Locality of information obtained from proximity-electron-tunneling spectroscopy

G. B. Arnold

Department of Physics, University of Notre Dame, Notre Dame, Indiana

E. L. Wolf

Ames Laboratory–U. S. Department of Energy and Department of Physics, Iowa State University, Ames, Iowa 50011

(Received 19 June 1981)

The locality of the information obtained by the technique of proximity-electron tunneling (PETS) is analyzed, with particular attention to the effects on the measured effectivephonon spectrum $a^2F(\omega)$ of disorder or impurities near the surface of the superconductor electrode. As in conventional tunnel junctions it is determined that the (energy-dependent) electron mean free path determines the maximum depth of the superconductor of which the measured phonon spectrum is characteristic. An averaging length L(E) is defined and found to be typically larger in proximity junctions than in conventional junctions. This can make PETS results inherently less susceptible than conventional results to surface disorder of the superconductor.

I. INTRODUCTION

The work of McMillan and Rowell¹ established superconducting tunneling as a useful probe of the properties of the electron-phonon interaction (EPI) in superconductors. The recent development of proximity-effect-tunneling spectroscopy (PETS)²⁻⁴ has allowed a similar investigation of EPI effects in materials which cannot be treated by the McMillan-Rowell technique.

These techniques allow determination of the effective-phonon spectrum $a^2F(\omega)$ and Coulomb pseudopotential μ^* ; these, via the Eliashberg equations, lead to the pair potential $\Delta(E)$ and renormalization function Z(E), fully describing the superconductivity of a homogeneous tunneling electrode. In either case, it is important to determine to what extent the properties obtained from tunneling are representative of the bulk metal.

The objectives of the present paper, therefore, are twofold. First, we extend the original analysis of locality given by McMillan and Rowell¹ for conventional junctions to the case of thin Nproximity junctions of the form used in PET spectroscopy. Second, we address in more detail the effect of surface or interfacial disorder on the measured $a^2F(\omega)$. Such defects, which are present to some extent in all tunnel junctions, are inherently more important in materials of short superconducting coherence length, such as A 15 compound superconductors or transition-metal alloys. A somewhat surprising prediction of our analysis is that the PET method applied to such materials should give results less affected by surface disorder than the conventional method.

In this paper we shall present some quantitative and qualitative arguments on the locality of superconducting tunneling as a probe of metal properties. The quantitative portions of the paper establish the properties which can, in principle, be reflected in the local self-energy functions. We then determine the range over which these local properties are averaged by a tunneling measurement. Thus, the intrinsic spatial sensitivity (range) of the tunneling probe is defined. The qualitative portion of this work discusses classes of spatial variations of the self-energy functions. The influence of these on the metal properties observed via tunneling is then assessed, based on the knowledge of the range of the tunneling probe $vis-\hat{a}-vis$ the spatial range and magnitude of the influence of each class of spatial variation.

II. LOCAL SELF-ENERGY FUNCTIONS

From standard diagrammatic perturbation theory, one finds the local, matrix-retarded self-energy due to the electron-phonon interaction (EPI) in the Migdal approximation (at T = 0 K)

25

1541

G. B. ARNOLD AND E. L. WOLF

$$\Sigma(x;\vec{k}_{||};E) = \int \frac{dE'}{2\pi} \int dx_1 \int dx_2 \sum_{\vec{q}_{||}} U(x-x_1;\vec{q}_{||}) D(x_1,x_2;\vec{q}_{||};E-E')\tau_3$$

$$\times G(x_1,x_2;\vec{k}_{||}-\vec{q}_{||};E')\tau_3 U(x_2-x;-\vec{q}_{||}), \qquad (2.1)$$

where $k_{||}$ and $\vec{q}_{||}$ are wave vectors lying in a plane which is parallel to the interfaces. Also involved in this expression are the two-dimensional Fourier transforms of the EPI potential, $U(x - x_1; \vec{q}_{\parallel})$, the dressedphonon Green's function $D(x_1, x_2; \vec{q}_{\parallel}; E - E')$, and the dressed-matrix Green's function $G(x_1, x_2; \vec{k}_{||} - \vec{q}_{||}; E')$. The diagonal Pauli matrix is denoted by τ_3 .

