Exact Results for the Kondo Problem: One-Body Theory and Extension to Finite Temperature

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Nozières and De Dominicis's one-body theory of the x-ray singularity is extended to the Kondo effect, and also to the finite-etmperature case. The Kondo problem is shown to be equivalent to the thermodynamics of charged rods moving on a circle, or to that of an Ising model with inverse-square interaction.

I. INTRODUCTION

THE substance of the present paper is an extension to the Kondo problem and to the finite temperatures of methods originally developed for another problem, known as the "x-ray problem." This has to do with the absorption of an x-ray photon by creating a deep hole, or the subsequent reemission when the hole is annihilated. The problem to be dealt with is how the response of the Fermi gas modifies this process; the hole is assumed to be completely immobile.

Mahan,[1] by a diagram summation, conjectures that the usual absorption edge becomes an $(E-E_0)^{-\epsilon}$ singularity (see Fig. 1), where ϵ depends on the electron-hole interaction strength. Fourier transforming, we find a $t^{-1-\epsilon}$ time decay, so that the hole lifetime is larger by a *time-dependent* factor of t^{ϵ} than it would be without the electron-hole interaction. The infinite lifetime at $t=\infty$ is what we expect from the Anderson infrared catastrophe[2] once the electron gas has adapted completely to the hole potential. The t^{ϵ} behavior was also conjectured by Anderson, and can also be obtained, at least to a crude approximation, by this approach: A measurement taking at time t can only give energies to within $\hbar/t$, and if we assume a Fermi surface smeared to that extent, a t^{ϵ} increase in lifetime (i.e., decrease in matrix elements) is obtained.

Nozières and Roulet and Gavoret[3,4] used Abrikosov's "drone-fermion" techniques[5] for this problem. This calculation confirms Mahan's $x^{-\epsilon}$ singular behavior.

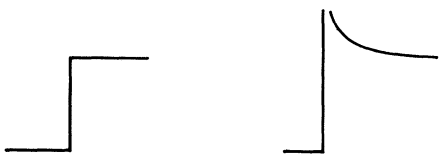

FIG. 1. Step-function and $(E-E_0)^{\delta}$ spectra.

It should be noted that Schotte and Schotte[6,7] have derived most of the results of this paper, using the Tomonaga model.[8] The Tomonaga model provides a useful physical feeling for the effects, but in our opinion its logical foundation is sufficiently mysterious that confirmation by other methods is important (see also Ferrell[9]).

II. NOZIÈRES–DE DOMINICIS METHOD

Nozières and De Dominicis[10] (ND) found an essentially exact solution of the x-ray problem. They used a time theory rather than an energy theory, calculating the probability amplitude for a hole lifetime of exactly t, which is the Fourier transform of that hole's energy spectrum. Once t is given, one only has to calculate a single numerical factor (i.e., the probability amplitude).[11] What is more, the calculation from this point onwards is done for an *independent-particle* system, since the behavior of the hole is assumed given, and the electrons can interact only with this hole. The expectation value for the process of creating an electron at the origin at time t_0 (when the hole appears) and annihilating one there at time t_1 (when it disappears) is, of course, just the one-particle Green's function, which is what we have ended up looking for; to be precise, we are looking for the origin-to-origin values of this function.

Since we are looking for an expectation value $\langle 0|\cdots|0\rangle$, where $|0\rangle$ is the many-body ground state, we have to multiply the one-body Green's function by $\langle 0|e^{iHt}|0\rangle$. This gives us the exponential of a closed-loop sum $e^{c(t)}$; ND calculate $c(t)$ from the one-body Green's function (see Sec. III C of their paper).

It turns out that the causal Green's function $\langle Ta^{\dagger}(t)a(t')\rangle$ is the one we should use. (For the time behavior of the hole, all the various functions give the same result because its creation *must* precede its annihilation.) For this Green's function, as for any

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[1] G. D. Mahan, Phys. Rev. **163**, 612 (1967).
[2] P. W. Anderson, Phys. Rev. Letters **18**, 1049 (1967).
[3] B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. **178**, 1072 (1969).
[4] P. Nozières, J. Gavoret, and B. Roulet, Phys. Rev. **178**, 1084 (1969).
[5] A. A. Abrikosov, Physics **2**, 5, 61 (1965).
[6] K. D. Schotte and U. Schotte, Phys. Rev. (to be published).
[7] K. D. Schotte and U. Schotte, Phys. Rev. (to be published).
[8] S. Tomonaga, Progr. Theoret. Phys. (Kyoto) **5**, 544 (1950).
[9] R. A. Ferrell, Phys. Rev. **186**, 399 (1969).
[10] P. Nozières and C. De Dominicis, Phys. Rev. **178**, 1097 (1969).
[11] This is essentially the same as a path integral approach, the only paths considered being creation of a pair consisting of a deep hole and a single electron at one time, and its annihilation at another.

