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[1]G. Högberg and H. Nordén, Phys. Status Solidi 33, K71 (1969); K. L. Merkle, L. R. Singer, and J. R. Wrobel, Appl. Phys. Lett. 17, 6 (1970).

[2]K. L. Merkle, *Radiation Damage in Reactor Materials* (International Atomic Energy Agency, Vienna, Austria, 1969), Vol. 1, p. 159.

[3]D. I. R. Norris, Philos. Mag. 19, 653 (1969); L. E. Thomas, T. Schober, and R. W. Balluffi, Radiat. Eff. 1, 257, 269 (1969); M. O. Ruault, B. Jouffrey, and P. Joyes, Philos. Mag. 25, 833 (1972).

[4]M. O. Ruault, B. Jouffrey, J. Chaumont, and H. Bernas, in *Application of Ion Beams to Metals*, edited by S. T. Picraux *et al.* (Plenum, New York, 1974), p. 459, and in Proceedings of the International Conference on Fundamental Aspects of Radiation Damage in Metals, Gatlinburg, Tennessee, October 1975 (to be published); M. O. Ruault, thesis, Université Paris-Sud, Orsay, 1974 (unpublished).

[5]K. B. Winterbon, P. Sigmund, and J. B. Sanders, K. Dan. Vidensk. Selsk., Mat.-Fys. Medd. 37, No. 14 (1970); K. B. Winterbon, *Ion Implantation Range and Energy Deposition Distributions* (Plenum, New York, 1975), Vol. II.

[6]P. Sigmund, Appl. Phys. Lett. 25, 169 (1974), and 27, 52 (1975).

[7]H. H. Andersen and H. Bay, Radiat. Eff. 19, 139 (1973), and J. Appl. Phys. 46, 2416 (1975).

[8]J. A. Moore, G. Carter, and A. H. Tinsley, Radiat. Eff. 25, 49 (1975); J. A. Davies, G. Foti, L. M. Howe, J. B. Mitchell, and K. B. Winterbon, Phys. Rev. Lett. 34, 1441 (1975).

[9]D. G. Beanland, J. H. Freeman, and C. A. English [Proceedings of the International Conference Ion Implantation in Materials, Institute of Nuclear Physics, Orsay, France, 1975 (to be published)] have observed multiple damage clusters in Cu and Ag targets bombarded with molecular Sb ions. The nature and depth distribution of these defects has not yet been reported, so that comparison with our findings is not yet possible.

[10]A doubly charged arsenic beam was used to ensure a low-current and high-purity beam.

[11]J. Chaumont, H. Bernas, M. Salomé, F. Lalu, and L. Thomé, Le Vide, Suppl. 171, 108 (1974).

[12]M. Rühle and M. Wilkens, Philos. Mag. 15, 1075 (1967).

[13]J. E. Westmoreland and P. Sigmund, Radiat. Eff. 6, 187 (1970).

[14]A. Seeger, in *Proceedings of the Second International Conference on the Peaceful Uses of Atomic Energy* (International Atomic Energy Agency, Vienna, Austria, 1958), Vol. 6, p. 250.

Superfluidity of Periodic Solids

W. M. Saslow

Department of Physics, Texas A & M University, College Station, Texas 77843

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Leggett's investigation of the superfluid density of solids has been extended. By employing plane waves as a basis set, one can obtain the superfluid fraction ρ_s/ρ_0 as a function of the localization parameter. Solid He^4 is estimated to have a ρ_s/ρ_0 between 0.05 and 0.2 at zero temperature. This approach also sheds light on the superfluidity of thin films and the "index of refraction" of fourth-sound chambers.

