# Quantum Mechanical Liouville Equation for a System in Contact with a Reservoir

CHARLES R. WILLIS*
*Boston University, Boston, Massachusetts*
AND
PETER G. BERGMANN
*Syracuse University, Syracuse, New York*
(Received April 3, 1962)

In this paper we derive the equations of motion satisfied by the density matrix of an arbitrary physical system in contact with an infinite thermal reservoir of quantum mechanical free particles. We show that for weak but sustained interactions between system and reservoir, the reservoir is represented by a linear time-independent kernel in the system density matrix space. We obtain the kernel for the three possible models of quantum mechanical free particles which are boson and fermion reservoirs in which the system-reservoir interaction conserves the number of particles of the reservoir and a boson reservoir in which reservoir "particles" may be created or destroyed. In order to derive the equations of motion without using the inconsistent "rerandomization of phases" after each interaction, we generalize the Wigner-Weisskopf theory of line broadening of spectral lines to the equations of motion for the density matrix. We next show that the kernel preserves the normalization, positive-definiteness, and Hermiticity of the system density matrix and causes the system to approach equilibrium monotonically. In the limit of a classical reservoir our results include a derivation, without the repeated use of random phasing, of Bloch's equations of motion for the density matrix of a spin system imbedded in a thermal reservoir.

## I. INTRODUCTION

IN this paper we extend a theory of irreversible Gibbsian ensembles from classical to quantum mechanics. In two previous papers Lebowitz and Bergmann[1,2] had obtained and discussed to some extent an integrodifferential equation in $\Gamma$ space which described nonequilibrium classical ensembles. In its derivation they had assumed that initially the reservoir and system were statistically uncorrelated; i.e., the initial distribution of system-plus-reservoir was the product of the system's distribution and the distribution of the reservoir. They considered impulse interactions ("collisions") between the system and individual components of the reservoir, which led to a canonical mapping of the joint phase space on itself. Immediately after a collision the reservoir component that was involved was discarded. Thus, the assumptions of independence referred to each reservoir component *before* collision; this assumed asymmetry between past and future led to irreversibility.

In quantum mechanics we can also start with a product distribution; but the boundary condition for impulsive interactions ties together the incoming and outgoing waves in such a manner that it is difficult to develop a consistent method for discarding the reservoir particle after collision. Intuitively, our difficulty may be formulated in terms of the uncertainty principle. If we let the time of interaction of system and reservoir particle go to zero, then the energy becomes indeterminate, and immediately "after" the collision there is no clearly defined reservoir particle energy.

There are two possible ways to remove this difficulty. One method would be to consider a system and reservoir each of a sufficiently low density that there is enough time between collisions to treat each individual collision by the $S$ matrix of the two-body problem. This method has the disadvantage of limiting the density of the system and the reservoir to nondegenerate quantum mechanical gases.

The second method, which we adopt in this paper, is to consider weak but sustained interactions. This alternative has the advantage of not limiting the density of the system and permitting reservoirs of moderate degeneration. The problem is to develop a method of consistently discarding the reservoir particle after collision.

Redfield[3] has shown that the first-order perturbation solution of the quantum mechanical Liouville equation for a system in contact with a reservoir may be represented for a restricted time interval by an integrodifferential equation whose solution for the same time interval agrees with the perturbation theory result. The difficulty with the derivations of Redfield and of Wangness and Bloch[4] is that after each time interval it is necessary to rerandom phase. Van Hove[5] has pointed out that derivations based on random phases at all times cannot hold true for nonequilibrium distributions. His argument which he gave for isolated systems holds also for systems in contact with a reservoir. The essence of his argument is the perturbative result for $\rho(t_0+\tau)$ is exactly equivalent to $\rho(t_0-\tau)$, where $\rho$ is the density matrix of system +reservoir and $\tau$ is the usual "long but not too long

* This work was supported, in part, by the Air Research and Development Command, Air Force Cambridge Research Center.
[1] P. G. Bergmann and J. L. Lebowitz, Phys. Rev. **99**, 578 (1955).
[2] J. L. Lebowitz and P. G. Bergmann, Ann. Phys. (New York) **1**, 1 (1957).
[3] A. G. Redfield, IBM J. Research Develop. **1**, 1 (1957).
[4] R. K. Wangsness and F. Bloch, Phys. Rev. **89**, 728 (1953).
[5] L. Van Hove in *The Theory of Neutral and Ionized Gases*, edited by C. DeWitt and J. F. Detoeuf (J. Wiley & Sons, Inc., 1960), p. 162.

time" of perturbation theory and thus $\partial\rho/\partial t=0$ for $t>t_0$.

Van Hove[6] gave a derivation of the Pauli equation for an isolated system which was no longer open to the above objection for certain classes of initial conditions and where the interaction satisfied the diagonal singularity condition. Our solution of the problem is different but related to Van Hove's method. First, since we are considering not an isolated system but a system in contact with a reservoir we do not make any restrictions on the initial density matrix for the system. However, the reservoir is considered in equilibrium; i.e., it is diagonal at all times.

Our method consists of a generalization of the Wigner-Weisskopf[7] and Heitler[8] theory of line broadening to the space of density matrices. Although we do not assume the diagonal singularity condition of Van Hove, we find that our generalization of the Wigner-Weisskopf theory, in effect, retains only those terms of the interaction which satisfy the diagonal singularity condition in the Hilbert space of the reservoir particles.

The Wigner-Weisskopf method applied to line broadening for an atom in a vacuum is equivalent to considering only those intermediate states in which there is only a single photon present at a time. Our generalization of their method leads to considering only those intermediate states of system+reservoir in which a single reservoir particle is present at a time. As a result we are able to discard consistently the spent reservoir particle after interaction.

Our model for a relaxing system consists of an arbitrary quantum mechanical system in interaction with a reservoir of free particles. We will consider three cases. Case 1 and 2 will represent fermion and boson reservoirs, respectively, with an interaction Hamiltonian that conserves the number of reservoir particles; in case 3, the interaction Hamiltonian does not conserve the number of bosons. We can not have a fermion reservoir with an interaction Hamiltonian linear in annihilation and creation operators because spin changes cannot be half-integral. The system in all three cases is completely arbitrary and occupies a fixed volume $\Omega_s$. In each case we first assume the reservoir consists of $N_R$ free particles (on the average) in a volume $\Omega_R$ with periodic boundary conditions. We then take the limit as $N_R\to\infty$ and $\Omega_R\to\infty$, such that $N_R/\Omega_R$ approaches a finite limit.

There are three important consequences of this limit. First, the number of reservoir particles that interact with the system is proportional to $\Omega_s$, the volume of the system, so the fraction of the reservoir that has interacted with the system is $\Omega_s/\Omega_R$ which vanishes in our limit. Thus, we may neglect the reservoir particles that have interacted with the system so the system "sees" an equilibrium reservoir before equilibrium. As a second consequence of the limit we may replace, with negligible error, the discrete sums over reservoir states by integrals over a continuous level density. Only in the case of a boson reservoir below its lambda point must the discrete level density be taken into account. Thirdly, we show the effect of the reservoir on the system is through a time-independent linear operator which depends on the density of the reservoir only through the chemical potential of the reservoir. We are thus able to carry out the integration over the reservoir explicitly.