other causal 1-particle one, the Dyson equation holds:

$$\twoheadrightarrow = \rightarrow + \twoheadrightarrow V \rightarrow,$$

where $\rightarrow$ is the unperturbed Green's function, and $\twoheadrightarrow$ the exact one. If the electron-hole potential V is a Dirac δ interaction (or any other separable potential), we find that the same equation holds when all arrows represent origin-to-origin Green's functions. In a space-time formulation, the equation reads

$$G(0,t';0,t)=G_0(0,t';0,t) + i\int_{t''} G(0,t';0,t'')V(t'')G_0(0,t'';0,t)dt''. \quad (1)$$

Usually, one avoids a convolution on t'' by Fourier-transforming the equation to an energy representation, where a convolution on t'' becomes a product. But here $V(t'')$ is time-dependent, and, in an energy representation, multiplication by $V(t'')$ becomes a convolution with its Fourier transform, so the cure is worse than the disease.

Instead of trying to avoid a convolution, ND managed to use it. They could do this because of the form of G_0. We assume an infinitely wide energy-band symmetric about E_F (for the consequences of relaxing this idealization see later); this makes the mathematics less messy without omitting any physical result.[12] Omitting the space coordinates (=0) and putting $E_F=0$, we find $G_0(t';t)=1/i(t-t')$. Dyson's equation, thus, becomes[13]

$$G(t',t)=\frac{1}{i(t-t')}+\text{P.P.}\int_{t''}\frac{1}{t'-t''}V(t'')G(t,t'')dt''. \quad (2)$$

Now $V(t'')$ is a function that can have two values. One of them is 0, and let the other be $\pi^{-1}\tan\delta$. Then, omitting the constant t,

$$G=[1/i(t-t')]+\tan\delta\,\text{H.T.}[S(t'')G(t'',t)], \quad (3)$$

where H.T. is the Hilbert transform[14] and $S(t'')$ is 1 when $V(t'')\neq 0$ and 0 otherwise. The solution of such an equation is found in Muskhelishvili's work.[15] We shall derive it in Sec. III.

III. MUSKHELISHVILI METHOD

Equation (3) is a singular integral equation with a kernel of the form $K(t'',t')=S(t'')/\pi(t'-t'')$. As Muskhelishvili pointed out, $\int K(t'',t')f(t')dt''$ is the Hilbert transform of $S(t)f(t)$. Since the Hilbert transform relates the real and imaginary part of any function which is analytic on a half-plane, we find we have an equation relating the real and complex parts of such a function on the real line. Instead of developing Muskhelishvili's general theory, we shall solve Eq. (3) directly using his methods.

We shall omit the variable t, and Hilbert transform the equation, giving [since H.T.$(1/\tau)=\delta(t)$]

$$\text{H.T.}G(t')=i\delta(t')+\tan\delta S(t')G(t'). \quad (4)$$

Now let $i^{-1}G$ be the imaginary part of a function Φ analytic in the upper half-plane, $i^{-1}G=\text{Im}\Phi$. Then, H.T.G is ReΦ, and Eq. (4) says that the phase of Φ on the real line is $\delta S(t')$ [we ignore the $i\delta(t')$ term for the moment]. If we make $-i^{-1}G=\text{Im}\Phi'$, with Φ' analytic in the lower half-plane, we find that, on the real line, Φ' has phase $-\delta S(t')$. In fact, Φ and Φ' join together to form an analytic function with a branch cut on the real axis, where the phase jumps by $2\delta S(t')$.

When we multiply two functions, their phases add, as do any jumps in these phases. Thus, all functions with a $2\delta S(t')$ phase jump across the real axis are obtained by multiplying any single such function by all analytic functions. Also, since $S(t')$ is of the form of Fig. 2, we can write $S(t')=\theta(t'-t_0)-\theta(t'-t_1)$, and get this branch cut by multiplying two fractions, one with a $\delta\theta(t'-t_0)$ phase jump and one with a $-\delta\theta(t'-t_1)$ one.

A $\delta\theta(t'-t_0)$ phase jump is immediately seen to occur for the function $(t'-t_0)^{-\delta/\pi}$, defined so as to be negative real for $t'-t_0<0$, and analytic in both half-planes. $(t'-t_1)^{+\delta/\pi}$ gives a cut of $-\delta\theta(t'-t_1)$ in the same way, and, thus, to get the right branch and structure, we have to multiply any analytic function by $[(t'-t_1)/(t'-t_0)]^{\delta/\pi}$. To get the $i\delta(t')$ term, we use the fact that $1/(t'\pm i\epsilon)=\text{P.P.}(1/t')\mp\pi\delta(t')$. Thus, $1/t'$ gives the right δ-function term in Eq. (4) (times $[(0-t_1)/(0-t_0)]^{\delta/\pi}$) and does not influence the branch-cut behavior, except for the pole it adds at the origin. The solution of Dyson's equation is, thus,

$$G(t')=G_0(t')[(t'-t_1)/(t'-t_0)(0-t_0)/(0-t_1)]^{\delta/\pi}.$$

For general t, time invariance gives

$$G(t',t)=G_0(t',t)[(t'-t_1)/(t'-t_0)(t-t_0)/(t-t_1)]^{\delta/\pi}.$$

Uncritical use of this form would give us a value of 0 or ∞ for $G(t_0,t_1)$, which is what the calculation is all about. This is because we have ignored band-structure effects, which give a time cutoff at $t\sim\xi_0=1/\text{bandwidth}$.

