Functional derivatives of the current jump at the superconducting gap

J. M. Coombes and J. P. Carbotte
Physics Department, McMaster University, Hamilton, Ontario L8S 4M1 Canada
(Received 22 September 1986)

A new method is developed to calculate the functional derivative of the real-axis gap function $\Delta(\omega)$ and its derivatives with frequency ω. It is tested against previous results for the functional derivative of the gap edge and applied to a calculation of the functional derivative with electron phonon $[\delta J_R/\delta\alpha^2F(\Omega)]$ and paramagnon $[\delta J_R/\delta P(\Omega)]$ spectral densities of the normalized quasiparticle current jump (J_R) at the gap edge in a tunneling junction.

I. INTRODUCTION

In a previous paper[1] we calculated within Eliashberg theory the jump, at the energy-gap voltage, in the quasiparticle current of a superconducting tunnel junction for many materials. The ratio of the jump to its weak-coupling limit, which we call J_R, is given by

$$J_R=\left[1+\frac{1}{2}\frac{d\Delta_1(\omega)}{d\omega}\bigg|_{\Delta_0}\right]^2, \tag{1}$$

where $\Delta_1(\omega)\equiv\mathrm{Re}[\Delta(\omega)]$, $\Delta(\omega)$ is the gap function for real frequencies ω and $\Delta_0=\Delta_1(\Delta_0)$ is the gap edge. Using the imaginary-axis formulation of the Eliashberg equations[2,3] with Padé approximants[4,5] we were able to determine $\Delta_1(\omega)$, its derivative and Δ_0. The results for J_R agreed well with the previous results of Harris *et al.*[6]

We now complement this work by determining the functional dependence of J_R on small changes in the electron-phonon spectral density $\alpha^2F(\Omega)$ and in the paramagnon spectral density $P(\Omega)$. The functional derivative shows which phonon or paramagnon frequencies in the spectral density influence the size of J_R the most. To do this we introduce in Sec. II a new method for calculating functional derivatives of functions of the gap. We derive new equations for the infinitesimal part of the perturbed Matsubara gaps. The infinitesimal part is basically the functional derivative of the gap. We obtain a set of inhomogeneous linear algebraic equations with the kernel and the inhomogeneous term dependent only on the unperturbed gaps and on $\alpha^2F(\Omega)$ and $P(\Omega)$. In Sec. III the analytic continuation from the functional derivatives of the Matsubara gaps to the real frequency axis is discussed and is based on Padé approximants.[7,8] In Sec. IV our new method is tested against the previous results of Mitrović *et al.*[7] for the gap edge although this is not the quantity of primary interest here. These authors carry out two separate calculations, one for the pure spectral density and another with its weight augmented by a small δ function like amount around some specific frequency. The comparison is successful and we proceed to calculate the functional derivative of the normalized jump for Pb, Nb_3Sn, V, Nb, V_3Si, and Nb_3Ge. As a further test, the brute force method of Mitrović *et al.*[7] is extended to the current jump and compared with our results for Pb and Nb_3Sn. In Sec. V we give a summary and draw conclusions.

II. DERIVATION OF BASIC EQUATIONS

In this section we derive a new method for calculating the functional derivative of functions of $\Delta(\omega)$. To begin we use a form of the imaginary-axis Eliashberg equations which combines the usual two[7,8] into one equation with the summation ranging from 1 to a cutoff N_c determined by the Coulomb repulsion pseudopotential μ^*:

$$\bar{\Delta}_n\left[(2n-1)+\sum_{m=1}^{N_c}[\lambda^+(n-m)-\lambda^+(n+m-1)]\frac{1}{(1+\bar{\Delta}_m^2)^{1/2}}\right]=\sum_{m=1}^{N_c}[\lambda^-(n-m)+\lambda^-(n+m-1)-2\mu^*]\frac{\bar{\Delta}_m}{(1+\bar{\Delta}_m^2)^{1/2}}\ . \tag{2}$$

The imaginary-axis gap function $\Delta_n\equiv\Delta(i\omega_n)$ is related to $\bar{\Delta}_n$ by

$$\bar{\Delta}_n=\Delta_n/|\omega_n| \tag{3}$$

where

$$i\omega_n\equiv i(2n-1)\pi T\quad(n=0,\pm1,\pm2,\ldots) \tag{4}$$

are the Matsubara frequencies at temperature T. For convenience we have set $k_B=\hbar=1$. The electron-phonon and paramagnon spectral densities enter via the parameters

$$\lambda^{\pm}(n-m)\equiv\int_0^\infty d\Omega[\alpha^2F(\Omega)\pm P(\Omega)]\times\frac{2\Omega}{\Omega^2+(2\pi T)^2(n-m)^2}\ . \tag{5}$$