In Sec. II we show the equations of motion for the density matrix of an arbitrary system in contact with a reservoir has the form

$$\frac{\partial}{\partial t}\langle\alpha|\rho|\beta\rangle+i\langle\alpha|[H_s+\chi,\rho]|\beta\rangle=\sum_\Delta K_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}\langle\alpha+\Delta|\rho|\beta+\Delta\rangle, \quad (1.1)$$

where $\chi$ is a potential that commutes with $H_s$ and $K_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}$ is the time-independent stochastic kernel that represents the effect of the reservoir on the system.

In Sec. III we carry out the explicit evaluation of the formal kernel derived in Sec. II for the case of a boson reservoir with a particle-conserving interaction. We also discuss the conditions on the reservoir that were imposed in the derivation of Eq. (1.1).

We show in Sec. IV that the kernel $\mathbf{K}$ preserves the normalization, Hermiticity, and positive definiteness of $\rho$. We also show the system approaches equilibrium at the temperature of the reservoir monotonically.

In Sec. V we give the results for the fermion reservoir and the boson reservoir with an interaction that does not conserve reservoir particles. We discuss our results and their relationship to other derivations in Sec. VI.

## II. BOSON RESERVOIR WITH CONSERVATION OF PARTICLES

In this section we derive an equation for a quantum mechanical model of irreversibility. We first treat in some detail a reservoir consisting of bosons whose number is conserved. The equations for the fermion reservoir whose number is conserved and for the boson reservoir for interactions that do not conserve reservoir particles are given without detail in Sec. V.

Consider an arbitrary system with Hamiltonian $H_s$ eigenstates

$$H_s|\alpha v'\rangle=E_\alpha|\alpha v'\rangle. \quad (2.1)$$

$(H_s,v)$ is a complete set of commuting observables.

In all that follows we suppress the degeneracy index $v'$. We can add it in the final form of the equations without difficulty. Therefore, we set $H_s|\alpha\rangle=E_\alpha|\alpha\rangle$, where Greek letters always denote states of the system and Latin letters refer to the reservoir. Also, for the sake of brevity, we confine ourselves to a Hamiltonian

[6] L. Van Hove, Physica **21**, 517 (1955).
[7] V. Weisskopf and E. Wigner, Z. Physik **63**, 54 (1930).
[8] W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, New York, 1954), 3rd ed., Chap. 4, Sec. 16.

$H_s$ with a discrete spectrum of eigenvalues by enclosing the system in a volume $\Omega_s$.

We describe the reservoir by second quantization. The Hamiltonian for a system of noninteracting bosons is then

$$H_R=\sum_k N_k\epsilon_k,$$

where the operators $N_k$ are, as usual,

$$N_k=a_k^\dagger a_k$$

and the $a_k$ satisfy the standard commutation relations:

$$a_k a_{k'}-a_{k'}a_{\prime}=0,\quad a_k^\dagger a_{k'}{}^\dagger-a_{k'}{}^\dagger a_k^\dagger=0,$$
$$a_k^\dagger a_{k'}-a_{k'}a_k^\dagger=\delta_{kk'}.$$

The $\epsilon_k$ are single-particle energy levels. When we take cyclic boundary conditions for a particle of mass $m$, we have

$$\epsilon_k=(k)^2/2m,\quad k=(2\pi N)/L_R,\quad N=0,\pm1,\pm2,\cdots$$

where we have set $\hbar=1$.

The eigenstates of $H_R$ are $|\mathbf{n}\rangle$ and they satisfy

$$H_R|\mathbf{n}\rangle=(\textstyle\sum_i n_i\epsilon_i)|\mathbf{n}\rangle,$$

where $\mathbf{n}$ represents the sequence $n_1n_2\cdots$.

The interaction Hamiltonian is

$$V=\lambda\textstyle\sum_{kk'}\langle k|\phi(\mathbf{xy})|k'\rangle a_k^\dagger a_{k'},\qquad(2.2)$$

where $\phi(\mathbf{xy})$ is the interaction between a single reservoir component at $\mathbf{y}$ and the system at the point $\mathbf{x}$ in its configuration space; $\lambda$ is a dimensionless constant.

The matrix elements of $V$ in the Fock space of the reservoir are $\langle\mathbf{n}|\mathbf{V}|\mathbf{m}\rangle$, where we have used boldface $\mathbf{V}$ to indicate that $\langle\mathbf{n}|\mathbf{V}|\mathbf{m}\rangle$ is an operator in the Hilbert space of the system. The explicit representation of $\langle\mathbf{n}|\mathbf{V}|\mathbf{m}\rangle$, which we will not need till later, is

$$\langle\mathbf{n}|\mathbf{V}|\mathbf{m}\rangle=\textstyle\sum_{kk'}\langle k|\phi(\mathbf{xy})|k'\rangle n_k^{1/2}(n_{k'}+1)^{1/2}\times\delta_{m_1n_1}\delta_{m_2n_2}\cdots\delta_{m_k,n_k-1}\cdots\delta_{m_{k'},n_{k'}+1}.\qquad(2.3)$$

The density matrix $\mu$ for the combined system + reservoir satisfies the Liouville equation,

$$\partial\mu/\partial t+i[H_s+H_R+V,\mu]=0.\qquad(2.4)$$

When we perform the unitary transformation that takes $\mu$ to the interaction representation, we obtain

$$\bar\mu=e^{i(H_s+H_R)t}\mu e^{-i(H_s+H_R)t},$$

where $\bar\mu$ satisfies

$$\partial\bar\mu/\partial t+i[\bar V(t),\bar\mu(t)]=0$$

and

$$\bar V(t)=e^{i(H_s+H_R)t}Ve^{-i(H_s+H_R)t}.$$

The bar over an operator indicates the operator is in the interaction representation. To find the density matrix, $\bar\rho$, of the system we take the trace of $\bar\mu$ over the reservoir, $\bar\rho=\mathrm{Tr}_n\bar\mu$.

The elements of $\bar\mu$ which are diagonal in the reservoir coordinates satisfy

$$(\partial/\partial t)\langle\mathbf{n}|\bar\mu|\mathbf{n}\rangle+i[\langle\mathbf{n}|\bar{\mathbf{V}}|\mathbf{m}\rangle\langle\mathbf{m}|\bar\mu|\mathbf{n}\rangle-\langle\mathbf{n}|\bar\mu|\mathbf{m}\rangle\langle\mathbf{m}|\bar{\mathbf{V}}|\mathbf{n}\rangle]=0,\qquad(2.5a)$$

and the off-diagonal elements satisfy

$$(\partial/\partial t)\langle\mathbf{m}|\bar\mu|\mathbf{n}\rangle-i[\langle\mathbf{m}|\bar{\mathbf{V}}|\mathbf{l}\rangle\langle\mathbf{l}|\bar\mu|\mathbf{n}\rangle-\langle\mathbf{m}|\bar\mu|\mathbf{l}\rangle\langle\mathbf{l}|\bar{\mathbf{V}}|\mathbf{n}\rangle]=0,\qquad(2.5b)$$

where we sum over repeated indices.

