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Mean-Value Point in the Brillouin Zone

A. Baldereschi
Bell Laboratories, Murray Hill, New Jersey 07974
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A new special point in the Brillouin zone is introduced. It is defined as the point such that the value which any given periodic function of wave vector assumes at this point is an excellent approximation to the average value of the same function throughout the Brillouin zone. This special point is termed the "mean-value point," and is dictated by the crystal symmetry. The coordinates of the mean-value point for cubic lattices are explicitly given.

Different kinds of special points in the Brillouin zone have been introduced since the existence of these zones was noticed in 1928.[1] After the work by Bouckaert *et al.*[2] on the symmetry properties of wave functions in crystals, the concept of high-symmetry points in the zone gained large popularity and is still one of the basic concepts in solid-state physics. Later, when deep interest arose in the thermodynamical and optical properties of solids, the concept of phonon (or electron) density of states became relevant and critical points were introduced by Van Hove[3] and studied in more detail by Phillips.[4]

Often, one is not interested in studying the properties of a single quasiparticle which belongs to a particular point of the Brillouin zone, but rather in studying the properties of all the quasiparticles of a certain kind which are present in the crystal in order to obtain crystal properties. In these studies one is usually faced with the problem of averaging quasiparticle properties (i.e., averaging over the Brillouin zone). It is well known that carrying out such averages is difficult and time consuming. It is useful in this respect to introduce a new special point in the Brillouin zone: the mean-value point.[5] Qualitatively, it is defined as the point such that the value which any given periodic function of wave vector assumes at this point is an excellent approximation to the average value of the same function throughout the Brillouin zone. It will be shown that the symmetry properties of crystals provide a way to uniquely define this point for any given lattice. The coordinates of the mean-value point in cubic lattices will be given together with two examples from semiconductor physics which will show how useful this new point can be.

While studying crystal properties, one often encounters Brillouin-zone integrals such as

$$I=\int_{\mathrm{BZ}} f(\vec{k})\,d^3k=\frac{(2\pi)^3}{\Omega}\,\bar{f}\,, \tag{1}$$

where the integrand $f(\vec{k})$ is a periodic function of wave vector and Ω is the primitive cell volume. As shown in (1), this integral can be expressed as the Brillouin-zone volume times the average value of

$f(\vec{k})$. Furthermore, without loss of generality, we can assume that $f(\vec{k})$ belongs to the completely symmetric irreducible representation of the crystal point group (this representation is usually denoted Γ_1), because, if this is not the case, we can decompose $f(\vec{k})$ into irreducible representations and it is easily demonstrated that only the Γ_1 representation contributes to integral (1).

Using the symmetry properties of $f(\vec{k})$ (Γ_1 symmetry and periodicity in $\vec{k}$ space), we can decompose it into symmetrized linear combinations of plane waves[6] with Γ_1 symmetry, as follows:

$$f(\vec{k}) = \sum_{i=0}^{\infty} a_i G_i^{(\Gamma_1)}(\vec{k}), \tag{2}$$

where $G_0^{(\Gamma_1)}(\vec{k}) \equiv 1$ and the summation index i runs over the stars of equivalent lattice vectors. Note that the functions $G_i^{(\Gamma_1)}(\vec{k})$ which appear in (2) depend on the lattice structure but not on the particular function $f(\vec{k})$. On the right-hand side of (2), only the coefficients a_i depend on the particular function f. Inserting (2) into (1), we obtain

$$I = \frac{(2\pi)^3}{\Omega} \bar{f} = \frac{(2\pi)^3}{\Omega} a_0, \tag{3}$$

since it is easily demonstrated that all terms in (2) but the first ($i = 0$) give vanishing contribution to the integral (1). We see, therefore, that the average value $\bar{f}$ is nothing but the first term in expansion (2). We must find a way to evaluate this term.