We note that, for the electron-phonon part alone of

$\lambda^{\pm}(n-m)$, the $n=m$ term drops out of Eq. (2) because it appears once on each side of the equation with the *same* sign. In contrast, for the paramagnon part, $\lambda^{+}(n-m)$ appears on one side and $\lambda^{-}(n-m)$ on the other resulting in opposing signs so that no cancellation can occur for the term $n=m$. This is very important because it implies that if we add an infinitesimal part $\epsilon\delta(\Omega-\Omega_0)$ at frequency Ω_0 with $\epsilon\to 0$ to the electron-phonon part, nothing happens to the gap functions as $\Omega_0\to 0$ because the change in $\lambda^{\pm}(n-m)$ for $n=m$ does not appear and for $n\neq m$ it is

$$\epsilon\frac{2\Omega_0}{\Omega_0^2+(2\pi T)^2(n-m)^2}, \quad n\neq m$$

which goes to zero as $\Omega_0\to 0$. This means that adding phonons at $\Omega_0=0$ does not affect the superconductivity in any way. On the other hand, a very different result arises when an infinitesimal term is added to the paramagnon spectral density. It leads to a $1/\Omega_0$ divergence in Eq. (2) from the term $\lambda^{\pm}(n-m)$ with $n=m$.

The functional derivative of a functional F of $G(\Omega)$ at some frequency Ω_0 is defined as

$$\frac{\delta F}{\delta G(\Omega_0)}=\lim_{\epsilon\to 0}\frac{1}{\epsilon}\{F[G(\Omega)+\epsilon\delta(\Omega-\Omega_0)]-F[G(\Omega)]\}\,|_t\ , \tag{6}$$

where $G(\Omega)$ is the spectrum, $\alpha^2F(\Omega)$ or $P(\Omega)$, in which one is interested and $t=T/T_c$ is the fraction of the critical temperature, T_c, at which one is working. Ordinarily for $F=\Delta(\omega)$ one wants the $t=0$ results, however these are impossible to attain with the imaginary axis equation, instead we work with $t\ll 1$ (usually $t=0.1$) and assume that $\Delta(\omega,T=tT_c)$ is very similar to $\Delta(\omega,T=0)$ for the frequency range ω of interest.

From Eq. (2) we note that $\bar{\Delta}_n$ is an explicit function of $G(\Omega)$ through the factors $\lambda^{\pm}$ as well as being a function of temperature T. When we keep the temperature fixed we will denote the variation in $\bar{\Delta}_n$ by $\delta\bar{\Delta}_n/\delta G(\Omega)$. It satisfies the equation

$$\sum_m H_{n,m}\frac{\delta\bar{\Delta}_m}{\delta G(\Omega)}=h_n \tag{7}$$

with

$$H_{n,m}=\delta_{n,m}\left[\frac{\omega_n}{\pi T}+\sum_{m'}[\lambda^{+}(n-m')-\lambda^{+}(n+m'-1)]\frac{1}{(1+\bar{\Delta}_{m'}^2)^{1/2}}\right]-\bar{\Delta}_n[\lambda^{+}(n-m)-\lambda^{+}(n+m-1)]\frac{\bar{\Delta}_m}{(1+\bar{\Delta}_m^2)^{3/2}}-[\lambda^{-}(n-m)+\lambda^{-}(n+m-1)-2\mu^*]\frac{1}{(1+\bar{\Delta}_m^2)^{3/2}}\ . \tag{8}$$

Note that this quantity can be constructed explicitly from the solution of the Eliashberg equation (2) and a knowledge of $\alpha^2F(\Omega)$ and $P(\Omega)$. In Eq. (7)

$$h_n=\sum_m\frac{2\Omega_0}{\Omega_0^2+(2\pi T)^2(n-m)^2}\frac{\{-\bar{\Delta}_n\pm\bar{\Delta}_m\}}{(1+\bar{\Delta}_m^2)^{1/2}}+\sum_m\frac{2\Omega_0}{\Omega_0^2+(2\pi T)^2(n+m-1)^2}\left[\frac{\bar{\Delta}_n\pm\bar{\Delta}_m}{(1+\bar{\Delta}_m^2)^{1/2}}\right] \tag{9}$$

which is also known once we have solutions to Eq. (2). Thus Eq. (7) is completely determined and yields $\delta\bar{\Delta}_m/\delta G(\Omega)$.

