Localized Dynamic Perturbations in Metals*

E. Müller-Hartmann,† T. V. Ramakrishnan, and G. Toulouse
Department of Physics, University of California, San Diego, La Jolla, California 92037
(Received 7 July 1970)

The effect of a localized time-dependent potential on a Fermi gas is discussed. A simple bosonlike model for the particle-hole excitations is developed. Its use appears justified for the dissipative part of the response of the Fermi gas to localized time-dependent potentials. General expressions are obtained for the probability that the Fermi gas remains in the ground state and for the energy spectrum of excited states. Several illustrative examples are discussed. We consider the effect of an exponentially switched-on localized potential. It is shown that the state reached when the potential attains its full strength V is orthogonal to the ground state of the Fermi gas with the potential V, no matter how slow the switching. It consists of a spectrum of excited states of the full Hamiltonian with a width proportional to the switching rate. Other aspects of this failure of adiabaticity such as nonreversibility and path dependence are investigated. Some possible applications are pointed out. The potential source may have a finite mass. The effect of its recoil is calculated for the special case of a suddenly switched-on potential. The probability of finding the Fermi gas in its final ground state after the perturbation is switched on is found to be $P_G = \exp[\tilde{V}^2 \ln\gamma/(1-\gamma^2)]$, where $\tilde{V} = V\rho_{\epsilon_F}$ and is a measure of the coupling of the localized perturbation to the electron gas. γ is the mass ratio m/M. The potential source is initially at rest. The above expression is critically discussed and corrections to it are calculated. They are found to be small. The spectrum of excitations produced is also calculated. In conclusion, connections are pointed out with other particle field problems exhibiting a similar infrared singularity.

I. INTRODUCTION

The problem of a static (fixed in space and stationary in time) ordinary localized potential in a Fermi sea has been thoroughly explored for some time.[1] Because of the simplicity of static properties, attention has been diverted early to the more puzzling problem of a "magnetic" impurity, overlooking the fact that the dynamic properties of an ordinary potential exhibit quite singular features.[2] Indeed, knowledge of these dynamic properties now appears to be a prerequisite for a real understanding of the spin fluctuations of a magnetic impurity,[2,3] as well as basic for the interpretation of many experimental data in metals.[2,4-6]

In this paper, we consider the response of a Fermi gas to a localized time-dependent potential whose source may have a finite mass. The physical reason for the anomalous behavior found for this response stems simply from the localized character of the perturbation considered and from the statistical nature of the perturbed particles. Because of the Pauli principle, each particle is surrounded by its Fermi hole; when an imbalance appears at some point of the medium, the particles all around it move to adjust to the local disturbance. During this process, they collide strongly against each other via their Fermi holes. Thus, even a weak perturbation results in a strong-coupling problem because of the continued turbulence induced in the Fermi sea.

Mathematically, the root of the anomalies may be found in the long-time behavior of the propagator,

$$G_0(t) = \langle 0 | a_0(t) a_0^\dagger(0) | 0 \rangle , \tag{1.1}$$

where $a_0^\dagger$ and a_0 are the creation and annihilation operators, respectively, for a localized Wannier orbital at the origin; the average is taken over the ground state of the Fermi sea. The propagator $G_0(t)$ contains information on the relaxation time of the system after an extra particle has been placed at the origin. Because of the Fermi statistics and because the added particle is prepared in a localized state, the decay of $G_0(t)$ takes the asymptotic form

$$G_0(t) \simeq 1/i\epsilon_F t \tag{1.2}$$

for long times $t(\epsilon_F t \gg 1)$, where ϵ_F is the Fermi energy. This asymptotic form shows a long scaleless relaxation for return to equilibrium after a sudden perturbation. The form (1.2) is trivially derived for independent fermions; for interacting fermions, the Landau quasiparticles of low energy E have a lifetime $\tau \simeq 1/E^2$ due to their interaction. Despite this added feature, the asymptotic dependence is still of the form (1.2). The reason for this insensitivity of $G_0(t)$ to the interaction among particles is clearly due to the fact that its long-time behavior is governed by the spectrum of low-lying excitations which is not qualitatively affected by the interaction. For simplicity, we shall hence-

forth consider only a gas of noninteracting fermions; thereby neglecting any effect associated with the high-frequency response of an electron gas (plasmons, etc.).

The anomalies, i.e., nonlinearities found for the response to a localized perturbation, do not jeopardize the standard linear-response theory for extended perturbations. The physical reason is simple. Suppose, for example, that the surface potential of a metal undergoes some variation. The electrons will be able to screen this perturbation in an orderly manner, thereby avoiding prolonged collisions among themselves. Mathematically, it is seen that the associated propagator exhibits exponential decay instead of the power law (1.2).

In Sec. II of this paper, a simple boson model is developed. The long-time (low-energy) dissipative response of the Fermi gas to localized dynamic perturbations is shown to be well described by such a model. The model is then applied to discuss several types of problems. In Sec. III, where the potential source is assumed to be infinitely massive, the effect of a slowly switched potential on the Fermi gas is examined; this allows a detailed discussion of adiabaticity. The effect on the Fermi gas of a potential turned on and then off is also studied; this is relevant for collision problems such as the scattering of an atom from a metal surface. In Sec. IV, a thorough discussion of the recoil effects due to the finite mass of a suddenly switched potential is presented; this is of interest in evaluating the influence of (initial-) final state interactions in the optical spectra of metals.

II. HAMILTONIAN AND ALTERNATIVE APPROACHES

A. Hamiltonian

The Hamiltonian of a system consisting of the Fermi gas and a time-dependent potential source of mass M interacting with it is given by

$$H=\sum_k \epsilon_k a_k^\dagger a_k+\frac{p^2}{2M}+\sum_{kk'} V_{kk'}(t)\, a_k^\dagger a_{k'} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}$$

$$=H_0+\sum_{kk'} V_{kk'}(t)\, a_k^\dagger a_{k'} e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}. \qquad (2.1)$$

Here ϵ_k is a quasiparticle energy and $V_{kk'}(t)$ is the time-dependent single-particle potential due to a source with coordinate R and kinetic energy $p^2/2M$.

The use of Hamiltonian (2.1) for a charge perturbation in an electron gas requires some justification. It is assumed that the screening of the charge due to Coulomb interactions occurs instantaneously, so that $V_{kk'}^{\mathrm{sc}}(t)=V_{kk'}(t)$ and $V_{kk'}^{\mathrm{unsc}}(t)$ have the same time dependence. Since the response of the electron gas to charge fluctuations has in fact a time scale of ω_p^{-1}, clearly our results will not describe properly the immediate response to potentials $V_{kk'}^{\mathrm{unsc}}(t)$ which vary appreciably on that time scale. We imply further that there are no long-time ($t\gg\omega_p^{-1}$) transient effects associated with the screening of the time-dependent potential by interacting electrons and that all transient effects arise from the response of the quasiparticles to the screened time-dependent potential. This is probably reasonable, for the low-energy electron-hole excitations responsible for long-time transient effects are not prominently involved in screening. Therefore, as discussed in the Introduction, we shall consider the quasiparticles to be noninteracting and the potential to be screened. Finally, the potential source is taken to have no internal structure; no "magnetic" effect is considered and the electron spin is ignored.

B. Outline

The aim is to determine the time evolution of the initial state $|\psi(t_0)\rangle$ (e.g., the ground state) of the system under the influence of the time-dependent perturbation. The state $|\psi(t)\rangle$ at a time t can be written as

$$|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle . \qquad (2.2)$$

The overlap of this with a given state (e.g., the initial state) is of interest. This ground-state overlap is the vacuum amplitude

$$A_G=\langle\psi(t_0)|U(t,t_0)|\psi(t_0)\rangle . \qquad (2.3)$$

The overlap with a state $|\psi_\alpha\rangle$ is

$$A_\alpha=\langle\psi_\alpha|U(t,t_0)|\psi(t_0)\rangle=\langle\psi(t_0)|U_\alpha^\dagger U(t,t_0)|\psi(t_0)\rangle , \qquad (2.4)$$

where $|\psi_\alpha\rangle$ is obtained from $|\psi(t_0)\rangle$ by the unitary transformation U_α. The time-dependent perturbation creates a large number of low-energy particle-hole pairs. The energy spectrum of these excitations with respect to the eigenstates of a Hamiltonian $\mathcal{H}$ is

$$S_t(\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau}\langle\psi(t)|e^{-i\mathcal{H}\tau}|\psi(t)\rangle \qquad (2.5)$$

and thus can be found if $|\psi(t)\rangle$ is known. Another class of effects, typified by threshold phenomena,[2,7] requires knowing the evolution of a singly excited initial state under the time-dependent perturbation. We shall not investigate this here.

The time evolution of the initial state will be found in two ways. In the first (Sec. II C), the evolution operator is written as an exponential and a systematic expansion of the exponent in powers of V is obtained. Averages of the evolution can be expressed as an exponential sum of cumulants. The procedure does not involve any approximation to the Hamiltonian (2.1) and is systematic. It is, however, cumbersome and does not give much

insight into the physical processes involved.

In the second method (Sec. IID), the particle-hole excitations are treated as bosons and the Hamiltonian H of (2.1) is replaced by a simpler boson model. The dissipative, low-energy (long-time) response of the Fermi gas to a localized perturbation is suitably represented in this model. The results are quantitatively accurate for weak potentials. The model is justified and its limitations are pointed out. In some cases, exact solutions can be obtained for arbitrary V, and this is used to suitably modify or to estimate the accuracy of the boson-approximation result (Secs. IID and III E). The cumulant expansion method will also be used to calculate higher-order corrections (Sec. IV B). In a simple soluble two-level model, the validity of the boson approximation can be discussed in detail (Appendix A).

C. Cumulant Method

We first discuss the cumulant method. In the interaction representation, the equation of motion for the evolution operator is

$$i\frac{\partial U(t,t_0)}{\partial t} = \tilde{V}(t)U(t,t_0), \tag{2.6}$$

where $U(t_0,t_0)=1$ and

$$\tilde{V}(t)=e^{iH_0t}\Big[\sum_{kk'} V_{kk'}(t)a_k^\dagger a_{k'}' e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}\Big]e^{-iH_0t}. \tag{2.7}$$

U can be expressed as an exponential operator

$$U=e^{-iF}; \tag{2.8}$$

the equation of motion for F as well as the first terms of an expansion of F in powers of the potential can be found in lecture notes of Gross.[8]

Knowing the evolution operator, one can evaluate various associated quantities; for example, the amplitude A_G that the system remain in its ground state under the action of the time-dependent perturbation is given by (2.3),

$$A_G(t)=\langle\psi(t_0)|\,e^{-iF(t,t_0)}\,|\psi(t_0)\rangle. \tag{2.9}$$

There exists a well-known cumulant expansion[9] for such an average,

$$\langle\psi|\,e^{-iF}\,|\psi\rangle=\exp[\textstyle\sum_n (c_n/n!)]. \tag{2.10}$$

The cumulants represent an expansion in terms of irreducible correlations between particle-hole operators (i.e., operators of the form $c_k^\dagger c_{k'}$). The expansion is useful if higher-order correlations are smaller than and/or qualitatively not different from the lower-order ones. For $A_G(t)$ in (2.9), the cumulants up to order V^2 are

$$c_1=-i\Big\langle\int_{t_0}^{t}\tilde{V}(\tau)\,d\tau\Big\rangle-\frac{1}{2}\Big\langle\int_{t_0}^{t}\Big[\tilde{V}(\tau),\int_{t_0}^{\tau}\tilde{V}(\sigma)\,d\sigma\Big]\,d\tau\Big\rangle, \tag{2.11a}$$

$$c_2=\Big\langle\Big\langle\int_{t_0}^{t}\tilde{V}(\tau)\,d\tau\Big\rangle\Big\rangle^2-\Big\langle\int_{t_0}^{t}\tilde{V}(\tau)\,d\tau\int_{t_0}^{t}\tilde{V}(\sigma)\,d\sigma\Big\rangle. \tag{2.11b}$$

This is the general way to obtain a cumulant expansion; in specific cases, simpler approaches can be followed (e.g., see Sec. IV B).