In 1970, Leggett considered the possible superfluidity of solids.[1] Analyzing only temperature $T=0$, he observed that if a modified crystal wave function [obtained by letting all single-particle states develop a phase $\varphi(\vec{r})$] were stable with respect to the decay of excitations (the Landau criterion[2]), then one can define a meaningful superfluid fraction ρ_s/ρ_0, where ρ_s and ρ_0 are the superfluid and average number densities. Observation of the moment of inertia of a macroscopically large rotating annulus of height h, inner radius R, and thickness $d \ll R$ might thus yield a nonclassical moment of inertia (NCMI) I, where $I = (1-\rho_s/\rho_0)I_0$, and I_0 is the classical value. Leggett developed an expression giving a variational upper limit for ρ_s/ρ_0, but he did not evaluate it, instead relying on an analogy of this effect to the nuclear-exchange effect in solid He^3.[1] (Both effects disappear in the classical limit.) This led to an estimate of ρ_s/ρ_0 on the order of 10^{-4}, thus suggesting that the effect would not readily be observed at finite T.[3] Recently, Fernandez and Puma[4] evaluated Leggett's expression, finding for hcp He^4, the low temperature phase of solid He^4, that ρ_s/ρ_0 lies between 0.2 and 0.4. They then went on to argue that the ground-state wave function Ψ_0 probably does not possess off-diagonal long-range order,[5] and hence that it cannot describe superfluidity. However, their argument was not rigorous. Because of the unclear status

of the theory, I believe that the only definitive arguments for or against the superfluidity of solid He^4 will come from experiment. Assuming superfluidity to be possible, the theory of ρ_s/ρ_0, and the expected value of ρ_s/ρ_0 for solid He^4, thus become relevant.

In the present paper, I derive in full generality the condition describing steady-state superflow of solids. Further, for periodic solids I obtain a formally exact expression for ρ_s/ρ_0 which, when evaluated approximately, yields an upper limit for that quantity. I compute a curve of ρ_s/ρ_0 as a function of the localization parameter (to be defined), and find results consistent with the calculation of Ref. 4, which was performed for only one value of the localization parameter. Having the curve of ρ_s/ρ_0 makes it possible to relate this work to the problem of the nonsuperfluid layer of He^4 which separates liquid He^4 from a substrate material. Most important, the results make it appear worthwhile to undertake experiments to measure ρ_s/ρ_0 for solid He^4. The general approach is also relevant to the problem of the "index of refraction" $n=(\rho_s/\rho_0)^{1/2}$ for superfluids in fourth-sound chambers.[6]

I first present a physical picture of the phenomenon of superfluidity in solids. The Ψ_0 for N particles has a series of quantum numbers specifying, in part, the crystalline sites. (The number M of such crystalline sites need not equal N.) Further, the density profile (which reflects the site positions) is somewhat delocalized, due to zero-point motion. In a conventional rotation experiment, the locations of the sites rotate, so the density profile rotates, the system thus developing angular momentum. On the other hand, in superfluid rotation, the locations of the sites do not change. Rather, the system develops angular momentum because of "superflow" or "phase flow," taking a flow pattern such that matter flows yet the density profile does not change.

Consider the energy E of a system when all the single-particle states develop the phase φ. As shown in Ref. 1, for a ground state with momentum zero one has

$$E=E_0+(m/2)\int \rho v_s^2 d^3r, \tag{1}$$

where E_0 is the ground-state energy, m is the particle mass, ρ is the ground-state number density, and the superfluid velocity $\vec{v}_s=(\hbar/m)\nabla\varphi$. By varying φ subject to the constraint of a fixed nonzero phase change $\Delta\varphi$ on traversing a given circuit (e.g., an annulus), one finds that the minimization condition is given, in general, by

$$\nabla\cdot\vec{j}=0, \tag{2}$$

where $\vec{j}=\rho\vec{v}_s$. In other words, number density is conserved in the steady state. Once $\vec{v}_s$ is determined, the superfluid density ρ_s can be obtained through the definition

$$(m/2)\rho_s v_0^2 V\equiv(m/2)\int \rho v_s^2 d^3r, \tag{3}$$

where v_0 is the average linear flow velocity along the path of the phase change, and V is the crystal volume.