In view of Eqs. (2) and (3) one might be tempted to define the mean-value point as the point $\vec{k}^*$ such that $G_i^{(\Gamma_1)}(\vec{k}^*) = 0$ for any positive integer i. In fact, if this can be done, then

$$f(\vec{k}^*) \equiv a_0 \equiv \bar{f}. \tag{4}$$

This is asking too much, of course. We have to be satisfied if we can find a point $\vec{k}^*$ for which the first equility in (4) is not strictly valid but is a reasonably good approximation. Since expansions similar to (2) are *generally* rapidly convergent, we define the mean-value point as the particular point $\vec{k}^*$ for which

$$G_i^{(\Gamma_1)}(\vec{k}^*) = 0 \quad (i = 1, 2, \ldots, n), \tag{5}$$

with n being the largest integer possible. The value of n is limited by the compatibility between different equations in system (5). In general, we expect $n = 3$, since the unknown variables in (5) are the three coordinates of $\vec{k}^*$. It might happen that system (5) has more than one solution and the system obtained by adding to (5) the $(n+1)$th equation $G_{n+1}^{(\Gamma_1)}(\vec{k}^*) = 0$ has no solutions at all. In this case we define the mean-value point as that particular solution of system (5) which minimizes the absolute value of the next term $|G_{n+1}^{(\Gamma_1)}(\vec{k})|$.

We can now determine the coordinates of the mean-value point for cubic lattices.

Simple cubic. In this case $n = 3$ and system (5) is

$$\begin{aligned} X + Y + Z &= 0, \\ XY + YZ + ZX &= 0, \\ XYZ &= 0, \end{aligned} \tag{6}$$

where $X = \cos(2\pi k_x)$ and similar definitions hold for Y and Z. System (6) uniquely defines the mean-value point $\vec{k}^* \equiv (\pi/a)(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, which lies halfway between the high-symmetry points Γ and R of the Brillouin zone.

Face-centered cubic. In this case $n = 2$. The resulting system has an infinite number of solutions, and, as already explained, we uniquely define the mean-value point as the one which minimizes the next term in expansion (2). The mean-value-point coordinates are[5] $\vec{k}^* \equiv (2\pi/a)(0.6223, 0.2953, 0)$.

Body-centered cubic. In this case, again we have $n = 2$ and minimization of the $i = 3$ term in expansion (2) is necessary. The mean-value point is $\vec{k}^* = (2\pi/a)(\frac{1}{6}, \frac{1}{6}, \frac{1}{2})$. The location of the mean-value point in the Brillouin zone of cubic lattices is shown in Fig. 1.

The mean-value point $\vec{k}^*$ that we have defined is really significant only if $f(\vec{k}^*)$ approximates closely the average value $\bar{f}$. We can say in general that the approximation is good if expansion (2) can be truncated after the term $i = 3$. This is generally the case, because, using tight-binding language, such truncation in expansion (2) means including interactions up through the third neighbors. How-

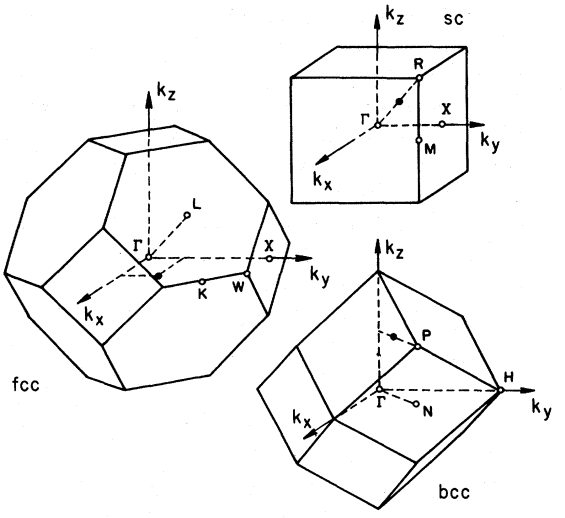

FIG. 1. Mean-value point in the Brillouin zone of different cubic lattices. Solid circles are the mean-value points, whereas open circles indicate high-symmetry points.