On the other hand, we can think of $\bar{\Delta}_n$ as an explicit function of $G(\Omega)$ and of $T=tT_c$ and consider keeping t constant rather than T. In this case we can write and complete variation as

$$\frac{\delta\bar{\Delta}_n}{\delta G(\Omega)}=\frac{\delta\bar{\Delta}_n}{\delta G(\Omega)}+\frac{\partial\bar{\Delta}_n}{\partial T}t\frac{\delta T_c}{\delta G(\Omega)}\ , \tag{10}$$

where $T(\partial\bar{\Delta}_n/\partial T)$ satisfies the equation

$$\sum_m H_{n,m}T\frac{\partial\bar{\Delta}_m}{\partial T}=g_n\ , \tag{11}$$

with

$$g_n=\sum_m[\Delta\lambda^{+}(n-m)-\Delta\lambda^{+}(n+m-1)]\frac{\bar{\Delta}_n}{(1+\bar{\Delta}_m^2)^{1/2}}-\sum_m[\Delta\lambda^{-}(n-m)+\Delta\lambda^{-}(n+m-1)]\frac{\bar{\Delta}_m}{(1+\bar{\Delta}_m^2)^{1/2}}\ , \tag{12}$$

where by definition

$$\Delta\lambda^{\pm}(n-m)=4\int_0^{\infty}d\Omega\frac{[\alpha^2F(\Omega)\pm P(\Omega)]\Omega}{[\Omega^2+(2\pi T)^2(n-m)^2]^2}\times(2\pi T)^2(n-m)^2\ . \tag{13}$$

As with h_n the new quantities g_n are known from solutions to Eq. (2) and the spectral densities for the material of interest. We note finally that the equation for $\delta\bar{\Delta}_n/\delta G(\Omega)$ is

$$\sum_m H_{n,m}\frac{\delta\bar{\Delta}_m}{\delta G(\Omega)}=h_n+g_n\frac{1}{T_C}\frac{\delta T_c}{\delta G(\Omega)}\ , \tag{14}$$

which involves explicitly the functional derivative of the critical temperature. This is a well known quantity since the pioneering work of Bergmann and Rainer[9,10] to whose work we refer for the appropriate formula. The formal solution to Eq. (14) is given by

$$\frac{\delta\bar{\Delta}_n}{\delta G(\Omega)}=\sum_m H_{n,m}^{-1}\left[h_m+g_m\frac{1}{T_c}\frac{\delta T_c}{\delta G(\Omega)}\right]\ . \tag{15}$$

We have generalized our original Eliashberg programs to compute $\delta\bar{\Delta}_n/\delta G(\Omega)$ in addition to Δ_n and want to construct from this information the functional derivative of the gap function $\Delta(\omega T)$ for real frequencies, namely $\delta\Delta(\omega,T)/\delta G(\Omega)$. This is the subject of Sec. III.

III. THE ANALYTIC CONTINUATION

We need now to analytically continue to the real frequency axis. First, we note that the $\bar{\Delta}_n$'s used in our numerical work are related to the Δ_n's by $\bar{\Delta}_n\omega_n=\Delta_n$ for positive n with the analytic continuation of Δ_n being $\Delta(\omega,T)$. Thus we have

$$\frac{\delta\Delta_n}{\delta G(\Omega)}=\omega_n\frac{\delta\bar{\Delta}_n}{\delta G(\Omega)}+\frac{\Delta_n}{T_c}\frac{\delta T_c}{\delta G(\Omega)} \ . \tag{16}$$

The Matsubara gaps for the system with the added piece $\epsilon\delta(\Omega=\Omega_0)$ are denoted by $\Delta'(i\omega_n')$ and related to those with $\epsilon=0$ by the equation

$$\Delta'(i\omega_n')=\Delta(i\omega_n)+\epsilon\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)} \ . \tag{17}$$

For t constant, T' and T are related by the ratio $(\delta T_c+T_c)/T_c=1+(\delta T_c/T_c)$ with $\delta T_c=\epsilon[\delta T_c/\delta G(\Omega)]$ so that we can write

$$\Delta'(i\omega_n)=\Delta[i\omega_n/(1+\delta T_c/T_c)]+\epsilon\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)} \ . \tag{18}$$

Both sides can now be analytically continued to get

$$\Delta'(\omega,T)=\Delta\left[\omega\left[1-\frac{\delta T_c}{T_c}\right],T\right]+\epsilon\mathcal{A}\left[\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)}\right] , \tag{19}$$

where the last term stands for analytical continuation using, in our case, Padé approximants. We get, on expanding (19)

$$\Delta'(\omega,T)=\Delta(\omega,T)-\omega\frac{\partial\Delta(\omega,T)}{\partial\omega}\frac{\delta T_c}{T_c}+\epsilon\mathcal{A}\left[\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)}\right] . \tag{20}$$