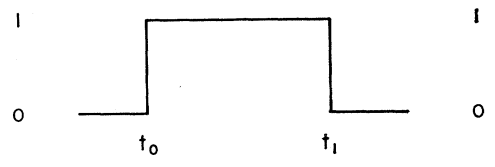

FIG. 2. Plot of $S(t)$.

[12] See ND for the case of an unsymmetric band.

[13] The principal part comes from the band-structure cutoff at small $t'-t''$ (see later).

[14] Defined as the convolution with $(1/\pi x)$, (principal part). See Erdely's *et al.* Bateman research project, Tables of Integral Transforms, Vol. 2.

[15] N. I. Muskhelishvili, *Singular Integral Equation* (Noordhoff: P. Noordhoff Ltd., Groningen, The Netherlands, 1953); cf. N. I. Mushkelishvili and D. A. Kveselava, Trudy Tbiliss. Mat. Inst. 11, 141 (1942).

This cutoff must be pure imaginary in order to give a real spectral density for the response function.[10] One sees how such a cutoff is obtained by making the hole appear and disappear only within a time ξ_0, rather than instantaneously, and constructing $C(t)$, not out of step functions (the phase function of X^δ), but out of arctan functions [the phase of $(X+i\epsilon)^\delta$].[1]

Whichever precise way we apply the cutoff, the $t^{\delta/\pi}$ factor, multiplying the usual time behavior, remains.

IV. EXTENSION TO FINITE TEMPERATURES

For $T\neq 0$, it is more convenient to use the standard-temperature Green's function. $G_0(\tau)$ is the Laplace transform of the smooth $\tanh\beta E$ Fermi factor [whereas for $T=0$, $G_0(t)$ was the Fourier transform of a sharp step-function Fermi factor]. It is easier to compute $G_0(t)$ first (real time) because the high-energy part can be disregarded there. The actual integration is done using the periodicity of the hyperbolic tangent modulo $i\pi$. Thus, $\int_{-\infty}^{\infty}\tanh\beta E e^{iEt}$ is $(1-e^{-\pi/\beta t})^{-1}$ times the integral on a loop (see Fig. 3). (The end segments can be disregarded because they fluctuate infinitely rapidly.) This loop integral equals the residue of the only pole inside the loop, which is $(1/\beta)2\pi i e^{-(\pi/2\beta)t}$. Thus,

$$G_0(t)=\frac{\pi/\beta}{\sinh(\pi/\beta)t}$$

and

$$G_0(\tau)=\frac{\pi/\beta}{\sin(\pi/\beta)\tau}.$$

G_0 satisfies the periodicity relation

$$G(\tau+\beta)=-G(\tau), \tag{5}$$

which the Green's functions must satisfy for $T\neq 0$ [Eq. (1-10) of Kadanoff and Baym[16]]. In the complex τ plane, G_0 can be used for dispersion relations: Let f be analytic on the upper-half plane and satisfy (5). Then,

$$\begin{aligned}\pi\,\mathrm{Im}f(x)&=\int_{-\infty}^{\infty}\frac{\mathrm{Re}[f(x')]dx'}{x-x'}\\&=\sum_{k=-\infty}\int_0^\beta\frac{\mathrm{Re}[f(x'+d\beta)]dx'}{x-x'-k\beta}\\&=\int_0^\beta G_0(x-x')\,\mathrm{Re}[f(x')]dx'.\end{aligned}\tag{6}$$

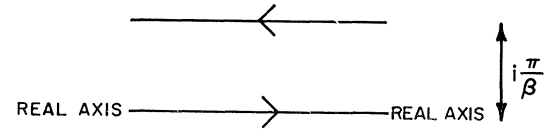

FIG. 3. Integration path for G_0.

[16] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W. A. Benjamin, Inc., New York, 1962).

Likewise, if f is analytic on the lower half-plane, this convolution gives $-\pi\,\mathrm{Im}f(x)$. Thus, Dyson's equation gives exactly the same branch cuts as before, except that the functions must obey Eq. (5) and the branch cuts must, thus, repeat periodically. We find

$$G(\tau,\tau')=G_0(\tau,\tau')\left(\frac{\sin(\pi/\beta)(\tau'-\tau_1)}{\sin(\pi/\beta)(\tau'-\tau_0)}\,\frac{\sin(\pi/\beta)(\tau-\tau_0)}{\sin(\pi/\beta)(\tau-\tau_1)}\right)^\delta. \tag{7}$$

As in the ground-state calculation, we can obtain an imaginary-time cutoff by pushing τ_0 and τ_1 a distance ϵ away from the real axis. The general Muskhelishvili solution can be extended to finite temperatures in the same way.