We now make our fundamental assumption which states that any time the equation of motion for $\langle\mathbf{m}|\bar\mu|\mathbf{n}\rangle$ depends only on the elements of $\bar\mu$ which are diagonal in the reservoir coordinates. The explicit form of this assumption is

$$\langle\mathbf{m}|\bar\mu|\mathbf{e}\rangle=\delta_{\mathbf{m}\mathbf{l}}P_{\mathbf{m}\mathbf{l}}\bar\rho(t)=\delta_{\mathbf{m}\mathbf{l}}P_{\mathbf{m}}e^{t\mathbf{K}}\bar\rho(0),\qquad(2.6)$$

where

$$P_{\mathbf{m}}=Z^{-1}e^{-\theta(H_R-\xi N)},\ Z=\mathrm{Tr}e^{-\theta(H_R-\xi N)},\quad\theta=(kT)^{-1},$$

and $\mathbf{K}$ is defined by $d\bar\rho/dt=\mathbf{K}\bar\rho$. Since $\bar\rho$ is the arbitrary density matrix for the system, we see that Eq. (2.5b) for the off-diagonal elements $\langle\mathbf{m}|\bar\mu|\mathbf{n}\rangle$ depends only on the diagonal elements of the reservoir but on both diagonal and off-diagonal elements of the system. The only assumption we make about the system is that in the interaction representation the system density matrix is determined by a time-independent kernel $K$ which, since it is an operator in the system density matrix space, has in general four indices.

Since the remaining derivation is straightforward but lengthy, we will outline it first. Our method is equivalent to a generalization of the Wigner-Weisskopf treatment of line broadening. They treated the problem of an atom in the radiation field of the vacuum by assuming that in the equations of motion for the amplitudes of the photons the amplitude of the atomic state was $e^{-\gamma t}$. This closed the chain of equations which allowed them to solve for the photon amplitude exactly. They then were able to solve for the amplitude of the atomic state which lead to a self-consistent condition to determine $\gamma$ of the form

$$-i\gamma=\sum_\lambda|V|^2\frac{[1-e^{it(\nu_0-\nu_\lambda-i\gamma)}]}{(\nu_0-\nu_\lambda-i\gamma)},\qquad(2.7)$$

where $\nu_0=E_b-E_a$ and $\nu_\lambda$ is the frequency of photons of wave number $\lambda$. In other words, the atom would decay from state $b$ to state $a$ with an amplitude $e^{-\gamma t}$ if a time-independent solution of Eq. (2.7) exists.

When we put Eq. (2.6) in the commutator of Eq. (2.5b), we are able to solve this equation exactly for $\langle\mathbf{m}|\bar\mu|\mathbf{n}\rangle$ which we use in Eq. (2.5a). We then sum Eq. (2.5a) over the states $\mathbf{n}$, and since

$$\textstyle\sum_{\mathbf{n}}\langle\mathbf{n}|\partial\bar\mu/\partial t|\mathbf{n}\rangle=\partial\bar\rho/\partial t=\mathbf{K}\bar\rho$$

we obtain an equation for the operator $\mathbf{K}$. We will have verified our ansatz if we can find a time-independent

solution of this equation for $\mathbf{K}$. We defer the discussion of the existence of a time-independent solution until we have obtained Eq. (2.12) for $\mathbf{K}$.

We substitute Eq. (2.6) into Eq. (2.5b) and obtain

$$(\partial/\partial t)\langle \mathbf{m}|\bar{\mu}|\mathbf{n}\rangle = i[P_{\mathrm{m}}e^{t\mathbf{K}}\bar{\rho}(0)\langle \mathbf{m}|\bar{\bar{V}}|\mathbf{n}\rangle - \langle \mathbf{m}|\bar{V}|\mathbf{n}\rangle P_{\mathrm{n}}e^{t\mathbf{K}}\bar{\rho}(0)], \quad (2.8)$$

where it is necessary to keep track of order of factors since all terms except $P_{\mathrm{m}}$ are operators in the system Hilbert space. To solve Eq. (2.8), we introduce the representation Eq. (2.1) of the system.

When we take the matrix elements in the energy representation, use the definition of $\bar{V}$, and integrate, we obtain

$$\langle \sigma\mathbf{m}|\bar{\mu}(t)|\mathbf{n}\nu\rangle = iP_{\mathrm{m}}\int_0^t dt'\, e^{i\omega_{mn}t'}\langle \sigma|e^{t'\mathbf{K}}\bar{\rho}(0)|\epsilon\rangle \times e^{i\omega_{\epsilon\nu}t'}\langle \epsilon\mathbf{m}|V|\mathbf{n}\nu\rangle - iP_{\mathrm{n}}\int_0^t dt' \times e^{i\omega_{mn}t'}\langle \epsilon|e^{t'\mathbf{K}}\bar{\rho}(0)|\nu\rangle e^{i\omega_{\sigma\epsilon}t'}\langle \sigma\mathbf{m}|V|\mathbf{n}\epsilon\rangle, \quad (2.9)$$

where

$$\omega_{mn}=E_{\mathrm{m}}-E_{\mathrm{n}}, \quad \omega_{\alpha\beta}=E_\alpha-E_\beta, \quad |\alpha\mathbf{n}\rangle\equiv|\alpha\rangle|\mathbf{n}\rangle,$$

and $\langle \epsilon\mathbf{m}|V|\mathbf{n}\nu\rangle$ is now a time-independent $c$ number.

We now explicitly perform the time integration in Eq. (2.9) and obtain

$$\langle \sigma\mathbf{m}|\bar{\mu}(t)|\mathbf{n}\nu\rangle = \left\langle \sigma\left|\left\{\frac{e^{it(\omega_{mn}+\omega_{\epsilon\nu}-i\mathbf{K})}-1}{\omega_{mn}+\omega_{\epsilon\nu}-i\mathbf{K}}\right\}\bar{\rho}(0)\right|\epsilon\right\rangle \times P_{\mathrm{m}}\langle \epsilon\mathbf{m}|V|\mathbf{n}\nu\rangle - \langle \sigma\mathbf{m}|V|\mathbf{n}\epsilon\rangle \times P_{\mathrm{n}}\left\langle \epsilon\left|\left\{\frac{e^{it(\omega_{mn}+\omega_{\sigma\epsilon}-i\mathbf{K})}-1}{\omega_{mn}+\omega_{\sigma\epsilon}-i\mathbf{K}}\right\}\bar{\rho}(0)\right|\nu\right\rangle. \quad (2.10)$$

