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Inversion Scheme for Obtaining the Fermi Surface from the de Haas–van Alphen Effect*

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The relationship between the recent inversion scheme of Mueller for obtaining the Fermi surface from de Haas–Van Alphen areas and the older scheme due to Lifshitz and Pogorelov is obtained. It serves as a simple derivation of the latter inversion scheme.

INTRODUCTION

MEASUREMENTS of the de Haas–van Alphen effect yield extremal cross sectional areas of the Fermi surface as cut by a plane perpendicular to the magnetic field. It is a problem of considerable interest to reconstruct the shape of the Fermi surface from such measured areas. If the Fermi surface has a center of symmetry, then at least one of the extremal areas is that on the plane through the center of symmetry; we shall call this the median area. If the Fermi surface has the additional property that any straight line through the center cuts the surface in only two symmetrically disposed points (so that the magnitude of the radius vector from the center to any point on the surface is a single-valued function of direction), in which case, also, a median plane cuts the surface in a simple closed curve, then Lifshitz and Pogorelov[1] (LP) have shown that the Fermi surface is uniquely determined by knowing of the median areas for all directions. In addition, they have given an elegant formula for reconstructing the surface from the median areas, but unfortunately this formula is not useful for practical calculation.

More recently, Mueller[2] has shown how the use of spherical harmonic expansions allows another form of the solution of the inversion problem of reconstructing the Fermi surface from median areas which not only has practical calculational advantages over the method of LP, but represents also a considerable improvement over an earlier employment of spherical harmonics in connection with the same problem by Shoenberg and Stiles.[3] Mueller makes no attempt to duscuss the relation of his result to that of LP. On the other hand, LP derive their result from an integral identity[4] for which no proof is given but which they state is readily verified by direct calculation. We have not been able to construct a simple direct verification of this identity for arbitrary functions defined on a sphere, but Kuerti[5] has supplied us with a proof for functions which can be written as polynomials in sines and cosines of the azimuth and colatitude. The exact class of functions for which the formula of LP is valid is thus not clearly defined.

In the present paper, we establish the connection between the results of Mueller and LP by beginning with the solution of the former and deriving the result of the latter. This establishes the result of LP for those cases where the radius of the Fermi surface as a function of direction can be uniformly approximated by a series of spherical harmonics. The connection between the two forms of the result depends on two identities for the Legendre polynomials which do not seem to be "immediate consequences" of any of the well-known identities satisfied by these polynomials but which can readily be established by induction using the recursion relation and the orthogonality relation for the polynomials. The proofs of these identities are given in the Appendix. The original identity of LP when applied to spherical harmonics yields a further, more recondite, identity for the Legendre polynomials for which no elementary proof has so far been obtained. In a sense, the present paper can be considered a "derivation for experimentalists" of the LP inversion formula.

DERIVATION

We designate the radius of the Fermi surface as measured from its center of symmetry in the direction of the unit vector $\hat{e}$ by $R(\hat{e})$ and define $\rho(\hat{e})$ by

$$\rho(\hat{e})=\pi R^2(\hat{e}). \tag{1}$$

Further, let $\sigma(\hat{\xi})$ be the median cross sectional area of the Fermi surface on the plane perpendicular to the unit vector $\hat{\xi}$. Then

$$\sigma(\hat{\xi})=\frac{1}{2\pi}\oint\delta(\hat{\xi}\cdot\hat{e})\rho(\hat{e})d\hat{e}, \tag{2}$$

where the integration is to be taken over all the directions of the unit vector $\hat{e}$ (over the area of the unit sphere). Mueller proceeds by introducing the spherical

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[1] I. M. Lifshitz and A. V. Pogorelov, Dokl. Akad. Nauk. SSSR **96**, 1143 (1954).

[2] F. M. Mueller, Phys. Rev. **148**, 636 (1966). An application is made in F. M. Mueller and M. G. Priestley, Phys. Rev. **148**, 638 (1966).

[3] D. Shoenberg and P. J. Stiles, Proc. Roy. Soc. (London) **A281**, 62 (1964).

[4] The identity as given in the paper of LP is not quite correct: The conditions $z^2<\lambda^2$ and $z^2<1-\lambda^2$ should be written, respectively, as $z<\lambda$ and $z<(1-\lambda^2)^{1/2}$.