The above discussion is valid for both crystals and amorphous materials. Let us now consider only the case of crystals, where one can write

$$\rho(\vec{r})=\textstyle\sum_G \rho_G \exp(i\vec{G}\cdot\vec{r}), \tag{4}$$

$$\vec{v}_s(\vec{r})=\vec{v}_0+\textstyle\sum_G{}' \vec{v}_G \exp(i\vec{G}\cdot\vec{r}), \tag{5}$$

with $\vec{v}_G=i\vec{G}\varphi_G$ for $\vec{G}\neq\vec{0}$, and φ_G is defined analogously to the definition of ρ_G in Eq. (4). (The $\vec{G}$'s are reciprocal-lattice vectors and $\sum_G'$ means that the $\vec{G}=\vec{0}$ component is deleted.) The quantity $\vec{v}_0$ is the average linear flow velocity with magnitude $v_0=(\hbar/m)\Delta\varphi/L$, where L ($=2\pi R$ for an unrolled annulus) is the path length over which $\Delta\varphi$ occurs. Use of Eqs. (4) and (5) permits Eq. (2) to be written as

$$\vec{G}\cdot\textstyle\sum_{G'}{}'\rho_{G-G'}\vec{v}_{G'}=-\vec{G}\cdot\rho_G\vec{v}_0. \tag{6}$$

[Here I have taken only the components of $\exp(i\times\vec{G}\cdot\vec{r})$.] This is a set of simultaneous linear equations for the unknowns $\vec{v}_{G'}$ (or $\varphi_{G'}$). Restriction to a finite number N_B of $\vec{G}$'s (i.e., plane waves) makes it clear that there are N_B equations in N_B unknown $\varphi_{G'}$. Use of Eq. (6) permits Eq. (3), after integration, to be written as

$$\rho_s/\rho_0=1-v_0^{-2}\vec{v}_0\cdot\textstyle\sum_G{}'\rho_{-G}\vec{v}_G. \tag{7}$$

If a finite number of $\vec{G}$'s is employed in determining $\vec{v}_s$ (but ρ is represented as accurately as is necessary) then Eq. (7) represents a variational upper limit on ρ_s.

In solving Eqs. (6) and (7) I have taken $\rho(\vec{r})$ to be made up of a sum of Gaussians about each lattice site: $\rho_{\text{site}}(\vec{r})=(\pi b^2)^{-3/2}\exp(-r^2/b^2)$, so $\rho_G=\rho_0\times\exp(-G^2b^2/4)$. For ease of calculation I consider an fcc lattice (with lattice constant a), which has the same number of nearest neighbors (12) as the hcp lattice. For each value of the localization parameter b, N_B was increased until convergence was obtained or until the available computer core was near saturation (values of $N_B=26$, 64, 112, and 234 were employed). Figure 1 and Table I

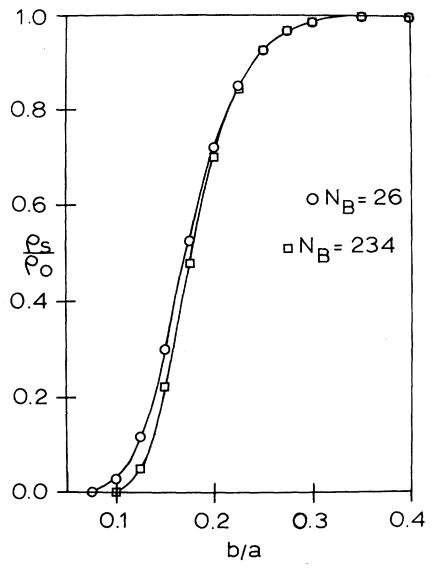

FIG. 1. Superfluid fraction ρ_s/ρ_0 plotted against b/a, the localization parameter divided by the lattice constant. N_B is the number of plane waves employed in the calculation. The circles are taken from Table I.