First, we approximate the EPI potential by a local potential

$$U(\mathbf{x} - \mathbf{x}_1; \mathbf{\vec{q}}_{\parallel}) \approx V(\mathbf{x}; \mathbf{\vec{q}}_{\parallel}) \delta(\mathbf{x} - \mathbf{x}_1) .$$

$$(2.2)$$

This should be a good approximation because the EPI potential is screened by conduction electrons. After this approximation, we introduce the spectral representations for the Green's functions and obtain, in the usual way, expressions for the diagonal and the off-diagonal components of the matrix EPI self-energy:

$$\phi^{\rm ph}(x;\vec{k};E) = \int_0^\infty dE' \int_0^\infty d\nu H(x;\vec{k}_{||};E')_{12} [(E'+E+\nu)^{-1} + (E'-E+\nu)^{-1}], \qquad (2.3)$$

$$Z^{\rm ph}(x;\vec{k};E)E = E - \int_0^\infty dE' \int_0^\infty d\nu H(x;\vec{k}_{||};E')_{11}[(E'+E+\nu)^{-1} - (E'-E+\nu)^{-1}], \qquad (2.4)$$

where

$$H(x;\vec{k}_{||};E')_{ij} = \sum_{\vec{q}_{||}} |V(x;\vec{q}_{||})|^{2} [-\mathrm{Im}D(x,x;\vec{q}_{||};\nu)] [-\mathrm{Im}G(x,x;\vec{k}_{||}-\vec{q}_{||};E')_{ij}].$$
(2.5)

In specular tunneling, only those electrons with wave vectors nearly perpendicular to the interfaces are important, so for those electrons we set $k_{\parallel} = 0$ in the above expressions.

Before presenting our general approximation for (2.5), we shall consider a very simple model in order to motivate the approximation. We shall use the bulk Green's functions calculated in the spherical model. For the phonon Green's function, a straightforward calculation yields

$$-\operatorname{Im}D(x,x;\vec{q}_{||}\nu) = \frac{1}{\hbar c_s} \operatorname{Re}\left[\frac{(\nu/\omega_D)}{\left[(\nu/\omega_D)^2 - (q_{||}/q_D)^2\right]^{1/2}}\right] \theta(1 - (\nu/\omega_D)), \qquad (2.6)$$

where $\theta(x)$ is the unit-step function and c_s is the sound velocity. For the matrix Green's function, a similar calculation gives

$$-\operatorname{Im} G(x,x;-\vec{q}_{\parallel};E) = \sum_{\pm} \operatorname{Re} \left[\frac{m}{2\hbar^2 K_{\pm}} \right] \operatorname{Re} \left[\frac{E \pm \Omega \tau_3 + \Delta \tau_1}{2\Omega} \right], \qquad (2.7)$$

where τ_1 is the real off-diagonal Pauli matrix and

$$K_{\pm} = \left[k_F^2 [1 - (q_{\parallel} / k_F)^2] \pm \frac{2m}{\hbar^2} Z(E) \Omega \right]^{1/2}, \qquad (2.8)$$
$$\Omega = (E^2 - \Delta^2)^{1/2}, \qquad (2.9)$$

with Δ as the pair potential and Z(E) as the renormalization function. If we compare the dependences on

 q_{\parallel} , we observe that each Green's function exhibits a potential square-root singularity. This is, of course, a reflection of the generally expected behavior for these quasi-one-dimensional spectral densities.

Noting that K_{\pm} is well approximated by

$$k_F [1 - (q_{\parallel}/k_F)^2]^{1/2} = k_F \cos\theta$$
,

we may write

$$-\operatorname{Im}G(x,x;-q_{||};E) \approx \rho(x,x;-q_{||};E)\operatorname{Re}\left[\frac{E+\Delta\tau_{1}}{\Omega}\right],$$
(2.10)

1542

where

$$\rho(x,x;-q_{\parallel},E) \equiv \left[\frac{1}{2\hbar v_F \cos\theta}\right], \qquad (2.11)$$

which is the normal-state local spectral density. Thus, in this case (2.5) may be written (for $k_{\parallel}=0$)

$$H(x;0;E')_{ij} = \int d(\cos\theta) \left[\frac{-\mathrm{Im}G(x,x;-\vec{q}_{||};E')_{ij}}{\rho(x,x;-\vec{q}_{||};E')} \right] \\ \times \sum_{\vec{q}_{||}} |V(x;\vec{q}_{||})|^2 \rho(x,x;-\vec{q}_{||};E') [-\mathrm{Im}D(x,x;\vec{q}_{||};\nu)] .$$
(2.12)

For convenience, we shall henceforth refer to the factor in large parentheses as the "local normalized density of states" when i = j, the "pair-density function" when $i \neq j$. Equation (2.12) is obviously correct for the simple case which we have considered. In the general case, where the matrix Green's function may contain dependences on q_{11} other than that of $\rho(x,x;-q_{||};E)$, the accuracy of this approximation may be questionable. This approximation has been made, implicitly, in all previous proximity-effect theories.⁵ We believe that, since it is clearly correct in the bulk case, it is accurate in any situation for which the matrixspectral density is very nearly equal to its bulk value, as in, for example, a thin N-metal proximity-effect sandwich.² In any event, we emphasize that (2.5) is the rigorously correct expression, against which the validity of (2.12) may be checked by explicit calculation.