When we substitute Eq. (2.10) into Eq. (2.5a), we obtain four terms:

$$\begin{aligned}-i\frac{\partial}{\partial t}\langle \alpha\mathbf{n}|\bar{\mu}|\mathbf{n}\beta\rangle &= \langle \alpha|\mathbf{c}(\omega_1)\bar{\rho}|\epsilon\rangle\langle \epsilon\mathbf{n}|V|\mathbf{m}\gamma\rangle\langle \gamma\mathbf{m}|V|\mathbf{n}\beta\rangle e^{i\omega_{\gamma\beta}t}P_{\mathrm{n}} \\ &\quad -\langle \alpha\mathbf{n}|V|\mathbf{m}\epsilon\rangle\langle \epsilon|\mathbf{c}(\omega_2)\bar{\rho}|\gamma\rangle\langle \gamma\mathbf{m}|V|\mathbf{n}\beta\rangle e^{i\omega_{\alpha\beta}t}P_{\mathrm{m}} \\ &\quad -\langle \alpha\mathbf{n}|V|\mathbf{m}\gamma\rangle\langle \gamma|\mathbf{c}(\omega_3)\bar{\rho}|\epsilon\rangle\langle \epsilon\mathbf{m}|V|\mathbf{n}\epsilon\rangle e^{i\omega_{\epsilon\beta}t}P_{\mathrm{m}} \\ &\quad +\langle \alpha\mathbf{n}|V|\mathbf{m}\gamma\rangle\langle \gamma\mathbf{m}|V|\mathbf{n}\epsilon\rangle\langle \epsilon|\mathbf{c}(\omega_4)\bar{\rho}|\beta\rangle e^{i\omega_{\alpha\gamma}t}P_{\mathrm{n}}, \end{aligned} \quad (2.11)$$

where the operator $\mathbf{c}(\omega)$ is

$$\mathbf{c}(\omega)=\frac{e^{it(\omega-i\mathbf{K})}-1}{(\omega-i\mathbf{K})}$$

and the $\omega_i$'s are

$$\omega_1=\omega_{nm}+\omega_{\epsilon\gamma}, \quad \omega_3=\omega_{mn}+\omega_{\epsilon\beta},$$
$$\omega_2=\omega_{nm}+\omega_{\alpha\epsilon}, \quad \omega_4=\omega_{mn}+\omega_{\gamma\epsilon}.$$

We use the relation $\bar{\rho}(0)=e^{-\mathbf{K}t}\bar{\rho}(t)$ and

$$\textstyle\sum_{\mathrm{n}}\langle \mathbf{n}|\partial\bar{\mu}/\partial t|\mathbf{n}\rangle = d\bar{\rho}/dt = \mathbf{K}\bar{\rho}$$

to obtain

$$\begin{aligned}&-i\langle \alpha|\mathbf{K}\bar{\rho}(t)|\beta\rangle \\ &=\textstyle\sum_{\mathrm{n}}\{\langle \alpha|\mathbf{C}(\omega_1)\bar{\rho}(t)|\epsilon\rangle\langle \epsilon\mathbf{n}|V|\mathbf{m}\gamma\rangle\langle \gamma\mathbf{m}|V|\mathbf{n}\beta\rangle P_{\mathrm{n}}e^{i\omega_{\epsilon\beta}t} \\ &\quad -\langle \alpha\mathbf{n}|V|\mathbf{m}\epsilon\rangle\langle \epsilon|\mathbf{C}(\omega_2)\bar{\rho}(t)|\gamma\rangle\langle \gamma\mathbf{m}|V|\mathbf{n}\beta\rangle P_{\mathrm{m}}e^{i(\omega_{\alpha\epsilon}+\omega_{\gamma\beta})t} \\ &\quad -\langle \alpha\mathbf{n}|V|\mathbf{m}\gamma\rangle\langle \gamma|\mathbf{C}(\omega_3)\bar{\rho}(t)|\epsilon\rangle\langle \epsilon\mathbf{m}|V|\mathbf{n}\beta\rangle P_{\mathrm{m}}e^{i(\omega_{\alpha\gamma}+\omega_{\epsilon\beta})t} \\ &\quad +\langle \alpha\mathbf{n}|V|\mathbf{m}\gamma\rangle\langle \gamma\mathbf{m}|V|\mathbf{n}\epsilon\rangle\langle \epsilon|\mathbf{C}(\omega_4)\bar{\rho}(t)|\beta\rangle P_{\mathrm{n}}e^{i\omega_{\alpha\epsilon}t}\}, \end{aligned} \quad (2.12)$$

where

$$\mathbf{C}(\omega)=[1-e^{-it(\omega-i\mathbf{K})}]/(\omega-i\mathbf{K}).$$

We now have a functional equation for the operator $\mathbf{K}$. Since $\mathbf{K}$ has been assumed independent of time it is necessary to find a time-independent solution of Eq. (2.12) for $\mathbf{K}$. There are two types of explicit time dependence in Eq. (2.12). To make the time dependence due to $e^{i\omega t}$ vanish we require $\omega_{\epsilon\beta}=0$ in the first term, $\omega_{\alpha\epsilon}+\omega_{\gamma\beta}=0$ in the second and third term and $\omega_{\alpha\epsilon}=0$ in the fourth term of Eq. (2.12). The second type of time dependence is due to the operators $\mathbf{C}(\omega)$. We see that for $\mathbf{K}\bar{\rho}<0$ and for $\omega\ll t\ll\lambda^{-2}$ there exists a time-independent solution of order $\lambda^2$ for $\mathbf{K}$ when we make the following substitution for $\mathbf{C}$:

$$\mathbf{C}(\omega)=\frac{1-e^{-i(\omega-i\mathbf{K})t}}{\omega-i\mathbf{K}}\to\frac{1}{\omega}-\!\!\!+i\pi\delta(\omega), \quad (2.13)$$

where $\mathcal{P}$ is the "principal part of."

More precisely, we take the limit as $\lambda\to 0$ and $t\to\infty$ such that $\lambda^2 t=\tau\ll 1$. We then find a solution for $\mathbf{K}$ which is proportional to $\lambda^2$ such that $\mathbf{K}\bar{\rho}$ is negative definite.

When Eq. (2.13) is used in Eq. (2.12), we obtain the time-independent solution for $\mathbf{K}$:

$$K_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}\equiv 2k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}-\delta_{\Delta 0}(\textstyle\sum_\gamma k_{\gamma\gamma}{}^{\alpha\alpha}+k_{\gamma\gamma}{}^{\beta\beta}), \quad (2.14)$$

where

$$k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}=\lambda^2\textstyle\sum_{\mathrm{n}}\pi\langle \alpha\mathbf{n}|V|\mathbf{m},\alpha+\Delta\rangle \times P_{\mathrm{m}}\langle \beta+\Delta,\mathbf{m}|V|\mathbf{n}\beta\rangle\delta(\Delta-\omega_{mn}) \quad (2.15)$$

and $\Delta$ is an energy,

$$\Delta=E_\gamma-E_\alpha=E_\epsilon-E_\beta.$$

In addition, we obtain a contribution from the principal part which can be written as a commutator of a temperature-dependent potential which we give in Sec. III. In Sec. III we shall explicitly evaluate $\mathbf{K}$, and in Sec. IV we shall prove $\mathbf{K}$ preserves the Hermiticity, positive definiteness, and normalization of $\rho$ and causes $\rho$ to approach equilibrium monotonically.