For a fixed value of ω this last equation tells us that on rearranging terms

$$\frac{\delta\Delta(\omega,T)}{\delta G(\Omega)}=\mathcal{A}\left[\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)}\right]-\omega\frac{\partial\Delta(\omega,T)}{\partial\omega}\frac{1}{T_c}\frac{\delta T_c}{\delta G(\Omega)} \ . \tag{21}$$

Also the gap $\Delta_0'=\Delta_0+\epsilon[\delta\Delta_0/\delta G(\Omega)]$ is obtained from the equation

$$\Delta_0'=\mathrm{Re}\Delta'(\omega=\Delta_0',T)\equiv\Delta_1'(\omega=\Delta_0',T) \tag{22}$$

which leads to

$$\frac{\delta\Delta_0}{\delta G(\Omega)}\equiv\Delta'(\Delta_0')-\Delta(\Delta_0)=\frac{\mathcal{A}_1\left[\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)}\right]\Big|_{\Delta_0}-\Delta_0\frac{\partial\Delta_1(\omega,T)}{\partial\omega}\Big|_{\Delta_0}\frac{1}{T_c}\frac{\delta T_c}{\delta G(\Omega)}}{\left[1-\frac{\partial\Delta_1(\omega,T)}{\partial\omega}\Big|_{\Delta_0}\right]} \ , \tag{23}$$

where $\mathcal{A}_1$ is the real part of the analytic continuation $\mathcal{A}$. This last formula can be evaluated directly in our programs which gives us $\mathcal{A}[\delta\Delta(i\omega_n)/\delta G(\Omega)]$ and $\Delta(\omega,T)$ through Padé approximants techniques. For this we follow the method of Vidberg and Serene.[4] The N-point Padé approximant to a complex function $u(z)$ of the complex variable z, whose N values u_i $(i=1,\ldots,N)$ are given at N complex points z_i $(i=1,\ldots,N)$ is defined[4,5] as a continued fraction:

$$C(N;\omega,T)=\cfrac{a_1}{1+\cfrac{a_2(\omega-z_1)}{1+\cfrac{a_3(\omega-z_2)}{1+\cfrac{\cdots a_{N-1}(\omega-z_{N-2})}{1+a_N(\omega-z_{N-1})}}}} \tag{24}$$

such that

$$C(N;z_i,T)=u_i, \quad i=1,\ldots,N \ . \tag{25}$$

The coefficients a_i are then given by the recursion

$$a_i=g_i(z_i), \quad g_1(z_i)=u_i, \quad i=1,\ldots,N \tag{26}$$

$$g_p(z)=\frac{g_{p-1}(z_{p-1})-g_{p-1}(z)}{(z-z_{p-1})g_{p-1}(z)}, \quad p\geq 2 \ . \tag{27}$$

It can be shown that

$$C(N;\omega,T)=\frac{A_N(\omega)}{B_N(\omega)} \ ,$$

where A_N and B_N are polynomials give by the recursion

$$A_{n+1}(\omega)=A_n(\omega)+(\omega-z_n)a_{n+1}A_{n-1}(\omega) \qquad n=1,2,\ldots,N-1 \tag{28}$$

$$B_{n+1}(\omega)=B_n(\omega)+(\omega-z_n)a_{n+1}B_{n-1}(\omega) \qquad n=1,2,\ldots,N-1$$

and

$$A_0=0, \quad A_1=a_1, \quad B_0=B_1=1 \ . \tag{29}$$

While formula (23) is the most useful for our work it can be rewritten in another way which is sometimes good for the purpose of discussion. Substituting (21) into (23) leads to

$$\frac{\delta\Delta_0}{\delta G(\Omega)}=\frac{\frac{\delta\Delta_1(\omega,T)}{\delta G(\Omega)}\Big|_{\Delta_0}}{\left[1-\frac{\partial\Delta_1(\omega,T)}{\partial\omega}\Big|_{\Delta_0}\right]} \ , \tag{30}$$

but at constant t we can rewrite

$$\frac{\delta\Delta_1(\omega,T)}{\delta G(\Omega)}=\frac{\delta\Delta_1(\omega,T)}{\delta G(\Omega)}+\frac{\partial\Delta_1}{\partial T}t\frac{\delta T_c}{\delta G(\Omega)} \tag{31}$$

leading to

$$\frac{\delta\Delta_0}{\delta G(\Omega)}=\frac{\left.\frac{\delta\Delta_1(\omega,T)}{\delta G(\Omega)}\right|_{\Delta_0}+T\left.\frac{\partial\Delta_1(\omega,T)}{\partial T}\right|_{\Delta_0}\frac{1}{T_c}\frac{\delta T_c}{\delta G(\Omega)}}{\left[1-\left.\frac{\partial\Delta_1(\omega,T)}{\partial\omega}\right|_{\Delta_0}\right]} . \tag{32}$$