One can obtain similar cumulant expansions for other quantities, such as the overlap with another state, or the spectrum. The procedure is to reduce the quantity to the ground-state expectation value of some operator [this can be done using expressions (2.4) and (2.5)] and then to write this as a single exponential operator using the Baker-Hausdorf[10] method. For the quantities of interest here, the general picture is as follows: The anomalous behavior will be governed by the term of second order in V in the cumulant expansion, henceforth called second cumulant. This, in turn, can be obtained through the boson model presented below.

D. Boson Approximation

We now discuss a simple model in which the particle-hole excitations of the Fermi gas are treated as bosons. The model appears to be suitable when the perturbation producing particle-hole excitations is of short range.

The boson approximation consists in replacing particle-hole operators with boson-creation and boson-annihilation operators. To be specific, we replace

$$a_{k_>}^\dagger a_{k'_<} \text{ by } b_j^\dagger, \tag{2.12}$$

where the subscripts $k_>$ and $k'_<$ mean that k is outside the Fermi sphere and k' is inside. The operator $a_{k_>}^\dagger a_{k'_<}$ applied to the ground state creates a hole k' and a particle k while imparting a momentum $k'-k$ to the potential source. The index j stands for the pair $k_>$, $k'_<$. The operators $b_j^\dagger$ are assumed to be bosons in the usual sense, i.e.,

$$[b_j, b_{j'}^\dagger]=\delta_{jj'},\quad [b_j, b_{j'}]=0. \tag{2.13}$$

Since

$$[H_0, a_k^\dagger a_{k'}]=(\epsilon_k-\epsilon_{k'})a_k^\dagger a_{k'},$$

we choose

$$H_0=\textstyle\sum_j \epsilon_j b_j^\dagger b_j, \tag{2.14}$$

where

$$\epsilon_j=\epsilon_{k_>}-\epsilon_{k'_<}. \tag{2.15}$$

The density of such boson excitations of energy E is

$$N(E)=\sum_j \delta(E-\epsilon_j)$$
$$=\sum_{k,k'} n_{k'}(1-n_k)\delta(E-\epsilon_{k_>}+\epsilon_{k'_<}). \quad (2.16)$$

The time-dependent potential can also be written in terms of the boson operators as

$$V(t)=\sum_j [V_j(t)b_j^\dagger e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}+V_j^*(t)b_j e^{-i(\vec{k}-\vec{k}')\cdot\vec{R}}], \quad (2.17)$$

where $V_j(t)=V_{kk'}(t)$ and $V_j^*(t)=V_{k'k}(t)$. We have omitted in (2.17) a part of $V(t)$:

$$V_1(t)=\Big(\sum_{k_<,k'_<}+\sum_{k_>,k'_>}\Big)V_{kk'}(t)e^{i(\vec{k}-\vec{k}')\cdot\vec{R}}a_k^\dagger a_{k'}, \quad (2.18)$$

i.e., the part which creates and destroys only particles or only holes. Clearly, this gives nothing when it acts on the ground state, except for the diagonal part which provides the first-order energy shift and can be lumped into H_0. Collecting the two terms (2.14) and (2.17), the boson approximation to the Hamiltonian (2.1) is

$$H=\sum_j \epsilon_j b_j^\dagger b_j+\sum_j [V_j(t)b_j^\dagger e^{i\vec{q}_j\cdot\vec{R}}+V_j^*(t)b_j e^{-i\vec{q}_j\cdot\vec{R}}]$$
$$+p^2/2M, \quad (2.19)$$

where $\vec{q}_j$ is the net momentum of the particle j (or k,k'), i.e., $\vec{q}_j=(\vec{k}-\vec{k}')$. Equation (2.21) describes the Hamiltonian of a piezoelectriclike polaron of mass M with a time-dependent coupling to the boson field.

The main basis for the applicability of the boson model is the localized short-range character of the potential perturbation. This means that $V_{k,k'}(t)$ is of order ϵ_F/N, so that each particle-hole mode is infinitesimally excited by the perturbation, i.e.,

$$\langle\psi(t)|b_j^\dagger b_j|\psi(t)\rangle\sim V_j/E_j\sim 1/N, \quad (2.20)$$

in general. Since the b_j, $b_j^\dagger$, etc., are actually fermion pair operators, expectation values of their products are subject to restrictions of the Pauli principle. For example, the maximum occupation number

$$\langle b_j^\dagger b_j\rangle_{\text{term}}\leq 1. \quad (2.21)$$

However, in a formal boson model there is no such upper limit. This difference in behavior is unlikely to lead to gross errors if the excited states of the system are such that the actual occupation number is $\sim 1/N$ as in the present case. On the other hand, if the potential is such that a few particle-hole modes are strongly excited (e.g., a long-range or extended perturbation), the boson approximation will be seriously in error.

The commutation relation satisfied by the b_j's is

$$[b_j, b_{j'}^\dagger]=a_{k'_<}a_{x'_<}\delta_{kx}-a_{x_>}^\dagger a_{k_>}\delta_{k'x'}, \quad (2.22)$$

where

$$b_j=a_{k'_<}^\dagger a_{k_>} \text{ and } b_{j'}^\dagger=a_{x_>}^\dagger a_{x'_<}.$$

Thus, if the indices j and j' are all different, we have

$$[b_j, b_{j'}^\dagger]=0, \quad (2.23)$$

i.e., b_j and $b_{j'}^\dagger$ commute. In the remaining cases when $k=x$ or $k'=x'$ or $j=j'$, the excited states for a short-range perturbation are such that

$$\langle[b_j, b_{j'}^\dagger]\rangle\sim\delta_{jj'}+O(1/N). \quad (2.24)$$

Equations (2.23) and (2.24) define the formal sense in which the operators b_j are bosonlike, i.e., the commutator averages have the correct values to $O(1/N)$. It cannot be concluded from this that our results are correct to relative order $(1/N)$ since summing over intermediate states can give an additional factor of N. We shall see later [Eqs. (2.26) and (2.27)] that the $1/N$ contributions do, in fact, add coherently but in a way which just leads to a renormalization of the coupling constant.

The lowest-order singular term for $\langle\psi_0|U(t,t_0)|\psi_0\rangle$ is the ground-state average of an operator of the form

$$\sum_j \int_{t_0}^t V_j(\tau)b_j(\tau)\,d\tau\int_{t_0}^t V_j^*(\sigma)b_j^\dagger(\sigma)\,d\sigma. \quad (2.25)$$

It is singular due to the large number of the excitations j and their excitation spectrum. The most singular terms in perturbation theory (in powers of V) arise from products of such operators. It is argued that for a short-range perturbation, the boson model gives reliable answers for the ground-state average of such many boson products. Thus, we can expect that the most singular long-time behavior in each order of perturbation theory will be correctly reproduced in the boson model. The errors due to the approximate commutation rules and due to the neglect of $V_1(t)$ [Eq. (2.18)] do not involve more singular terms. They can be estimated by looking at the cumulant expansion (2.10).

In some special cases (when $M=\infty$), it is possible to obtain exact solutions. An example is the suddenly switched-on potential studied by Nozières and De Dominicis.[2] The boson model is found to give the correct form of the long-time behavior. For instance, the long-time overlap for a zero-range potential V has the exact value

$$(1/t)^{(\delta/\pi)^2}, \quad (2.26)$$

where δ is the s-wave phase shift at the Fermi level, and the boson-approximation result is

$$(1/t)^{(V\rho_{\epsilon_F})^2}. \tag{2.27}$$

(Note that $-V\rho_{\epsilon_F}$ is the first term in the Born expansion of δ/π, so that the boson result is exact for weak potentials.) Thus, in this case, using the boson model and then the correspondence $-V\rho_{\epsilon_F} \to (\delta/\pi)$ would lead to the exact result. For a generally time-dependent potential, it is not possible to make such a correspondence. In one such case where exact results can be found (see Sec. III E) the boson result is obtained for weak potentials, i.e., $|V\rho_{\epsilon_F}| \ll 1$.

The reactive part of the response of the Fermi gas to the localized perturbation results in an energy shift which appears as a phase factor in the vacuum amplitude. For example, in case of a steady zero-range potential V, the energy shift is

$$\Delta E = -(1/\pi)\int_{-\infty}^{\epsilon_F} \delta(E)\,dE,$$

where

$$\delta(E) = -\tan^{-1}\left(\frac{\pi V\rho(E)}{1 - V\mathrm{Re}\mathcal{F}(E)}\right).$$

Here $\rho(E)$ is the density of states and $\mathcal{F}(E)$ is its Hilbert transform. In the boson approximation, however, we see that $\Delta E = -\sum_j (V_j^2/E_j)$, which is the correct second-order contribution to the energy shift but may be a qualitatively wrong estimate of the actual energy shift. This observation is true of the reactive response to time-dependent perturbations as well. The reason for the inadequacy of the boson model as regards energy shifts is the following. The reactive response involves (virtual) excitations of all energies, and the boson model is good only for quantities sensitively dependent on low-energy excitations.

The Hamiltonian (2.1) can be reduced to the Hamiltonian of an electron gas with one (radial) dimension if $M = \infty$ and V is of zero range[11] (s-wave scattering). Tomonaga[12] has shown that the low-lying excitations of such a (one-dimensional electron-gas) system are approximate bosons. The Tomonaga boson-creation operator is

$$b_q^\dagger = (1/\sqrt{q})\sum_k a_k^\dagger a_{k-q}, \tag{2.28}$$

where k and $k-q$ are radial quantum numbers. It is thus a coherent superposition of particle-hole operators. In this case, the Hamiltonian can be rewritten in terms of Tomonaga boson operators and the physical effects of a time-dependent potential can be calculated. This might be a formally more satisfactory way of obtaining the boson model, but it is restricted to the special case of $M = \infty$ and zero range. Moreover, the physical reasons (discussed above) for the applicability of the boson model are not brought out. In fact, the Tomonaga linear superposition, when used (where applicable) in this problem, appears just as an unnecessary intermediate step in the calculation.

To conclude this section, we observe that the model Hamiltonian (2.19) is of intrinsic interest as example of a particle interacting with a boson field. In many systems, the low-lying excitations are bosonlike (e.g., phonons, magnons) and their interaction with a time-dependent perturbation can be represented by a similar Hamiltonian.

III. GENERAL TIME DEPENDENCE AND ADIABATICITY

A. Outline

In this section, the potential source is assumed not to recoil on exciting a particle-hole pair, i.e., it is taken to be infinitely massive. Using the approximation introduced in Sec. II, we discuss in detail the cases of a potential turned on from $t = -\infty$ to $t = 0$ and of a potential turned on and switched off between $t = -\infty$ and $t = +\infty$. The results are used to elucidate the nature of the response of the Fermi gas to time-dependent perturbations. The response to a localized perturbation appears to be never adiabatic in the strict usual sense. This failure is due to the comparatively high density of low-lying excitations and is discussed in some detail. Temperature effects are finally mentioned; a formula for the nonadiabatic part of the temperature-dependent evolution operator is presented.

B. Density of Excitations

We first discuss the density of particle-hole excitations, the low-energy behavior of which plays a crucial role in the effects considered here. This density $\rho(\omega)$ is given by

$$\rho(\omega) = \sum_j \delta(\omega - \omega_j) = \sum_{k,k'} n_{k'}(1 - n_k)\delta(\omega - \epsilon_k + \epsilon_{k'}). \tag{3.1}$$

The potential V_j is here assumed for simplicity to be of zero range and thus couples equally to all excitations. The dependence on the range of the potential is most simply taken into account by redefining $\rho(\omega)$ as

$$V^2\rho(\omega) = \sum_{k,k'} |V_{kk'}|^2 n_{k'}(1 - n_k)\delta(\omega - \epsilon_k + \epsilon_{k'}). \tag{3.2}$$

The nonzero range of the potential will have the effect of greatly reducing this $\rho(\omega)$ beyond an energy $\sim(\hbar^2/2ma^2)$, where a is the range of the potential. The band structure of the metal also provides a cutoff of the order of electronic energy. A crude way of considering these effects is to use an upper cutoff $\omega_c(\sim\epsilon_F)$. We shall do so where necessary. The characteristic features of our results depend on the density of low-energy ($\omega \ll \epsilon_F$) excitations and thus are not qualitatively affected by such approximations for the high-energy region.

