NOTIZEN

The Inversion of the Tunneling Conductance Formula

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Inversion formulas are given for determining the density of states by tunneling conductance measurements.

The finite-temperature tunneling current between two metals with densities of states $N_1(x)$ and $N_2(x)$ is proportional to

$$I(v) \propto \int_{-\infty}^{+\infty} dx\, N_1(x)\, N_2(x+v)\, \big(f(x) - f(x+v)\big) \quad (1)$$

where $f(x)$ denotes the Fermi function.

When one of the two metals has a slowly-varying density of states at the Fermi level the normalized tunneling conductance can be written as

$$\sigma(v) = \frac{dI/dv}{\langle dI/dv \rangle} = \frac{1}{4T} \int_{-\infty}^{+\infty} dx\, N(x)\, \mathrm{sech}^2 \frac{x+v}{2T}. \quad (2)$$

The density of states is connected with the single-particle Green's function via [1]

$$N(x) = -\frac{1}{\pi}\, \mathrm{sign}(x-\mu) \int d^3\boldsymbol{r}\, \mathrm{Im}\, G(\boldsymbol{r}, \boldsymbol{r}, x). \quad (3)$$

In terms of the retarded and advanced Green's functions, which are analytic in the upper and lower half planes respectively, the density of states is given as

$$N(x) = \frac{1}{2\pi i} \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \big(G_A(\boldsymbol{p}, x) - G_R(\boldsymbol{p}, x)\big). \quad (4)$$

The tunneling conductance can be represented by the difference of the two functions

$$\sigma_{R,A}(v) = \frac{1}{8\pi i T} \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \int_{-\infty}^{+\infty} dx\, G_{R,A}(\boldsymbol{p}, x)\, \mathrm{sech}^2 \frac{x+v}{2T}. \quad (5)$$

The hyperbolic secant is a meromorphic function with simple poles on the imaginary axis. Making use of the relation

$$\pi^2 \mathrm{sech}^2 \pi x = \psi'(\tfrac{1}{2} + i x) + \psi'(\tfrac{1}{2} - i x) \quad (6)$$

where $\psi'(x)$ is the first derivative of the digamma function, which has poles on the negative real axis, we get

$$\sigma_{R,A}(v) = \frac{T}{(2\pi)^3 i} \int \frac{d^3\boldsymbol{p}}{(2\pi)^3} \int_{-\infty}^{+\infty} dx\, G_{R,A}(\boldsymbol{p}, x)\, \psi'\left(\frac{1}{2} \pm i \frac{v+x}{2\pi T}\right). \quad (7)$$

The sign in the argument of the digamma function stands for the retarded and advanced case respectively. We have here omitted that part of the integrand which has no poles in the analytical region of $G_A(G_R)$ and gives no contribution to $\sigma_R(\sigma_A)$. Applying the functional equation

$$\psi'(x) - \psi'(1+x) = x^{-2} \quad (8)$$

we find

$$\sigma(x + i\pi T) - \sigma(x - i\pi T) = 2\pi i T\, (dN/dx). \quad (9)$$

Another inversion formula is obtained by expanding (9) in powers of temperature and integration over v

$$N(v) = \sigma(v) - \frac{(\pi T)^2}{3!} \frac{d^2\sigma}{dv^2} + \frac{(\pi T)^4}{5!} \frac{d^4\sigma}{dv^4} \mp \dots \quad (10)$$

In the general case of the formula (1) the density of states of the one metal can be obtained by means of Fourier transform when that of the other is known. Performing (1) we find

$$I(v)\, \mathrm{cosech}(v/2T) \propto \int_{-\infty}^{+\infty} dx\, N_1(x)\, \mathrm{sech}(x/2T) \cdot N_2(x+v)\, \mathrm{sech}\big((x+v)/2T\big). \quad (11)$$

This equation can be solved by Fourier transformation [2].

$$\mathcal{I}(y) \propto \mathcal{N}_1(y) \cdot \mathcal{N}_2(y),$$
$$\mathcal{N}_{1,2}(y) = \int_{-\infty}^{+\infty} dx\, e^{ixy} N_{1,2}(x)\, \mathrm{sech}(x/2T), \quad (12)$$
$$\mathcal{I}(y) = \int_{-\infty}^{+\infty} dx\, e^{ixy} I(x)\, \mathrm{cosech}(x/2T).$$

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[1] A. A. ABRIKOSOV, L. P. GORKOV, and I. YE. DZYALOSHINSKII, Quantum Field Theoretical Methods in Statistical Physics, Pergamon Press, New York 1965.

[2] E. C.. TITCHMARSH, Introduction to the Theory of Fourier Integrals, Oxford 1959.