the reasonable value

$$|\langle {}^2T_1 \,|\, V(C_i) \,|\, {}^2E \rangle| \simeq 200 \text{ cm}^{-1}$$

and the energy denominator to be identical to that of ruby, g' may be as large as 4 for certain choices of ${}^2E$.

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Magnetic Relaxation in an Exactly Soluble Model

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Some nonequilibrium properties of an impurity in a linear chain of spins with nearest-neighbor interaction of the isotropic X-Y type are studied. It is shown that under certain conditions its behavior is in agreement with the general principles of statistical mechanics. The relaxation in the presence of a transverse field is also studied, and it is found that in the weak coupling region the approach to equilibrium is described by a sum of exponentials. However, the results do not agree with the solution of the Bloch equations.

I. INTRODUCTION

The magnetic relaxation in a spin system which is isolated from the lattice vibrations has been the subject of interest in the past years.[1-3] In the theoretical considerations, one normally assumes that the methods which are employed in nonequilibrium statistical mechanics also apply in this situation. On the other hand, it was recently demonstrated that a nontrivial model such as the X-Y

model[4] does not satisfy the usual assumptions of statistical mechanics.[5-8] In this paper we study a slightly different model which is also exactly soluble. The model consists of a linear array of spin-$\frac{1}{2}$ particles with nearest-neighbor interaction of the isotropic X-Y type. In contrast to the X-Y model, we assume that one of the spins is an impurity in the sense that the interaction with its neighbors is different in strength and also that it may be coupled differently to the external field. It will be shown in this model that, under certain conditions, the motion of the impurity spin is well in accordance with what one expects on general grounds. The physical reason for this is that the other spins can act as a thermal bath for this impurity.

One particular way to describe the behavior of a magnetic system is by the Bloch equations.[9] As is well known, these equations play a very important role in the macroscopic description of relaxation in the presence of an external magnetic field. The equations essentially imply that there are no coherence effects between the external field and the relaxation process, even for relatively strong fields. If we suppose that a magnetic field with components $(h_1, 0, H)$ is applied to the impurity, then the Bloch equations have the form

$$\frac{d}{dt}M^x = -\frac{M^x}{T_2} + HM^y \ ,$$
$$\frac{d}{dt}M^y = -HM^x - \frac{M^y}{T_2} + h_1 M^z \ , \qquad (1.1)$$
$$\frac{d}{dt}M^z = -h_1 M^y - \frac{M^z - M_0}{T_1} \ ,$$

where M^α is the αth component of the magnetization of the impurity, and M_0 is the equilibrium value. In the microscopic derivation of Eqs. (1.1), one usually assumes that in addition to the weak coupling approximation the system can be completely described by the observables M^α. The validity of the above set of equations can readily be studied in this model for the case that the impurity is at one of the ends of the chain. It is found that they are not valid in this model, although the time dependence of the magnetization is described by a sum of exponentials. The reason for this failure is that the observables M^α are not sufficient to characterize completely the behavior of the system.

The organization of this paper is as follows: In Sec. II we describe the model and the method used to diagonalize the Hamiltonian. Furthermore, an expression is derived for the time dependence of the longitudinal magnetization of the impurity. The long-time behavior of this expression is studied in detail in Sec. III. In particular, it is shown that the value of the magnetization for $t\to\infty$ is well in accordance with the canonical distribution only for a limited range of values of the external field which is applied on the impurity. Section IV deals with the autocorrelation functions for the impurity. Finally, Sec. V, the magnetization is determined in the presence of a transverse field.

II. MODEL

Let us consider a linear chain of spin-$\frac{1}{2}$ particles with nearest-neighbor interaction. Although the results in this section can readily be extended to the case that the impurity is situated anywhere in the chain, we shall assume for notational convenience that its position is at the beginning of the chain. The Hamiltonian of the system is given by

$$\mathcal{H}(H) = \mathcal{H}_0(H) + V \ , \qquad (2.1)$$

with

$$\mathcal{H}_0(H) = -HS_0^Z - H_L \sum_{i=1}^{N} S_i^Z + J\sum_{i=1}^{N-1}(S_i^X S_{i+1}^X + S_i^Y S_{i+1}^Y) \ ,$$
$$V = g(S_0^X S_1^X + S_0^Y S_1^Y) \ . \qquad (2.2)$$

Here, S_i^α is the αth component of the spin operator of the ith spin, while the impurity spin is supposed to be the zeroth spin. Let us, for convenience, assume that the parameters g, J, and H_L in Eqs. (2.2) are positive. As is well known, we may rewrite the Hamiltonian in terms of Fermi operators by defining the operators S_i^+, S_i^-

$$S_i^X = \frac{S_i^+ + S_i^-}{2} \ , \quad S_i^Y = \frac{S_i^+ - S_i^-}{2i} \ , \quad S_i^Z = S_i^+ S_i^- - \tfrac{1}{2} \ , \qquad (2.3)$$

and introducing the Fermi operators $c_i, c_i^\dagger$ through the relation

$$S_i^+ = c_i^\dagger \exp\left(i\pi \sum_{k=0}^{i=-1} c_k^\dagger c_k\right) \ . \qquad (2.4)$$

Equations (2.2) then become

$$\mathcal{H}_0(H) = -Hc_0^\dagger c_0 - H_L \sum_{i=1}^{N} c_i^\dagger c_i + \tfrac{1}{2}J\sum_{i=1}^{N-1}[c_i^\dagger c_{i+1} + \text{H.c.}] + \tfrac{1}{2}(H + NH_L) \ ,$$
$$V = \tfrac{1}{2}g[c_0^\dagger c_1 + \text{H.c.}] \ . \qquad (2.5)$$

To diagonalize this Hamiltonian, we closely follow the method of Ullersma[10] used in his studies of Brownian motion. The diagonalization procedure consists of two steps. The first step is to diagonalize the operator $\mathcal{H}_0$ by the canonical transformation

$$c_m = \sum_{\nu=1}^{N} U_{m\nu}\eta_\nu \ , \quad m = 1, \ldots, N \qquad (2.6)$$

with

$$U_{m\nu}=[2/(N+1)]^{1/2}\sin[m\nu\pi/(N+1)] \ .$$

In terms of the Fermi operators $\eta_\nu, \eta_\nu^\dagger$ the expressions in Eqs. (2.5) become

$$\mathcal{H}_0(H)=-Hc_0^\dagger c_0+\sum_{\nu=1}^{N}\Lambda_\nu\eta_\nu^\dagger\eta_\nu+\tfrac{1}{2}(H+NH_L) \ , \qquad V=\sum_{\nu=1}^{N}\alpha_\nu[c_0^\dagger\eta_\nu+\eta_\nu^\dagger c_0] \ , \tag{2.7}$$

with

$$\Lambda_\nu=-H_L+J\cos[\nu\pi/(N+1)] \ , \ \alpha_\nu=\tfrac{1}{2}gU_{1\nu} \ .$$