This last formula involves the temperature derivative of the real gap $\partial\Delta_1(\omega,T)/\partial T$ which is not evaluated directly here. If we assume that it is finite, however, we see from (32) that the second term drops out as $T\to 0$ because it contains an explicit factor of temperature leaving us with the formula

$$\frac{\delta\Delta_0}{\delta G(\Omega)}=\frac{\left.\frac{\delta\Delta_1(\omega,T)}{\delta G(\Omega)}\right|_{\Delta_0}}{\left[1-\left.\frac{\partial\Delta_1(\omega,T)}{\partial\omega}\right|_{\Delta_0}\right]}, \quad T\to 0 . \tag{33}$$

This tells us that at low temperature it does not matter whether we keep T or t constant as we would expect. Our numerical work confirms this as well and suggests that working with $t=0.1$ is good enough.

To obtain the functional derivative of J_R first note that

$$\frac{\delta J_R}{\delta G(\Omega)}=J_R^{1/2}\frac{\delta}{\delta G(\Omega)}\left[\left.\frac{d\Delta_1(\omega)}{d\omega}\right|_{\Delta_0}\right] . \tag{34}$$

To find the functional derivative of $[d\Delta_1(\omega)/d\omega]|_{\Delta_0}$ we simply take the derivative with respect to ω of both sides of the real part of (20), evaluate at Δ_0', and expand to first order in ϵ. This gives

$$\begin{aligned}\frac{\delta}{\delta G(\Omega)}\left[\left.\frac{d\Delta_1(\omega)}{d\omega}\right|_{\Delta_0}\right]=&\left[\left.\frac{d}{d\omega}\mathcal{A}_1\left[\frac{\delta\Delta(i\omega_n)}{\delta G(\Omega)}\right]\right]\right|_{\Delta_0}+\left.\frac{d^2\Delta_1(\omega,T)}{d\omega^2}\right|_{\Delta_0}\left.\frac{\delta\Delta_0}{\delta G(\Omega)}\right|_{\Omega_0}\\&-\left[\left.\frac{d\Delta_1(\omega,T)}{d\omega}\right|_{\Delta_0}+\Delta_0\left.\frac{d^2\Delta_1(\omega,T)}{d\omega^2}\right|_{\Delta_0}\right]\frac{1}{T_c}\left.\frac{\delta T_c}{\delta G(\Omega)}\right|_{\Omega_0} .\end{aligned} \tag{35}$$

IV. RESULTS

In this section we present results for Pb, Nb_3Sn, V, Nb, V_3Si, and Nb_3Ge. As a check, the results for Pb and Nb_3Sn are compared to those found using the method of Mitrović *et al.*[7] In that method the Eliashberg equations are solved for a given material spectrum and $\Delta(\omega)$ determined. Next the equations are solved again but with a δ function of finite weight A added to either $\alpha^2F(\Omega)$ or $P(\Omega)$, as desired, at some frequency Ω. The critical temperature is found by keeping μ^* unchanged. At the same reduced temperature t, the new $\Delta'(\omega)$ is determined. The difference between the gap edges, or between the derivatives at the gap edge, divided by A gives the approximate functional derivative of each of those quantities. Of course A must be small enough that there is an approximately linear dependence on A. To check the linearity two or more values of A must be used for each frequency Ω. The main advantage of the method proposed in Secs. II and III is that only one calculation need be done for each value of Ω. As well, decisions on a choice of A and on how constant the functional derivative is with varying A are no longer present. We will not present results for $\delta\Delta_0/\delta G(\Omega)$ as we found that the results from the two methods agreed to within approximately 2% and because the Mitrović *et al.*[7] paper thoroughly discusses that functional derivative. We note that 2% is the level of agreement that is obtained when the direct ("brute force") method of Mitrović *et al.*[7] is applied to the calculation of the functional derivative of the critical temperature and compared with the results for the same quantity based on the analytic formulas given in Bergmann and Rainer.[9]