The pair potential is a local function given by

$$\Delta(E,x) = \phi(E,x) / Z(E,x) , \qquad (2.13)$$

where, adopting the approximation (2.12), and in-

$$K_{\pm}(E,E',x) = \int_0^\infty d\omega \, \alpha^2(\omega,x) F(\omega,x) [(E'+E+\omega)^{-1} \pm (E'-E+\omega)^{-1}] - \mu^*(x) \theta(E_B-E') \theta(\pm 1) , \quad (2.18)$$

where $\theta(x)$ is the unit step function and E_B is a cutoff energy. This is the local electron-phonon interaction (EPI) kernel. Its spatial variation depends on the spatial variations of (i) The EPI parameter $a^2(\omega, x)$ (involving local EPI matrix elements) and the Coulomb pseudopotential parameter $\mu^*(x)$. One observes, on physical grounds, that these functions may vary over a distance as small as a screening length, i.e., on an atomic scale. (ii) The local phonon density of states $F(\omega, x)$. The importance of spatial variation in this function will be discussed later.

The pair density, f(E',x) is a function which is sharply peaked at the local value of the energy gap cluding the screened Coulomb interaction:

$$\phi(E,x) = \int_0^\infty dE' f(E',x) K_+(E,E',x) \qquad (2.14)$$

$$Z(E,x)E = E - \int_0^\infty dE' N(E',x) K_{-}(E,E',x) .$$
(2.15)

The "pair-density function" f(E,x), and the local normalized density of states N(E,x) were introduced above. They are defined in terms of the retarded Nambu-matrix Green's function by

$$f(E',x) = \int_0^1 d(\cos\theta)(-2\hbar v_F \cos\theta) \\ \times \operatorname{Im} G(x,x,E')_{12}$$
(2.16)

and

$$N(E',x) = \int_0^1 d(\cos\theta)(-2\hbar v_F \cos\theta) \times \operatorname{Im} G(x,x,E')_{11}, \qquad (2.17)$$

where θ is the angle between an electron wave vector and the normal to the interface planes. At T=0 K the kernel functions in (2.14) and (2.15) are

and varies with x on the scale of a coherence length. The local density of states, N(E',x), is also sharply peaked at the local gap, and varies on the same scale as f(E',x). We conclude that the pair potential may vary with x over a distance as large as a coherence length or as small as a lattice constant.

III. TUNNELING DENSITY OF STATES

The tunneling density of states is the local density of states⁶ at the interface separating the tunnel-

<u>25</u>

1544

ing barrier from the metal being "tunneled into," i.e., the "tunneling interface." For specular tunneling at T=0 K, it is equal to²

$$D(0,E) = \frac{-2\hbar v_F}{\pi} \operatorname{Im} G(0,0,E)_{11}, \qquad (3.1)$$

where E = eV, V being the bias voltage, and v_F is the Fermi velocity in the metal located adjacent to the tunneling interface (at x = 0).

The Green's function required to calculate the tunneling density of states is the solution to

$$\left[Z(x)E + \frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial x^2} + k_F^2 \right] \tau_3 - \phi(x)\tau_1 \right] G(x, x', E)$$
$$= \delta(x - x') , (3.2)$$

where the τ_i are the Pauli matrices. Assumption of spatial invariance in the y and z directions has reduced the original three-dimensional problem to a one-dimensional problem. In accord with the assumption of specular tunneling, we have assumed that the (implicit) wave-vector dependence of the Green's function is that appropriate to propagation with k vector normal to the interface planes.