In the second step the total Hamiltonian $\mathcal{H}$ is diagonalized with the aid of another canonical transformation

$$\eta_0=c_0=\sum_{k=0}^{N}V_{0k}\xi_k \ , \qquad \eta_\nu=\sum_{k=0}^{N}V_{\nu k}\xi_k \ , \quad \nu=1,\ldots,N \tag{2.8}$$

with $V_{\nu k}$ real. Here $\xi_k, \xi_k^\dagger$ are again Fermi operators. In order that (2.8) be canonical, it is necessary that the following orthonormality condition is satisfied:

$$\sum_{\nu=0}^{N}V_{\nu k}V_{\nu k'}=\delta_{kk'} \ . \tag{2.9}$$

Dropping the constant term $\frac{1}{2}(H+NH_L)$ the Hamiltonian can be expressed as

$$\mathcal{H}(H)=\textstyle\sum_k\lambda_k\xi_k^\dagger\xi_k \ . \tag{2.10}$$

It should be noted that since the eigenvalues λ_k determined by Eq. (2.13) below can in general have positive and negative values, the equilibrium ground state is given by that state where the modes with $\lambda_k<0$ are occupied. The corresponding ground-state energy is given by

$$E_0=\tfrac{1}{2}(H+NH_L)+\textstyle\sum_k'\lambda_k \ ,$$

where the summation is restricted to the eigenvalues λ_k with $\lambda_k<0$. In order that $\mathcal{H}$ have the form (2.10), the coefficients $V_{\nu k}$ should satisfy the following set of linear equations:

$$-HV_{0k}+\sum_{\nu=1}^{N}\alpha_\nu V_{\nu k}=\lambda_k V_{0k} \ , \qquad \alpha_\nu V_{0k}+\Lambda_\nu V_{\nu k}=\lambda_k V_{\nu k} \ , \quad \nu=1,\ldots,N \ . \tag{2.11}$$

Substituting Eqs. (2.8) into the Hamiltonian given by Eqs. (2.7) with the term $\frac{1}{2}(H+NH_L)$ dropped, one, indeed, easily verifies [using Eqs. (2.9) and (2.11)] that $\mathcal{H}$ has the form (2.10). From the second equation in (2.11) we have

$$V_{\nu k}=[\alpha_\nu/(\lambda_k-\Lambda_\nu)]V_{0k} \ . \tag{2.12}$$

On substituting this in the first equation of (2.11) we obtain the secular equation

$$\lambda_k+H-\sum_{\nu=1}^{N}\frac{\alpha_\nu^2}{\lambda_k-\Lambda_\nu}=0 \tag{2.13}$$

for the eigenvalues λ_k. Finally, we have to determine V_{0k}. Inserting Eq. (2.12) into Eq. (2.9) gives

$$V_{0k}^2=\left(1+\sum_{\nu=1}^{N}\frac{\alpha_\nu^2}{(\lambda_k-\Lambda_\nu)^2}\right)^{-1} \ . \tag{2.14}$$

To illustrate how this diagonalization procedure can be applied in an actual calculation, we determine the time dependence of the longitudinal magnetization of the impurity. Let us assume that for $t<0$ there is an external magnetic field $H+h$ present along the z axis and that the system is in statistical equilibrium. Then the system can be described by the density matrix

$$\rho_{H+h}=e^{-\beta\mathcal{H}(H+h)}/\mathrm{Tr}\,e^{-\beta\mathcal{H}(H+h)} \ , \tag{2.15}$$

with $\beta=1/kT$. If we now suppose that at $t=0$ the field h is suddenly switched off, then the time-dependent behavior for $t\geq 0$ of the longitudinal magnetization of the impurity is determined by

$$\langle S_0^z(t)\rangle=\mathrm{Tr}\rho_{H+h}S_0^z(t) \tag{2.16}$$

with

$$S_0^z(t)=e^{i\mathcal{H}(H)t}S_0^z e^{-i\mathcal{H}(H)t} \ . \tag{2.17}$$

In view of the relation

$$S_0^z=c_0^\dagger c_0-\tfrac{1}{2} \ ,$$

we may evaluate Eq. (2.17), using Eqs. (2.8) and the property

$$\xi_k(t)=e^{-i\lambda_k t}\xi_k \ , \tag{2.18}$$

to obtain

$$S_0^z(t)=-\tfrac{1}{2}+\sum_{k_1,k_2}V_{0k_1}V_{0k_2}\xi_{k_1}^\dagger\xi_{k_2}\exp[i(\lambda_{k_1}-\lambda_{k_2})t] \ . \tag{2.19}$$

In order to simplify matters somewhat, we replace the density matrix ρ_{H+h} in Eq. (2.16) by

$$\rho^{(0)}(H+h)=e^{-\beta\mathcal{H}_0(H+h)}/\mathrm{Tr}\,e^{-\beta\mathcal{H}_0(H+h)} \ . \tag{2.20a}$$

In doing this we do not expect to change the main features of the time behavior of Eq. (2.16) drastically for small values of g. Moreover, since we will in particular be concerned with the weak coupling limit, i.e., $g\to 0$, $t\to\infty$, such that g^2t is kept constant, the approximation (2.20a) becomes exact in this limit. Of course, the calculations can also be performed with Eq. (2.15) (see the Appendix). The expressions become more lengthy, but it can, indeed, be verified that our results do not change qualitatively. To find Eq. (2.16) we have to compute

$$\langle \xi^\dagger_{k_1} \xi_{k_2} \rangle = \mathrm{Tr}\rho^{(0)}(H+h)\,\xi^\dagger_{k_1}\xi_{k_2} \ . \tag{2.20b}$$

This is done by applying the inverse transformation of Eq. (2.8),

$$\xi_k = \sum_{\nu=0}^{N} V_{\nu k}\eta_\nu \ . \tag{2.21}$$

We find, using relation (2.12),

$$\langle \xi^\dagger_{k_1}\xi_{k_2}\rangle = V_{0k_1}V_{0k_2}\left(\frac{f_1(\lambda_{k_1})-f_1(\lambda_{k_2})}{\lambda_{k_2}-\lambda_{k_1}} + \frac{1}{1+e^{-\beta(H+h)}}\right) , \tag{2.22}$$

with

$$f_1(\lambda) = \sum_{\nu=1}^{N}\frac{\alpha_\nu^2}{\lambda-\Lambda_\nu}\,[1+e^{\beta\Lambda_\nu}]^{-1} \ .$$

Noting now that in the limit of $\beta=0$, Eq. (2.16) trivially reduces to zero, we may as well subtract the expression for $\beta=0$ from Eq. (2.16). In so doing, and by virtue of Eqs. (2.19) and (2.22), we obtain

$$\langle S_0^z(t)\rangle = \tfrac{1}{2}\sum_{k_1,k_2} V^2_{0k_1}V^2_{0k_2}\exp i(\lambda_{k_1}-\lambda_{k_2})t \times\left(\frac{f(\lambda_{k_1})-f(\lambda_{k_2})}{\lambda_{k_1}-\lambda_{k_2}} + \tanh\tfrac{1}{2}\beta(H+h)\right) \tag{2.23}$$

with

$$f(\lambda) = \sum_{\nu=1}^{N}\frac{\alpha_\nu^2}{\lambda-\Lambda_\nu}\tanh\tfrac{1}{2}\beta\Lambda_\nu \ . \tag{2.24}$$