V. MUSKHELISHVILI METHODS FOR KONDO PROBLEM

We will now show that the Kondo problem can be viewed as an infinite succession of x-ray problems, with the spin flip S_+s_- and S_-s_+ playing the part of ND's perturbation $H_x=\sum_k W_k a_k^\dagger b e^{-i\omega t}$ [Eq. (2) of their paper] while the S_zs_z term plays the part of the last term $\sum_{kk'} V_{kk'}a_k^\dagger b_{k'}bb^\dagger$ of their Eq. (1). We use the Kondo Hamiltonian[17] dividing it as follows:

$$H=H_0+H_1', \tag{8}$$

$$H_0=\sum_{k\sigma}\epsilon_k n_{k\sigma}+JS_z\sum_{kk'\sigma\sigma'}C_{k\sigma}^\dagger(S_z)_{\sigma\sigma'}C_{k'\sigma'}, \tag{9}$$

$$H_1'=J\sum_{k\sigma}C_{k\sigma}^\dagger C_{k'\sigma'}[S_+(s_-)\sigma\sigma'+S_-(s_+)_{\sigma\sigma'}]. \tag{10}$$

H_0 conserves S_z, and for a given value ($+\frac{1}{2}$ or $-\frac{1}{2}$) of S_z, its eigenstates are independent-particle states in the presence of a potential (due to S_z). Let $\psi_{0\uparrow}$ be its lowest eigenstate with $S_z=+\frac{1}{2}$.

Following ND, we now want to find the system's behavior from an appropriate response function.[10] We switch H_1 on for a time t and ask how the ground-state–to–ground-state amplitude $F(t)=\langle\psi_{0\uparrow}|e^{iHt}|\psi_{0\uparrow}\rangle$ depends on t. As $F(t)=\sum_\omega|\langle\psi_{0\uparrow}|\psi_\omega\rangle|^2e^{i\omega t}$ (summing over eigenstates of H), its time behavior is closely related to the energy spectrum of the Kondo Hamiltonian. In particular, the energy at which the spectrum of F begins is the ground-state energy. This is so, despite Anderson's infrared catastrophe, because there is a non-zero matrix element between ψ_0 and the ground state of the system in an arbitrarily large box, and this latter ground state has an energy which approaches the infinite-gas ground-state energy as the size of the box tends to infinity.

In the interaction representation

$$F(t)=\langle\psi_{0\uparrow}|e^{iH_0t}T\left\{\exp\left[i\int_0^t H'(t')dt'\right]\right\}|\psi_{0\uparrow}\rangle, \tag{11}$$

[17] J. Kondo, Progr. Theoret. Phys. (Kyoto) **32**, 37 (1964).

where $H'(t')$ is defined as $e^{-iH_0t}H'e^{iH_0t}$ in the usual way. Expanding the exponential,

$$F(t)=\sum_{n=0}^{\infty}\langle\psi_{0\uparrow}|\int_{0<t_1<\cdots<t}dt_1\cdots dt_{2n}e^{iH_0(t-t_{2n})}\times iH'e^{iH_0(t_{2n}-t_{2n-1})}iH'\cdots iH'e^{iH_0t_1}|\psi_{0\uparrow}\rangle. \quad (12)$$

(H' must appear an even number of times, because it flips S_z each time.)

If we normalize our energies to make $\langle\psi_{0\uparrow}|H_0|\psi_{0\uparrow}\rangle=0$, we can drop the first and last factors, $e^{iH_0(t-t_{2n})}$ and $e^{iH_0t_1}$, because they have no effect.

The effect of H' is to flip S_z each time it occurs, downwards at t_{2k-1} and upwards at t_{2k}. At odd times t_{2k-1}, H' creates an electron of spin up and destroys one of spin down; at even times t_{2k}, it creates one of spin down and destroys one of spin up. Because of the changes in S_z with time, these electrons and holes are perturbed in a way similar to that of ND. [For $n=2$, $F(t)$ is a double time integral over the squared amplitude of an ND x-ray problem. For $n>2$, the problem gets more complicated.] To get an amplitude

$$\langle\psi_{0\uparrow}|iH'e^{iH_0(t_{2n}-t_{2n-1})}\cdots e^{iH_0(t_2-t_1)}iH'|\psi_{0\uparrow}\rangle,$$

we multiply the two amplitudes this term gives us for the spin-up and spin-down electrons separately. Each of these two amplitudes is the sum of $n!$ terms, found by matching the n creation operators (at odd times, for spin-up electrons) with the n annihilation operators (at even times, for spin-up electrons) into n pairs (see Fig. 4).