The density $\rho(\omega)$ of particle-hole excitations is easily calculated from the explicit form (3.1) to be

$$\rho(\omega)=\tfrac{1}{4}\rho_{\epsilon_F}^2\,\epsilon_F\left[(2+\tilde{\omega})(1+\tilde{\omega})^{1/2}-(2-\tilde{\omega})(1-\tilde{\omega})^{1/2}-\tilde{\omega}^2\ln\left(\frac{1+(1+\tilde{\omega})^{1/2}}{1+(1-\tilde{\omega})^{1/2}}\right)\right]\quad\text{if }\tilde{\omega}\le 1$$

$$=\tfrac{1}{4}\rho_{\epsilon_F}^2\,\epsilon_F\left[(2+\tilde{\omega})(1+\tilde{\omega})^{1/2}-\tilde{\omega}^2\ln\left(\frac{1+(1+\tilde{\omega})^{1/2}}{(\tilde{\omega})^{1/2}}\right)\right]\qquad\text{if }\tilde{\omega}\ge 1\,,\tag{3.3}$$

where ρ_{ϵ_F} is the density of states at the Fermi energy and $\tilde{\omega}$ is the dimensionless excitation energy in units of ϵ_F. A numerical calculation shows that

$$\rho(\omega)=\epsilon_F\,\rho_{\epsilon_F}^2\,\tilde{\omega}\tag{3.4}$$

quite closely. This is exact for $\tilde{\omega}\ll 1$ and is higher than the true value only by 5% at $\tilde{\omega}=0.6$. For $\tilde{\omega}\gg 1$, (3.4) greatly overestimates the density of particle-hole excitations; from (3.3) we see that

$$\rho(\omega)=\tfrac{2}{3}\rho_{\epsilon_F}^2\,\epsilon_F\,\tilde{\omega}^{1/2}.\tag{3.5}$$

We shall use the form (3.4) for $\rho(\omega)$ throughout this section. The upper cutoff ω_c removes any artificial ultraviolet divergences that may result from this usage.

C. Solution

In the case $M=\infty$, the boson model (2.19) is exactly soluble. The solution is derived here and general expressions are found for some quantities of physical interest. In the interaction representation, the equation of motion for the evolution operator is

$$i\frac{\partial U(t,t_0)}{\partial t}=\sum_j\left[V_j(t)\,e^{iE_jt}\,b_j^\dagger+V_j^*(t)\,e^{-iE_jt}\,b_j\right]U(t,t_0)\,.\tag{3.6}$$

The form of this clearly suggests that U is an exponential operator with exponent linear in $b^\dagger$ and b. We therefore make the ansatz

$$U(t,t_0)=\exp[i\textstyle\sum_j\phi_j(t,t_0)]\times\exp\{-\sum_j[f_j(t,t_0)b_j^\dagger-f_j^*(t,t_0)b_j]\}\,,\tag{3.7}$$

where $\phi_j(t,t_0)$ and $f_j(t,t_0)$ are c numbers, and substitute in (3.6) to find equations for them. They are solved to give

$$\phi_j(t,t_0)=\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\,V_j(t')V_j(t'')\sin E_j(t'-t'')\tag{3.8}$$

and

$$f_j(t,t_0)=i\int_{t_0}^{t}V_j(t')e^{iE_jt'}\,dt'.\tag{3.9}$$

The reactive response to the time-dependent perturbation is represented by the phase factor $\sum_j\phi_j(t,t_0)$. This describes the energy shift in the ground state. The integrated displacement between t_0 and t of each oscillator j is given by $f_j(t,t_0)$ and is a measure of the degree of excitation of that mode.

The spectral distribution of the state $|\psi(t)\rangle$ is given by (2.5), i.e., by

$$S_t(\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{i\omega\tau}\times\langle\psi(t_0)|\,U^\dagger(t,t_0)U_{\mathcal{K}}^\dagger\,e^{-iH_0\tau}U_{\mathcal{K}}U(t,t_0)\,|\psi(t_0)\rangle\,d\tau\,,\tag{3.10}$$

where the spectrum is with respect to the eigenvalues of $\mathcal{K}$, itself related to H_0 by the unitary transformation

$$\mathcal{K}=U_{\mathcal{K}}^\dagger H_0U_{\mathcal{K}}\,.\tag{3.11}$$

This can be written compactly as

$$S_t(\omega)=\frac{1}{2\pi}\int e^{i\omega\tau}\langle\psi(t_0)|\,A^\dagger(\tau)A\,|\psi(t_0)\rangle\,d\tau\,,\tag{3.12}$$

with

$$A=U_{\mathcal{K}}U(t,t_0)\quad\text{and}\quad A^\dagger(\tau)=e^{iH_0\tau}A^\dagger\,e^{-iH_0\tau}\,.\tag{3.13}$$

One important particular case is the case $\mathcal{K}=H_0$; then the spectrum is

$$S_t(\omega)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{i\omega\tau}\exp\left(\sum_j c_j(\tau)\right)d\tau\,,\tag{3.14}$$

where

$$c_j(\tau)=(e^{-iE_j\tau}-1)\,|\,f_j(t,t_0)\,|^2\tag{3.15}$$

and $f_j(t,t_0)$ is defined in (3.9).

The probability for the perturbation leaving the Fermi gas in its ground state is given by the $\delta(\omega)$ part of the spectrum and is therefore

$$P_G^0(t)=\exp[\textstyle\sum_j c_j(\tau=\infty)]=\exp[-\sum_j|f_j(t,t_0)|^2]\,,\tag{3.16}$$

since as $\tau\to\infty$, the exponential sum in $\sum_j c_j(\tau)$ rapidly oscillates to zero. Several sum rules can be derived for the spectrum from the form (3.14) for $S_t(\omega)$. Clearly, we have

$$\int_{-\infty}^{+\infty}S_t(\omega)\,d\omega=1\,.\tag{3.17}$$

This just expresses conservation of probability. The moments are useful in discussing the energy spread of excitations. The first two are seen to be

$$\langle\omega\rangle=i\textstyle\sum_j\dot{c}_j(0)\,,\tag{3.18}$$

$$\langle\omega^2\rangle=\langle\omega\rangle^2-\textstyle\sum_j\ddot{c}_j(0)\,.\tag{3.19}$$

D. Switching On

Consider a localized potential which is switched on exponentially, i.e.,

$$V_{kk'}(t) = V_{kk'}\, e^{\eta t}\,, \quad \eta > 0. \tag{3.20}$$

At $t = -\infty$, the Fermi gas is assumed to be in its unperturbed ground state. One would like to know how the state at $t = 0$, when the localized potential attains its full strength $V_{kk'}$, is related to the true ground state in the presence of the potential $V_{kk'}$.

In the boson approximation of Sec. IID, the state at $t = 0$ is

$$|\psi_\eta\rangle = U_\eta(0, -\infty)\,|\psi_0\rangle\,, \tag{3.21}$$

where from (3.7) to (3.9), we see that

$$U_\eta(0, -\infty) = \exp\left(\tfrac{1}{2} i \sum_j \frac{|V_j|^2 \epsilon_j}{\eta(\epsilon_j^2 + \eta^2)}\right) \times \exp\left[-\sum_j \left(\frac{V_j}{\epsilon_j - i\eta}\, b_j^\dagger - \frac{V_j^*}{\epsilon_j + i\eta}\, b_j\right)\right]. \tag{3.22}$$

In (3.22), $V_j = V_{kk'}$ and $\epsilon_j = \epsilon_k - \epsilon_{k'}$. As mentioned above, one is interested in the relation of $|\psi_\eta\rangle$ to the eigenstates of the full Hamiltonian

$$H = H_0 + \sum_{kk'} V_{kk'}\, a_k^\dagger a_{k'} = H_0 + \sum_j (V_j\, b_j^\dagger + V_j^*\, b_j)\,, \tag{3.23}$$

i.e., the Hamiltonian with the localized potential $V_{kk'} = V_j$ present. This can be obtained from Eq. (2.4). We need to know the canonical transformation relating H to H_0. In the independent boson approximation, we easily see that

$$H = U_v^\dagger\,(H_0 + \Delta E)\, U_v\,, \tag{3.24}$$

with

$$U_v = \exp[\textstyle\sum_j (V_j\, b_j^\dagger - V_j^*\, b_j)/\epsilon_j]\,. \tag{3.25}$$

From (3.10), (3.9) and (3.22), we see that

$$S_\eta(\omega) = (1/2\pi) \int e^{i\omega\tau} \exp[\textstyle\sum_j c_j^\eta(\tau)]\, d\tau\,, \tag{3.26}$$

where

$$c_j^\eta(\tau) = (e^{-i\epsilon_j\tau} - 1)\,|V_j|^2 \left(\frac{1}{\epsilon_j^2} - \frac{1}{\epsilon_j^2 + \eta^2}\right)\,. \tag{3.27a}$$

In particular, the overlap of the state $|\psi_\eta\rangle$ with the ground state $|\psi_v\rangle$ of the Hamiltonian H (3.23) is given by

$$|\langle\psi_\eta|\psi_v\rangle|^2 = \exp[\textstyle\sum_j c_j^\eta(\tau = \infty)]\,, \tag{3.27b}$$

where

$$\sum_j c_j^\eta(\tau = \infty) = -\int_0^\infty V^2 \rho(\omega) \left(\frac{1}{\omega^2} - \frac{1}{\omega^2 + \eta^2}\right) d\omega\,. \tag{3.27c}$$

The overlap (3.27b) can be written as

$$|\langle\psi_\eta|\psi_v\rangle|^2 = |\langle\psi_v|\psi_0\rangle|^2 / |\langle\psi_\eta|\psi_0\rangle|^2\,. \tag{3.28}$$

For a system with finite volume Ω, there is a low-energy cutoff coming from the fact that a given mode cannot accommodate more than one excitation (see, e.g., Appendix A),

$$V^2/\omega^2 \Rightarrow V^2/(\omega^2 + \alpha V^2), \quad V \simeq \Omega^{-1}\,.$$

Therefore, we obtain

$$|\langle\psi_v|\psi_0\rangle|^2 = e^{-\tilde{V}^2 \ln\Omega} \tag{3.29}$$

which is the Anderson result[13] with the proper coefficient (for small phase shift). In the overlap $|\langle\psi_\eta|\psi_0\rangle|^2$, the effective cutoff is the maximum of two competing cutoffs, one related to the volume, the other related to the switching time:

$$|\langle\psi_\eta|\psi_0\rangle|^2 = \exp(\tilde{V}^2 \ln\max|\Omega^{-1}, \eta|)\,. \tag{3.30}$$

Thus, in the limit of infinite volume, no matter how small η is ($\Omega \to \infty$ first, then $\eta \to 0$), the switched state never reaches the true ground state of the final Hamiltonian

$$|\langle\psi_\eta|\psi_v\rangle|^2 \equiv 0\,. \tag{3.31}$$

The spectrum of excitations with respect to the final ground state is formally given by

$$S_\eta(\omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{i\omega t}\, e^{B(\tau)}\, d\tau\,, \tag{3.32a}$$

$$B(\tau) = \tilde{V}^2 \int_0^{\omega_c} (e^{-i\omega\tau} - 1)\left(\frac{1}{\omega} - \frac{\omega}{\omega^2 + \eta^2}\right) d\omega\,. \tag{3.32b}$$