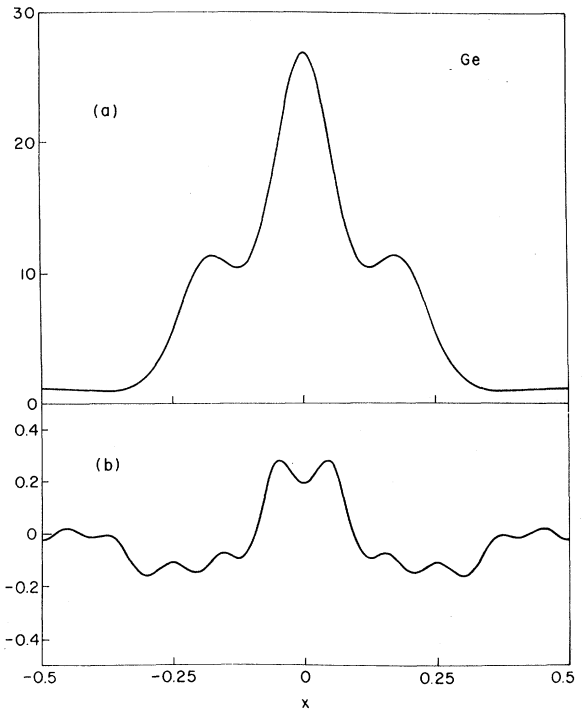

FIG. 2. (a) Valence charge density in Ge along the bond direction as obtained using the mean-value-point method. The origin is halfway between the two atoms and units are electrons per primitive cell. (b) Difference between the valence charge densities in Ge as obtained by Walter and Cohen (Ref. 7) and by the mean-value-point method. Note the change in scale between (a) and (b).

ever, special cases might happen in which $f(\vec{k})$ varies so strongly in the Brillouin zone that a large number of terms have to be retained in expansion (2) and the mean-value point becomes meaningless. We believe that these special cases, though not impossible, occur only rarely.

We now present two examples from semiconductor physics in order to give convincing evidence of the elegance, power, and usefulness of the mean-value-point technique in making averages over the Brillouin zone. Both examples make use of the mean-value point defined for face-centered-cubic lattices.

The first example is the calculation of the valence-electron charge density in semiconductors. We define

$$f(\vec{k}) = e\sum_v |\psi_v(\vec{k}, \vec{r})|^2, \tag{7}$$

where the band index v runs over all valence bands and $\psi_v(\vec{k}, \vec{r})$ are Bloch functions. Valence-electron charge densities for a few semiconductors have been calculated by Walter and Cohen,[7] using a grid of 3360 sample points in the Brillouin zone. Using the same wave functions, we have calculated the valence-electron charge density in Ge with the mean-value-point technique. The result along the (1, 1, 1) direction is shown in the upper portion of Fig. 2. It was our intention to compare our result with that of Walter and Cohen in the same graph, but since the two results agree to within 1%, differences between them could hardly be appreciated. Therefore, we have represented in the lower portion of the figure, *using a magnified scale*, the difference between the two results.

TABLE I. Average energy per electron in the valence bands. Different approximations of the Kleinman–Phillips (KP) method are compared with the mean-value-point method. The zero of energy is at the top of the valence bands (Γ point) and energy units are eV.

	KP			Mean-value
	8 points	64 points	512 points	point
Ge	−4.76	−5.07	−5.09	−5.18
GaAs	−4.66	−4.94	−4.95	−5.01
ZnSe	−4.59	−4.80	−4.80	−4.85

The equilibrium lattice constant and the bulk modulus of crystals may be calculated from the total crystal energy as a function of lattice constant. One of the terms which enters the total crystal energy is the sum of the one-electron energies over all occupied states. We define

$$f(\vec{k}) = \sum_v E_v(\vec{k}), \tag{8}$$

where the band index v runs over the valence bands and $E_v(\vec{k})$ are the one-electron energies. We use the pseudopotential method to compute $E_v(\vec{k})$ for Ge, GaAs, and ZnSe. We obtain for the sum of the one-electron energies the results shown in Table I. In this case the mean-value-point method is compared with a method due to Kleinman and Phillips,[8] which is based on a procedure for successive approximations.

The above examples serve to demonstrate the accuracy of the mean-value-point technique. One comment on Table I is in order. The Kleinman–Phillips eight-point approximation is inadequate in averaging over the Brillouin zone and this approximation is nothing but the commonly used weighted average on the high-symmetry points Γ, X, and L. When 512 points are used, our mean-value-point method agrees with the Kleinman–Phillips method within 2%.