To calculate a particular term, we multiply the n Green's functions[18] of the creation-annihilation pair in it. Since the time ordering has already been done,

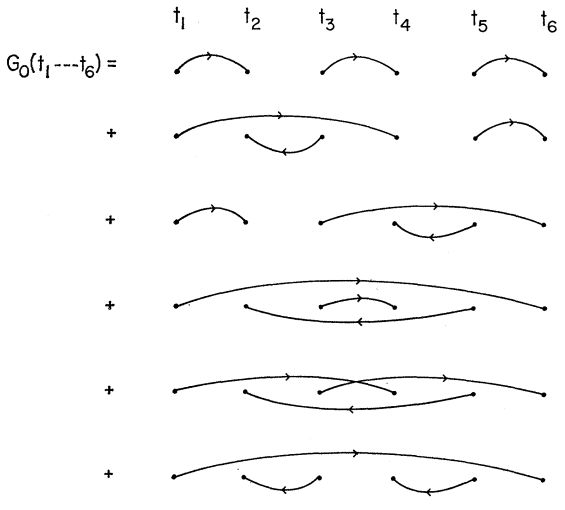

FIG. 4. Example of diagram contributing to G_0. The contribution of one set of times.

[18] All Green's functions here are origin-to-origin.

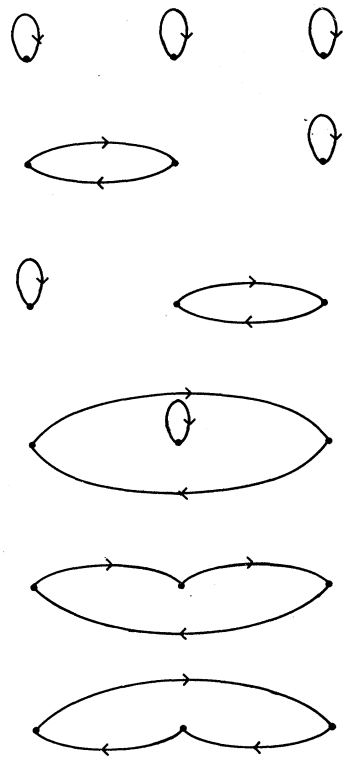

FIG. 5. The equivalent permutations.

the -1 factor one usually puts in $G_0(t_1;t_2<t_1)$ is absent. Thus, we add a phase factor of $(-1)^{\text{No. of hole lines}}$. Also, for each pair of lines that cross, whatever direction the arrows on them, we add a factor of -1, because we have to interchange two fermion operators before they separate into pairs.

Now the $n!$ ways to match the $2n$ creation and annihilation operators are equivalent to the $n!$ permutations P of the n pairs of operators. We get this equivalence (Fig. 5) by identifying t_{2k-1} and t_k and drawing the diagram as before. The phase factor turns out to be the parity $(-1)^P$ of the permutation P. This can be seen by following its behavior when any permutation is multiplied by a pair interchange. Since any permutation can be built up of such interchanges, and since the phase factor for the unit permutation is $+1$, we have

$$\langle\psi_{0\uparrow}|iH'e^{iH_0(t_{2n}-t_{2n-1})}\cdots e^{iH_0(t_2-t_1)}iH'|\psi_{0\uparrow}\rangle$$
$$=[\sum_P(-1)^PG(t_1,t_{2P(1)})G(t_3,t_{2P(2)})G(t_5,t_{2P(3)})\cdots]^2$$
$$=[\mathrm{Det}G(t_{2k-1},t_{2L})]^2. \quad (13)$$

Another way to check the phase factor is to sum up over the $n!^2$ ways to match pair of operators for both spins. The product of the two parity factors is then -1^n times the usual loop factor -1^L, where L is the number of loops.

For independent particles, without the H' term, $G(t_1,t_2)=i/(t_1-t_2)$, and the determinant $i^n\,\mathrm{Det}|1/$

$(t_{2k-1}-t_{2k})|$ is a Cauchy determinant[19] with value

$$\prod_{k>k'}(t_{2k-1}-t_{2k'-1})\prod_{k>k'}(t_{2k}-t_{2k'})/\prod_{k,k}(t_{2k-1}-t_{2L})$$
$$=\exp[\sum_{j>k}(-)^{j-k}\ln|t_j-t_k|\,]. \quad (14)$$

Because of H', the various Green's functions must now be found from the Dyson equation. This has the form discussed in Sec. II, except that $C(t)$ now changes its value $2n$ times rather than twice. The branch cut is still a sum of step functions, and we find that multiplying the unperturbed Green's function by the various fractional powers that give each step in $C(t)$ gives the solution of Dyson's equation.[20] Thus, in complete analogy with the x-ray case, we find

$$G(t',t)=G_0(t)\left(\frac{\prod(t'-t_i)\prod(t-t_k)}{\prod(t'-t_k)\prod(t-t_i)}\right)^{\delta/\pi}, \quad (15)$$

where i runs over the odd-numbered flips and k over the even.