The comparison for $\delta\ln J_R/\delta\alpha^2F(\Omega)$ as a function of Ω/T_c is given in Fig. 1 and for $\delta\ln J_R/\delta P(\Omega)$ in Fig. 2. The solid and dashed curves in each figure were obtained using formulas (34) and (35) of Sec. III while the $\times$'s represent results of direct calculations ("brute force"). That is, J_R is calculated twice, once for the desired spec-

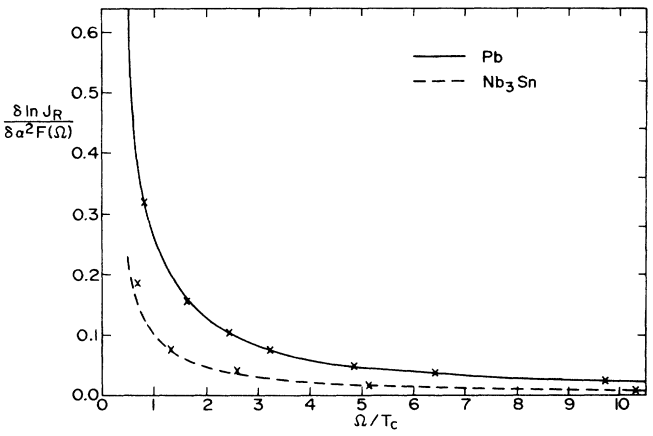

FIG. 1. The functional derivative, with respect to $\alpha^2F(\Omega)$, the electron-phonon spectral density, of the ratio of the jump, at the gap edge Δ_0, in the quasiparticle current of a superconducting tunnel junction to its weak coupling limit, $\delta\ln J_R/\delta\alpha^2F(\Omega)$, plotted against Ω/T_c for Pb (solid line) and Nb_3Sn (dashed line) using the method of Secs. II and III of this paper. For comparison, values of $\delta\ln J_R/\delta\alpha^2F(\Omega)$ determined by an extension of the method of Mitrović *et al.* (Ref. 7) are also given ($\times$).

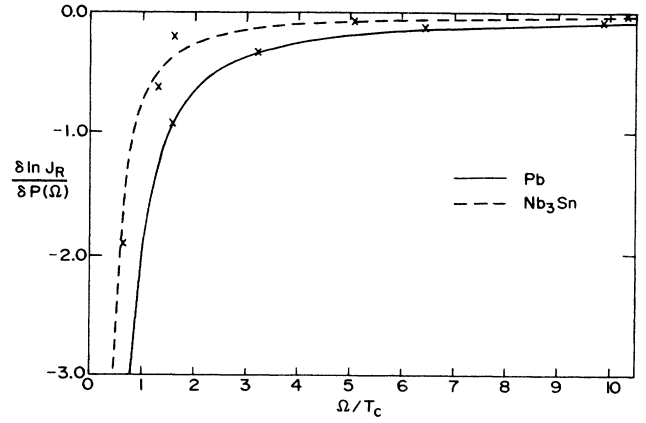

FIG. 2. Same as Fig. 1, but for the functional derivative with respect to $P(\Omega)$, the paramagnon spectral density.

trum and again for an augmented spectrum with a delta function of small weight A added. As might be expected, since the derivative is much smaller than for the gap edge and by the nature of the analytic continuation less accurate, the difference between the two methods is greater, roughly 5%. In Nb_3Sn, for the $P(\Omega)$ functional derivative, the difference at the low frequencies is actually worse, about 10%, but at these frequencies the linear dependence on A was not as consistent as at higher frequencies or as in Pb. In fact, the figure of 5% also describes the consistency of the values of $\delta J_R/\delta G(\Omega)$ found by the method of Mitrović *et al.*[7] due to a lack of linearity in results as a function of the weight A.

In Figs. 3 and 4 we show results for $\delta \ln J_R/\delta\alpha^2F(\Omega)$ and $\delta \ln J_R/\delta P(\Omega)$, respectively, for V, Nb, V_3Si, and Nb_3Ge. For reasons of numerical accuracy we were not able to calculate values at the very lowest values of Ω/T_c. The method of Mitrović *et al.*[7] also has this problem but at even higher frequencies. This deficiency is unfortunate, for as can be seen, it is the phonons of frequency about $\Omega \simeq 0.25T_c$ that influences J_R the most. On the other hand the very low ω region corresponds to the sound regime where the phonon frequency distribution is very small for any physical situation. It is therefore of little physical interest. Since we know from our previous discussion that the Matsubara gaps and consequently $\delta \ln J_R/\delta\alpha^2F(\Omega)$ will go to zero as $\Omega \to 0$ we expect the curve to peak somewhere below $0.25T_c$ and then drop towards zero. The peak is resolved only in the case of V. While we could have attempted to increase accuracy at low ω we felt it was of no physical interest to do so. The large values obtained for $\delta \ln J_R/\delta\alpha^2F(\Omega)$ at and above $\Omega/T_c \simeq 0.25$ suggests that shifting phonon weight to these lower frequencies should increase the jump appreciably, a result that could be tested experimentally.