The summations over k_i can now be converted into integrals by applying Cauchy's theorem. Introducing the function

$$R(\lambda) = [\lambda + H - f_0(\lambda)]^{-1} \tag{2.25}$$

with

$$f_0(\lambda) = \sum_{\nu=1}^{N}\frac{\alpha_\nu^2}{\lambda-\Lambda_\nu} \ , \tag{2.26}$$

we may write, in view of Eqs. (2.13) and (2.14),

$$\langle S_0^z(t)\rangle = \tfrac{1}{2}(1/2\pi i)^2\oint d\lambda\oint d\lambda' R(\lambda)R(\lambda') \times e^{i(\lambda-\lambda')t}\{(\lambda-\lambda')^{-1}[f(\lambda)-f(\lambda')] + \tanh\tfrac{1}{2}\beta(H+h)\} \ , \tag{2.27}$$

where the integration path encircles in the counterclockwise direction all the poles of $R(\lambda)$, which are situated on a part of the real axis in the λ plane. Up to now, all considerations apply for a finite number of spins. We now take the thermodynamic limit $N\to\infty$. Then, the summations in Eqs. (2.24) and (2.26) are replaced by integrations. We get

$$f(\lambda) = \frac{g^2}{2\pi}\int_0^\pi \frac{\sin^2 x\,dx}{\lambda + H_L - J\cos x}\tanh\tfrac{1}{2}\beta(J\cos x - H_L), \tag{2.28}$$

$$f_0(\lambda) = \frac{g^2}{2\pi}\int_0^\pi\frac{\sin^2 x\,dx}{\lambda+H_L-J\cos x} = \frac{g^2}{2J^2}\{\lambda+H_L - [(\lambda+H_L)^2-J^2]^{1/2}\} \ , \tag{2.29}$$

where the square root is defined to be positive for positive arguments. Evidently in the process of letting $N\to\infty$ the poles of $R(\lambda)$ become a dense set on the real axis, so that, at the end, they constitute a branch cut. As is obvious from Eq. (2.29), this cut extends from $-H_L-J$ to $-H_L+J$. In addition, notice that for a sufficiently large field H, $R(\lambda)$ has a pole in the first Riemann sheet. This happens if λ is a solution of the secular equation $R(\lambda)^{-1}=0$, with λ real and outside the cut, i.e., $\lambda > -H_L+J$ or $\lambda < -H_L - J$. Notice, also, that the analytic structure of $R(\lambda)$ is simple. Apart from the square-root branch points at $\lambda = -H_L \pm J$, the only singularities of $R(\lambda)$ are two poles. We may distinguish between two possibilities: (i) Both poles are in the second sheet; they can then be either real or complex, depending on the value of H. In the complex case, the poles are complex conjugate of each other. (ii) One pole is in the first sheet while the other one is in the second sheet. Both of them are real.

III. ASYMPTOTIC BEHAVIOR OF LONGITUDINAL MAGNETIZATION

In Sec. II we derived an expression for the time dependence of the longitudinal magnetization of the impurity spin which we should like to study in detail in this section. In particular, we would like to examine the behavior for asymptotic large times. To do this, we introduce the Laplace transform

$$\hat{g}(p) = \int_0^\infty e^{-pt}dt\,\langle S_0^z(t)\rangle \ \text{ with } \mathrm{Re}\,p>0 \ . \tag{3.1}$$

From Eq. (2.27), we obtain, by deforming the contours in the λ and λ' planes,

$$\hat{g}(p) = -(1/4\pi i p)\int_{-\infty}^{\infty}d\lambda R(\lambda - i\epsilon)R(\lambda+ip) \times[f(\lambda-i\epsilon)-f(\lambda+ip) - ip\tanh\tfrac{1}{2}\beta(H+h)] \tag{3.2}$$

with $\epsilon \downarrow 0$. Using the identity

$$R(\lambda)R(\lambda') = [R(\lambda)-R(\lambda')]\,[\lambda'-\lambda+f_0(\lambda)-f_0(\lambda')]^{-1} \ , \tag{3.3}$$

which follows immediately from Eq. (2.25), the expression (3.2) can also be written as

$$\hat{g}(p) = (1/4\pi i p) \int_{-\infty}^{\infty} d\lambda [R(\lambda - i\epsilon) - R(\lambda + ip)] I(\lambda, p)$$

with (3.4)

$$I(\lambda, p) = [ip \tanh\tfrac{1}{2}\beta(H+h) + f(\lambda+ip) - f(\lambda - i\epsilon)] \times [ip - f_0(\lambda + ip) + f_0(\lambda - i\epsilon)]^{-1} \quad . \tag{3.5}$$

Let us first consider the limiting value of $\langle S_0^z(t)\rangle$ for $t \to \infty$. It is simply given by the residue of the pole of $\hat{g}(p)$ at $p = 0$, i.e.,

$$\lim_{t\to\infty}\langle S_0^z(t)\rangle = \frac{1}{4\pi i}\int_{-\infty}^{\infty} d\lambda [R(\lambda - i\epsilon) - R(\lambda + i\epsilon)] \lim_{p\downarrow 0} I(\lambda, p) \;. \tag{3.6}$$

If the general assumptions of statistical mechanics are valid, then we anticipate that this quantity is equal to the expectation value of S_0^z taken over a canonical distribution corresponding to the situation where there is an external field H present. This distribution is described by the density matrix ρ_H. By straightforward application of the method described in Sec. II, we get

$$\mathrm{Tr}\rho_H S_0^z = -(1/4\pi i)\int_{-\infty}^{\infty} d\lambda [R(\lambda - i\epsilon) - R(\lambda + i\epsilon)] \tanh\tfrac{1}{2}\beta\lambda \;, \tag{3.7}$$

which holds for any given value of g. To compare this with the expression (3.6), let us first assume that the only singularity of $R(\lambda)$ in the first sheet is given by the branch cut between $-H_L - J$ and $-H_L + J$. Then the only contribution to Eq. (3.6) comes from the cut. For this region, we have, according to Eq. (3.5),

$$\lim_{p\downarrow 0} I(\lambda, p) = [f(\lambda - i\epsilon) - f(\lambda + i\epsilon)]\,[f_0(\lambda + i\epsilon) - f_0(\lambda - i\epsilon)]^{-1}.$$

In view of Eqs. (2.28) and (2.29), this reduces to

$$\lim_{p\downarrow 0} I(\lambda, p) = -\tanh\tfrac{1}{2}\beta\lambda \;,$$

so that we, indeed, see that Eq. (3.6) is the same as Eq. (3.7). We now turn to the case that $R(\lambda)$ has an additional pole λ_1 in the first sheet, which is outside the cut and on the real axis. In the presence of the pole λ_1, the expressions (3.6) and (3.7) will no longer be identically the same because of the contribution from this pole. In fact, we have

$$\lim_{p\downarrow 0} I(\lambda_1, p) = \left(\frac{df(\lambda_1)}{d\lambda_1} + \tanh\tfrac{1}{2}\beta(H+h)\right)\left(-\frac{df_0(\lambda_1)}{d\lambda_1} + 1\right)^{-1}, \tag{3.8}$$

which depends explicitly on the previous history of the system through the presence of the second term in the numerator on the right-hand side of Eq. (3.8).