[5] G. Kuerti (private communication). The method consists in an appropriate parametrization of the integrals so that the integrations involved in the identity can be readily carried out for functions of the trignometric form referred to above. We are grateful to Professor Kuerti for informing us of his results.

harmonic expansions of $\sigma(\hat{\xi})$ and $\rho(\hat{\epsilon})$:

$$\sigma(\hat{\xi})=\sum_{lm} \alpha_l^m Y_l^m(\hat{\xi}), \tag{3}$$

$$\rho(\hat{\epsilon})=\sum_{lm} \beta_l^m Y_l^m(\hat{\epsilon}). \tag{4}$$

We shall require the identity for $-1<u<1$,

$$\delta(\hat{\epsilon}\cdot\hat{\xi}-u)=2\pi\sum_{lm} P_l(u)Y_l^{m*}(\hat{\epsilon})Y_l^m(\hat{\xi}), \tag{5}$$

which is the generalization of the same formula for $u=0$ given by Mueller[2] and which can be derived by the same method. By the use of the addition theorem for the spherical harmonics,

$$\sum_m Y_l^{m*}(\hat{\epsilon})Y_l^m(\hat{\xi})=\frac{2l+1}{4\pi}P_l(\hat{\epsilon}\cdot\hat{\xi}); \tag{6}$$

Eq. (5) can also be written as

$$\delta(\hat{\epsilon}\cdot\hat{\xi}-u)=\tfrac{1}{2}\sum_l (2l+1)P_l(\hat{\epsilon}\cdot\hat{\xi})P_l(u), \tag{7}$$

which for $\hat{\epsilon}\cdot\hat{\xi}=0$ takes the form

$$\delta(u)=\tfrac{1}{2}\sum_l (2l+1)P_l(0)P_l(u). \tag{8}$$

Returning now to Eq. (2), substituting the expansions (3) and (4), together with (5) for $u=0$, and using the orthogonality relation for the spherical harmonics one finds with Mueller[2] that

$$\alpha_l^m=P_l(0)\beta_l^m, \tag{9}$$

whence

$$\begin{aligned}\rho(\hat{\epsilon})&=\sum_{lm}{}'\frac{\alpha_l{}^m}{P_l(0)}Y_l^m(\hat{\epsilon})\\&=\sum_{lm}{}'\frac{1}{P_l(0)}\oint\sigma(\hat{\xi})Y_l^{m*}(\hat{\xi})Y_l^m(\hat{\epsilon})d\hat{\xi}\\&=\sum_l{}'\frac{2l+1}{4\pi P_l(0)}\oint\sigma(\hat{\xi})P_l(\hat{\xi}\cdot\hat{\epsilon})d\hat{\xi},\end{aligned} \tag{10}$$

where the prime on the summation indicates that only *even* values of l are to be included.

To continue, we rewrite (10) as

$$\rho(\hat{\epsilon})=\sum_l{}'\frac{2l+1}{2P_l(0)}\int_{-1}^{1}\chi(\hat{\epsilon},u)P_l(u)du, \tag{11}$$

where

$$\chi(\hat{\epsilon},u)=\chi(\hat{\epsilon},-u)=\frac{1}{2\pi}\oint\sigma(\hat{\xi})\delta(\hat{\epsilon}\cdot\hat{\xi}-u)d\hat{\xi}. \tag{12}$$

Then, since, from (8),

$$\chi(\hat{\epsilon},0)=\sum_l{}'\tfrac{1}{2}(2l+1)P_l(0)\int_{-1}^{1}\chi(\hat{\epsilon},u)P_l(u)du, \tag{13}$$

where we have used the fact that χ is an even function of u to limit the summation to even values, we may rewrite (11) as

$$\rho(\hat{\epsilon})=\chi(\hat{\epsilon},0)+\sum_l{}'\tfrac{1}{2}(2l+1)\left[\frac{1}{P_l(0)}-P_l(0)\right]\times\int_{-1}^{1}\chi(\hat{\epsilon},u)P_l(u)du. \tag{14}$$

We now require one of the identities referred to in the Introduction and derived in the Appendix, namely, (A6), to write

$$\rho(\hat{\epsilon})=\chi(\hat{\epsilon},0)+\sum_l\tfrac{1}{2}(2l+1)\int_{-1}^{1}\int_0^1\chi(\hat{\epsilon},u)\times\frac{P_l(v)P_l(u)-P_l(0)P_l(u)}{u^2}dvdu. \tag{15}$$