On comparing various materials the magnitude of the curves obtained correlates well with the strength of the material's' electron-phonon coupling; the weaker this coupling, the larger the functional derivative. This is similar to what was found for $\delta \ln T_c/\delta\alpha^2F(\Omega)$

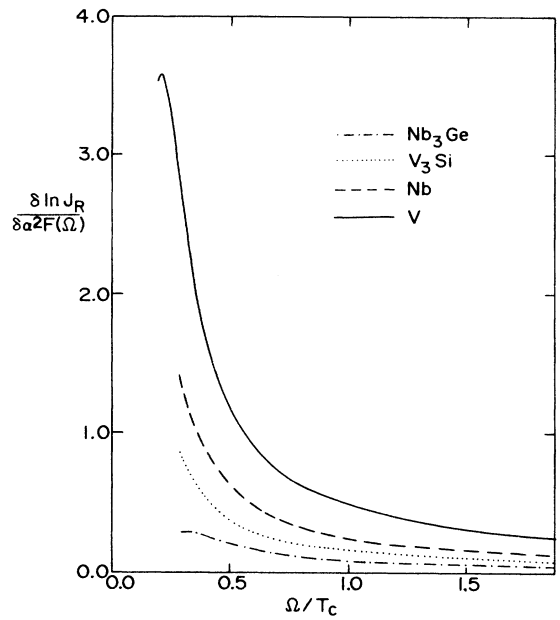

FIG. 3. Plots of $\delta \ln J_R/\delta\alpha^2F(\Omega)$ vs Ω/T_c for V (solid line), Nb (dashed line), V_3Si (dotted line), and Nb_3Ge (dashed-dotted line).

and $\delta \ln \Delta_0/\delta\alpha^2F(\Omega)$. The major difference of $\delta \ln J_R/\delta\alpha^2F(\Omega)$ compared to $\delta \ln T_c/\delta\alpha^2F(\Omega)$ and $\delta \ln \Delta_0/\delta\alpha^2F(\Omega)$ is that the peaks occur at considerably smaller frequencies. The heights of the peaks are also several times larger than those of $\delta \ln T_c/\delta\alpha^2F(\Omega)$ or $\delta \ln \Delta_0/\delta\alpha^2F(\Omega)$. The curves for $\delta \ln J_R/\delta P(\Omega)$ differ lit-

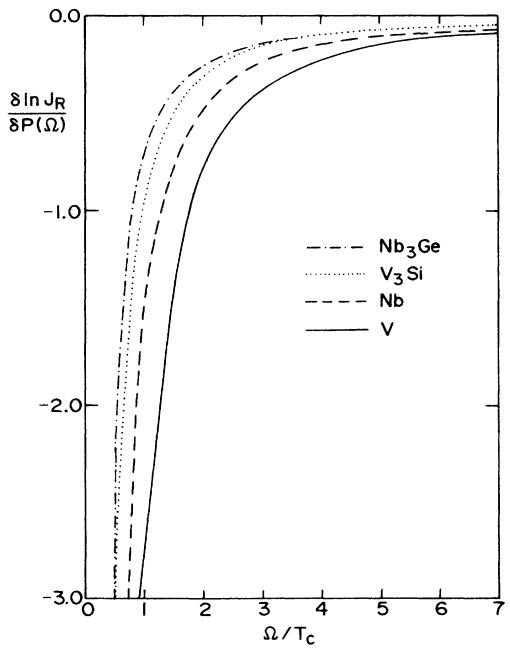

FIG. 4. Same as Fig. 3 but for $\delta \ln J_R/\delta P(\Omega)$.

tle from $\delta \ln T_c/\delta P(\Omega)$ and $\delta \ln \Delta_0/\delta P(\Omega)$. The curves start from zero at $\Omega/T_c=\infty$ and smoothly approach $-\infty$ at $\Omega/T_c=0$. In general, weaker coupling the material, the faster it falls to infinity, at least in the range shown. This is the same behavior as $\delta \ln T_c/\delta P(\Omega)$ and $\delta \ln \Delta_0/\delta P(\Omega)$. The only difference is again in the sensitivity, at a given Ω/T_c the absolute value of $\delta \ln J_R/\delta P(\Omega)$ is several times larger than $\delta \ln T_c/\delta P(\Omega)$ or $\delta \ln \Delta_0/\delta P(\Omega)$.