We proceed to discuss the behavior of the magnetization for long times. From now on, we restrict ourselves to the high-temperature approximation, i.e., we retain only terms up to linear in β in the expression (3.5). The results on the time dependence of $\langle S_0^z(t)\rangle$ in the high-temperature limit will be valid on time scales such that t/β is large. The reason is that, for finite temperatures, we get additional exponentially decaying functions of t with arguments which are proportional to β^{-1}. Their origin is in the poles of the hyperbolic-tangent function. For a discussion of this, we refer to Ref. 8. In the high-temperature limit, Eq. (3.5) reduces to

$$I(\lambda, p) = \tfrac{1}{2}\beta[ip(H+h) + (\lambda + ip) f_0(\lambda + ip) - \lambda f_0(\lambda - i\epsilon)] \times [ip - f_0(\lambda + ip) + f_0(\lambda - i\epsilon)]^{-1} \;. \tag{3.9}$$

Let us, for the moment, consider the case where the poles of $R(\lambda)$ are complex. Denote them by λ_1 and λ_2 with $\mathrm{Im}\lambda_1 > 0$ and $\lambda_1 = \lambda_2^*$. The following properties of $\hat{g}(p)$ readily can be inferred from Eq. (3.4). It is regular in the p plane, except for a pole at $p = 0$ and a cut with logarithmic branch points at $\pm 2iJ$. Furthermore, the function $\hat{g}(p)$ can be written as the sum of two terms, one of which, when it is continued analytically from right to left through the above-mentioned cut into the second Riemann sheet, yields another branch cut between $i(H_L + J + \lambda_1)$ and $i(H_L - J + \lambda_1)$. The branch points are of a square-root type. Similarly, the other term has a branch cut between $-i(H_L + J + \lambda_2)$ and $-i(H_L - J + \lambda_2)$. Finally, the analytic continuation through these cuts into the "third" sheet yields, as singularities in this sheet, poles at $p = 0$ and $-2\,\mathrm{Im}\lambda_1$. To determine the long-time behavior of the magnetization, we make use of the above analytic structure of $\hat{g}(p)$. For $t > 0$, we have

$$\langle S_0^z(t)\rangle = \frac{1}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon} dp\, e^{pt}\hat{g}(p) \tag{3.10}$$

with $\epsilon > 0$. In the case that the branch cuts in the second sheet of the p plane intersect the real axis, and the pole at $-2\,\mathrm{Im}\lambda_1$ is far away from the various branch points, i.e.,

$$\mathrm{Im}\lambda_1 \ll \mathrm{Min}(2J, |H_L \pm J + \lambda_1|) \;, \tag{3.11}$$

the expression (3.10) can be computed by deforming the integration path into the second and third sheet, as, for example, shown in Fig. 1 for one of the terms of $\hat{g}(p)$. For long times, the main contributions come from the poles and branch points. As a result, we find for

$$t \gg \mathrm{Max}(|J|^{-1}, H_L \pm J + \lambda_1|^{-1}) \;,$$

$$\langle S_0^z(t)\rangle = A + Be^{-2\,\mathrm{Im}\lambda_1 t} + t^{-3/2}\,\mathrm{Im}\{C_+ \exp[i(H_L + J + \lambda_1)t + \tfrac{1}{4}i\pi] - C_- \exp[i(H_L - J + \lambda_1)t - \tfrac{1}{4}i\pi]\} + D\sin 2Jt/t^3 \tag{3.12a}$$

with

$$A = -(\beta/8\pi i)\int_{-\infty}^{\infty} d\lambda[R(\lambda - i\epsilon) - R(\lambda + i\epsilon)]\lambda \ , \quad (3.12b)$$

$$B = \frac{\beta\alpha^2 |(\lambda_1 + H_L)^2 - J^2|}{4(1-2\alpha)^2(\mathrm{Im}\lambda_1)^3}\,\mathrm{Im}\lambda_1[H + h + \bar{f}_0(\lambda_1)] \ , \quad (3.12c)$$

$$C_\pm = \frac{-\beta\alpha^2[2J(J^2 - (\lambda_1 + H_L)^2)]^{1/2}}{4\pi^{1/2}} \times \frac{(\mp J - H_L)(H_L - H \pm J) + (H+h)(\lambda_1 + H_L \pm J) + \lambda_1 \bar{f}_0(\lambda_1)}{(\lambda_1 + H_L \pm J)(H - H_L \mp J)^2(1-2\alpha)\,\mathrm{Im}\lambda_1} \quad (3.12d)$$

$$D = \frac{\beta\alpha^2 J[2H + h - H_L(2-\alpha)]}{4\pi[(H - H_L)^2 - J^2(1-\alpha)^2]^2} \ , \quad (3.12e)$$

where $\alpha = g^2/2J^2$ and $\bar{f}_0(\lambda)$ is the analytic continuation of $f_0(\lambda)$ into the second sheet. For fixed g, the second and third terms in Eqs. (3.12) are exponentially small for $t \gg 1/g^2$ and should be dropped. Hence, for times long compared to $1/g^2$, the system is governed by a nonexponential time behavior given by

$$\langle S_0^z(t)\rangle = A + D\sin 2Jt/t^3 \ .$$

Since the validity of rate equations is expected to hold in the so-called weak coupling limit, [11] we turn to study this situation. Physically, the weak coupling limit describes the behavior of the system in time for sufficiently weak g on time scales of the order of $1/g^2$. In this case, the above-mentioned terms in Eq. (3.12) are not exponentially small in

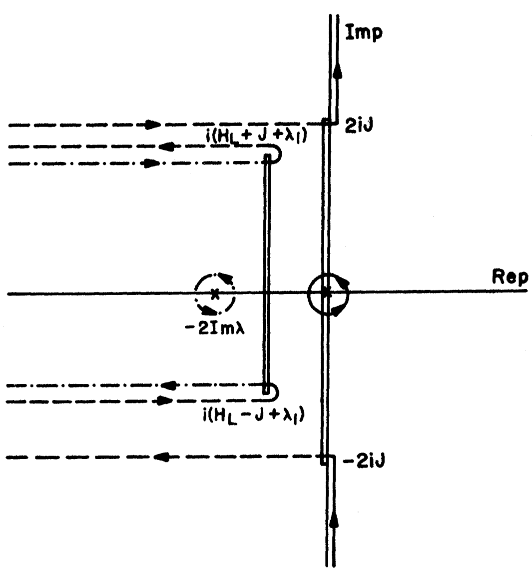

FIG. 1. Contour for evaluating the asymptotic behavior of one of the terms in Eq. (3.10). Solid line: first Riemann sheet. Broken line: second Riemann sheet. Broken dotted line: third Riemann sheet.

this limit. For sufficiently weak g, the poles of Eq. (2.25) are simply given by

$$\lambda_1 = \lambda_2^* = -H + \alpha\{-H + H_L + i\sqrt{[J^2 - (H_L - H)^2]}\} \ . \quad (3.13)$$