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Cyclotron Resonance and the Cohen Nonellipsoidal Nonparabolic Model for Bismuth. III. Experimental Results*

Robert J. Dinger† and A. W. Lawson
Department of Physics, University of California, Riverside, California 92502
(Received 11 April 1972; revised manuscript received 7 December 1972)

Complete measurements of the anisotropy of the central-orbit cyclotron effective masses by Azbel'–Kaner cyclotron resonance have been taken at a frequency of 24.03 GHz and a temperature of 1.15 °K for the magnetic field in the three crystallographic planes of Bi. Deviations of up to 10% from ellipsoidal behavior were observed for the electron-effective-mass anisotropies. Except in one instance, the various effective-mass anisotropies give a good fit to the Cohen nonellipsoidal nonparabolic (NENP) model and the fit is clearly superior to the Lax ellipsoidal nonparabolic model fit. The ratio of the Fermi energy to the L-point band-gap energy, E_F/E_g, was determined from fitting the NENP model and found to be 1.5 ± 0.4, in good agreement with other measurements. The fit to the NENP model also indicated that m_2/m_2' is approximately 1, implying that the L-point valence and conduction bands have identical parameters. The cyclotron effective masses agree within 3% with the values obtained by Edel'man and Khaikin, and disagree by as much as 30% with the values obtained by Kao. Quantum oscillations of the microwave surface impedance similar in nature to de Haas–Schubnikov oscillations have also been observed, but periods arising from the large cross-sectional areas could not be detected and no conclusions regarding the NENP model could be made. Magnetoplasma oscillations due to standing Alfvén waves have also been observed. The mass-density values derived from these measurements agree with the values obtained by other investigators. However, the carrier concentration derived from the Alfvén-wave periods differs by nearly 12% with the value derived from the Azbel'–Kaner cyclotron-resonance measurements. This difference may be due to nonellipsoidal effects.

I. INTRODUCTION

In spite of a wealth of experimental measurements on the electron Fermi surface of Bi, the exact shape of the surface is still somewhat uncertain. Two recent papers, for example, are at odds with each other. Herrmann *et al.*,[1] from rf-size-effect measurements, obtain data which supports the Cohen nonellipsoidal nonparabolic (NENP) model[2] of the electron Fermi surface, whereas the magneto-optical results of Maltz and Dresselhaus[3] support the Lax ellipsoidal nonparabolic (ENP) model.[4] In two earlier papers[5,6] (hereafter referred to as I and II, respectively), we analyzed the Azbel'–Kaner cyclotron-resonance (AKCR) data of Edel'man and Khaikin[7] (hereafter, EK) and Kao[8] and, with a few exceptions, found reasonable agreement with the NENP model. The various discrepancies between experiments and the Fermi-surface models for Bi have been reviewed in I and II.

In hopes of clarifying the situation, we undertook further measurements of cyclotron resonance in Bi. At the outset, we were motivated by our ability to observe quantum oscillations (QO) of the microwave surface impedance similar in origin to de Haas–Shubnikov oscillations and magnetoplasma oscillations of the Alfvén-wave type, in addition to cyclotron resonance. All three phenomena were observed during the same liquid-helium run, with no basic change in measurement method required, a circumstance which had the potential to reveal fine deviations of the Fermi surface from ellipsoidality. For example, by forming the ratio of the cyclotron effective mass m^* and the extremal cross-sectional area A_{ext} (the parameter obtained from the QO), the deviations expected for the NENP model are about 20% instead of the 10% or so expected in either m^* or A_{ext} alone. The fact that the phenomena were observable simultaneously meant that errors due to sample handling, misalignment, temperature variations, and the like would not be present, as they might be if data from different investigators were combined.

Unfortunately, in spite of the fact that QO were observable over a large angular range, it turned out that at the crucial angles where the ratio might be expected to show up the deviations, the QO disappeared, apparently because of a lack of sufficient resolution in our apparatus. Hence, our original motivation for undertaking the present set