V. CONCLUSIONS

We have developed a new method for calculating the functional derivative of the gap $\Delta(\omega)$ on the real frequency axis and of its derivative with respect to frequency ω. The method is based on imaginary axis equations that deal directly with the change in the Matsubara gaps $\Delta(i\omega_n)$ with spectral weight $G(\Omega)$ namely $\delta\Delta(i\omega_n)/\delta G(\Omega)$. Here $G(\Omega)$ can be the electron-phonon $[\alpha^2F(\Omega)]$ or the paramagnon spectral density $[P(\Omega)]$. The coefficients in our equations, which are a set of linear inhomogeneous algebraic equations, require only the material parameters of the particular superconductor under consideration and the solutions of the Eliashberg equations at the Matsubara energies. The functional derivative of the gap edge on the real axis $\delta\Delta_0/\delta G(\Omega)$ then follows on analytical continuation of the $\delta\Delta(i\omega_n)/\delta G(\Omega)$ and $\Delta(i\omega_n)$ which is accomplished by the method of Padé approximates. Comparison with results obtained by the brute force method of Mitrović *et al.*[7] shows that our new method is accurate in all cases considered while it is much faster and more direct.

We have used our new methods to calculate $\delta \ln J_R/\delta\alpha^2F(\Omega)$ and $\delta \ln J_R/\delta P(\Omega)$ as a function of Ω/T_c for Pb, Nb_3Sn, V, Nb, V_3Si, and Nb_3Ge, where J_R is the normalized jump in the current at the gap edge (Δ_0) in a tunneling junction. To our knowledge this quantity has never before been calculated. Although, for reasons of numerical accuracy, we were not able to continue our calculations beyond $\Omega/T_c \simeq 0.25$ at which point $\delta \ln J_R/\delta\alpha^2F(\Omega)$ is still rising as Ω is lowered (except for V), we argue that the curve starts from zero at $\Omega/T_c=0$ increases to a maximum at some approximately universal value of Ω/T_c and then decrease to zero at infinity. This shape for $\delta \ln J_R/\delta\alpha^2F(\Omega)$ is similar to that previously found for $\delta \ln T_c/\delta\alpha^2F(\Omega)$ and $\delta \ln \Delta_0/\delta\alpha^2F(\Omega)$ but the magnitude is greater and the peak is at much lower frequencies $\lesssim 0.25T_c$. In general, weaker coupling materials have higher values of $\delta \ln J_R/\delta\alpha^2F(\Omega)$ indicating that in weak coupling materials J_R is more sensitive to a given small change in $\alpha^2F(\Omega)$ than is the case for strong coupling materials.

Our results for the functional derivative of the current jump at the gap edge with electron-paramagnon spectral density $P(\Omega)$ are even more similar to its $\delta \ln T_c/\delta P(\Omega)$ and $\delta \ln \Delta_0/\delta P(\Omega)$ counterparts. The curves start at zero at infinite frequency, are negative for all finite frequency increasing steadily in absolute value and diverging as $1/\Omega$ for $\Omega \to 0$. This indicates that paramagnons of any frequency reduce the jump J_R with the lowest frequencies having proportionally the largest effect.

ACKNOWLEDGMENT

This research was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC).

[1] J. M. Coombes and J. P. Carbotte, Phys. Rev. B **34**, 4622 (1986).

[2] G. M. Eliashberg, Zh. Eksp. Teor. Fiz. **38**, 966 (1960) [Sov. Phys.—JETP **11**, 696 (1960)]; **39**, 1437 (1961) [**12**, 1000 (1961)].

[3] P. B. Allen and B. Mitrović, in *Solid State Physics,* edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1982), Vol. 37, p. 1.

[4] H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. **29**, 179 (1977).

[5] B. Mitrović, H. G. Zarate, and J. P. Carbotte, Phys. Rev. B **29**, 184 (1984).

[6] R. E. Harris, R. C. Dynes, and D. M. Ginsberg, Phys. Rev. **14**, 993 (1976).

[7] B. Mitrović, C. R. Leavens, and J. P. Carbotte, Phys. Rev. B **21**, 5048 (1980).

[8] J. M. Daams and J. P. Carbotte, J. Low Temp. Phys. **40**, 135 (1980).

[9] G. Bergmann and D. Rainer, Z. Phys. **263**, 59 (1973).

[10] D. Rainer and G. Bergmann, J. Low Temp. Phys. **14**, 501 (1974).