Here the prime has been removed from the sum since χ is an even function of u and hence the integral vanishes for odd l. Finally, if we set $\hat{\epsilon}\cdot\hat{\xi}=v$ in Eq. (7), we see that the sum on l in (15) yields the result of LP:

$$\begin{aligned}\rho(\hat{\epsilon})&=\chi(\hat{\epsilon},0)+\int_{-1}^{1}\int_0^1\chi(\hat{\epsilon},u)\frac{\delta(v-u)-\delta(u)}{v^2}dvdu\\&=\chi(\hat{\epsilon},0)+\int_0^1\frac{\chi(\hat{\epsilon},v)-\chi(\hat{\epsilon},0)}{v^2}dv.\end{aligned} \tag{16}$$

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APPENDIX

The first identity which we require,

$$\int_0^1\frac{P_l(u)}{u}du=\frac{1}{lP_{l-1}(0)},\quad (l \text{ odd and } \geq 1) \tag{A1}$$

serves only as a lemma for the proof of the second identity (A6). The proof by induction proceeds as follows: From the recurrence relation for the Legendre polynomials

$$(l+2)P_{l+2}(u)-(2l+3)uP_{l+1}(u)+(l+1)P_l(u)=0, \tag{A2}$$

we have

$$\int_0^1\frac{P_{l+2}(u)}{u}du=\frac{2l+3}{l+2}\int_0^1P_{l+1}(u)du-\frac{l+1}{l+2}\int_0^1\frac{P_l(u)}{u}du. \tag{A3}$$

For odd l, the first term on the right can be written as half the integral from -1 to 1; for $l\geq 1$, the resultant integral vanishes by the orthogonality relation for the Legendre polynomials Now if we assume the identity (A1) to be valid for l, we then have

$$\int_0^1 \frac{P_{l+2}(u)}{u}du = -\frac{l+1}{(l+2)lP_{l-1}(0)}. \tag{A4}$$

But from the recursion relation (A2) for $u=0$ it follows that

$$P_{l+1}(0) = -\frac{l}{l+1}P_{l-1}(0), \tag{A5}$$

which substituted into (A4) yields (A1) for l replaced by $l+2$. Since (A1) clearly holds for $l=1$, the proof by induction is complete.

The second identity is

$$\int_0^1 \frac{P_l(u)-P_l(0)}{u^2}du = P_l(0) - \frac{1}{P_l(0)} \qquad (l \text{ even and } \geq 0). \tag{A6}$$

From the recurrence relation one again has

$$\int_0^1 \frac{P_{l+2}(u)-P_{l+2}(0)}{u^2}du = \frac{2l+3}{l+2}\int_0^1 \frac{P_{l+1}(u)}{u}du - \frac{l+1}{l+2}\int_0^1 \frac{P_l(u)-P_l(0)}{u^2}du = \frac{2l+3}{l+2}\,\frac{1}{(l+1)P_l(0)} - \frac{l+1}{l+2}\int_0^1 \frac{P_l(u)-P_l(0)}{u^2}du, \tag{A7}$$

where we have used the first theorem to evaluate the first integral on the right. Then assuming the validity of (A6) and using again (A5) we have

$$\int_0^1 \frac{P_{l+2}(u)-P_{l+2}(0)}{u^2}du = \frac{2l+3}{(l+2)(l+1)P(0)} - \frac{l+1}{l+2}\left[P_l(0) - \frac{1}{P_l(0)}\right] = P_{l+2}(0) - \frac{1}{P_{l+2}(0)}. \tag{A8}$$

Since the identity is trivially valid for $l=0$, its validity for all even l is established by induction.

The third identity which can be derived from the identity of LP, but for which no simple direct proof has yet been obtained, can be written in the following two equivalent forms:

$$P_l(0)\int_\lambda^1 \frac{P_l(u)udu}{(u^2-\lambda^2)^{1/2}} = \int_0^{(1-\lambda^2)^{1/2}} P_l(u)du, \qquad (l \text{ even and } \geq 0) \tag{A9}$$

$$P_l(0)\int_0^{(1-\lambda^2)^{1/2}} P_l(\lambda^2+u^2)^{1/2}du = \int_0^{(1-\lambda^2)^{1/2}} P_l(u)du. \tag{A10}$$

[*Note added in proof.* Identities (A1) and (A6) can be derived by use of the generating function for the Legendre polynomials but require an awkward power series expansion; the same is presumably true of (A9). A conversation on this point with Professor J. W. Weinberg is gratefully acknowledged.]