We conclude this section with some remarks about the treatment of the time dependence of Eq. (2.12). The reason that the time derivative of the matrix element $\langle\alpha|\rho|\beta\rangle$ depends only on matrix elements of the form $\langle\alpha+\Delta|\rho|\beta+\Delta\rangle$ instead of on the general matrix element $\langle\gamma|\rho|\delta\rangle$, where $\gamma$ and $\delta$ are arbitrary is a consequence of our requirement that $\mathbf{K}$ be time independent. We did not take an unrestricted limit as $t\to\infty$ in Eq. (2.13) because in that case the left-hand side of Eq. (2.12) would vanish since it is necessary that $\mathbf{K}\rho(\infty)=0$ and we would have been unable to determine $\mathbf{K}$. The limit $\lambda\to 0$ and $t\to\infty$ such that $\lambda^2 t=\tau\ll 1$ permits us on the one hand to replace $\mathbf{C}$ by a delta function and on the other hand to obtain an explicit solution for $\mathbf{K}$ up to terms of order $\tau$. The virtue of our model is that for smoothly varying potentials we are able to show explicitly that a time exists such that there is a time-independent solution for $\mathbf{K}$.

## III. SOLUTIONS FOR THE KERNELS

In this section we obtain the explicit equation satisfied by the density matrix of a system in contact with the reservoir. We first obtain the dependence of the kernel $\mathbf{K}$ on the temperature and chemical potential of the reservoir. To do this we perform the trace over the reservoir coordinates in Eq. (2.15). When we use the definition of $V$ in terms of annihilation and creation operators in Eq. (2.5), we obtain

$$k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}=\pi\lambda^2\sum_{n_r}\sum_{n_{r'}}\sum_r\sum_{r'}\langle\alpha r|\phi|r',\alpha+\Delta\rangle \times\langle\beta+\Delta,r'|\phi|r\beta\rangle n_{r'}(n_r+1) \times P(n_r n_{r'})\delta(\epsilon_{r'}-\epsilon_r+\Delta). \quad (3.1)$$

We perform the sum over the occupation numbers $n_r$ and $n_{r'}$ and obtain

$$\sum_{n_r}\sum_{n_{r'}} n_{r'}(n_r+1)P(n_r n_{r'})=\langle n_{r'}\rangle\{\langle n_r\rangle+1\},$$

where

$$\langle n_r\rangle=1/[e^{\theta(\epsilon_r-\xi)}-1].$$

Since we have taken the limit as $\Omega_R\to\infty$, we may replace the discrete sum over reservoir state, $\sum_r(\cdots)$, by the integral $\int(\cdots)g(\epsilon)d\epsilon$, where $g(\epsilon)d\epsilon$ is the number of single-particle states with energy between $\epsilon$ and $\epsilon+d\epsilon$. With this substitution we obtain for Eq. (3.1)

$$k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}=\lambda^2\pi\int d\epsilon d\epsilon'\, g(\epsilon)g(\epsilon')\langle\alpha\epsilon|\phi|\epsilon',\alpha+\Delta\rangle \times\langle\beta+\Delta,\epsilon'|\phi|\epsilon\beta\rangle\langle n(\epsilon')\rangle\{\langle n(\epsilon)\rangle+1\}\delta(\epsilon'-\epsilon+\Delta). \quad (3.2)$$

At this point it is worth remarking that we could have performed the summation over the occupation numbers of the reservoir and introduced the level density in Eq. (2.9). We deferred the summation until now, because the relationship of our method to the diagonal singularity condition of Van Hove and the Wigner-Weisskopf theory is somewhat more transparent in the occupation number representation. Furthermore, as we show in Eq. (4.4), the form of Eq. (2.15) before summation is easier to identify as the form that is needed for an $H$ theorem.

We now show that $k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}$ is independent of the volume of the reservoir. Since the state of a single reservoir particle is

$$|\epsilon\rangle=\Omega_R^{-\frac{1}{2}}\exp(-i\mathbf{k}\cdot\mathbf{r}),$$

where $\epsilon=k^2/(2m)$, the matrix element, $\langle\alpha\epsilon|\phi|\epsilon',\alpha+\Delta\rangle \sim\Omega_R^{-1}$, and the density of states $g(\epsilon)\sim\Omega_R$ is independent of the volume of the reservoir. As a result, $k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}$ depends only on the density of the reservoir through $\xi$, the chemical potential. From the discussion of the preceding two paragraphs we see that the first limit we take is the limit as $N_R\to\infty$ and $\Omega_R\to\infty$ such that the density of the reservoir is constant. This allows us to treat the reservoir as always presenting a canonical distribution to the system. The second limit, $\lambda^2\to 0$, allows us to solve for $\mathbf{K}$ directly. The limit as $t\to\infty$ such that $\lambda^2 t=\tau\ll 1$ allows us to introduce the delta function in Eq. (2.13).

We must now examine the "slowly varying" condition that is implicit in replacing Eq. (2.13) by a delta function. This requirement means physically that $F(\epsilon)$ should be slowly varying over $\epsilon^*=t^{-1}$ where $t$ is large enough to contain many periods of the reservoir. We thus have

$$\Delta=\epsilon_r-\epsilon_{r'}\gg t^{-1}\equiv\epsilon^*=\lambda^2\tau^{-1},$$

which implies $\tau\Delta\gg\lambda^2$. For $\Delta$ finite, we can satisfy this condition by taking the limit $\lambda\to 0$. However, since $\Delta\sim\theta^{-1}=kT$, we see that as $T\to 0$ we cannot satisfy this condition for any finite $\lambda$. This means that we must exclude degenerate reservoirs because both boson and fermion reservoirs are not slowly varying as $T\to 0$. This is no real restriction on the derivation because as $\theta^{-1}$ goes to zero the specific heat of the reservoir also goes to zero; i.e., it cannot emit energy, it can only absorb energy and can not physically serve as a reservoir.

We now show that the contribution of the principal part to Eq. (2.12) can be written as the commutator of a potential that commutes with the Hamiltonian $H_s$. The contributions of the principal parts of the second and third term cancel each other. For the imaginary part of the first and fourth terms of Eq. (2.12), we obtain $\langle\beta|\chi|\beta\rangle\langle\alpha|\bar{\rho}|\beta\rangle$ and $-\langle\alpha|\chi|\alpha\rangle\langle\alpha|\bar{\rho}|\beta\rangle$, where

$$\langle\beta|\chi|\beta\rangle=\lambda^2\mathcal{P}\int d\epsilon d\epsilon'\frac{|\langle\beta\epsilon|\phi|\epsilon'\gamma\rangle|^2}{\epsilon'-\epsilon-\omega_{\gamma\beta}}g(\epsilon)g(\epsilon') \times\langle n(\epsilon')\rangle\{\langle n(\epsilon)\rangle+1\}. \quad (3.3)$$

Thus, $\langle\beta|\chi|\beta\rangle$ is a second-order level shift of the state $\beta$ due to the interaction of the system with the reservoir

weighted by the equilibrium distribution of the reservoir.