For simplicity, we neglect the spatial variation of the renormalization function $[Z(x)=Z_N]$ and let

$$\phi(x) = \phi_N + Z_N \delta \Delta(x) , \qquad (3.3)$$

where N is a label characterizing the metal layer adjacent to the tunneling barrier and Z_N has an implicit energy dependence. We shall further restrict our treatment to energies E satisfying $E >> \Delta_{\max}(E)$, where $\Delta_{\max}(E)$ is the maximum value of the spatially varying pair potential at energy E. In this regime a perturbation expansion in powers of Δ/E is appropriate. The zeroth-order Green's function is available from previous work,² so the calculation is straightforward. Neglecting terms which oscillate over a spatial range of k_F^{-1} or less, one finds [to order $(\Delta/E)^2$]

$$D(0,E) = \operatorname{Re}[1 + \frac{1}{2}I(E)^2/E^2], \qquad (3.4)$$

where $\Delta_N(E)$ is the pair potential at energy E in the metal adjacent to the tunneling barrier and

$$I(E) = -i(\Delta K) \int_0^\infty dx \exp(i\Delta Kx) \times [\delta\Delta(x) + \Delta_N(E)], \quad (3.5)$$

where $\Delta K = 2Z_N(E)E/(\hbar v_{FN})$. A very similar calculation is presented in Ref. 1.

Up to this point, our arguments have been quite general. Note that ΔK in Eq. (3.5) has a real and a positive imaginary part due to $Z_N(E)$. The integral I(E) contains information on the Re ΔK Fourier component of the spatially varying pair potential. From (3.5) one also observes that the maximum depth from which Andreev-reflected quasiparticles can emerge and produce interference at the tunneling interface (x = 0) is of the order of $(\text{Im}\Delta K)^{-1}$, which is equal to the mean free path in the N metal. The typical range over which a spatially varying pair potential is averaged by a tunneling measurement is (as we will show below) $L(E) = \Delta K^{-1}$. In what follows, we shall present a model for the spatial variation of the pair potential. This will allow us to make quantitative arguments concerning the effects of a spatially varying pair potential. Our conclusions, however, will be model dependent only to the extent that we shall consider only monotonic spatial variations. For the NS geometry, the length

$$L(E) = |\Delta K^{N}|^{-1} = \frac{n v_{FN}}{2 |Z_{N}(E)|E}$$
$$= \left[\left(\frac{2E}{\hbar v_{FN}} \operatorname{Re} Z_{N}(E) \right)^{-2} + l_{\mathrm{ph}}(E)^{2} \right]^{1/2}.$$

The first quantity is the square of the energydependent coherence length in N. The second is the square of the mean free path due to phonon scattering in N.

We propose the following model form for $\delta \Delta(x)$:

$$\delta\Delta(x) = \begin{cases} 2\delta\Delta_N(E)\{\exp[-2(x-d)/\xi_N] + 1\}^{-1} & 0 < x < d \\ \Delta_S(E) - \Delta_N(E) - 2\delta\Delta_S(E)\{\exp[2(x-d)/\xi_S] + 1\}^{-1} & d < x \end{cases}$$
(3.6)

The spatial dependence resulting from this model is shown in Fig. 1. The similarity between the spatially varying parts of $\delta\Delta(x)$ and statistical Fermi distributions allows one to investigate various limits easily.

First, consider the case wherein $\xi_{S,N}/2 >> L(E)$, $\xi_N/2$, $\xi_N/2 >> d$. This is the "slow-variation limit." Note that if ξ_S is a coherence length, then

$$\frac{L(E)}{\xi_s} \left| \frac{\Delta_s}{2Z_N(E)E} \right| <<1 ,$$

since the validity of our work is restricted to this energy regime. In the slow-variation limit we find

$$I(E) \approx \delta \Delta_N(E) \{ [1 - \exp(i\Delta Kd)] [1 + i(\Delta K\xi_N)^{-1}] + d/\xi_N \}$$

+
$$[\Delta_s(E) - \Delta_N(E)] \exp(i\Delta Kd) - \delta \Delta_s(E) \exp(i\Delta Kd) [1 - i(\Delta K\xi_s)^{-1}] + \Delta_N(E) .$$
(3.7)

Neglecting the small corrections, we find

$$D(0,E) \approx \operatorname{Re}\left(1 + \frac{1}{2} \left\{ \Delta_N(E) + \delta \Delta_N(E) + \left[\Delta_s(E) - \delta \Delta_s(E) - \Delta_N(E) - \delta \Delta_N(E) \right] \exp(i\Delta Kd) \right\}^2 / E^2 \right).$$
(3.8)

Note that only the values of the pair potentials at the NS interface are involved here. In this limit, tunneling samples provide the local values of the pair potentials at the NS interface. Thus, the properties inferred from tunneling measurements are local interface properties to the extent that $d < L(E) < \xi_{S,N}/2$ is true.