It is difficult to evaluate the integral $B(\tau)$ exactly. We therefore make an approximation to it. In the integrand, the exponential $e^{-i\omega\tau}$ oscillates rapidly for larges values of ω. The effect of this (together with the decrease of the multiplying function as $1/\omega^2$ for $\omega \gg \eta$) is to greatly reduce the contribution of the exponential in the region $\omega > 1/\tau$. We assume a sharp cutoff at $\omega = 1/\tau$. Further, for $\omega < 1/\tau$, we approximate $e^{-i\omega\tau}$ by unity. In this approximation, we find

$$B(\tau) = -\tilde{V}^2 \int_{1/\tau}^{\omega_c} \left(\frac{1}{\omega} - \frac{\omega}{\omega^2 + \eta^2}\right) d\omega = -\tfrac{1}{2}\tilde{V}^2 \ln(1 + \eta^2\tau^2) \tag{3.33}$$

for $\eta \ll \omega_c$. However, this $B(\tau)$ does not have the right analytic properties which are that it should be analytic and bounded in the lower half-plane (lhp) as a function of complex τ, and purely real on the imaginary line in the lhp. These result from the fact that the excitation energies are positive. The simplest modification of (3.33) consistent with these requirements is

$$B(\tau) = -\tilde{V}^2 \ln(1 + i\eta\tau)\,. \tag{3.34}$$

This clearly has also the same functional form as

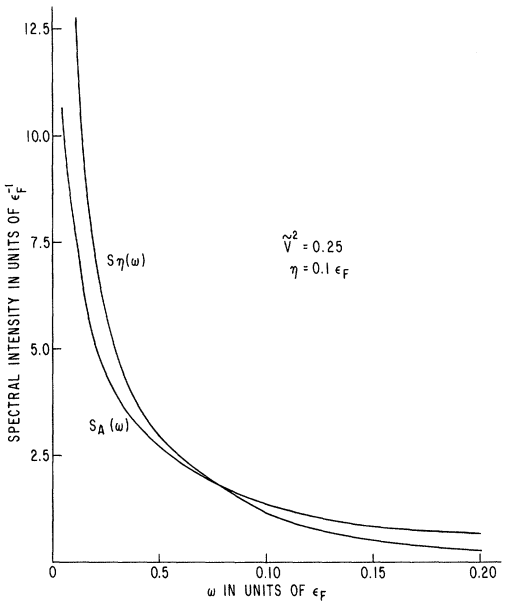

FIG. 1. Spectrum of particle-hole excitations, the localized perturbation V being switched on exponentially at a rate $\eta = 0.1\,\epsilon_F$. The spectrum is of the eigenstates of the Hamiltonian with V. The ground state is at zero energy. For comparison, the spectrum of the unperturbed Hamiltonian is also plotted. Here $\tilde{V}^2 = 0.25$.

(3.33) for long and short times τ. The spectrum calculated using the form (3.34) for $B(\tau)$ is

$$S_\eta(\omega) = \frac{1}{\Gamma(\tilde{V}^2)}\,\frac{1}{\omega}\,e^{-\omega/\eta}\left(\frac{\omega}{\eta}\right)^{\tilde{V}^2}. \tag{3.35}$$

$\Gamma(\tilde{V}^2)$ is a Γ function. The spectrum is plotted in Fig. 1 for $\tilde{V}^2 = 0.25$. The power-law divergence for small ω has exactly the same form as that of the excitation spectrum (with respect to the ground state of H_0) of the ground state of $H = H_0 + V$. The latter spectrum is given by[2,11]

$$S(\omega) = \frac{1}{\Gamma(\tilde{V}^2)}\,\frac{1}{\omega}\left(\frac{\omega}{\omega_c}\right)^{\tilde{V}^2}. \tag{3.36}$$

We see that the slow switching has introduced an exponential cutoff at energies $\omega \gtrsim \eta$ in the spectrum (3.35) as compared to (3.36); this is balanced by an enhanced strength of the divergent part at low energies to preserve the sum rule (3.17).

The sum rules (3.18) and (3.19) can be used to obtain results about the spectrum independent of the approximation (3.34) for $B(\tau)$. We find that

$$\langle\omega\rangle = \tfrac{1}{2}\pi\,\tilde{V}^2\eta \tag{3.37}$$

and that

$$\langle\omega^2\rangle - \langle\omega\rangle^2 = \tilde{V}^2\eta^2\ln(\omega_c/\eta). \tag{3.38}$$

The mean excitation energy thus decreases linearly with η. This is in accord with the scaling of the spectrum with η seen above in (3.35). The first moment calculated from (3.35) differs only by a factor $\frac{1}{2}\pi$ from (3.37). The logarithmic dependence on ω_c in (3.38) shows, however, that the approximation (3.34) is not correct at energies $\omega \gtrsim \omega_c$.

E. Switching On and Off

We next consider the case of a localized potential which is turned on and then is turned off. Thus, there is no localized potential initially ($t = -\infty$) and also finally ($t = +\infty$). Initially, the system is in the Fermi ground state. One would like to know whether it finally returns to the ground state. We shall see that the probability that it does so is always less than unity. The remainder goes into excited states whose spectrum is discussed for a special case.

Consider for concreteness a potential turned on exponentially at a rate η_1 and turned off at a rate η_2, i.e.,

$$V_j(t) = V_j\left[e^{\eta_1 t}\theta(-t) + e^{-\eta_2 t}\theta(t)\right]. \tag{3.39}$$

In the boson approximation, the state at $t = \infty$ is

$$|\psi_\infty\rangle = U_{\eta_{12}}(\infty, -\infty)\,|\psi_0\rangle,$$

where

$$U_{\eta_{12}}(\infty, -\infty) = e^{i\phi_{12}} \times \exp\left[-i\sum_j\left(\frac{V_j}{i\epsilon_j + \eta_1} + \frac{V_j}{i\epsilon_j - \eta_2}\right)b_j^\dagger + \text{H.c.}\right]. \tag{3.40}$$

The overlap of this with the original ground state is given by the probability

$$P_G^0 = \exp\left[-\sum_j |f_i|^2\right] = \exp\left[-\tilde{V}^2\left(\frac{\eta_1+\eta_2}{\eta_1-\eta_2}\right)\ln\left(\frac{\eta_1}{\eta_2}\right)\right]. \tag{3.41}$$

It is a function only of the ratio (η_1/η_2), i.e., it does not depend on the absolute switching rate (since the high-energy cutoff has been taken to be infinite; see below). As a function of this ratio, it has a maximum for $(\eta_1/\eta_2) = 1$, i.e., the symmetric case, and its value there is

$$P_G^0 = e^{-2\tilde{V}^2}. \tag{3.42}$$

As a function of (η_1/η_2), the overlap decreases monotonically and symmetrically around this value. The probability P_G^0 is thus always less than unity.

For the symmetric case, the probability (3.42) is seen to be independent of η. From the expression (3.16) for the ground-state overlap and Eq. (3.9), we see that if the time-dependent potential can be written as $V(\eta t)$, the ground-state overlap is independent of η (to a relative accuracy of η/ω_c in the exponent). The reason for this result is the

use of a linear spectrum for particle-hole excitations and the constant coupling of the potential to them.

The excitation spectrum is difficult to calculate explicitly, at least for the nonsymmetric case. However, it can be shown to begin linearly for small ω. From the sum rules (3.18) and (3.19), it is seen that

$$\langle\omega\rangle = \tfrac{1}{2}\pi\tilde{V}^2(\eta_1+\eta_2), \tag{3.43a}$$

$$\langle\omega^2\rangle - \langle\omega\rangle^2 = \tfrac{1}{2}\tilde{V}^2\frac{\eta_1+\eta_2}{\eta_1-\eta_2}\left[\eta_1^2\ln\left(\frac{\omega_c}{\eta_1}\right) - \eta_2^2\ln\left(\frac{\omega_c}{\eta_2}\right)\right]. \tag{3.43b}$$

The excitations have an average energy of the same size as the switching rate times the coupling of the excitations to the localized potential. This is in conformity with the result (3.37) for the mean energy. For the symmetric case, (3.43) becomes

$$\langle\omega\rangle = \pi\tilde{V}^2\eta, \tag{3.44a}$$

$$\langle\omega^2\rangle - \langle\omega\rangle^2 = 2\tilde{V}^2\eta^2\ln\left(\frac{\omega_c}{\eta}\right). \tag{3.44b}$$

For illustrative purposes, we mention the results for a different path, namely, the Gaussian

$$V_j(t) = V_j[e^{-1/2(t/\tau_1)^2}\theta(-t) + e^{-1/2(t/\tau_2)^2}\theta(t)]. \tag{3.45}$$

The probability of returning to the ground state is in this case

$$P_G^0 = e^{-\pi\tilde{V}^2} \tag{3.46}$$

for $\omega_c \gg 1$ if the switching is symmetric. In contradistinction to exponential switching, the probability P_G^0 is minimum instead of maximum in the symmetric case.

The ground state probability P_G^0 can be calculated directly for a generally time-dependent potential.[14] The method used is due originally to Nozières and De Dominicis[2] who investigated the case of a suddenly turned-on potential. They found that the Dyson equation for the one electron propagator $G(tt')$ was a singular integral equation. The ground-state overlap is simply related to the equal time limit of this propagator. In our case, the Dyson equation is

$$G(tt') = G^0(tt') - g\rho_{\epsilon_F} \times \int_{\tau_i}^{\tau_f} P(1/t-t'')V(t'')G(t''t')\,dt'', \tag{3.47}$$

where the potential $g\,V(t'')$ is turned on at τ_i and is turned off at τ_f. The band of electronic states is assumed to be symmetric with respect to the Fermi energy. The chief approximation made in (3.47) is to assume that the free propagator

$$G^0(tt') = \langle T[\textstyle\sum_k a_k^\dagger(t)\sum_{k'} a_{k'}(t')]\rangle \tag{3.48}$$

has the form

$$G^0(tt') = \rho_{\epsilon_F}/i(t-t') \tag{3.49}$$

for time intervals $(t-t') \gg \rho_{\epsilon_F}$ and in using this in the kernel of (3.47). This "asymptotic approximation" is equivalent to assuming that the density of particle-hole excitations is given by Eq. (3.4) without a cutoff. The integral equation can be solved following Muskhelishvili.[14,15] We find $G(tt)$ and thence A_G using the expression

$$A_G = \exp[-i\int_0^1 dg \int_{\tau_i}^{\tau_f} V(tt)G(tt^+)\,dt]. \tag{3.50}$$

The expression obtained for P_G^0 is

$$P_G^0 = e^{-C(\tau_f,\tau_i)}, \tag{3.51}$$

where

$$C(\tau_f,\tau_i) = \int_{\tau_i}^{\tau_f} dt \int_{\tau_i}^{\tau_f} dt' P\left(\frac{1}{t-t'}\right) V(t)\frac{dV(t')}{dt'} \times\left(\frac{1}{V^2(t)-V^2(t')}\right)\ln\left(\frac{1+\rho_{\epsilon_F}^2V^2(t')}{1+\rho_{\epsilon_F}^2V^2(t)}\right). \tag{3.52}$$

If the time scale of the potential is determined by a single parameter η, and the times τ_i, τ_f are $\mp\infty$, respectively, it is clear from (3.52) that the ground-state probability is independent of η. We have seen above that this is true in the boson model also for $\eta \ll \omega_c$. Here the cutoff $\omega_c = \infty$, so that the (spurious) scaling is found for all η.

For weak potentials such that $V(t)\rho_{\epsilon_F} \ll 1$, the logarithmic term in the integrand can be expanded in powers of V. Retention of only the first term leads to the boson result (3.16). It is difficult to calculate (3.52) in general. For the symmetric special case of (3.39), it can be shown that the ground-state probability goes as $e^{-(1/4)\ln\ln\tilde{V}^2}$ if $\tilde{V}^2 \gg 1$. Thus, for strong potentials the overlap slowly goes to zero.

F. Adiabaticity

We now examine the implications of the above results for the nature of the response of the Fermi gas to a localized time-dependent perturbation:

(a) We first briefly summarize the established ideas of adiabaticity as used in many-body theory for interacting Fermi systems.[16] The system is initially ($t = -\infty$) in the ground state of the Hamiltonian H_0. To the actual interaction Hamiltonian H_1, a factor $e^{\eta t}$ is added. This means that the interaction is turned on exponentially and attains its actual strength at $t = 0$. By means of a diagrammatic analysis, mainly utilizing the fact that the "correlation time" of a diagram is $\sim 1/\epsilon_F$, it is

shown that the state at $t=0$ is

$$|\psi_\eta\rangle = U_\eta(0,-\infty)|\psi_0\rangle \tag{3.53a}$$

$$= U_{\eta L}(0,-\infty)|\psi_0\rangle e^{U_{\eta c}(0,-\infty)}, \tag{3.53b}$$

where

$$U_{\eta c}(0,-\infty) = (a/\eta) + b + O(\eta) \tag{3.53c}$$

is a c number and $U_{\eta L}(0,-\infty)$ is an operator. The terms a (purely imaginary) and b are extensive quantities proportional to the volume Ω of the system. One is interested in the state obtained when the perturbation is switched on very slowly, i.e., the limit $\eta \to 0$. This limit is not well defined for (3.53c) because of the factor a/η. A state free of this factor is

$$|\psi_\eta\rangle_n = e^b U_{\eta L}(0,-\infty)|\psi_0\rangle . \tag{3.54}$$

It is shown that $\lim|\psi_\eta\rangle_n$ as $\eta \to 0$ is an eigenstate of H and its energy is

$$E = E_0 + i\frac{da}{dg}\bigg|_{g=1}, \tag{3.55}$$

where E_0 is the unperturbed ground-state energy and g is a factor multiplying the interaction H_1. The eigenstate of H thus reached is taken to be its ground state. This is the adiabatic assumption. Then the Gell-Mann–Low theorem (3.55) gives the ground-state energy shift.