We, thus, find that each product in the Cauchy determinant for G_0 is multiplied by $G_0^{-\delta/\pi}$, and the determinant—their sum—is multiplied by the same factor. The closed-loop sum $C(\delta,t)$ is trickier. ND have shown

$$e^{C(\delta,t)}=\left(\frac{t_1-t_0}{\tau_{\text{cutoff}}}\right)^{-(\delta/\pi)^2}.$$

If we extend their method to the case of arbitrarily many-time pairs, we find that the contribution of a time t to the integral which gives C (or, to be more precise, $\lambda\partial C/\partial\lambda$, where λ multiplies the vertices of a diagram of ND) is of the form $D(t)E(\delta)$, where $E(\delta)$ has exactly the same form as in ND's paper. The tricky integrations over δ, thus, give us nothing new, and a comparison of the different integrals over $D(t)$ gives us $l^{C(\delta,t)}=G_0^{(\delta/\pi)^2}$. Thus,

$$F_{2n}(t_1,\ldots,t_{2n})=[G_0(t_1,\ldots,t_{2n})]^{1-\epsilon}$$
$$=G_0(t_1,\ldots,t_{2n})^{1-2\delta/\pi+(\delta/\pi)^2}.$$

Transforming to imaginary times $t_k=i\beta_k$, we find

$$F(i\beta)=\sum_{n=0}^{\infty}J^{2n}\int d\beta_1,\cdots,d\beta_{2n}$$
$$\times\exp[(2-2\epsilon)\sum_{n>n'}-1^{n-n'}\ln(\beta_n-\beta_{n'}/\tau)],$$
$$n\text{ even},\quad 0<\beta_1-\tau<\cdots<\beta-2n^{\tau}<\beta-(2n+1)^{\tau}. \quad (16)$$

For a finite-temperature calculation, we replace our ground-state–to–ground-state amplitudes $\langle 0|\ldots|0\rangle$ by a thermodynamic average. The partition function Z satisfies

$$Z=\mathrm{Tr}e^{-\beta(H+H')}=\mathrm{Tr}\left(e^{-\beta H}T\exp i\int_0^{i\beta}H'(\tau')d\tau'\right).$$

This is completely analogous to the expression (11) for $F(t)$ when $t=i\beta$, and the integrand in it is again the amplitude of a generalized x-ray problem.

Dyson's equation is solved as in Sec. IV. (The analyticity and branch-cut conditions are the same as for the ground-state calculation, except for periodicity modulu $i\beta$.)

The same arguments as before shows $(G_0)_{2n}$ to be the determinant $|\beta/\sin[(\tau_{2k-1}-\tau_{2L})/\beta]|$. This equals

$$\left|\frac{2\beta i/\pi}{\exp[(i/\beta\pi)(\tau_{2k-1}-\tau_{2L})]-\exp[(i/\beta\pi)(\tau_{2L}-\tau_{2k-1})]}\right|=\left|\frac{2\beta i\exp(i/\beta\pi)\tau_{2k-1}\exp(i/\beta\pi)\tau_{2L}}{\exp(2i/\beta\pi)\tau_{2k-1}-\exp(2i/\beta\pi)\tau_{2L}}\right|,$$

and is, thus, equivalent to a Cauchy determinant, with the value

$$\left(\frac{2}{-\beta i}\right)^N\prod_k\exp\frac{i}{\pi\beta}\tau_{2k-1}\prod_L\exp\frac{i}{\pi\beta}\tau_{2L}$$
$$\times\prod_{k<k'}\left(\exp\frac{2i}{\pi\beta}\tau_{2k-1}-\exp\frac{2i}{\pi\beta}\tau_{2k'-1}\right)\prod_{L<L'}\left(\exp\frac{2i}{\pi\beta}\tau_{2L}-\exp\frac{2i}{\pi\beta}\tau_{2L'}\right)\Big/\prod_{k,L}\left(\exp\frac{2i}{\pi\beta}\tau_{2k-1}-\exp\frac{2i}{\pi\beta}\tau_{2L}\right),$$

which in turn equals

$$\prod_{k<k'}\frac{\beta}{\pi}\sin\left(\frac{\tau_{2k-1}-\tau_{2k'-1}}{\pi\beta}\right)\prod_{L<L'}\frac{\beta}{\pi}\sin\left(\frac{\tau_{2L}-\tau_{2L'}}{\pi\beta}\right)\Big/\prod_{k,L}\frac{\beta}{\pi}\sin\left(\frac{\tau_{2k-1}-\tau_{2L}}{\pi\beta}\right)$$

in complete analogy with the result we had before.[21] We, thus, get

$$F(i\beta)=\sum_{n=0}^{\infty}J^{2n}\int d\beta_1,\ldots,d\beta_n$$
$$\times\exp\left\{(2-2\epsilon)\sum_{n>n'}-1^{n-n'}\ln\left[\frac{\sin(\beta_n-\beta_{n'}/\beta)}{\sin\tau/\beta}\right]\right\},$$
$$n\text{ even},\quad 0<\beta_1,\ldots,<\beta_{2n}<\beta. \quad (17)$$

Both the formulas for $F(i\beta)$ have the form of a classical grand partition-function integral, with J^{2n} serving for the chemical-potential term $e^{-2\mu n}$, and $e^{\text{expression}}$ being a Boltzmann factor $e^{-E/kT}$. For $kT=1$,

[19] G. Polya and Szegö, *Aufgabe und Lehrsatze aus per Analysis* (Dover Publications, Inc., New York, 1945), Vol. 2. p. 97.