When we combine Eqs. (2.14) and (3.3), we obtain

$$(\partial/\partial t)\langle\alpha|\bar{\rho}|\beta\rangle+i\langle\alpha|[\chi,\bar{\rho}]|\beta\rangle=(\mathbf{K}\bar{\rho})_{\alpha\beta}.$$

If we now return from the interaction representation for the system to the original representation, we obtain the final form of our equation for the density matrix. This is

$$\begin{aligned}(\partial/\partial t)\langle\alpha|\rho|\beta\rangle+i\langle\alpha|[H_s+\chi,\rho]|\beta\rangle&=(\mathbf{K}\rho)_{\alpha\beta}\\ &\equiv\textstyle\sum_\Delta 2k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}\langle\alpha+\Delta|\rho|\beta+\Delta\rangle\\ &\quad-(k_{\alpha+\Delta,\alpha+\Delta}{}^{\alpha\alpha}+k_{\beta+\Delta,\beta+\Delta}{}^{\beta\beta})\langle\alpha|\rho|\beta\rangle,\end{aligned}\tag{3.4}$$

where we have used the property

$$\bar{K}_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}=e^{it(E_\alpha-E_\beta+E_\gamma-E_\delta)}K_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}.$$

However, since our requirement that $\mathbf{K}$ be time independent leads to the condition $E_\alpha-E_\beta+E_\gamma-E_\delta=0$, we have the result $\bar{\mathbf{K}}=\mathbf{K}$. Thus, the assumption that $\mathbf{K}$ in the interaction representation is independent of time, coupled with the use of perturbation theory, leads to a time-independent kernel in the original representation. In Sec. IV we show that $\mathbf{K}$ satisfies the necessary and sufficient conditions that must be satisfied if Eq. (3.4) is to serve as an equation for the time evolution of a system in contact with a reservoir.

## IV. APPROACH TO EQUILIBRIUM

We now show that the kernel $\mathbf{K}$ preserves the normalization, positive definiteness, and Hermiticity of the density matrix $\rho$. If $\mathbf{K}$ is to represent a thermal reservoir, it is necessary to show that Eq. (3.4) approaches equilibrium monotonically. In a previous paper[9] we proved that the necessary and sufficient condition that a kernel of the form

$$\begin{aligned}\mathbf{K}\rho=\mathrm{Tr}_R\{&2\mathbf{O}P_R{}^{\frac{1}{2}}\rho P_R{}^{\frac{1}{2}}\mathbf{O}^\dagger-e^{\theta/2H_s}\rho e^{\theta/2H_s}P^{\frac{1}{2}}\mathbf{O}^\dagger\mathbf{O}P^{\frac{1}{2}}\\ &-P^{\frac{1}{2}}\mathbf{O}^\dagger\mathbf{O}P^{\frac{1}{2}}e^{\theta/2H_s}\rho e^{\theta/2H_s}\},\end{aligned}\tag{4.1}$$

where

$$P_R{}^{\frac{1}{2}}=Z^{-1}e^{-\theta(H_R-\xi N)},\quad P=e^{-\theta H_s}P_R,\quad Z=\mathrm{Tr}e^{-\theta(H_R-\xi N)},$$

and $\mathbf{O}$ is an arbitrary operator, approach equilibrium monotonically was

$$\mathbf{K}e^{-\theta H_s}=0;\tag{4.2}$$

i.e., equilibrium is a solution. In I we showed that any kernel of the form of Eq. (4.1) satisfied the normalization, Hermiticity, and positive definiteness conditions. We now show that Eq. (3.4) satisfies Eq. (4.2) and that $\mathbf{K}\rho$ is of the form of Eq. (4.1). This will complete the demonstration that $\mathbf{K}$ possesses the necessary and sufficient conditions to be a kernel representing a reservoir.

Although Eqs. (4.1) and (4.2) do not imply any local symmetry principles, we first show that, because our model uses weak interactions, $\mathbf{K}$ satisfies the detailed-balance condition for a system in the presence of a reservoir:

$$k_{\alpha\alpha}{}^{\alpha+\Delta,\alpha+\Delta}=e^{\theta\Delta}k_{\alpha+\Delta,\alpha+\Delta}{}^{\alpha\alpha}.\tag{4.3}$$

From the definition of $k$, Eq. (3.2), we obtain

$$\begin{aligned}&k_{\alpha\alpha}{}^{\alpha+\Delta,\alpha+\Delta}\\ &=\pi\lambda^2\int d\epsilon\, g(\epsilon)g(\epsilon-\Delta)\\ &\qquad\times|\langle\alpha\epsilon|\phi|\epsilon-\Delta,\alpha+\Delta\rangle|^2\langle n(\epsilon-\Delta)\rangle[\langle n(\epsilon)\rangle+1]\\ &=\pi\lambda^2\int d\epsilon\, g(\epsilon)g(\epsilon-\Delta)\\ &\qquad\times|\langle\alpha\epsilon|\phi|\epsilon-\Delta,\alpha+\Delta\rangle|^2\langle n(\epsilon-\Delta)\rangle\langle n(\epsilon)\rangle e^{\theta\epsilon},\end{aligned}$$

where we have used the identity

$$\langle n(\epsilon-\Delta)\rangle[\langle n(\epsilon)\rangle+1]=e^{\theta\epsilon}\langle n(\epsilon-\Delta)\rangle\langle n(\epsilon)\rangle.$$

We change the variable of integration from $\epsilon$ to $\epsilon+\Delta$ to obtain

$$\begin{aligned}&k_{\alpha\alpha}{}^{\alpha+\Delta,\alpha+\Delta}\\ &=\pi\lambda^2e^{\theta\Delta}\int d\epsilon\, g(\epsilon+\Delta)g(\epsilon)\\ &\qquad\times|\langle\alpha,\epsilon+\Delta|\phi|\epsilon,\alpha+\Delta\rangle|^2\langle n(\epsilon)\rangle[\langle n(\epsilon+\Delta)\rangle+1]\\ &=e^{\theta\Delta}k_{\alpha+\Delta,\alpha+\Delta}{}^{\alpha\alpha}.\end{aligned}$$

We prove that $\rho=Z^{-1}e^{-\theta H_s}$ is a solution of Eq. (3.4) by direct substitution. This gives the following:

$$\begin{aligned}[H_s+\chi,e^{-\theta H_s}]_{\alpha\alpha}=\textstyle\sum_\Delta(&2k_{\alpha\alpha}{}^{\alpha+\Delta,\alpha+\Delta}e^{-\theta(E_\alpha+\Delta)}\\ &-2k_{\alpha+\Delta,\alpha+\Delta}{}^{\alpha\alpha}e^{-\theta E_\alpha}).\end{aligned}$$

The left-hand side vanishes since $\chi$ is diagonal, and the right-hand side vanishes by use of Eq. (4.3).