Other important notions for the adiabatic hypothesis are those of reversibility and uniqueness. Consider the perturbation H_1 decreased progressively from $t=0$ to $t=+\infty$ as $e^{-\eta t}$. The state $U_\eta(+\infty,-\infty)|\psi_0\rangle$ differs from the original ground state by only a phase factor $e^{2a/\eta}$:

$$U_\eta(+\infty,-\infty)|\psi_0\rangle = e^{2a/\eta}|\psi_0\rangle . \tag{3.56}$$

This is "proved" in perturbation theory again, if the intermediate state energies are always positive. Thus, the adiabatic switching of the perturbation is reversible, i.e., no transitions to excited states occur in the course of this process. This reversibility also implies uniqueness, i.e., the state of time $t=0$ does not depend on the precise way the interaction is turned on, in the slow or $\eta \to 0$ limit.

(b) We now compare the results for a localized perturbation with those mentioned above. The equations corresponding to (3.53) are (3.21) and (3.22). From this we see that

$$|\psi_\eta\rangle = \exp\left[\frac{a}{\eta}+b\right]\exp\left(-\sum_j \frac{V_j}{\epsilon_j - i\eta}\, b_j^\dagger\right)$$

$$\times\exp\left(\sum_j \frac{V_j^*}{\epsilon_j + i\eta}\, b_j\right)|\psi_0\rangle , \tag{3.57a}$$

where

$$a = \tfrac{1}{2} i \tilde{V}^2 \omega_c \tag{3.57b}$$

and

$$b = -\tfrac{1}{4}\tilde{V}^2 \ln\left(\frac{\omega_c^2+\eta^2}{\eta^2+\alpha\Omega^{-2}}\right) \tag{3.57c}$$

$$\simeq -\tfrac{1}{2}\tilde{V}^2 \ln\Omega . \tag{3.57d}$$

a is independent of volume, as the energy shift, since the perturbation is localized. However, the normalization coefficient b is anomalous, being proportional to $\ln\Omega$. This is the infrared catastrophe first noted by Anderson.[13] The overlap of the normalized state

$$|\psi_\eta\rangle_n = \exp\left(-\sum_j \frac{V_j}{\epsilon_j - i\eta}\, b_j^\dagger + \sum_j \frac{V_j^*}{\epsilon_j + i\eta}\, b_j\right)|\psi_0\rangle \tag{3.58}$$

with the true ground state

$$|\psi_v\rangle = \exp\left(-\sum_j \frac{V_j b_j^\dagger - V_j^* b_j}{\epsilon_j}\right)|\psi_0\rangle \tag{3.59}$$

has been calculated in Sec. III D and found to be zero (3.31) for a potential slowly switched on in an infinite volume.

Thus the state attained is *orthogonal* to the true ground state rather than being identical with it. From Sec. III D we know that $|\psi_\eta\rangle$ consists of excited states of H with a spectrum given by (3.35). Now, the spread of the excitations itself shrinks as $\eta \to 0$, so $|\psi_\eta\rangle$ consists of very low-lying excited states (over an energy range η) in such a way that the conclusions of the Gell-Mann–Low theorem for the energy shift remain valid. From the results for the switched-on and switched-off potential (Sec. III E), we see that reversibility and uniqueness do not hold. When the interaction is slowly turned off, the system does not return entirely to its original ground state; excited states are produced with a certain probability. We have also seen that this probability is path dependent. The standard "adiabatic hypothesis" is not confirmed.

G. Temperature Effects

(a) The notions of adiabaticity and reversibility are clearly tied to entropy considerations. The slow switching of a localized potential in a Fermi sea involves two kinds of entropy change:

(i) a reversible entropy change ΔS_1 which is the static entropy difference between the final and initial states and cannot be calculated in the boson approximation:

$$\Delta S_1 \simeq \Delta\gamma T , \quad \Delta\gamma = \frac{\pi}{3}\frac{d\delta(E)}{dE}\bigg|_{\epsilon_F} ;$$

(ii) an irreversible entropy change due to the creation of real particle-hole excitations and which can be estimated (for $T \ll \epsilon_F$) as

$$\Delta S_2 \simeq \langle \omega \rangle / T \ .$$

For an exponential switching $Ve^{\eta t}$ between $-\infty$ and 0, $\langle \omega \rangle$ is given by (3.37), i.e.,

$$\Delta S_2 \simeq \tfrac{1}{2} \pi \tilde{V}^2 \eta / T \ . \tag{3.60}$$

Thus, the value of the irreversible entropy production is shown to depend on the ratio of the switching rate to the temperature.

(b) The finite-temperature generalization of the formulas of the preceding sections is easily obtained in the boson model; for temperatures low enough, the density of excitations can be assumed to remain unaffected. The averages over the ground state are replaced by thermodynamic averages. In a formula like (3.15), the temperature effect is obtained through the replacement

$$e^{-iEt} - 1 \ \Rightarrow \ (\cos Et - 1)(1 + 2\bar{n}) - i \sin Et \ , \tag{3.61}$$

where

$$\bar{n} = 1/(e^{\beta E} - 1)$$

is the Bose distribution function.

In particular, the δ-function weight or overlap P_G^0 in formula (3.16) becomes

$$P_G^0 = \exp(-\textstyle\sum_j |f_j|^2) \Rightarrow \ \exp[-\textstyle\sum_j (2\bar{n}_j + 1)|f_j|^2], \tag{3.62}$$

as intuitively expected, with stimulated emission and absorption adding to spontaneous emission.

The effect of temperature in the various spectra considered above is not expected to be very spectacular for $T \ll \epsilon_F$. One essentially will get a smearing out of the singular part of the spectra.

(c) In the functional-integral method for dilute magnetic alloys,[3] use is made of the temperature-evolution operator $U(\beta)$ which obeys the differential equation

$$\frac{\partial U}{\partial \beta} = -\overline{V}(\beta)\, U(\beta), \quad \overline{V}(\beta) = e^{\beta H_0} V(\beta) e^{-\beta H_0} \ .$$

For constant $V(\beta) = V$, $U(\beta)$ gives the thermodynamic quantities in the presence of the potential V at temperature β^{-1}, through the thermal average $Z/Z_0 = \langle U(\beta) \rangle$. However in the functional integral technique, knowledge of $U(\beta)$ for arbitrary paths $V(\beta)$ is required.

In the boson model, the thermal average $\langle U(\beta) \rangle$ for one boson mode of energy E is easily obtained as

$$\langle U(\beta) \rangle = \exp\Big[\int_0^\beta V(\beta') e^{-\beta' E} d\beta' \int_0^{\beta'} V(\beta'') e^{\beta'' E} d\beta'' + \bar{n} \int_0^\beta V(\beta') e^{-\beta' E} d\beta' \int_0^\beta V(\beta'') e^{\beta'' E} d\beta''\Big] \ .$$

Now, for constant V, we know that $\langle U(\beta) \rangle$ may be written as

$$\langle U(\beta) \rangle = e^{-\beta \Delta U + \Delta S} = e^{L} \ ,$$

with

$$\Delta S = L(\beta) - \beta \frac{\partial L(\beta)}{\partial \beta} \ .$$

We see that L contains an energy shift part and an entropy part. Along the same lines of reasoning as in Sec. II D, we expect that the energy shift of the fermion problem will not be correctly described by the boson model but that the nonadiabatic part will be adequately described by summing the boson entropy change over the appropriate density of states.

The recipe to obtain the nonadiabatic (NA) contribution for a given path $V(\beta')$ is therefore to calculate

$$L(\beta, E) = \int_0^\beta d\beta' \int_0^{\beta'} d\beta'' \, V(\beta') \, V(\beta'') \times [(1 + \bar{n}) e^{-(\beta' - \beta'')E} + \bar{n} e^{(\beta' - \beta'')E}] \ ; \tag{3.63a}$$

then we have

$$T(\beta, E) = L(\beta, E) - \beta \frac{\partial L}{\partial \beta}(\beta, E) \tag{3.63b}$$

and finally integrate over the appropriate density of states to find

$$\langle U(\beta) \rangle_{\rm NA} \simeq \exp[\int N(E)\, T(\beta, E)\, dE] \ . \tag{3.63c}$$

Compared to the formula which can be obtained directly via Muskhelishvili technique, formula (3.63) has the drawback of being valid only for small V, but it has the advantage of allowing one to include recoil effects through the density of states; it may also have computational advantages for given paths through the flexibility in the order of integrations over temperature and energy variables.

IV. RECOIL EFFECTS

A. Solution

In this section, we investigate the effect of the recoil of the potential source on the transient phenomena discussed above. The general effect of the recoil is to mute the infrared divergence, though strong final-state interaction effects are still present. For simplicity, we confine ourselves to the case of a suddenly switched-on potential. This describes the situation in a photoemission experiment, for example.[6,17]

We want to compare the ground state of the Hamiltonian without the potential to the eigenstates with the potential present or to obtain the behavior of the state after the sudden switching. For instance, we have

$$\langle \psi_0 | \psi(t) \rangle = \langle \psi_0 | e^{-i(H_0 + V)t} | \psi_0 \rangle = \textstyle\sum_n \langle \psi_0 | \psi_v^n \rangle \langle \psi_v^n | \psi_0 \rangle \, e^{-iE_n t}, \tag{4.1}$$

where $|\psi_v^n\rangle$ is an eigenstate of the Hamiltonian

H_0+V with energy E_n. The long-time value of (4.1) is

$$\langle\psi_0|\psi(t)\rangle=\langle\psi_0|\psi_v^G\rangle\langle\psi_v^G|\psi_0\rangle=|\langle\psi_0|\psi_v^G\rangle|^2\ , \quad (4.2)$$

with $|\psi_v^G\rangle$ being the ground state of H_0+V. The excited-state contributions drop out because of the oscillatory factor [for $\rho(\omega)\simeq\omega^\alpha$, $\alpha\geq 1$]. In particular, one is interested in finding the ground state of the final Hamiltonian

$$H=\sum_j \epsilon_j b_j^\dagger b_j+\sum_j (V_j b_j^\dagger e^{i\vec{q}_j\cdot\vec{R}}+V_j^* b_j e^{-i\vec{q}_j\cdot\vec{R}})+\frac{p^2}{2M}\ . \quad (4.3)$$

This is a basic problem in polaron theory[18] and the there exist several approximations depending on the coupling strength. The simplest way of estimating the latter is to equate it with the number of virtual bosons present in the ground state. A simple perturbation theoretic estimate of the latter is

$$\tfrac{1}{2}\alpha=\sum_j\langle b_j^\dagger b_j\rangle=\sum_j\frac{|V_j|^2}{(\epsilon_j+q_j^2/2m)^2}=-\tilde{V}^2\frac{\ln\gamma}{1-\gamma^2}\ ,$$

where $\gamma=m/M$. This is of order unity, so that we are in a regime where the intermediate coupling approximation is suitable. One first transforms the system through a unitary operator U_1 to the rest frame of the potential source so that (4.3) becomes

$$H=\sum_j\epsilon_j n_j+(\vec{K}-\sum_j\vec{q}_j n_j)^2/2M+\sum_j(V_j b_j^\dagger+V_j^* b_j)\ . \quad (4.4)$$