Another simple limit is that in which $\xi_{S,N}/2 \ll L(E)$. In this case, both pair potentials vary rapidly over the length scale L(E). We find

$$I(E) \approx \exp(i\Delta K d) [\Delta_s(E) - \Delta_N(E) - \delta \Delta_s(E) i\Delta K \xi_s C(\infty) - \delta \Delta_N(E) i\Delta K \xi_N C(2d/\xi_N)] + \Delta_N(E) , \qquad (3.9)$$

where

$$C(x) = -x / [\exp(x) + 1] - \ln\{[1 + \exp(-x)]/2\}.$$
(3.10)

Since the maximum value of C(x) is equal to ln2, neglect of small first-order corrections leads to [assuming $\delta \Delta_{N,S}(E) \leq \Delta_{N,S}(E)$]

$$D(0,E) \approx \operatorname{Re}(1 + \frac{1}{2} \{ \Delta_N(E) + [\Delta_s(E) - \Delta_N(E)] \exp(i\Delta Kd \}^2 / E^2) .$$
(3.11)

Here we observe that variations in the pair potentials which are rapid compared to the length scale L(E) do not affect the measured density of states. In this case, the true bulk (asymptotic) pair potentials are sampled by tunneling.

It may happen that $\delta\Delta_N(E) > \Delta_N(E)$ due to enhancement of the N-metal superconductivity near the NS interface by the proximity effect and/or more favorable local electron-phonon interaction parameters (a^2F,μ^*) near the interface. In this case, one should maintain the lowest-order correction in $\xi_N/L(E)$ [the next highest order is smaller by a factor of $\xi_N/L(E)$] so that

$$D(0,E) \approx \operatorname{Re}\left(1 + \frac{1}{2} \left\{ \Delta_N(E) + \left[\Delta_s(E) - \Delta_N(E) - \delta \Delta_N(E) i \Delta K \xi_N C \left(\frac{2d}{\xi_N}\right)\right] \exp(i \Delta K d) \right\}^2 / E^2 \right).$$
(3.12)

In this case, the information obtained on the N metal involves a composite of the asymptotic pair potential $\Delta_N(E)$, and a contribution from the local value of the pair potential at the NS interface.

A remaining limit is that in which $\xi_{S,N}/2 >> L(E)$ and $d >> \xi_N/2$. In this case we may use the result of the slow-variation limit for the integral I(E) over the range where x > d; but for x between 0 and d we recognize that over most of the integration range $\exp[2(d-x)/\xi_N] >> 1$, and find (neglecting first-order corrections)

$$I(E) \approx [\Delta_s(E) - \delta \Delta_s(E) - \Delta_N(E) - \delta \Delta_N(E)] \exp(i\Delta Kd) + \Delta_N(E) , \qquad (3.13)$$

so that

$$D(0,E) \approx \operatorname{Re}\left(1 + \frac{1}{2} \left\{ \Delta_N(E) + \left[\Delta_s(E) - \delta \Delta_s(E) - \Delta_N(E) - \delta \Delta_N(E)\right] \exp(i\Delta Kd) \right\}^2 / E^2 \right).$$
(3.14)

Note that this result indicates that the N-metal pair potential measured by tunneling is a true *composite* of the local NS interface value and the asymptotic value. The information obtained on the

local value is a result of Andreev scattering, hence is modulated by the factor $\exp(i\Delta Kd)$.

It is also possible that other combinations of the limits considered above will be relevant. However,

1545

25



FIG. 1. Spatial dependence of the pair potential as described by Eq. (3.6) of the text. The lower sketch illustrates the limit of (3.6) for d = 0, $\Delta_N = \delta \Delta_N = 0$.

we feel that consideration of the three cases mentioned should be sufficient to extract the basic behavior expected for the tunneling density of states in most situations of experimental interest. A feature of all three limits is the comparison between the scale of spatial variation in the pair potentials (over the lengths ξ_S and ξ_N) and the *energy*-dependent length $|\Delta K|^{-1} = L(E)$. Thus, L(E) is the spatial resolution of the probe in a tunneling experiment. If it is desired that bulk properties be measured, then one requires that L(E)be very long compared to ξ_S and ξ_N over the energy range of interest.