Using this in Eqs. (3.12a)–(3.12d) we see that, for sufficiently weak g and t of the order of $1/g^2$, the contributions which do not vanish are (3.12a) and (3.12b). We obtain in this limit the purely exponential behavior

$$\langle S_0^z(t)\rangle = \tfrac{1}{4}\beta(H + he^{-t/T_1}) \ , \quad (3.14)$$

where the longitudinal relaxation time T_1 is given by

$$T_1^{-1} = (g^2/J^2)[J^2 - (H - H_L)^2]^{\frac{1}{2}} \ . \quad (3.15)$$

Let us write down what we get for T_1 according to perturbation theory. One way to perform the calculation is to use a master equation approach. [2] We then find

$$(T_1^{-1})_{\text{pert}} = [\langle S_0^z(0)\rangle - \langle S_0^z(\infty)\rangle]^{-1} \times \int_{-\infty}^{\infty} d\tau \langle[[S_0^z, \bar{V}(\tau)], V]\rangle \ , \quad (3.16)$$

with

$$\bar{V}(\tau) = e^{i\mathcal{H}_0(H)\tau} V e^{-i\mathcal{H}_0(H)\tau} \ .$$

It is easily verified by explicit calculation of Eq. (3.16) that it indeed agrees with Eq. (3.15).

We conclude this section by discussing briefly the cases different from Eq. (3.11). For a fixed value of g, we may vary, for example, the magnitude of the field H. Correspondingly, the poles λ_i of $R(\lambda)$ move along the cut until they are near one of the branch points. In this situation we do not expect that the exponential behavior given by Eq. (3.16) is valid any more, since the influence of the branch point near the pole $-2\,\mathrm{Im}\lambda_1$ will be important. The contributions from both singularities should then be treated together. Varying H even further leads to the case that both poles are on the real axis. This corresponds to the situation where the poles and branch cuts of $\hat{g}(p)$ have moved to the imaginary axis of the p plane. As was discussed in Sec. II, one of the poles of $R(\lambda)$ can also appear in the first sheet. In this case, something qualitatively new happens with the behavior of $\langle S_0^z(t)\rangle$. The appearance of the pole of $R(\lambda)$ in the first sheet has as a consequence that the pole of $\hat{g}(p)$ at $p = 0$ which was in the third sheet also shows up in the first sheet of the p plane. It is precisely the appearance of this pole which causes the discrepancy with the "canonical" answer for $\lim\langle S_0^z(t)\rangle$ as $t \to \infty$.

IV. AUTOCORRELATION FUNCTIONS

As is well known, according to the Kubo-Tomita[12] theory the linear response to an oscillating magnetic field which is applied to the impurity is, at high temperatures, simply related to the Fourier transform of the autocorrelation functions. They are defined by

$$C_1(t) = \mathrm{Tr} S_0^+(t) S_0^- / \mathrm{Tr} 1 \tag{4.1}$$

and

$$C_2(t) = \mathrm{Tr} S_0^z(t) S_0^z / \mathrm{Tr} 1 \ . \tag{4.2}$$

This section is devoted to the study of the time dependence of these functions. It should be remarked that, in contrast with the previous sections, most of the results in the remaining part of this paper are only valid for the situation that the impurity is at one of the ends of the chain.

By virtue of Eq. (2.4) we may rewrite the correlation functions in terms of Fermi operators. Introducing again the Laplace transforms of these functions,

$$\hat{C}_i(p) = \int_0^\infty e^{-pt} dt\, C_i(t) \quad \text{with } \mathrm{Re} p > 0 \,, \tag{4.3}$$

applying the canonical transformation (2.7), and taking the thermodynamic limit $N \to \infty$ gives

$$\hat{C}_1(p) = (1/2i) R(-ip) \tag{4.4}$$

and

$$\hat{C}_2(p) = (1/8\pi i p) \int_{-\infty}^{\infty} d\lambda R(\lambda - i\epsilon) R(\lambda + ip) \times [2ip + f_0(\lambda - i\epsilon) - f_0(\lambda + ip)] - 1/4p \tag{4.5}$$

Let us first consider $C_1(t)$. For sufficiently weak g and

$$H_L - J < H < H_L + J \ , \tag{4.6}$$

we may compute the asymptotic long-time behavior by deforming the integration path as shown in Fig. 2. The main contributions come from the pole at λ_1 given by Eq. (3.13) and from the branch points at $-H_L \pm J$. Since the latter are of the order g^2, we have

$$C_1(t) = e^{i\,\mathrm{Re}\lambda_1 t} e^{-t/T_2} + O(g^2) \ , \tag{4.7}$$

where the transversal relaxation time T_2 is given by

$$1/T_2 = (g^2/2J)[J^2 - (H - H_L)^2]^{1/2}. \tag{4.8}$$

Similarly, under the condition (4.6) and weak coupling, we get

$$C_2(t) = e^{-t/T_1} + O(g^2) \ , \tag{4.9}$$

where T_1 is given by Eq. (3.15). From this we see that in this model the relaxation times are simply related by

$$T_2 = 2T_1 \ . \tag{4.10}$$

Some comments are in order on the situation where the pole λ_1 of $R(\lambda)$ is in the first Riemann sheet. Instead of Eqs. (4.8) and (4.10), we then

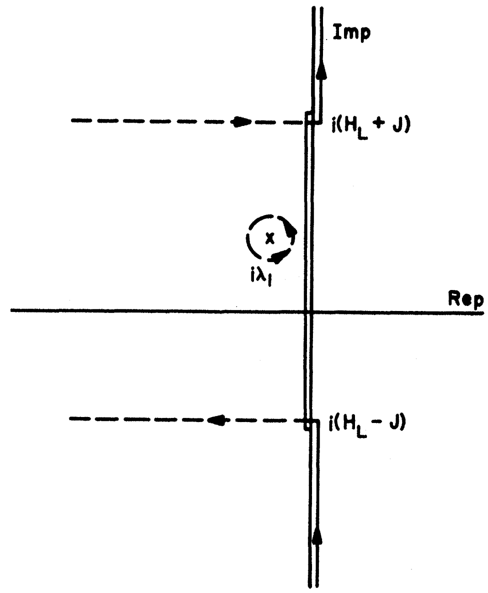

FIG. 2. Contour for evaluating the asymptotic behavior of $C_1(t)$. Solid line: first Riemann sheet. Broken line: second Riemann sheet.

get

$$C_1(t) = \tfrac{1}{2} e^{i\lambda_1 t} + O(g^2) \ ,$$

$$C_2(t) = \tfrac{1}{4} + O(g^2)$$

with λ_1 real. In the absence of g, we see from Eq. (3.13) that λ_1 is just the Larmor frequency of the impurity. The effect of g, in general, is not only to shift the Larmor frequency, but also to damp this frequency mode. However, if λ_1 is in the first sheet, then this mode persists in time, and as a consequence S_0^z is up to order g^2 a constant of motion. Because of this fact, we should not expect canonical considerations to hold in this case.