This is the Hamiltonian of an assembly of displaced oscillators except for the middle term. K is the eigenvalue of the total momentum which is a constant of the motion; from now on in this section, we shall take $K=0$, which corresponds to a source potential initially at rest (the case $K\neq 0$ is discussed in Sec. III C). Then, a displacement is so chosen as to minimize the ground-state energy. The canonical transformation which does this is

$$U_2=\exp[\textstyle\sum_j\bar{f}_j(b_j^\dagger-b_j)]\ , \quad (4.5a)$$

$$\bar{f}_j=\frac{V_j}{(\epsilon_j+q_j^2/2M)}\ . \quad (4.5b)$$

The Hamiltonian (4.4) then becomes[8]

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_1$$

$$=\left[E_G+\sum_j\epsilon_j n_j+\frac{1}{2M}\left(\sum_j\vec{q}_j n_j\right)^2\right]$$

$$+\left[\frac{1}{2M}\sum_{jj'}(\vec{q}_j\cdot\vec{q}_{j'})(b_j^\dagger b_{j'}^\dagger\,\bar{f}_j\bar{f}_{j'}+\text{c.c.}+2b_j^\dagger b_{j'}\,\bar{f}_j\bar{f}_{j'}^*)\right.$$

$$\left.+\frac{1}{2M}\sum_{jj'}(\vec{q}_j\cdot\vec{q}_{j'})(b_j^\dagger b_j\,b_{j'}\,\bar{f}_{j'}^*+b_{j'}^\dagger\,b_j^\dagger\,b_j\,\bar{f}_{j'})\right]. \quad (4.6)$$

On neglecting the effect of $\mathcal{H}_1$ (intermediate-coupling approximation), the ground state of $\mathcal{H}_0$ is seen to be the vacuum, so that

$$|\bar{\psi}\rangle=U_2U_1|\psi_0\rangle\ . \quad (4.7)$$

This is identical with the ground-state wave function of an independent boson model. The correlations between bosons are contained in the nondiagonal term $\mathcal{H}_1$ of (4.6). In the present case, they give rise to small corrections to the ground-state overlap starting in order V^4 and independent of γ (i.e., not of order $\ln\gamma$).

The independent boson Hamiltonian which has the ground state (4.7) and the same low excited states as $\mathcal{H}_0$ is

$$H=\textstyle\sum_j E_j b_j^\dagger b_j+\sum_j(V_j b_j^\dagger+V_j^* b_j), \quad (4.8)$$

with an energy of the boson j given by

$$E_j=\epsilon_k-\epsilon_{k'}+(\vec{k}-\vec{k}')^2/2M\ . \quad (4.9)$$

Thus, the density of particle-hole excitations is now given by

$$\rho_M(\omega)=\sum_{k,k'}n_{k'}(1-n_k)\,\delta\left(\omega-\epsilon_k+\epsilon_{k'}-\frac{(\vec{k}-\vec{k}')^2}{2M}\right)\ .$$

Comparing $\rho_M(\omega)$ and $\rho(\omega)$ (3.1), we see that there is an additional positive definite term in the excitation energy. The size of this increases with the square of the exchanged momentum and is of order $\gamma\epsilon_F$. Thus, for total excitation energies less than $\gamma\epsilon_F$, this recoil-energy term restricts the volume of k,k' space available for particle-hole excitations. This will reduce the density of the states characteristically for $\omega\lesssim\gamma\epsilon_F$. In terms of the density of particle-hole excitations $\rho(\epsilon,q)$ of energy ϵ and momentum $\vec{q}$ (imaginary part of the Lindhard function), we have

$$\rho(\omega)=\textstyle\sum_q\rho(\omega,\vec{q})\ ,$$

$$\rho_M(\omega)=\textstyle\sum_q\rho(\omega-(q^2/2M),\vec{q})\ .$$

The expression for $\rho(\omega)$ is given in (3.3); $\rho_M(\omega)$ is easily calculated too and has different analytic forms for $\tilde{\omega}\leq 4\gamma$ and $\tilde{\omega}\geq 4\gamma$, where $\tilde{\omega}=\omega/\epsilon_F$; for $\gamma\ll 1$, it simply becomes

$$\rho_M(\omega)=\rho_{\epsilon_F}^2\,\epsilon_F\,\tilde{\omega}^2/8\gamma, \qquad \tilde{\omega}\leq 4\gamma \quad (4.10a)$$

$$=\rho_{\epsilon_F}^2\,\epsilon_F\,(\tilde{\omega}-2\gamma), \quad 4\gamma\leq\tilde{\omega}\lesssim\omega_c\ . \quad (4.10b)$$

The density of low-energy particle-hole excitations behaves like $\tilde{\omega}^2$ rather than $\tilde{\omega}$, i.e., it is depleted due to recoil.

We now examine the effect of this reduction in the density of states. Consider the case of a potential suddenly switched on at $t=0$. The probability that the Fermi gas remains in the ground state at a subsequent time t is

$$P_G^0(t)=e^{-C(t)}\ ,$$

where

$$C(t) = 2V^2 \int \frac{\rho_M(\omega)}{\omega^2} \ (1 - \cos\omega t) \ .$$

For long times t, the oscillatory cosine term in the integrand contributes negligibly to $C(t)$, so that

$$C(\infty) = C = 2V^2 \int_0^{\omega_c} \frac{\rho_M(\omega)}{\omega^2} \ d\omega \ .$$

Using the form (4.10) which is valid for $\gamma \ll 1$ and $\tilde{\omega} < \tilde{\omega}_c$, we see that

$$C \cong 2\tilde{V}^2 \ln(\tilde{\omega}_c/4\gamma) \quad \text{and} \quad P_G^0(t=\infty) = P_G^2,$$

with

$$P_G = e^{-\tilde{V}^2 \ln(\tilde{\omega}_c/4\gamma)} = (4\gamma/\tilde{\omega}_c)^{\tilde{V}^2} \ . \tag{4.11}$$

The ground-state probability is nonzero because of the finiteness of the mass M. The result (4.11) means that when recoil of the potential source is considered, the ground states of the Fermi gas with and without the potential have a nonzero overlap. This overlap goes to zero as $M \to \infty$, which is the result found by Anderson.[13] The difference is directly due to the change in the density of low-energy excitations; in the former case $\rho_M(\omega) \alpha \omega^2$ while in the latter $\rho(\omega) \alpha \omega$ thus leading to an infrared divergence.

The result (4.11) is valid only for $\gamma \ll 1$ because the form (4.10) has been used for the density of excitations. The exact expression for $\rho_M(\omega)$ yields on integration the overlap

$$P_G = \exp\left[\tilde{V}^2 \left(\frac{\ln\gamma}{1-\gamma^2} \right) \right] \ . \tag{4.12}$$

This agrees with (4.11) in the limit of small γ. We notice that here P_G does not depend on the cutoff ω_c; this is because the density of high-energy excitations goes actually as $\omega^{1/2}$ [see (3.1)] rather than ω, the value used in the approximate result (4.10). This lower density obviates the need for a cutoff. The result can be rephrased by saying that there is no ultraviolet divergence. Typically, $P_G \simeq 0.5$; for example, with $\gamma = 0.1$ and $\tilde{V}^2 = 0.25$, P_G is 0.56. The overlap is thus substantial.

The overlap progressively increases from near zero for $\gamma \ll 1$ to unity for $\gamma \gg 1$. The latter is understandable since for very small M the potential source behaves as a highly mobile free particle only weakly coupled to the Fermi gas which is therefore excited very little.

We shall see later (Sec. IV B) that for $\gamma \ll 1$, the correction (due to correlations, etc.) to the independent boson result for P_G is small. For $\gamma \gg 1$, we can calculate the overlap from the exact Hamiltonian (2.1), treating the interaction V as perturbation. To the first nonvanishing order in V, this is

$$P_G = 1 - \tilde{V}^2 (\ln\gamma)/\gamma^2$$

and is identical with (4.12) in that limit. Thus, the independent boson result (4.12) for the overlap is exact in the two limits $\gamma \ll 1$ and $\gamma \gg 1$, and interpolates smoothly between these two limits. Therefore, it is probably a reliable estimate throughout.

We now discuss the energy spectrum of excited states. For the density of states $\rho_M(\omega)$ given by (4.10), the quantity $B(\tau)$ (3.32a) is calculated to be

$$B(\tau) \simeq -\tilde{V}^2 \ln(\gamma - i/8\epsilon_F\tau), \quad \epsilon_F\tau/\gamma \gg 1 \ . \tag{4.13}$$

The resulting spectrum $S(\omega)$ has the following features. There is a δ-function peak at $\omega = 0$; this has been discussed above. The excitation spectrum starts with a constant nonzero value for small ω:

$$S(\omega) = P_G \tilde{V}^2/8\gamma\epsilon_F \quad \text{for } \tilde{\omega} \ll 4\gamma \ . \tag{4.14}$$

This is in contrast to the power-law singularity of the spectrum for small energies $\tilde{\omega}$ when $M = \infty$. It also differs from the usual phonon sideband spectrum where the strength goes to zero as the excitation energy $\omega \to 0$. The spectral intensity smoothly passes over into that for the recoilless case (Fig. 2). The reduction in the inelastic strength over the infinite-mass case occurs mainly for $\tilde{\omega} \lesssim 4\gamma$; the fact that the low-energy reduction is found to be equal to the restored elastic peak weight and the existence of the sum rule (3.17) for the total area confirm that result.

The features of the spectrum for the class of effective density of states

$$V^2(E)\,\rho(E) \simeq E^{\alpha}$$

are sketched in Appendix B.

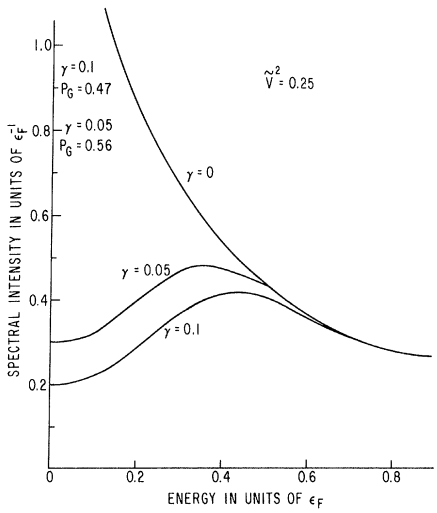

FIG. 2. Spectrum of particle-hole excitations after the sudden switching of a localized potential V. The potential source has a mass M. The general form of the spectrum is shown for $\gamma (= m/M) = 0.1$ and 0.05.

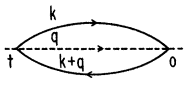

FIG. 3. Second-order diagram for $\Gamma(t)$. The dotted line represents the potential source (of initial and final momentum $\vec{K}=0$). The solid lines show a particle and a hole.

B. Discussion

The effect of a suddenly switched-on potential of mass M can be discussed without making an approximation for the fermion Hamiltonian (2.1). This can be done either as a systematic expansion outlined in Sec. IIC or more directly as follows.[19] One is interested in the average

$$A_G(t)=\langle U(t)\rangle_0=\langle e^{iH_0t}e^{-i(H_0+V)t}\rangle_0 . \tag{4.15}$$

This can be formally rewritten as an exponent:

$$A_G(t)=\exp[-i\int_0^t \Gamma(t')\,dt']=e^{B(t)} , \tag{4.16}$$

where

$$\Gamma(t)=\langle V(t)\,U(t)\rangle_0/\langle U(t)\rangle_0 . \tag{4.17}$$

One can thus obtain a power series (in V) expansion for $\Gamma(t)$ and thence for the exponent $B(t)$. The second-order term in V leads to an expression for $A_G(t)$ which is identical with the independent boson result (4.12). The second-order term in $\Gamma(t)$ is represented by the diagram of Fig. 3.

The third-order term in $\Gamma(t)$ can be represented by the two time-ordered diagrams of Fig. 4. The corresponding $B^{(3)}(t)$ as $t\to\infty$ is seen to be the higher (V^3) Born term in the expansion of $(\delta/\pi)^2$ in powers of V for a zero-range potential.