TABLE I. Superfluid fraction (ρ_s/ρ_0) as a function of localization parameter (b) and number of plane waves employed in the calculation (N_B). a is the fcc lattice constant.

b/a \ N_B	26	64	112	234
0.5	0.999 999	0.999 999		
0.45	0.999 983	0.999 983		
0.40	0.999 789	0.999 789		
0.35	0.998 017	0.998 015		
0.30	0.986 058	0.985 976	0.985 972	0.985 972
0.275	0.966 920	0.966 523	0.966 478	0.966 474
0.25	0.927 162	0.925 624	0.925 260	0.925 223
0.225	0.851 444	0.846 778	0.844 645	0.844 368
0.20	0.721 405	0.710 687	0.701 644	0.699 969
0.175	0.528 457	0.511 004	0.484 828	0.477 835
0.150	0.301 894	0.283 879	0.238 025	0.221 925
0.125	0.117 682	0.107 383	0.066 507	0.051 401
0.10	0.027 335	0.024 394	0.008 376	0.004 081
0.075	0.003 226	0.002 848	0.000 375	0.000 092

represents the results, which were computed for $\vec{v}_s$ along [100] and [111]. As expected for a cubic lattice, the results were independent of the direction of $\vec{v}_s$.

There are three notable aspects to the results. First, ρ_s/ρ_0 begins to deviate from unity only when b is about half of the nearest-neighbor distance $a/2^{1/2}$, so that hcp and fcc lattices, with the same close-packing ratio, are likely to give very similar results.[7] Second, ρ_s/ρ_0 falls off very rapidly, going from 0.925 to less than 0.051 as b/a goes from 0.25 to 0.125. Third, $(\rho_s/\rho_0) < 10^{-4}$ for $b/a \leq 0.075$, so that highly localized systems (e.g., conventional solids) will have a negligible ρ_s/ρ_0. Taking the Gaussians employed in Ref. 4 for the hcp lattice, and transcribing them to the fcc lattice, one finds $(b/a) \simeq 0.15$.[8] This is at the limit of convergence of the calculations, which for $N_B = 234$ give $\rho_s/\rho_0 \simeq 0.22$, and are consistent with $0.2 < (\rho_s/\rho_0) < 0.4$ as determined in Ref. 4. This ρ_s/ρ_0 value is sufficiently large to give encouragement that an NCMI might be observable. Note, however, that considerations of exchange (e.g., as described in Ref. 3) give $b/a \simeq 0.125$, which has $\rho_s/\rho_0 \simeq 0.05$. A ρ_s/ρ_0 of this magnitude is still encouraging, but will be somewhat harder to measure.

The above calculations also provide a semiquantitative explanation of the nonsuperfluid layer of He^4 separating liquid He^4 from a substrate material.[9] In this case it is believed that the first layer feels a Van der Waals attraction to the substrate which is stronger than the He^4-He^4 attraction in solid He^4. As a consequence one can expect this layer to be more localized than in solid He^4, and thus to behave as if $\rho_s/\rho_0 \simeq 0$. Other layers, being significantly further from the substrate, are more delocalized, and therefore may possess a $\rho_s/\rho_0 > 0$.

Finally, note that if one considers the powder within a fourth-sound chamber to consist of regularly packed spheres of radius b, it should be possible to apply the above methods to obtain n.[6] Preliminary calculations for an fcc lattice with $b/a = 0.3$ (corresponding to a porosity $P = 0.55$) give $n = 1.11$ (the results for $N_B = 64$ and 112 are very close, so I believe this to be a convergent result). This is not in good agreement with the empirical result $n^2 = 2 - P$,[10] indicating that an fcc model is inappropriate for the description of an irregularly packed powder.

In another article I will consider both fourth sound and ρ_s/ρ_0 at finite T.[11] Note that Andreev and Lifshitz have discussed fourth sound and related questions.[12] It is my opinion that, since their work has not incorporated the considerations of Ref. 1, there is a need to rederive a number of their results. The theory of the transition temperature T_c for the disappearance of superfluidity, and of the effect of superfluidity on the thermal and transport properties, remains undeveloped. Such investigations might well explain

why superfluidity of solids, if it does exist, has failed to manifest itself, although it should be noted that so far there has been no explicit attempt to measure ρ_s/ρ_0 in solid He^4.

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[1]A. J. Leggett, Phys. Rev. Lett. 25, 1543 (1970).