Conversely, one may wish to study local properties at an interface. In this case, one would require L(E) small compared to ξ_S and ξ_N in the energy range of interest. If one is interested in an energy range which is far above the energy gap of the *S* metal, then it should always be possible to employ tunneling as a probe of metal properties near the *NS* interface.

It is now easy to obtain the results analogous to those above for the case of a conventional junction; one simply takes the limit $d \rightarrow 0$. For convenience, we list the results (neglecting first-order corrections):

$$\xi_{s}/2 >> L_{s}(E) ,$$

$$D(0,E) \approx \operatorname{Re}\{1 + \frac{1}{2} [\Delta_{s}(E) - \delta \Delta_{s}(E)]^{2}/E^{2}\} ,$$

$$\xi_{s}/2 << L_{s}(E) ,$$

$$D(0,E) = \operatorname{Re}\{1 + \frac{1}{2} A^{2}(E)/E^{2}\} .$$

$$(2.16)$$

$$D(0,E) \approx \operatorname{Re}[1 + \frac{1}{2}\Delta_s^2(E)/E^2]$$
. (3.16)

The appropriate length scale in this case is

$$L_{S}(E) = [2 | Z_{S}(E) | E / (\hbar v_{FS})]^{-1}$$

When the pair potential varies slowly on this scale, the *local* value of the S-metal pair potential (at x = 0) is reflected by tunneling. Numerous sample-dependent factors may affect this local value. We shall discuss these in the next section.

At this point, it is interesting to compare the utility of proximity-effect tunneling (PET) as a probe of bulk (asymptotic) S-metal properties, with that of the conventional tunneling experiment. The ratio of the spatial resolution in PET to that in conventional tunneling provides a measure of the improved ability of PET to probe bulk properties in the S metal. The ratio is equal to

$$Q(E) = \frac{L(E)}{L_s(E)} = \frac{|Z_s(E)| v_{FN}}{|Z_N(E)| v_{FS}} .$$
(3.17)

If the S metal is Nb and the N metal is Al, then at 24 mV (approximately the position of the longitudinal-acoustic phonon peak in the Nb a^2F function), $Z_S(24) \approx 2.8$, $Z_N(24) \approx 1.6$, and $v_{FN}/v_{FS} = 2/0.61$ (using the free-electron value for Al and 0.61×10^8 cm/sec for Nb),⁷ so that we estimate the ratio to be 5.8. Thus, at this energy, the PET probe averages information over a range which is 5.8 times larger than the range of the conventional tunneling probe. For an absolute comparison, note that $L_S(E) \approx 28$ Å for Nb at 24 mV in the conventional experiment, while $L(E) \approx 165$ Å in the PET case.

The situation for the A 15 compounds is even more dramatic. In these materials the coherence length is shorter than that in Nb (~400 Å) by a factor of 10. For example, in Nb₃Sn the value of v_{FS} is (for material having a T_c of 17.9 K) 0.2×10^8 cm/sec⁸ and $\lambda = Z_S(0) - 1 = 1.78$,⁹ thus, the ratio is at least [since $Z_S(E) > Z_S(0)$] equal to 11. On an absolute scale, $L_S(E)$ is thus at most (at 20 mV) of the order of 10 Å. This is to be compared to $L(20) \approx 200$ Å for an Al-Nb₃Sn PET geometry. Clearly, if metallurgical difficulties can be avoided, the PET experiment should give a far better characterization of the bulk properties of this material. Similarly, by implication, a PET study of any of the A15 metals should be intrinsically less sensitive to surface damage of the A15 metal than a conventional tunneling study.

IV. CLASSIFICATION OF SOURCES OF SPATIAL VARIATIONS AND THEIR INFLUENCES

We have demonstrated that the spatial resolution of the tunneling probe is L(E). Since the pair potentials which are probed in tunneling may differ from their bulk values within a distance of L(E)or more from the tunneling interface and/or the NS interface, one must inquire into both the source and the nature of the difference. We shall classify the sources of spatial variations into two groups: "ideal" and "nonideal" variations.