To prove $\mathbf{K}\rho$ can be written in the form of Eq. (4.1) we set $\mathbf{O}=\mathbf{D}V$ where $\mathbf{D}$ is a projection operator that picks out the state of the reservoir particle that conserves the energy of reservoir+system.

With this substitution Eq. (4.1) becomes

$$\begin{aligned}&\langle\alpha|\mathbf{K}\rho|\beta\rangle\\ &=\mathrm{Tr}_m{}'[2\textstyle\sum_\Delta\langle\alpha\mathbf{m}|V|\mathbf{n},\alpha+\Delta\rangle P_{\mathbf{n}}\rho\langle\beta+\Delta,\mathbf{n}|V|\mathbf{m}\beta\rangle\\ &\qquad-\langle\alpha|\rho|\beta\rangle P_{\mathbf{m}}(|\langle\alpha\mathbf{m}|V|\mathbf{n},\alpha+\Delta\rangle|^2\\ &\qquad+|\langle\beta\mathbf{m}|V|\mathbf{n},\beta+\Delta\rangle|^2)],\end{aligned}\tag{4.4}$$

where $\mathrm{Tr}_m{}'$ is restricted to states that conserve energy. The restriction of the double sum over intermediate states of the system to a single sum over $\Delta$ is a consequence of the two projection operators which require both the following equations to be satisfied:

$$\Delta=E_{\mathbf{m}}-E_{\mathbf{n}}=E_\gamma-E_\alpha,\quad\Delta=E_{\mathbf{m}}-E_{\mathbf{n}}=E_\delta-E_\beta.$$

Thus, the double sum over intermediate states is restricted to a single sum because of the relationship $E_\gamma-E_\alpha=E_\delta-E_\beta$.

This completes the proof that $\mathbf{K}$ has the form of Eq.

[9] C. R. Willis, Phys. Rev. **127**, 1405 (1962); referred to as I.

(4.1) since Eq. (4.4) is equivalent to Eqs. (2.14) and (2.15). Thus, $\mathbf{K}$ preserves the normalization, Hermiticity, and positive definiteness of $\rho$ and causes $\rho$ to approach equilibrium monotonically.

## V. OTHER INTERACTIONS

We can obtain the results of a fermion reservoir which conserves the number of particles of the reservoir by replacing $\langle n(\epsilon)\rangle[\langle n(\epsilon')\rangle+1]$ by $\langle n(\epsilon)\rangle[\langle n(\epsilon')\rangle-1]$ in Eq. (3.2) and replacing $[e^{\beta(\epsilon-\xi)}-1]^{-1}$ by $[e^{\beta(\epsilon-\xi)}+1]^{-1}$. All the derivations and proofs of Secs. II through IV proceed without modification for the fermion reservoir.

We now consider the case of a boson reservoir with a linear interaction with the system, for example, a black-body reservoir. The interaction Hamiltonian is

$$V=\sum_k \sum_i f_k{}^i a_k+f_k{}^{i*}a_k{}^\dagger,$$

where

$$f_k{}^i=(e/c)\Omega_R{}^{-\frac{1}{2}}\sum_j P_j\cdot\epsilon_k{}^i \exp(i\mathbf{k}\cdot\mathbf{x}_j).$$

The sum over $j$ is a sum over the charged particles of the system and the superscript denotes the direction of polarization.

The derivations proceed in the same way as for the previous two cases. The only difference is that the kernels depend on $g(\epsilon)$ and $[n(\epsilon)+1]$ instead of on $g(\epsilon)g(\epsilon')$ and $n(\epsilon)[n(\epsilon')+1]$. The kernels are still independent of the volume of the reservoir since the matrix elements of $V$ are proportional to $\Omega_R{}^{-\frac{1}{2}}$; thus, the term $V^2\propto\Omega_R{}^{-1}$ just cancels the single power of the volume that occurs in a density over states.

The rate equation for a system linearly coupled to a boson reservoir is

$$\frac{\partial}{\partial t}\langle\alpha|\rho|\beta\rangle+i\langle\alpha|[H_s+\chi,\rho]|\beta\rangle$$
$$=\sum_\Delta[2k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}\langle\alpha+\Delta|\rho|\beta+\Delta\rangle$$
$$-(k_{\alpha+\Delta,\alpha+\Delta}{}^{\alpha\alpha}+k_{\beta+\Delta,\beta+\Delta}{}^{\beta\beta})\langle\alpha|\rho|\beta\rangle], \quad (5.1)$$

where

$$k_{\alpha\beta}{}^{\alpha+\Delta,\beta+\Delta}\equiv\langle\langle\alpha|f^*(\Delta)|\alpha+\Delta\rangle\langle\beta+\Delta|f(\Delta)|\beta\rangle\rangle_{\mathrm{av}}F(\Delta);$$

the "av" indicates an average over the random orientation of the polarization vectors $\epsilon_k{}^i$, and

$$F(\Delta)=\{\langle n(\Delta)\rangle+1\}g(\Delta) \quad \text{for} \quad \Delta>0 \text{ emission},$$
$$F(\Delta)=\langle n(\Delta)\rangle g(\Delta) \quad \text{for} \quad \Delta<0 \text{ absorption}.$$
$$n(\Delta)=1/(e^{\beta\Delta}-1), \quad g(\Delta)=(\Omega_R/\pi^3c^3)\Delta^2,$$

and

$$f(\Delta)=\sum_{\mathbf{k}}{}' f_k{}^1(\Delta)+f_k{}^2(\Delta),$$

where

$$f_k{}^i(\Delta)\equiv(e/c)\Omega_R{}^{-\frac{1}{2}}\sum_j \mathbf{p}_j\cdot\epsilon_k{}^i\exp(i\mathbf{k}\cdot\mathbf{x}_j).$$

The primed $\mathbf{k}$ sum indicates a sum over $|\mathbf{k}|=\Delta/c$.

## VI. DISCUSSION

The requirement that our kernel be time independent in the interaction representation has reduced the number of indices needed to specify $\mathbf{K}$ from four to three. A consequence of this reduction is the separation of the effects of the reservoir on the diagonal and off-diagonal matrix elements of the system. In order to see this, we take the diagonal matrix elements of Eq. (3.4) which are

$$(\partial/\partial t)\langle\alpha|\rho|\alpha\rangle=2\sum_\Delta k_{\alpha,\alpha+\Delta}\langle\alpha+\Delta|\rho|\alpha+\Delta\rangle$$
$$-k_{\alpha+\Delta,\alpha}\langle\alpha|\rho|\alpha\rangle, \quad (6.1)$$

where

$$k_{\alpha,\alpha+\Delta}\equiv k_{\alpha\alpha}{}^{\alpha+\Delta,\alpha+\Delta}.$$

Equation (6.1) is just the master equation for a system in contact with a reservoir. The reservoir connects an arbitrary matrix element $\langle\alpha|\rho|\beta\rangle$ with only those matrix elements that have the form $\langle\alpha+\Delta|\rho|\beta+\Delta\rangle$. The reservoir thus has the effect of dividing the matrix elements into mutually exclusive sets that relax among themselves.