In the fourth order, $\Gamma(t)$ is given by the time-ordered diagrams of Fig. 5. The terms for the limiting exponent $B^{(4)}(\infty)$ can be classified into two groups. The first (class a) consists of fourth-order Born corrections to $(\delta/\pi)^2$ similar to the third-order correction mentioned above. [These fourth-order Born corrections have energy denominators $\epsilon_k-\epsilon_{k'}+(\vec{k}-\vec{k}')^2/2M$ occurring instead of $(\epsilon_k-\epsilon_{k'})$ as is usual for scattering from a rigid potential.] The second class (class b) would vanish except for the momentum correlation between successive particle-hole pairs. Its contribution can be calculated by assigning a correlation energy phase factor to the full

FIG. 4. The third-order diagrams for $\Gamma(t)$.

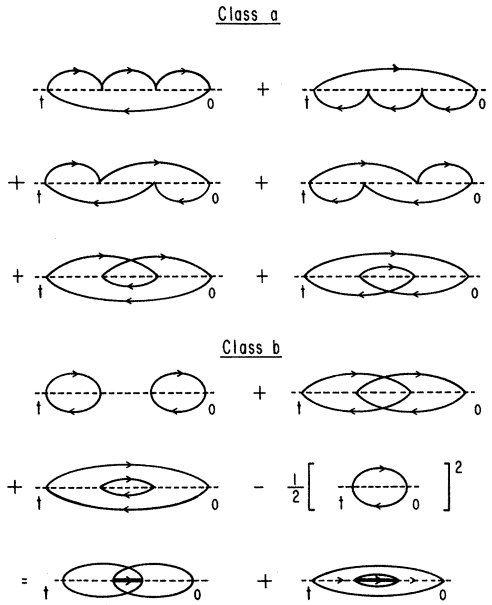

FIG. 5. Fourth-order diagrams for $\Gamma(t)$. The contribution of class b can be condensed into the two "correlation" diagrams shown at the end.

thick line in the second part of class b diagrams (Fig. 5). It corresponds exactly to the fourth-order corrections in the polaron model (Sec. IVA), i.e., it is of order $\tilde{V}^4$. [This term vanishes identically for $\gamma=0$, i.e., in the limit $\lim_{t\to\infty}\lim_{\gamma\to 0}B(t)$.] It is thus small compared to the leading term $\tilde{V}^2\ln\gamma$ and will be neglected. On the basis of the Born-expansion behavior of the remaining terms up to order $\tilde{V}^4$, one can rewrite (4.12) as

$$P_G=\exp\left(\frac{\delta^2}{\pi^2}\,\frac{\ln\gamma}{1-\gamma^2}\right) . \tag{4.18}$$

C. Nonzero Momentum

We now consider the case when the potential source has initially a nonzero momentum $\vec{K}$. Some qualitatively new features appear because the initial state is an excited state of the noninteracting system. The source can (through the coupling to the Fermi gas) make real transitions to other states $\vec{K}'$ by creating particle-hole pairs of the right energy and momentum. Thus, instead of the δ-function line at $\omega=0$ which one has for $\vec{K}=0$, one finds here a peak. The width of this peak is the inverse relaxation time for the source having an initial momentum $\vec{K}$. The spectrum of excitations extends down to $\omega=-E_K=-\vec{K}^2/2M$ (for $\vec{K}\le 2k_F$) on the low-energy side, and has a general resemblance to the $\vec{K}=0$ inelastic spectrum (with a shift E_K) on the high-energy side. Thus, it has the form shown in Fig. 6. We discuss below some of its essential

features, namely, the threshold behavior at $\omega = -E_K$, the width and strength of the elastic peak at $\omega = 0$.

The density of particle-hole excitations of energy ω, including the effect of source recoil is given by

$$\rho_M(\omega, K) = \sum_{k,q} f_k^- f_{k+q}^+ \, \delta(\omega - \epsilon_{k+q} + \epsilon_k - E_{K-q} + E_K) \, . \tag{4.19}$$

This vanishes for $\omega \leq -E_K$ ($K \leq 2k_F$). The lower limit corresponds to the source coming to rest (i.e., losing its energy E_K), the momentum being taken up by a particle-hole pair of zero-excitation energy. The behavior of the inelastic spectrum near the threshold depends on $\rho_M(\omega, \vec{K})$ for $\omega \gtrsim -E_K$. This is calculated from (4.19) to be

$$\rho_M(\omega, \vec{K}) = \rho^2_{\epsilon_F} \epsilon_F \frac{1}{15\gamma^{3/2}} \frac{k_F}{K} \left(\frac{\omega + E_K}{\epsilon_F} \right)^{5/2} . \tag{4.20}$$

In the threshold region, the inelastic spectrum can be calculated by treating V as a perturbation because there the excitation energy is not vanishingly small, i.e., $|\omega| \simeq E_K$. In the lowest nonvanishing order, the threshold spectrum is found to be

$$S(\omega) = \frac{16}{15} \frac{\tilde{V}^2}{\epsilon_F} \frac{1}{\gamma} x^{5/2}, \quad x = \frac{\omega + E_K}{E_K} . \tag{4.21}$$

This is valid for $x \ll 1$; an upper limit is $x = (\gamma/\tilde{V}^2)^{2/5}$, around which perturbation theory breaks down.

As mentioned before, the potential source can make real transitions to other states $\vec{K}'$. The transition probability in second-order perturbation theory is

$$\Gamma = 2\pi V^2 \rho_M(0, \vec{K}) \tag{4.22a}$$

$$= (2\pi/15) \gamma \tilde{V}^2 \epsilon_F (K/k_F)^4, \quad K < k_F, \quad \gamma < 1 \, . \tag{4.22b}$$

The E_K^2 behavior is a well-known consequence of Fermi statistics. The transition probability is seen to be generally much smaller than the energy E_K of the source, so that the elastic peak is narrow and well defined (see, for example, Fig. 6).

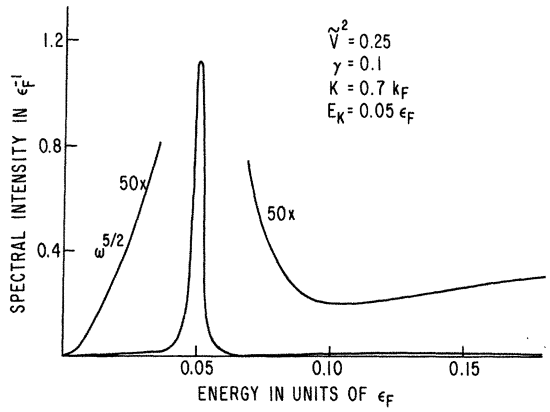

FIG. 6. Elastic peak and spectrum of particle-hole excitations after the sudden switching of a localized potential V. The potential source of mass $10m$ has an initial momentum $K = 0.7k_F$. The interaction $\tilde{V}^2 = 0.25$.

For the case $\vec{K} = 0$, the independent boson model was used to calculate the inelastic spectrum in detail. Its use here leads to a qualitative error on the low-energy side. The reason is as follows: As we saw in (4.19), the excitation spectrum extends down to $\omega = -E_K$. If these excitations are considered boson-like and many boson processes are treated by considering them to be independent, we will obtain [on using a formula of the type (3.14)] an inelastic spectrum extending down to $\omega = -\infty$. But we know (4.20) that the true spectrum starts from $\omega = -E_K$. On the high-energy side, however, it is likely that the spectrum is reliably obtained from the model.

A quantity of direct physical interest is the elastic peak. One would like to compare its strength to that of the δ function obtained for $\vec{K} = 0$. To calculate it, we proceed as follows. The vacuum amplitude has the form (for long times)

$$\langle U(t, 0) \rangle = e^{B(t)} = \exp(-\lambda t + \Delta + \kappa/t + \cdots) \, , \tag{4.23}$$

where λ has the value $\frac{1}{2}\Gamma$ (4.22). For long times, κ/t and succeeding terms may be omitted. The elastic peak is then seen to be a Lorentzian of strength e^{Δ}. We calculate Δ in the independent boson model. Its defect pointed out on the previous paragraph concerns the low inelastic energy spectrum which is determined by κ/t and succeeding terms in (4.23). Thus, we expect the Δ calculated below to be as reliable as the result (4.12) or (4.18) for $\vec{K} = 0$.

In the boson model, we have

$$B(t) = V^2 \int_{-E_K}^{\omega_c} \frac{(e^{-i\omega t} - 1)}{\omega^2} \rho_M(\omega, \vec{K}) \, d\omega \, . \tag{4.24}$$

For long times, $B(t)$ is easily shown to be

$$B(t) = -\tfrac{1}{2}\Gamma t + \Delta + O(1/t) \, , \tag{4.25}$$

with

$$\Delta = -V^2 \int_{-\infty - i\epsilon}^{+\infty - i\epsilon} \frac{\partial}{\partial \omega} \{\rho_M(\omega, \vec{K})\} \frac{d\omega}{\omega} \, . \tag{4.26}$$

The imaginary part of Δ gives rise to an asymmetric contribution in addition to the Lorentzian, but this is very small. The real part turns out to be

$$\Delta = \tilde{V}^2 \left[\frac{\ln\gamma}{1 - \gamma^2} \left(1 - \tfrac{1}{3} \frac{K^2}{k_F^2} \right) + \frac{1}{3} \frac{K^2}{k_F^2} \ln\left(\frac{K}{k_F} \right) + O(\gamma^2, K^2) \right] \, . \tag{4.27}$$

Thus, for $\vec{K} = 0$, we recover the strength (4.12) of the elastic δ peak, whereas except for quite small $K \lesssim \gamma k_F$ the area under the Lorentzian tends to ex-

ceed the strength of the δ peak for $\vec{K}=0$. The difference is, however, small.

The substantial final-state interaction found here after taking into account the effect of hole recoil may be relevant to the common occurrence of indirect ($\vec{k}$-nonconserving or inelastic) transitions in photoemission.

V. CONCLUSION

The boson model considered above provides probably the simplest (soluble) example of a particular class of strong-coupling problems, namely, infrared divergences. Although the interaction contains a small coupling constant, here $\tilde{V}$, it turns out that in a perturbation expansion the real coupling constant is $\tilde{V}^2 \ln E$, which may be arbitrarily large for small energies. The consequent breakdown of perturbation methods is in fact a signature of infrared divergence problems. Consideration of source recoil changes the coupling constant to $\tilde{V}^2 \ln\gamma$, which is not small but is of order unity.

The main application here has been to the problem of a time-dependent localized charge perturbation in a metal. This problem is relevant for the interpretation of several types of experimental effects. Some examples, such as x-ray photoemission spectra of metals and atom or ion scattering from metals have already been mentioned. The motion (slowing down) of an ion in a metal or in He^3 may also show strong-coupling effects. The response of an electron gas to a local Einstein oscillator, including corrections to the Born-Oppenheimer approximation, will be described in a later publication.

A more complicated but obviously germane problem is the study of a time-dependent localized spin perturbation in a metal. This has been done in relation to the Kondo effect by Anderson and Yuval[3] and by Hamann.[3,14] In several phenomena involving hyperfine interactions, sudden spin flips occur. One expects transients or after effects due to these. Examples are the Mössbauer effect, perturbed angular correlations, and ion implantation experiments.[20]

As made clear by Hopfield,[21] infrared divergences are likely to occur whenever the coupling constant $V(E)$ and the density of excitations $N(E)$ are such that $V^2(E)N(E)\simeq E$ for small energy E. Besides the examples listed by Hopfield, it is likely that (ferromagnetic) magnons and surface phonons may also provide singular satellite spectra in some situations. As before, the observability will depend on the size of the natural cutoffs.

Outside the realm of solid-state theory, it is easy to see that the scalar fixed-source meson-nucleon model exhibits[22] the same singularities (besides uv divergences) with a natural cutoff provided by the nonzero meson mass. Finally, a few words should be said about the famous infrared divergence of quantum electrodynamics (qed).[23] In that case, the historical effort has been to show that in each order of perturbation theory, addition of virtual and real singular contributions gives a well-behaved sum. Their cancellation is obvious in our model, as it is built into the sum rule. The weight of the elastic peak plus the area of the satellite spectrum must add to unity. The infrared divergence of qed manifests itself in a bremsstrahlung experiment which is the equivalent of a sudden switching situation in our model. The slow-switching anomalies have apparently received little attention, probably for lack of experimental impetus.