For an ideal variation, we assume that the EPI spectral function and Coulomb pseudopotential are given by their bulk values up to the interfaces. Thus, in the ideal case, spatial variations in the pair potential arise solely from the pair-density function f(E,x) and the normalized density of states N(E,x) [or, in the more general case, from the two independent components of the matrix in the large parentheses of Eq. (2.12)]. As mentioned previously, these two functions vary on the scale of a coherence length. Thus, the variation of the pair potential due to these functions is slow compared to L(E) (recall, we assume $E >> \Delta$). When assessing the influence of the spatial variations due to these functions, one must determine the degree to which they are depressed below their bulk values within L(E) of the interfaces. For example, in the bulk S metal

$$f(E,x) = \operatorname{Re}\left[\frac{\Delta_s}{\Omega_s}\right],$$
$$N(E,x) = \operatorname{Re}\left[\frac{E}{\Omega_s}\right],$$

where $\Omega_S = [E^2 - \Delta_s(E)^2]^{1/2}$. At the NS interface, in the thin N-metal limit $(d << \hbar v_{FN}/\Delta_S)$, these functions are smaller than their bulk values, and the "energy gap," meaning the energy at which these functions are sharply peaked, is below the bulk value.² As the N metal is made more thick, the depression of the pair potential at the NS interface increases.

The qualitative influence of ideal variations on the pair potential probed by tunneling is thus a uniform decrease in magnitude without any change in energy dependence, since the kernel functions are assumed to be the same at the interfaces as they are in the bulk.

For PET in the thin N-metal limit, it was shown

in Ref. 2 that the change in magnitude at the interface is of order $R\Delta_S = 2d\Delta_S / (\hbar v_{FN}) << 1$, where Δ_S is the bulk-energy gap. Thus, for ideal variations in the thin *N*-metal limit, even though the scale of variation is large compared to the resolution of the tunneling probe L(E), the size of the variation is negligibly small, so the bulk *S*-metal properties are indeed probed by the experiment to an excellent approximation.

For the conventional experimental geometry, one may employ the results of Ref. 2 to determine the degree of depression of Δ_S at the tunneling interface by identifying d as the tunnel-barrier width, setting $\Delta_N = 0$, and changing $\hbar v_{FN}$ to $i\hbar^2 K/m$ where Kd is real and large compared to unity, and m is the electron mass. The thin N-metal layer is thus converted to a thin-insulating barrier layer. The change in magnitude of Δ_S at the S-metal barrier interface is then $2d\Delta_S/(\hbar^2 K/m)$ $<<2md^2\Delta_S/\hbar^2$, which is negligibly small for d less than 40 Å or so. We conclude that in the conventional geometry as well as in the thin N-metal PET geometry, ideal variations have little influence on the pair potential measured by tunneling.

Under nonideal variations, we consider three classes: variations in $a^2(\omega, x)F(\omega, x)$ and $\mu^*(x)$ at interfaces due to (i) boundary conditions, (ii) changes in metal structure near interfaces, and (iii) imperfections near the interfaces. In the first class of nonideal variations, we confront changes in the local electron and phonon densities of states which occur solely due to the absence of translational invariance in one direction. Yaniv¹⁰ has obtained the local electron density of states at a metal-metal interface for tight-binding electrons in a simple cubic lattice. His results show that by the third atomic layer away from the interface, the local electron density of states is very close to its bulk value.

It is not difficult to use the analog of the tightbinding electron calculations of Yaniv to obtain the local *phonon* density of states at a metal-metal interface, as long as one considers only nearestneighbor coupling. One finds in this case that the local phonon density of states also reaches its bulk value within a few layers of the interface.

We may conclude from these model calculations that the first class of nonideal variations leads to a rapid change in the local EPI spectral function and Coulomb pseudopotential as one moves away from an interface. At a distance of only a few atomic layers, these functions have nearly attained their bulk values. Because this scale of variation is always much smaller than L(E), such variations have negligible effects on the measured tunneling density of states, according to the results presented in Sec. III.

In accounting for the second class of nonideal variations, we confront the possibility of a mismatch in lattice potential and structure at the interface. In this case, however, the "healing length" for the lattice structure and potential should be of the order of an atom layer or so, due to electronic screening. We conclude that the rapid changes produced by these variations will not be resolved by the tunneling probe. This leaves the third class of nonideal variations. We shall argue below that variations of this sort may lead to changes in the pair potential which are sensitively probed by a tunneling measurement, either of conventional or of thin *N*-metal PET variety.

When there is structural disorder (dislocations, vacancies, many grain boundaries) near interfaces, the "healing length" need not be the ideal value of two or three atomic layers, but may extend more than L(E) from an interface. The same remark also applies to impurities. If one metal is a metallic compound, one has the additional possibility that the metallic region adjacent to the interface is rich in one component of the compound. To be definite, we shall say that the impurities or disorder extend through a region of width h. Beyond this distance, we shall assume that the metal is in its pure, ordered bulk state. From remarks already made, it is clear that if $h \ll L(E)$, then the spatial variation in this layer will not be probed by tunneling, i.e., the energy dependence reflected by tunneling will still be characteristic of the bulk metal. We may therefore consider only the case for which h > L(E).