[2]I believe that the Fermi system of solid He^3 may more easily violate the Landau criterion than the Bose system of solid He^4. Therefore, I consider solid He^4 as my prototype. Since solid He^3 is more "quantum" than solid He^4, this errs on the pessimistic side.

[3]See R. A. Guyer, Phys. Rev. Lett. 26, 174 (1971), for a tunneling analogy which lowers ρ_s/ρ_0 to $O(10^{-6})$.

[4]J. F. Fernandez and M. Puma, J. Low Temp. Phys. 17, 131 (1974). Their calculation was done for superflow along the hexagonal c axis. These authors employ the important observation that Leggett's variational solution gives the exact value of a lower limit on ρ_s/ρ_0.

[5]C. N. Yang, Rev. Mod. Phys. 34, 644 (1962); D. Sherrington and W. Kohn, Rev. Mod. Phys. 42, 1 (1970).

[6]For a recent summary see D. J. Bergman, B. I. Halperin, and P. C. Hohenberg, Phys. Rev. B 11, 4253 (1975).

[7]The fact that ρ_s/ρ_0 deviates from unity only for strongly localized systems makes it likely that no correction for this effect need be made for superconducting electrons flowing in a metal.

[8]This value is consistent with the representative calculations of L. H. Nosanow, Phys. Rev. 146, 120 (1966); C. Ebner and C. C. Sung, Phys. Rev. A 4, 269 (1971); J. P. Hansen and E. L. Pollock, Phys. Rev. A 5, 2651 (1972). It is also consistent with the "experimental" estimate of the rms displacement $\langle r^2\rangle^{1/2}=\frac{3}{2}\hbar(mk_B\Theta_D)^{-1/2}$, where Θ_D is the experimental Debye temperature, as obtained by D. O. Edwards and R. C. Pandorf, Phys. Rev. 140, A816 (1965). See R. A. Guyer, Solid State Phys. 23, 413 (1969).

[9]M. H. W. Chan, A. W. Yanof, and J. D. Reppy, Phys. Rev. Lett. 32, 1347 (1974); T. E. Washburn, J. E. Rutledge, and J. M. Mochel, Phys. Rev. Lett. 34, 183 (1975).

[10]M. Kriss and I. Rudnick, J. Low Temp. Phys. 3, 339 (1970).

[11]W. M. Saslow, to be published.

[12]A. F. Andreev and I. M. Lifshitz, Zh. Eksp. Teor. Fiz. 56, 2057 (1969) [Sov. Phys. JETP 29, 1107 (1969)].

Tight-Binding Calculation of a Core-Valence-Valence Auger Line Shape: Si(111)†

Peter J. Feibelman and E. J. McGuire
Sandia Laboratories, Albuquerque, New Mexico 87115

and

K. C. Pandey
Bell Laboratories, Murray Hill, New Jersey 07974

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The shape of the $L_{2,3}VV$ Auger line has been calculated for a Si(111) surface and found to be in excellent agreement with the data of Houston and Lagally. By contrast, the experimental line shape scarcely resembles the self-fold of the occupied Si density of states, a fact which the calculation shows to be the result of matrix-element angular momentum dependence and *not* of "many-body" effects.

This Letter reports the first complete one-body calculation (i.e., including matrix elements) of a core-valence-valence Auger line shape for a solid. The case treated, the ($L_{2,3}VV$) line associated with Auger emission from Si $2p$ core holes through a clean Si(111) surface, is of particular interest because (see Fig. 1) the experimental line shape[1] is in rather poor agreement with the weighted self-fold of the occupied density of states (WSFDOS) for this surface (the weighted SFDOS is calculated by summing the self-fold of the occupied local DOS for each crystal layer times a factor[2] which accounts for inelastic damping of the Auger electrons). Until now it has not been known whether such a discrepancy is an indication of "many-electron effects" or, more simply, of a variation across the valence band of one-electron model Auger matrix elements,[3] because neither of these effects has heretofore been studied quantitatively. In fact, our results show for Si(111) that the simpler explanation is correct, i.e., that apart from the absence of a sharp dangling-bond surface-state peak in the data,[4] the discrepancy can be largely explained as a conse-