ACKNOWLEDGMENTS

The authors wish to express their deep gratitude to Professor H. Suhl for his advice, support, and hospitality. One of the authors (E. M.-H.) gratefully acknowledges a travel grant from the Fulbright Commission and partial support by the Heinrich-Hertz-Stiftung des Landes Nordrhein-Westfalen, Germany.

APPENDIX A

The effects considered in this paper can be viewed as transitions induced in a Fermi system by a perturbation which couples the levels pairwise. The simplest example of this class of systems has two levels and the problem is described by the Hamiltonian

$$H=\tfrac{1}{2}E(c_1^\dagger c_1 - c_2^\dagger c_2)+V(t)c_1^\dagger c_2+V^*(t)c_2^\dagger c_1 \ . \quad \text{(A1)}$$

The perturbation $V(t)$ causes transitions between the levels 1 and 2 which have energies $\pm\frac{1}{2}E$, respectively. Though the Hamiltonian in its general time-dependent form has not been solved exactly, special forms have been widely studied in connection with problems of magnetic resonance, molecular predissociation, atomic collision, interband tunneling in solids, etc.

TABLE I. Strength of δ line and sideband for various densities of states (Appendix B).

	Strength of δ line	Sideband for $\omega \to 0$
$\alpha>1$	$\frac{1}{\epsilon_f} e^{-\tilde{V}^2/(\alpha-1)}$	$\frac{1}{\epsilon_F}\tilde{V}^2\left(\frac{\omega}{\epsilon_F}\right)^{\alpha-2}$
$\alpha=1$	0	$\frac{1}{\epsilon_F}\tilde{V}^2\left(\frac{\omega}{\epsilon_F}\right)^{\tilde{V}^2-1}$
$\alpha=\frac{1}{2}$	0	$\frac{1}{\epsilon_F}\tilde{V}^2\left(\frac{\epsilon_F}{\omega}\right)^{3/2}\exp\left[-\pi\tilde{V}^4\left(\frac{\epsilon_F}{\omega}\right)\right]$

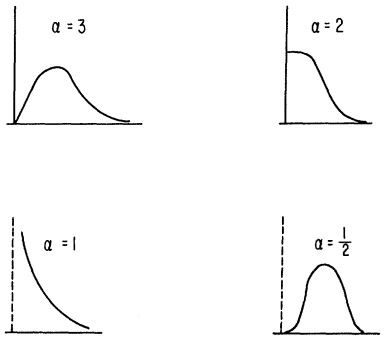

FIG. 7. Excitation spectrum for various effective density-of-states functions.

Let us consider here the special case $V(t) = V$ in which the Hamiltonian can be exactly diagonalized and compare the results obtained in various approximations. When V is time independent, the Hamiltonian H is diagonalized by the unitary operator

$$U_{fe} = \exp[-\tfrac{1}{2}\tan^{-1}(2V/E)(c_1^\dagger c_2 - c_2^\dagger c_1)] \ . \qquad \text{(A2)}$$

Born approximation for the exponent of the unitary operator would lead to

$$U_{fB} = \exp[-(V/E)(c_1^\dagger c_2 - c_2^\dagger c_1)] \ . \qquad \text{(A3)}$$

Changing from Fermi to Bose variables in U_{fB} leads to

$$U_{bB} = \exp[-(V/E)(b^\dagger - b)] \ . \qquad \text{(A4)}$$

The various expressions for U can be compared through their expectation values in the ground state, i.e., the state 2. This is $A_G = \langle 0 | c_2 U_f c_2^\dagger | 0\rangle$ for Fermi operator forms, and $A_G = \langle 0 | U_b | 0\rangle$ for Bose operator form

$$\langle 0 | c_2 U_{fe} c_2^\dagger | 0\rangle = \cos[\tfrac{1}{2}\tan^{-1}(2V/E)] , \qquad \text{(A5)}$$

$$\langle 0 | c_2 U_{fB} c_2^\dagger | 0\rangle = \cos(V/E) , \qquad \text{(A6)}$$

$$\langle 0 | U_{bB} | 0\rangle = \exp(-\tfrac{1}{2} V^2/E^2) \ . \qquad \text{(A7)}$$

We see that for $V/E \ll 1$, all forms agree. For large V/E, the exponentiated Born approximation (A6) is qualitatively wrong, leading to an amplitude oscillating in sign. The corresponding boson approximation (A7) is somewhat better with a positive ground-state amplitude. Thus, the two steps of Born exponentiation and boson approximation tend to cancel errors. Furthermore, by introducing a cutoff for the energy denominator, i.e., replacing

$$V^2/E^2 \to V^2/(E^2 + \alpha V^2) \ , \quad \alpha \simeq 1 \qquad \text{(A8)}$$

the boson result (A7) can be improved in the limit $V/E \gg 1$ without affecting the other one $V/E \ll 1$. The boson result (A7) with the renormalization (A8) is, in fact, a very good approximation to (A5). The same features are also obtained for the S-matrix elements $\langle 0 | c_2 U(+\infty, -\infty) c_2^\dagger | 0\rangle$ in an on-off passage, where the exact formula has been surmised by Rosen and Zener.[24]

APPENDIX B

Here we discuss how the form of the spectrum (3.14) depends on the density of low-lying excitations. The spectrum $S(\omega)$ is given by

$$S(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, e^{it\omega} \times \exp\left(V^2 \int_0^\infty dE\, \rho_{\rm eff}(E)\, \frac{e^{-itE} - 1}{E^2} \right) .$$

We assume an effective density of states

$$V^2 \rho_{\rm eff}(E) = V^2(E)\rho(E) = V^2 \rho_{\epsilon_F}^2 \epsilon_F (E/\epsilon_F)^\alpha \quad (\alpha > 0)$$

for small energies. Thus, large α means a low density of excitations and vice versa. The spectrum quite generally may consist of a δ-function line at zero energy and a positive-energy sideband. Actually, the presence of the δ line and the shape of the sideband sensitively reflect the exponent α. As α decreases, the sideband progressively consumes the δ line and swallows it at $\alpha = 1$ where the infrared divergence sets in. The characteristic features are listed in Table I and are exemplified in Fig. 7.

The case $\alpha = 3$ is familiar from phonon sidebands (with dilatational coupling[21]): $\alpha = 2$ is found for a recoiling localized perturbation considered in this paper; the limit of infinite mass corresponds to $\alpha = 1$.

---

*Research supported by the Air Force Office of Scientific Research, Office of Aerospace Research, U. S. Air Force, under AFOSR Grant No. AF-AFOSR-67-0610A.

†On leave from Institut f. Theoretische Physik der Universität Köln, Germany.

[1]J. Friedel, Advan. Phys. 3, 446 (1954).

[2]B. Roulet, J. Gavoret, and P. Nozières, Phys. Rev. 178, 1072 (1969); 178, 1084 (1969); P. Nozières and C. T. De Dominicis, *ibid.* 178, 1097 (1969).

[3]P. W. Anderson and G. Yuval, Phys. Rev. Letters 23, 89 (1969); D. R. Hamann, *ibid.* 23, 95 (1969).

[4]Threshold singularities in the soft x-ray spectra of metals: G. D. Mahan, Phys. Rev. 163, 612 (1967); Ref. 2 quoted above; G. A. Ausman and A. J. Glick, *ibid.* 183, 687 (1969). For experimental results (up to 1968), see *Soft X-Ray Band Spectra*, edited by D. J. Fabian (Academic, New York, 1968). See also R. Haensel

et al., Phys. Rev. Letters 23, 528 (1969).
[5]Overlap singularities: see, for example, S. Doniach and M. Sunjic, J. Phys. C 3, 284 (1970).
[6]S. Doniach, Phys. Rev. B (to be published).
[7]J. Gavoret, P. Nozières, B. Roulet, and M. Combescot, J. Phys. (Paris) 30, 987 (1969).
[8]E. P. Gross, in *Mathematical Methods in Solid State and Superfluid Theory* (Oliver and Boyd, Edinburgh, 1967), p. 46.
[9]R. Kubo, J. Phys. Soc. Japan 17, 1100 (1962).
[10]R. M. Wilcox, J. Math. Phys. 8, 962 (1967).
[11]K. D. Schotte and U. Schotte, Phys. Rev. 182, 479 (1969).
[12]S. Tomonaga, Progr. Theoret. Phys. (Kyoto) 5, 544 (1950).
[13]P. W. Anderson, Phys. Rev. Letters 18, 1049 (1967).
[14]See D. R. Hamann, Phys. Rev. B 2, 1373 (1970).
[15]N. I. Muskhelishvili, *Singular Integral Equations* (P. Noordhoff, Ltd., Groningen, The Netherlands, 1953), Chap. 14.
[16]See, for instance, P. Nozières, *Interacting Fermi Systems* (Benjamin, New York, 1964), Chap. 5.
[17]See, for example, W. E. Spicer, Phys. Rev. 154, 385 (1967) and references therein for an account of photoemission experiments.
[18]See, for example, *Polarons and Excitons* (Oliver and Boyd, Edinburgh, 1962).
[19]K. D. Schotte and U. Schotte, Phys. Rev. 185, 509 (1969).
[20]See, for example, *Hyperfine Structure and Nuclear Radiation*, edited by E. Matthias and D. A. Shirley (North-Holland, Amsterdam, 1968).
[21]J. J. Hopfield, Commun. Solid State Phys. 11, 40 (1969).
[22]S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1961), Chap. 12.
[23]D. R. Yennie, in *Lectures on Strong and Electromagnetic Interactions*, edited by K. W. Ford (Brandeis Lecture Notes, Boston, 1964), p. 165.
[24]N. Rosen and C. Zener, Phys. Rev. 40, 502 (1932).

PHYSICAL REVIEW B VOLUME 3, NUMBER 4 15 FEBRUARY 1971

Lattice Thermal Conductivity of Plastically Deformed Copper plus 10 Atomic Percent Aluminum Specimens in the Temperature Range 1–4 °K*

M. A. Mitchell,† P. G. Klemens, and C. A. Reynolds
Physics Department and Institute of Materials Science, University of Connecticut, Storrs, Connecticut 06268
(Received 5 June 1970)

The total thermal and electrical conductivities of seven polycrystalline rods of copper plus 10 at.% aluminum, which were in a total of 25 different states of recovery from plastic deformation at 77 °K, and one commercially pure nickel single crystal were measured in the liquid-helium temperature range. The low-temperature lattice thermal conductivity of a specimen which had been plastically deformed 9% recovered slowly as it was annealed between 300 and 700 °K, and then rapidly recovered to its prestrain magnitude after being annealed between 700 and 800 °K. The recrystallization temperature was 725 °K. Metallographic grain-size studies supported these conclusions. An application of the theory of Klemens and Ackerman and Klemens to the variation of the dislocation lattice thermal resistivity with annealing temperature (below 700 °K) due to impurity atmospheres made it possible to determine the fractional atomic-volume difference α between the aluminum and copper atoms to be 0.23. When the same theory was compared with variation of the dislocation lattice thermal resistivity with aluminum concentration found by Charsley, Salter, and Leaver, it was found that $\alpha = 0.24$. From the experimental x-ray data, α is 0.20. A later theory of Klemens which treated the variation of dislocation resistivity with annealing time at fixed annealing temperature was found to be inconsistent with the data of this work, but the experimental error was large. The theory contained the assumption that a unique diffusion constant could be defined for the deformed alloys, but this may not have been true, since plastic deformation generates excess vacancies. An anomalous departure of the phonon-electron lattice thermal resistivity from a T^{-2} temperature dependence was thought to be an effect associated with the small electron mean free paths in these alloys. The theory of Lindenfeld and Pennebaker qualitatively explained the anomaly.

I. INTRODUCTION

The lattice conductivity of a metal is sensitive to defects in the crystal structure. The different types of defect give rise to lattice thermal resistivities[1] which have their own characteristic temperature dependences. Plastic deformation generates dislocations; these produce a lattice thermal resistivity which is proportional to T^{-2}. Charsley *et al.*[2] found that the thermal resistivity per dislocation had a concentration dependence in copper-aluminum alloys which could not be explained by the