However, this does not mean there is no interaction between diagonal and off-diagonal matrix elements. The evolution of the density matrix is through the Hamiltonian of the system interrupted by collisions with the reservoir. The direct time evolution of the full Hamiltonian of the system connects diagonal and off-diagonal matrix elements of the system. Frequently this reversible dephasing of the off-diagonal matrix elements is more important than the irreversible relaxing of the off-diagonal matrix elements.

If we take the classical limit, the reservoirs lose their degeneracy and go over into a classical reservoir. We then obtain for our arbitrary system an equation of the same functional form as Eq. (3.4) but where the reservoirs are now classical. Our method of proof does not depend in any way on the statistics or temperature of the reservoir so the classical limit is valid.

Since we have said nothing about the statistics of the system, the kernels take the same form independent of the statistics of the system. No changes are required in any derivation. The states of the system $|\alpha\rangle$ are just the properly symmetrized wave functions of the system. Throughout the derivations we have left the sum over intermediate states of the system as formally a discrete sum. If a density of states for the system exists, it can be introduced in the final Eqs. (3.4) and (5.1). The important point is that essentially no properties of the system are required in any derivation. The nearest we come to a requirement on the system is that the interaction between reservoir and system is sufficiently smooth which is only very indirectly a requirement on the system.

If for our system we take a system of spins and go over to the limit of a classical reservoir, we obtain Bloch and Wangness'[4] equations. The one point of difference is that their kernels depend on three indices instead of four because of special properties of magnetic systems instead of our requirement that the kernel be time independent in the interaction representation. Consequently, our proofs constitute, as a special case,

a proof of the Bloch-Wangness equations that is free of the random phase inconsistency pointed out by Van Hove.[5]

We conclude with some remarks about the diagonal singularity condition of Van Hove.[6] In the Wigner-Weisskopf theory of line broadening the method consists of an exact solution of a problem where the only states considered are those in which only one photon at a time appears in any intermediate state and the photons in successive intermediate states are independent of each other. A consequence of our derivation is that we consider only those intermediate states of the system+reservoir interaction in which only one reservoir particle appears at a time and the reservoir particles in successive intermediate states are independent of each other. This allows us to effectively discard the spent reservoir particle and the system "sees" a canonically distributed reservoir before each collision.

We can see the connection between the above discussion and the diagonal singularity condition by considering the $j$th term in the expansion of the time evolution operator of the system, $e^{t\mathbf{K}}$, which is

$$(1/j!)t^j\mathbf{K}^j = (1/j!)(\lambda^2 t)^j[\sum_{\mathbf{n}}\langle\mathbf{n}|V|\mathbf{m}\rangle P_{\mathbf{m}}\langle\mathbf{m}|V|\mathbf{n}\rangle]^j. \quad (6.2)$$

The intermediate states of the system in Eq. (6.2) are arbitrary. However, in the reservoir Hilbert space where the system operators are $c$ numbers, Eq. (6.2) is of the form $[\sum(VAV)_d]^j$, where $A=P$ is diagonal in the reservoir coordinates and where $d$ indicates "take the diagonal matrix element of $(\cdots)$." This is just the term that the diagonal singularity condition for internal relaxation gives for the coefficient of $(\lambda^2 t)^j$. Thus, our derivation which starts with the assumption that the off-diagonal matrix elements of the system +reservoir density matrix are determined by $Pe^{t\mathbf{K}}$ has, as a consequence, that in the reservoir Hilbert space the interaction between system and reservoir satisfies the diagonal singularity condition of Van Hove.

PHYSICAL REVIEW VOLUME 128, NUMBER 1 OCTOBER 1, 1962

# Lorentz-Invariant Equations of Motion of Point Masses in the General Theory of Relativity

PETER HAVAS*
*Department of Physics, Lehigh University, Bethlehem, Pennsylvania*
AND
JOSHUA N. GOLDBERG
*Aeronautical Research Laboratory, Wright-Patterson Air Force Base, Ohio*
(Received April 5, 1962)

After a general discussion of the problem of motion in the general theory of relativity a simple derivation of the law of motion is given for single poles of the gravitational field, which is based on a method originally developed by Mathisson. This law follows from the covariant conservation law for the matter energy-momentum tensor alone, without reference to any field equations, and takes the form of a geodesic of the (unknown) metric. Expanding this metric in terms of a power series in a parameter $\lambda$ and using the Minkowski proper time to parametrize the world lines of the particles, the (Lorentz-invariant) form of the approximate laws of motion follows. A method is developed to obtain the equations of motion (including the explicit form of the metric in terms of the particle variables) from Einstein's field equations. A systematic linearization procedure leads to a series of second-order differential equations for the metric; the $n$th order approximation of the equations of motion, as well as the explicit form of the matter tensor in $(n+1)$st order, is obtained as an integrability condition on the $(n+1)$st order opproximation for the metric. No coordinate conditions are required to obtain the general form of the equations of motion; they are needed only to reduce the approximation equations to wave equations and thus to allow their explicit integration in terms of retarded or symmetric potentials. In developing the approximation method it is shown that consistency requires that any set of approximate equations is solved "up to" rather than "in" $n$th order; this implies that the form of the lower-order metric be maintained, but with the motion corresponding to the $n$th order solutions rather than to lower order ones. In particular, the equations for the first-order metric imply zero-order equations of motion which restrict the particles to zero acceleration; the equations for the second-order metric imply first-order equation of motion involving the first-order metric, but without the previous restriction. In the retarded case the equations of motion contain retarded interactions and radiation reaction terms of the form familiar from electrodynamics; no such terms appear in the symmetric case. The equations of the symmetric case are derivable from a Fokker-type variational principle. The relation of the results obtained to work on Lorentz-invariant equations by other authors is discussed. In Appendix I a discussion of alternative derivations is presented; Appendix II contains remarks on Wheeler-Feynman type considerations for general relativistic equations of motion.

## I. INTRODUCTION

WITHIN the conceptual framework of Newtonian particle mechanics there is a sharp division between laws of motion and force laws. The laws of motion ($F=ma$) are assumed to be the same for all matter; the force laws (Newton's law of gravitation, Coulomb's law etc.) are different for different types of particles, their specific form to be determined by experiment.[1]

* Research supported in part by the National Science Foundation.

[1] In the following we shall call "laws of motion" the expressions relating the variation of some particle variables to the (unspeci-