V. RELAXATION IN PRESENCE OF A TRANSVERSE FIELD

To study the validity of the Bloch equations in this model, we consider the following situation. Suppose that, for $t < 0$, there is a field H present along the z direction and that the system is in equilibrium. Similarly, as in Sec. II, let us use, for simplicity, instead of the initial density matrix ρ_H, the operator $\rho^{(0)}(H)$. Let us now assume that at $t = 0$ a field h_1 is switched on along the x direction and that it only acts on the impurity. Then, for $t > 0$ the magnetic moment is determined by

$$\langle S_0^\alpha(t) \rangle = \mathrm{Tr} \rho^{(0)}(H) S_0^\alpha(t) \tag{5.1}$$

with

$$S_0^\alpha(t) = e^{i\bar{\mathcal{H}}t} S_0^\alpha e^{-i\bar{\mathcal{H}}t} \quad , \tag{5.2}$$

where

$$\bar{\mathcal{H}} = \mathcal{H}(H) - \tfrac{1}{2}h_1 (S_0^+ + S_0^-) \quad . \tag{5.3}$$

In order to diagonalize Eq. (5.3) we replace $\bar{\mathcal{H}}$ by a new Hamiltonian

$$\mathcal{H}_t = \mathcal{H}(H) - \tfrac{1}{2}h_1 (S_0^+ + S_0^-)(S_{-1}^+ + S_{-1}^-) \quad , \tag{5.4}$$

where we have enlarged the Hilbert space by introducing a fictitious spin at the position to the left of the impurity. It can easily be seen that, with this new Hamiltonian, we have to compute, instead of Eq. (5.1),

$$\langle S_0^\alpha(t)\rangle = \langle\langle S_0^\alpha(t)\rangle\rangle + \langle\langle S_0^\alpha(t)(S_{-1}^+ + S_{-1}^-)\rangle\rangle \tag{5.5}$$

with

$$\langle\langle A\rangle\rangle = \mathrm{Tr}\rho^{(0)}(H)A \quad .$$

Here, the trace should, of course, be taken with respect to the $(N+2)$ spins.

We now turn to the diagonalization of Eq. (5.4). First, we rewrite $\mathcal{H}_t$ in terms of Fermi operators in the same way as in Sec. II, except that the summation in Eq. (2.4) now starts from -1. Next, we apply the two canonical transformations (2.6) and (2.8) to diagonalize $\mathcal{H}(H)$. Defining

$$\xi_{-1}^\dagger \equiv S_{-1}^+ \quad ,$$

we get

$$\mathcal{H}_t = \sum_{k,l=-1}^{N} [\xi_k^\dagger A_{kl}\xi_l + \tfrac{1}{2}(\xi_k^\dagger B_{kl}\xi_l^\dagger + \text{H. c.})] \tag{5.6}$$

with

$$A = \begin{pmatrix} 0 & \beta_0 & \cdots & \beta_N \\ \beta_0 & \lambda_0 & & 0 \\ \vdots & & & \\ \beta_N & 0 & & \lambda_N \end{pmatrix}, \quad B = \begin{pmatrix} 0 & \beta_0 & \cdots & \beta_N \\ -\beta_0 & 0 & & \\ \vdots & & & \\ -\beta_N & & & \end{pmatrix} , \tag{5.7}$$

and

$$\beta_k = -\tfrac{1}{2}h_1 V_{0k} \quad . \tag{5.8}$$

Finally, the Hamiltonian (5.6) can be diagonalized by using the canonical transformation

$$\zeta_k = \sum_{i=-1}^{N} (g_{ki}\xi_i + h_{ki}\xi_i^\dagger) \tag{5.9}$$

with g_{ki}, h_{ki} real and where ζ_k, $\zeta_k^\dagger$ are Fermi operators. Then

$$\mathcal{H}_t = \textstyle\sum_k E_k \zeta_k^\dagger \zeta_k + \text{const.} \tag{5.10}$$

If we introduce

$$\begin{aligned} \phi_{ki} &= g_{ki} + h_{ki} \quad , \\ \psi_{ki} &= g_{ki} - h_{ki} \quad , \end{aligned} \tag{5.11}$$

then the eigenvalue equations become

$$\begin{aligned} \phi_{kj}(A-B)_{ji} &= E_k \psi_{ki} \quad , \\ \psi_{kj}(A+B)_{ji} &= E_k \phi_{ki} \quad , \end{aligned} \tag{5.12}$$

which yield, by virtue of Eq. (5.7) and the orthonormality condition for ψ,

$$\left.\begin{aligned} \psi_{ki} &= \frac{2\beta_i\lambda_i}{E_k^2-\lambda_i^2}\psi_{k,-1} \\ \phi_{ki} &= \frac{2\beta_i E_k}{E_k^2-\lambda_i^2}\psi_{k,-1} \end{aligned}\right\} \quad \text{for } i = 0, \ldots, N,$$

$$\psi_{k,-1}^2 = \left(1 + \sum_i \frac{4\beta_i^2\lambda_i^2}{(E_k^2-\lambda_i^2)^2}\right)^{-1} \quad , \tag{5.13}$$

$$E_k\phi_{k,-1} = 0.$$

Substituting the first two expressions into Eq. (5.11) gives

$$\left.\begin{aligned} g_{ki} &= \beta_i(E_k-\lambda_i)^{-1}\psi_{k,-1} \\ h_{ki} &= \beta_i(E_k+\lambda_i)^{-1}\psi_{k,-1} \end{aligned}\right\} \text{ for } i = 0, \ldots, N. \tag{5.14}$$

The eigenvalues E_k are determined by the secular equation

$$R_1^{-1}(E_k) = 0 \tag{5.15}$$

with

$$R_1^{-1}(E) = E\left(1 - \sum_{i=0}^{N}\frac{4\beta_i^2}{E^2-\lambda_i^2}\right) \quad . \tag{5.16}$$

We distinguish between two possibilities: (i) $E_k \neq 0$, then $\phi_{k,-1} = 0$; (ii) $E_k = 0$, then $\phi_{k,-1} = 1$. From Eq. (5.15) we see that, if E_k is a solution, then $-E_k$ is also. We now have the freedom to choose all E_k to be non-negative. Notice that Eq. (5.16) can be rewritten as

$$R_1^{-1}(E) = E + \tfrac{1}{2}h_1^2[R(-E) - R(E)] \quad . \tag{5.17}$$

We now proceed to compute the transversal magnetization, i.e.,

$$\langle S_0^-(t)\rangle = \langle\langle S_0^-(t)\rangle\rangle + \langle\langle S_0^-(t)(S_{-1}^+ + S_{-1}^-)\rangle\rangle \quad . \tag{5.18}$$

Since the first term in Eq. (5.18) is odd in the number of Fermi operators, it simply vanishes. The second term is rewritten as

$$\langle\langle S_0^-(t)(S_{-1}^+ + S_{-1}^-)\rangle\rangle = \langle\langle[-\xi_{-1}(t) + \xi_{-1}^\dagger(t)]\eta_0(t)\rangle\rangle \quad ,$$

which can be calculated by applying the canonical transformations (2.8) and the relation

$$\zeta_k(t) = e^{-iE_k t}\zeta_k \quad .$$

As a result, we obtain after some algebra for the Laplace transform of the transversal magnetization,

$$\langle\hat{S}_0^-(p)\rangle = \tfrac{1}{2}h_1 \sum_{k=-1}^{N}\sum_{l=-1}^{N}\psi_{k,-1}^2\psi_{l,-1}^2 \times\left(\frac{R(-E_l)F(E_k,E_l)}{p+iE_k-iE_l}+\frac{R(-E_l)F(-E_k,E_l)}{p-iE_k-iE_l}+\frac{R(E_l)F(E_k,-E_l)}{p+iE_k+iE_l}+\frac{R(E_l)F(-E_k,-E_l)}{p-iE_k+iE_l}\right) \quad (5.19)$$

with

$$F(E,E')=[h_1^2/4(E-E')][R(E)R(E')C(E,E')+R(-E)R(-E')C(-E,-E')], \quad (5.20)$$

$$C(E,E')=\tfrac{1}{2}[f(E)-f(E')+(E-E')\tanh\tfrac{1}{2}\beta H] . \quad (5.21)$$