[20] The full complexity of Muskhelishvili's inhomogeneous equation solution is not needed, because we can write

$$G(t',t)=1/(t-t')+\tan\delta\,[\text{H.T.}[S(t'')G(t,t'')]]$$
$$=\tan\delta\,\{\text{H.T.}[S(t'')+\alpha\delta(t-t')]G(t'',t)\},$$

where α is an unknown factor. In this form, the equation becomes homogeneous, and the solution must then be normalized.

[21] It is clear that the phases cancel each other out, because the determinant of a real matrix is real.

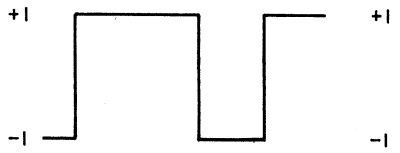

FIG. 6. Plot of $f(t)$.

we find

$$E=-(2-2\epsilon)\sum_{n>n'}-1^{n-n'}\ln\frac{\beta_n-\beta_{n'}}{\tau},$$

with an equivalent expression for the finite-temperature case. The statistical mechanics of a similar gas (without the $-1^{n-n'}$ factor and without the cutoff) has been done before.[22]

Instead of summing over pairs of spin flips, we can transform to a double integral over the spin $S_z(t)$ at different times, using

$$\int (f')_{x_1}(f')_{x_2}\ln(x_1-x_2)dx_1dx_2 = \int f_{x_1}f_{x_2}\frac{1}{(x_1-x_2)^2}dx_1dx_2. \quad (18)$$

[f' changes sign each time, so the $-1^{n-n'}$ factor is accounted for; f as, in Fig. 6, gives an f' integral equal to the sum we need].

If we discretize this integral over f and turn it into a sum over discrete times (by forbidding the flip to occur except at these times), we find ourselves with an Ising model with $1/(m-n)^2$ interaction, or rather, with the $2n$-flip term of such a model. The sum $\sum J^{2n}F_{2n}$ gives us the partition function (*not* the grand partition function) of a one-dimensional Ising model with an interaction term $J_{mn}=(2-2\epsilon)/(m-n)^2$ plus a nearest-neighbor term μS_nS_{n+1} ($\mu=-\ln J_\pm$ as before).

APPENDIX: BAND-STRUCTURE EFFECTS AND CUTOFFS

The $1/it$ Green's function discussed above is unrealistic: It corresponds to an infinitely wide structureless band. A more realistic band structure would give a different Green's function, without the $1/t$ singularity at the origin. For instance, for a flat band, symmetric about the Fermi level, we find $G_0(t)=(1/it)(1-e^{i|t/\tau_0|})$, where the bandwidth is $2/\tau_0$.

The effect of such a Green's function on the determinant [Eq. (13)] of the free Green's functions is clearly that of a cutoff, forbidding the time denominator to be less than about τ_0. As long as only one pair of times t_i, t_k is close enough to make band-structure effects important, we can write

$$G_0(t_i,t_k)=[1/i(t_k-t_i)]+\{G_0(t_i,t_k)-[1/i(t_k-t_i)]\},$$

and the determinant in [Eq. (13)] becomes the sum of two Cauchy determinants as follows. If, for convenience, we set $i=1$, $k=2$, we have

$$G^{\text{free}}=\begin{vmatrix} G_0(1-2) & \frac{1}{1-4} & \frac{1}{1-6} & \cdots \\ \frac{1}{3-2} & \frac{1}{3-4} & \cdots & \end{vmatrix}$$

$$=(\text{Cauchy})+\left(G_0-\frac{1}{1-2}\right)\begin{vmatrix} \frac{1}{3-4} & \frac{1}{3-6} & \cdots \\ \frac{1}{5-4} & \cdots & \end{vmatrix}$$

and, introducing the product representation of the Cauchy determinant, we get

$$G^{\text{free}}=\begin{vmatrix} \frac{1}{3-4} & \frac{1}{3-6} & \cdots \\ \frac{1}{5-4} & \cdots & \end{vmatrix}$$

$$\times\left\{G_0-\frac{1}{1-2}\left[1-\pi\left(\frac{(t_1-t_3)}{(t_2-t_3)}\frac{(t_1-t_5)}{(t_2-t_5)}\frac{(t_2-t_4)}{(t_1-t_4)}\right)\cdots\right]\right\}.$$

Again, using our assumption that only t_1-t_2 is small, the bracket is

$$\{\ \}\simeq\left\{G_0-\frac{1}{t_3}+\frac{1}{t_4}-\frac{1}{t_5}+\cdots\right\}.$$

This is essentially the same result and we would obtain if we were to insert a cutoff function in place of $1/t_1-t_2$ in the Cauchy product from (14).

