\mathbf{k})$ were calculated over the cubic domain $-2\pi/a \leq k_x, k_y, k_z \leq +2\pi/a$ by the formula

$$\begin{aligned}
 C(\mathbf{R}_{ij}) &= \frac{a^3}{(4\pi)^3} \int_{-2\pi/a}^{2\pi/a} dk_x \int_{-2\pi/a}^{2\pi/a} dk_y \int_{-2\pi/a}^{2\pi/a} dk_z \varepsilon(k_x, k_y, k_z) \\
 &\quad \times \cos(a[k_x X_{ij} + k_y Y_{ij} + k_z Z_{ij}]) \\
 &= \int_0^1 dx \int_0^1 dy \int_0^1 dz \varepsilon(2\pi[2x-1]/a, 2\pi(2y-1)/a, 2\pi(2z-1)/a) \\
 &\quad \times \cos(2\pi[(2x-1)X_{ij} + (2y-1)Y_{ij} + (2z-1)Z_{ij}]), \quad (5)
 \end{aligned}$$

where $a(X_{ij}, Y_{ij}, Z_{ij})$ are rectangular coordinates of b.c.c. lattice vectors, a is the lattice constant. Three-dimensional integral over the unit cube was calculated by Korobov's method, optimal coefficients $\alpha_1, \alpha_2, \alpha_3$ have been taken from the tables of [5]. Coefficients $C(\mathbf{R}_{ij})$ obtained by (5) do not yield symmetry requirements. Thus their averages C_l over coordination spheres were considered.

Table 2
Accuracy of global approximation of the model spectra by Korobov's method (in 10^4 Ry)

number of sites	one-band model			two-band model					
	s-band			band number 1			band number 2		
	m	Δm	Δ_s	m	Δm	Δ_s	m	Δm	Δ_s
102	3	0.0	0.0	10	430	84	10	560	130
152	3	0.0	0.0	18	260	60	22	310	84
308	3	0.0	0.0	24	140	36	26	160	59
524	3	0.0	0.0	31	86	19	33	95	28

3. Results and Discussion

Results of studying the accuracy of the global interpolation of the model functions by Korobov's method are listed in Table 2. These data include numbers of coordination spheres (m) kept in the sum (1) for the best accuracy and maximum (Δ_m) and root mean square (r.m.s.) (Δ_s) errors obtained in this case for different nets. Errors were calculated using 150 points of the binary-rational net [8], distributed in the cube $0 \leq k_x, k_y, k_z \leq 2\pi/a$. The arrangement of the binary-rational net sites differs from that of both Korobov's and used regular nets and therefore is more suitable to analyse the accuracy obtained. Data of Table 2 show that Korobov's nets having 308 and more sites provide an acceptable accuracy (5×10^{-3} Ry).

To approximate $\varepsilon(\mathbf{k})$ functions in regular meshes local linear or quadratic interpolations are commonly used. It is of interest to compare them with Korobov's method of interpolation. Maximum and r.m.s. errors of linear and quadratic interpolations of the model bands are presented in Table 3. Both spectra were calculated in regular nets having 140, 285, and 506 points in the irreducible part of b.c.c. Brillouin zone and the errors were estimated for the binary-rational net, taking into account the symmetry of $\varepsilon(\mathbf{k})$.

Data of Table 3 show that if the numbers of sites are approximately equal, then the accuracy of global interpolation by Korobov's method is slightly better than the piecewise linear one and is comparable to the piecewise quadratic one.

Table 3
Accuracy of piecewise linear and piecewise quadratic interpolations of the model spectra (in 10^{-4} Ry)

number of sites	one-band model				two-band model							
	s-type band				band number 1				band number 2			
	linear		quadratic		linear		quadratic		linear		quadratic	
	Δm	Δ_s	Δm	Δ_s	Δm	Δ_s	Δm	Δ_s	Δm	Δ_s	Δm	Δ_s
140	181	58	49	15	332	76	192	32	281	60	221	36
285	76	22	19	4	240	44	149	21	20	36	128	19
506	60	17	9	2	148	31	74	9	131	26	59	10

4. Conclusion

The presented results make it possible to propose Korobov's method of interpolation of the one-electron energies $\varepsilon(\mathbf{k})$ using theoretical-numerical nets together with widely applying local interpolation methods.

References

- [1] K. K. CHIA, A. P. CRACNELL, and R. J. WALKER, J. Phys. F 4, 1121 (1974).
- [2] J. B. KETERSON, F. M. MUELLER, and L. R. WINDMILLER, Phys. Rev. 186,656 (1969).
- [3] L. L. BOYER, Phys. Rev. B 19,2824 (1979).
- [4] W. R. FEHLER and S. H. VOSKO, Canad. J. Phys. 55, 2041 (1977),
- [5] N. M. KOROBOV, Teoretiko-chislovye metody v priblizhonnym analize, Nauka, Moskva 1963.
- [6] J. C. SLATER and G. F. KOSTER, Phys. Rev, 94,1498 (1954).
- [7] L. L. BOYER, D. A. PAPACONSTANTOPOULOS, and B. M. KLEIN, Phys. Rev, B 15, 3685 (1977).
- [8] I. M. SOBOL, Mnogomernye kwadraturnye formuly i funktsii Haara, Izd. Nauka, Moskva 1969,

(Received May 3, 1990)