To change the summations in Eq. (5.19) into integrals, we make use of the Cauchy theorem. It is not difficult to show that Eq. (5.19) can be rewritten as

$$\langle\hat{S}_0^-(p)\rangle = [h_1/2(2\pi i)^2]\oint dE\oint dE' R_1(E)R_1(E')\{h_1^2R(E)R(E')R(-E')C(E,E') + R(-E)R(-E')[h_1^2R(E')-2E']C(-E,-E')\}[(E-E')(p+iE-iE')]^{-1} . \quad (5.22)$$

Here the integration path encircles in the counterclockwise direction all the poles of the function R_1. In order not to pick up contributions from the singularities of $R(E')$ in the integrations in Eq. (5.22) we have made use of Eq. (5.15) before the conversion of the summations. Now, one of the integrals in Eq. (5.22) can be explicitly carried out so that we get

$$\langle\hat{S}_0^-(p)\rangle = (h_1/4\pi ip)\int_{-\infty}^{\infty} dE\, R_1(E-i\epsilon)R_1(E_p)R(-E+i\epsilon)\{h_1^2R(E-i\epsilon)R(E_p)C(E_p,E-i\epsilon) + [h_1^2R(E-i\epsilon)-2E]R(-E_p)C(-E_p,-E+i\epsilon)\} \quad (5.23)$$

with $E_p=E+ip$.

Finally, let us turn to the calculation of the longitudinal magnetization

$$\langle S_0^z(t)\rangle = \langle\langle S_0^z(t)\rangle\rangle + \langle\langle S_0^z(t)(S_{-1}^+ + S_{-1}^-)\rangle\rangle .$$

In this case, the second term vanishes so that

$$\langle S_0^z(t)\rangle = \langle\langle c_0^\dagger c_0(t)\rangle\rangle - \tfrac{1}{2} .$$

This can again be evaluated using the described diagonalization procedure. The final result for its Laplace transfor is

$$\langle\hat{S}_0^z(p)\rangle = -(1/8\pi ip)\int_{-\infty}^{\infty} dE\, R_1(E-i\epsilon)R_1(E_p)R(-E+i\epsilon)R(-E_p)\{h_1^4R(E-i\epsilon)R(E_p) \times C(E_p,E-i\epsilon)+[h_1^2R(E-i\epsilon)-2E][h_1^2R(E_p)-2E_p]C(-E_p,-E+i\epsilon)\} . \quad (5.24)$$

To discuss the validity of the Bloch equations we have to study the weak coupling approximation to Eqs. (5.23) and (5.24). This approximation essentially amounts to taking a sufficiently large value of J for a given g and h_1. The discussion proceeds along lines similar to those in the previous sections. For this case, the only important contributions come from the poles of $R_1(E)$ which are determined by

$$E(E-\lambda_1)(E+\lambda_2)-\tfrac{1}{2}h_1^2(2E-\lambda_1+\lambda_2)=0 , \quad (5.25)$$

where λ_i are given by Eq. (3.13). From Eq. (5.25) we see that there are three poles. Let us denote them by E^n. Because of the factor $R_1(E+ip)$ in Eqs. (5.23) and (5.24), each one of these poles gives rise to three poles in the p plane for $\hat{S}_0^\alpha(p)$, so that the time dependence of the magnetization is in general governed by nine exponentials. The locations of the corresponding poles are given by

$$P_{nm}=i(E^n+E^m) , \quad (5.26)$$

so that we see that there are, in fact, only six exponentials. On the other hand, if the Bloch equations were valid for this model, then according to Eqs. (1.1) we should have three poles in the Laplace transform of M^α. Hence, we have to conclude that Eqs. (1.1) cannot be a correct description for the system. From Eq. (5.5) we see that in order to describe the magnetization of the impurity we also need to know the motion of the fictitious spin. Therefore, we expect that in a macroscopic description the degrees of freedom of the fictitious spin should also play an important role, so that it is not surprising that there are more than three exponentials present in this case. Of course, it should be emphasized that this is probably a special feature of the situation studied here. In particular, it is, for example, not clear that the above conclusions are also valid for the case where the impurity is in the middle of the chain.

APPENDIX

In this Appendix we give for the convenience of the reader some results for $\mathscr{g}(p)$ in the case that we do not make the approximation (2.20). The only difference in the calculation is that we have to compute, instead of Eq. (2.20a),

$$\langle \xi_{k_1}^\dagger \xi_{k_2} \rangle = \mathrm{Tr}\rho_{H+h} \xi_{k_1}^\dagger \xi_{k_2} \quad . \tag{A1}$$

Using canonical transformations described in Sec. II, we find

$$\langle \xi_{k_1}^\dagger \xi_{k_2} \rangle = V_{0k_1} V_{0k_2} (\lambda_{k_1} - \lambda_{k_2})^{-1} [F(\lambda_{k_1}) - F(\lambda_{k_2})] \tag{A2}$$

with

$$F(\lambda_{k_1}) = \tfrac{1}{2} h \textstyle\sum_k \overline{V}_{0k}^2 \tanh\tfrac{1}{2}\beta \overline{\lambda}_k (\overline{\lambda}_k - \lambda_{k_1})^{-1} \times [f_0(\lambda_{k_1}) - f_0(\overline{\lambda}_k) + \overline{\lambda}_k - \lambda_{k_1}] \quad . \tag{A3}$$

Here, the barred quantity $\overline{\lambda}_k$ is defined as a solution of the secular equation

$$\overline{R}^{-1}(\overline{\lambda}_k) \equiv \overline{\lambda}_k + H + h - \sum_{\nu=1}^{N} \frac{\alpha_\nu^2}{\overline{\lambda}_k - \Lambda_\nu} = 0 \tag{A4}$$

and

$$\overline{V}_{0k}^2 = \left(1 + \sum_{\nu=1}^{N} \frac{\alpha_\nu^2}{(\overline{\lambda}_k - \Lambda_\nu)^2}\right)^{-1} \quad . \tag{A5}$$

The summation in (A3) can also be converted into an integral using Cauchy's theorem. We have

$$F(\lambda_{k_1}) = (h/4\pi i) \oint d\lambda \tanh\tfrac{1}{2}\beta\lambda \overline{R}(\lambda) (\lambda - \lambda_{k_1})^{-1} \times [f_0(\lambda_{k_1}) - f_0(\lambda) + \lambda - \lambda_{k_1}] \quad , \tag{A6}$$

where the contour of integration is taken to be around the poles of $\overline{R}(\lambda)$ in the counterclockwise direction. Equation (A6) can be rewritten in a more convenient form by making use of the following identity:

$$\overline{R}^{-1}(\lambda) - \overline{R}^{-1}(\lambda_{k_1}) = f_0(\lambda_{k_1}) - f_0(\lambda) + \lambda - \lambda_{k_1} \quad .$$