The effect of the band-structure on the Dyson equation is much harder to handle. If the potential $V(t)$ is a *single* step function, we find that, whatever the form of $G(t)$, the Dyson equation is of the Muskhelishvili form *in frequency space*. With this potential, the solution is the same as before, except for a cutoff at times of order τ_0. For small δ, the cutoff region becomes the same as that of $G(t)$.

We expect the same sort of behavior in the solution for a more general $V(t)$. However, since the equation is no longer singular, it becomes much harder to make rigorous statements on its solution.

As for the closed-loop sum c, its leading (second-order) term, for any form of G, equals

$$\sin^2\delta\int_{V(t_1)\neq0}dt_1\int_{V(t_2)\neq0}dt_2G_0^2(t_1-t_2).$$

This leading term is all we need within the approxima-

[22] F. J. Dyson, J. Math. Phys. **3**, 140 (1962); **3**, 156 (1962); **3**, 166 (1962); **3**, 1191 (1962); K. G. Wilson, *ibid.* **3**, 1040 (1962); J. Gunson, *ibid.* **3**, 752 (1962).

tion $\sin^2\delta=\delta^2$. Thus, very directly for this term, we obtain the form (18), in which the interaction between different times is given not by the singular function $1/(x_1-x_2)^2$ but by $G_0^2(x_1-x_2)$, which has the singular behavior cutoff at $x_1-x_2=\tau$. To within this approximation, we can, thus, show that a cutoff at time τ_0 appears again. Higher-order terms are about as straightforward as any Feynman diagram of the same order, and are unlikely to give us drastically different results.

Thus, in at least three distinct cases, we can work out the mathematics of the cutoff precisely. None of the results are identical in detail, but all behave in very similar fashion. Further effort in elucidating the numerical nature of the cutoff is physically unwarranted, since in fact we are seldom or never confronted with known form factors and band structures; it is only the Fermi-surface-dependent features of the problem which are of any real physical interest.

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Band Structure of the Holes in Bismuth

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A study of the band structure for the holes in Bi has been by the magnetoacoustic effect in a Sn-doped Bi sample. The existence of a singular point of the saddle type is confirmed and a new pocket of holes is found. The analysis of the experimental results supports the Golin band calculation in Bi.

1. INTRODUCTION

In a previous paper,[1] the existence of a singular point of the saddle type for the holes in bismuth was postulated to explain some experimental results. The main feature of the experiments was the disappearance of the oscillations of the ultrasound absorption coefficient as a function of the magnetic field strength when the hole Fermi surface was investigated.

To confirm and clarify the hole-band structure of bismuth a new set of measurements has been carried out in a sample of Sn-doped Bi, with a concentration of impurity of 4.5×10^{18} cm^{-3}, in order to have only hole carriers.[2] The interpretation of the experimental results, in particular the location of the double-conic point along the binary direction, is consistent with the Golin band-structure calculation[3] of bismuth.

The present work is concerned with measurements, by means of the magnetoacoustic effect, of the cross-sectional area S of the Fermi surface and of the phase factor γ of the semiclassical quantization rule, $S(\epsilon_F,k_H)=(n+\gamma)(2\pi eH/c\hbar)$, for various magnetic-field and sound-wave vector directions.

In Sec. 2 the theoretical background is outlined; in Sec. 3 the experimental results are presented; in Sec. 4 a dispersion law and a model of the hole Fermi surface are deduced from the experimental measurements.

2. THEORY

In this section some particular aspects of the existence of a singular point of saddle type in the **k** space are analyzed.

Around a saddle point the dispersion law of the carriers can be approximated as follows:

$$\epsilon=\epsilon_0+\alpha_1k_1^2+\alpha_2k_2^2+\alpha_3k_3^2, \tag{1}$$

with the coefficients α_1, α_3 having sign opposite to α_2 and choosing k_1, k_2, k_3 as the bisector, binary, and trigonal axis, respectively.

In this case one of the authors[4] has shown, with semiclassical arguments, that the relation

$$S(\epsilon,k)=2\pi(eH/c\hbar)(n+\gamma) \tag{2}$$

is still valid and γ assumes the value of $\frac{3}{4}$. This result has been obtained when the magnetic field is along the k_3 axis and in relation with all the values of the momentum k_3 that do not lead in the **k** space to self-intersecting orbits for carriers. In the case of self-intersecting orbits, the semiclassical arguments, in fact, are not valid.[5]

The value $\gamma=\frac{3}{4}$ follows from the structure of the differential equation derived from Eq. (1) by means of the Luttinger and Kohn[6] procedure in the presence of

[1] M. Giura, R. Marcon, T. Papa, and F. Wanderlingh, Phys. Rev. **179**, 645 (1969).
[2] J. M. Noothoven Van Goor, Phys. Letters **21**, 603 (1966).
[3] S. Golin, Phys. Rev. **166**, 643 (1968).
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[5] M. Giura and F. Wanderlingh, Phys. Rev. Letters **20**, 445 (1968).
[6] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).