A layer of imperfections influences the pair potential by changing a^2F and μ^* and producing scattering. Both a^2 and μ^* may fluctuate on the scale of a lattice constant, but such rapid changes are averaged over the length L(E) in a tunneling measurement. These parameters may, however, exhibit a progressive average decrease as the interface is approached, causing the pair potential to decay accordingly.

Such decreases in the magnitude of the pair potential probed by tunneling may lead to anomalously small ratios of measured gap values to $k_B T_C$ if the extent of the imperfect layer is greater than a coherence distance (the range of the tunneling probe at the energy gap). Indeed, this condition may be difficult to avoid in certain A15 compound superconductors, because of their relatively short coherence lengths. In principle, the probe range L(E) might be increased by constructing a proximity-effect sandwich from the A15 material, thereby yielding a more bulklike result.

But the energy dependence of $a^2(\omega,x)$ and $F(\omega,x)$ is affected by the presence of imperfections as well. The origin of changes in the energy variation of $a^2(\omega,x)$ involves details of the EPI-matrix elements which are not, at present, well understood. Because of this we shall neglect the possibility of significant alterations in the energy variation of this function, and concentrate on changes in the local-phonon density of states, $F(\omega,x)$, within the layer of imperfections.

It will certainly be true that if there exists sharp Van Hove singularity-associated structure in the local phonon density of states for a pure material; then the effect of imperfections will be to broaden this structure by the introduction of a phonon lifetime. The extent of the effects of such broadening depends on the value of the phonon lifetime, $\tau_{\rm ph}(E)$, at the relevant energy. When $\hbar/\tau_{\rm ph}(E)$ is comparable to or larger than the characteristic width of the Van Hove peak structure, then such broadening will decrease the peak height as well as shift the peak to a lower energy [because $F(\omega, x)$ is normalized and the phonon spectrum has a cutoff]. In addition, the phonon lifetime is certainly a decreasing function of energy, so that the effects of imperfections will be most severe at the higher energies (corresponding to higher q values, say $q > h^{-1}$), especially those near the cutoff of the spectrum.

We conclude that nonideal variations of class III, i.e., imperfections, can significantly affect tunneling measurements of the energy-dependent pair potential when the spatial extent of the damaged region exceeds L(E). The nature of the effect is to decrease the magnitude of the pair potential measured and possibly alter the shape of the local phonon density of states, especially at energies near the phonon-spectrum cutoff.

ACKNOWLEDGMENTS

This work has been supported by NSF Grant No. DMR80-19739. The research at Ames Laboratory, operated for the U. S. Department of Energy by Iowa State University under Contract No. W-7405-Eng-82, was supported by the Director for Energy Research, Office of Basic Energy Sciences, WPAS-KC-02-02-02.

- ¹W. L. McMillan and J. M. Rowell, in *Superconductivi ty*, edited by R. Parks (Dekker, New York, 1969), p. 561.
- ²Gerald B. Arnold, Phys. Rev. B <u>18</u>, 1076 (1978).
- ³E. L. Wolf, J. Zasadzinski, J. W. Osmun, and Gerald B. Arnold, J. Low Temp. Phys. <u>40</u>, 19 (1980).
- ⁴Gerald B. Arnold, J. Zasadzinski, J. W. Osmun, and E. L. Wolf, J. Low Temp. Phys. <u>40</u>, 227 (1980).
- ⁵See, for example, W. L. McMillan, Phys. Rev. <u>175</u>, 559 (1968).

- ⁶Gerald B. Arnold, Phys. Rev. B <u>17</u>, 3576 (1978).
- ⁷B. Chakraborty, W. E. Pickett, and P. B. Allen, Phys. Rev. B <u>14</u>, 3227 (1976).
- ⁸T. P. Orlando, E. J. McNiff, Jr., S. Foner, and M. R. Beasley, Phys. Rev. B <u>19</u>, 4545 (1979).
- ⁹E. L. Wolf, Johm Zasadzinski, G. B. Arnold, D. F. Moore, J. M. Rowell, and M. R. Beasley, Phys. Rev. B <u>22</u>, 1214 (1980).
- ¹⁰A. Yaniv, Phys. Rev. B <u>17</u>, 3904 (1978).