We then find

$$F(\lambda_{k_1}) = \tfrac{1}{2} h \overline{R}^{-1}(\lambda_{k_1}) \tilde{F}(\lambda_{k_1}) \tag{A7}$$

with

$$\tilde{F}(\lambda_{k_1}) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{d\lambda}{\lambda_{k_1} - \lambda} \times [\overline{R}(\lambda - i\epsilon) - \overline{R}(\lambda + i\epsilon)] \tanh\tfrac{1}{2}\beta\lambda \quad . \tag{A8}$$

The derivation now proceeds along the same lines as those following Eq. (2.22) with the only difference being that Eq. (2.22) is replaced by Eq. (A2). The final result is

$$\mathscr{g}(p) = (-1/4\pi i p) \int_{-\infty}^{\infty} d\lambda R(\lambda - i\epsilon) R(\lambda + ip) \times \overline{R}^{-1}(\lambda - i\epsilon) \overline{R}^{-1}(\lambda + ip) \times [\tilde{F}(\lambda - i\epsilon) - \tilde{F}(\lambda + ip)] \quad . \tag{A9}$$

In deriving (A9) we have also made use of the identity

$$\overline{R}^{-1}(\lambda) - R^{-1}(\lambda) = h \quad . \tag{A10}$$

A special limiting case of Eq. (A9) is when $h \to 0$; then $\overline{R} \to R$, so that we get

$$\mathscr{g}(p) = (-1/4\pi i p) \int_{-\infty}^{\infty} d\lambda [\tilde{F}(\lambda - i\epsilon) - \tilde{F}(\lambda + ip)] \quad . \tag{A11}$$

Shifting the path of integration for the second term in (A11) and making use of the relation

$$\tilde{F}(\lambda - i\epsilon) - \tilde{F}(\lambda + i\epsilon) = [\overline{R}(\lambda - i\epsilon) - \overline{R}(\lambda + i\epsilon)] \tanh\tfrac{1}{2}\beta\lambda, \tag{A12}$$

we get back precisely Eq. (3.7), as we should, in the case $h = 0$.

Let us now study the limiting value of $\langle S_0^z(t) \rangle$ for $t \to \infty$. Suppose that the two poles of $R(\lambda)$ are in the second Riemann sheet; then we have, according to (A9),

$$\langle S_0^z(\infty) \rangle = (-1/4\pi i) \int_{-\infty}^{\infty} d\lambda R(\lambda - i\epsilon) R(\lambda + i\epsilon) \times \overline{R}^{-1}(\lambda - i\epsilon) \overline{R}^{-1}(\lambda + i\epsilon) \times [\tilde{F}(\lambda - i\epsilon) - \tilde{F}(\lambda + i\epsilon)] \quad . \tag{A13}$$

With the aid of (A12) we get

$$\langle S_0^z(\infty) \rangle = (-1/4\pi i) \int_{-\infty}^{\infty} d\lambda R(\lambda - i\epsilon) R(\lambda + i\epsilon) \times [\overline{R}^{-1}(\lambda + i\epsilon) - \overline{R}^{-1}(\lambda - i\epsilon)] \tanh\tfrac{1}{2}\beta\lambda \quad , \tag{A14}$$

which is, indeed, the same as the "canonical" answer (3.7) in view of Eq. (3.3) and the definitions of R and $\overline{R}$. Similarly, if $R(\lambda)$ has a pole in the first sheet, one can readily show that the above equality does not hold any longer. Again, the contributions of this pole to $\langle S_0^z(\infty) \rangle$ and Eq. (3.7) will be different.

Finally, let us consider the high-temperature limit of (A9). We get

$$\tilde{F}(\lambda) = \tfrac{1}{2}\beta [\lambda \overline{R}(\lambda) - 1] \quad ,$$

so that (A9) reduces to

$$\mathscr{g}(p) = (-\beta/8\pi i p) \int_{-\infty}^{\infty} d\lambda R(\lambda - i\epsilon) R(\lambda + ip) \times [\lambda \overline{R}^{-1}(\lambda + ip) - (\lambda + ip) \overline{R}^{-1}(\lambda - i\epsilon)] \quad . \tag{A15}$$

From the definitions of R and $\bar{R}$ it follows immediately that

$$\lambda\bar{R}^{-1}(\lambda+ip)-(\lambda+ip)\bar{R}^{-1}(\lambda-i\epsilon) = -iph+\lambda R^{-1}(\lambda+ip)-(\lambda+ip)R^{-1}(\lambda-i\epsilon) \quad . \tag{A16}$$

Substituting this into (A15) yields, after some algebra,

$$\hat{g}(p)=\beta h\,\hat{c}_2(p)+\beta H/4p \quad , \tag{A17}$$

where $\hat{c}_2(p)$ is the longitudinal autocorrelation function defined in Sec. IV. Of course, the same result could have been found by noting that we have, by expanding Eq. (2.16) to linear terms in β,

$$\langle S_0^z(t)\rangle = -\beta\,\mathrm{Tr}\,\mathcal{H}(H+h)\,S_0^z(t)/\mathrm{Tr}\,1 \quad . \tag{A18}$$

Equation (A18) can also be rewritten as

$$\langle S_0^z(t)\rangle = \beta\left[h\,\mathrm{Tr}\,S_0^z S_0^z(t) - \mathrm{Tr}\,\mathcal{H}(H)\,S_0^z(t)\right]/\mathrm{Tr}\,1 \;, \tag{A19}$$

which, indeed, agrees with (A17).

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Correlation between Lifetime and Momentum for Positron Annihilations in Teflon

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A novel technique has made it possible to correlate the three components in the lifetime distribution of positrons in Teflon with the angle between the γ rays resulting from the annihilation. The intensity of the intermediate component was found to be virtually independent of this angle, whereas the intensity of the longest-lived component was greatly enhanced for angles corresponding to higher momentum. Apparently the intermediate component does not result from the annihilation of orthopositronium, because the momentum associated with this component is too small. The intermediate component could be caused by free-positron annihilation or by annihilation of positrons which are bound in Teflon molecules.

INTRODUCTION AND HISTORY OF PROBLEM

As early as 1956 it was suggested[1,2] that many details of positron interactions with matter could be clarified by an experiment in which the positron lifetime was correlated with the angle between the two γ rays resulting from the annihilation. Experimental techniques needed for such a measurement were not developed until several years later. In 1964, preliminary results were reported[3] which showed for the first time the angular dependence of the long-lived component in the lifetime spectrum of positrons in Teflon.

Additional measurements, using some refinements in technique and with improved statistics, were reported by one of us (V. F. W.).[4] These results indicated that the angular correlation of radiation from "pick-off" annihilation of positrons in positronium (Ps) atoms is significantly broader than the angular correlation of annihilation radia-