much lesser extent for Lyman-β. For higher lines the broadening in the discharge will be very large because of the Stark effect. Accordingly only the first or the first two excited states are expected to be appreciably populated, which would correspond to exciting about 40 or 70% of the atoms in the ambient gas before the shock reaches the point of observation. This also explains why, e.g., no appreciable precursor radiation at H_β could be observed photoelectrically.

CONCLUSIONS

The experiments have shown that magnetically driven shock waves propagating into hydrogen or helium of about 1 mm Hg pressure encounter an ambient gas which is drastically influenced by the arc producing the shock wave. Consistency between spectroscopically measured temperatures and densities and those calculated from shock theory can be achieved if radiative energy transfer from the arc to the cold gas and magnetic fields produced by the arc in the cold gas are taken into account.

Certainly not only the conservation equations will be affected but also any relaxation phenonoma, which will be much less critical now than expected for a shock going into a gas at room temperature. While the influence of the radiative energy transfer on temperatures and densities will be less important for much faster shocks leading to temperatures in the million degree range it may still be of great value to overcome relaxation effects also in such experiments, and make possible the production of plasmas in LTE in magnetic shock tubes, expecially in the 1–10 mm Hg pressure and 1–10 ev temperature range, which is very important for the measurement of transition probabilities and damping constants of astrophysical interest.

PHYSICAL REVIEW VOLUME 120, NUMBER 4 NOVEMBER 15, 1960

Dielectric Formulation of Quantum Statistics of Interacting Particles*

F. Englert† and R. Brout
Laboratory of Atomic and Solid-State Physics and Department of Physics, Cornell University, Ithaca, New York

(Received February 25, 1960)

Formal relations between the free energy, the "dielectric constant" which expresses the response of the system to an external perturbation, and the two-particle Green's function in temperature space are derived. Connection with perturbation expansion for free energy and for general admittance tensors are established. These results are applied to a general discussion of the random-phase approximation at finite temperature and it is shown that the sum on ring diagrams corresponds to the calculation of the dielectric constant in the approximation of the neglect of local field corrections.

I. INTRODUCTION

THE purpose of this article is twofold. In the first sections we set forth some interesting general relations connecting the dielectric constant with the two-particle Green's function in temperature space and with the thermodynamic functions derived from quantum statistical mechanics. The reason for setting them out here is not only to make a convenient tabulation, but also to show how they may be put to use in approximate many-body theory, which brings us to the second purpose of this paper.

There are now several studies which exist on the generalization of the random-phase approximation (RPA) of the electron correlation problem to finite temperature. Since this theory gives the correct high-density limit at zero temperature and both correct high- and low-density behavior in the classical or high-temperature limit, such studies are very much in order. These theories have taken two forms: (a) an approximate evaluation of the partition function obtained by a selection of a special class of diagrams (called ring diagrams) in analogy to Gell-Mann and Brueckner[1] and Mayer[2]; (b) a dynamical model for the equation of motion of the one-particle density matrix in analogy to the theory of Sawada *et al.*[3] In this paper, we show directly the connection between these approaches through the abovementioned formal relations.

Section 2 recalls the definition of the dielectric functions and summarizes their formal properties, in particular the fluctuation-dissipation theorem. In Sec. 3, we express the free energy in terms of the dielectric constant. We show how to formulate RPA for the dielectric constant at finite temperature, in analogy to Nozières and Pines.[4] When this is substituted into the

* This work has been supported in part by the Office of Naval Research.

† On leave of absence from Université Libre de Bruxelles, Brussels, Belgium.

[1] M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957).

[2] J. E. Mayer, J. Chem. Phys. **18**, 1426 (1950).

[3] K. Sawada, Phys. Rev. **106**, 372 (1957); K. Sawada, K. A. Brueckner, W. Fukuda, and R. Brout, Phys. Rev. **108**, 507 (1957); R. Brout, Phys. Rev. **108**, 515 (1957).

[4] P. Nozières and D. Pines, Nuovo cimento **9**, 470 (1958).

formal relation for the free energy, one recovers the result obtained[5,6] by summation over ring diagrams.

In Sec. 4, we introduce the two-particle Green's function in temperature space and show how its Fourier decomposition gives rise to coefficients which are in fact the dielectric constant evaluated at various imaginary frequencies. The connection with perturbation theory is also established. Section 5 is devoted to a complete discussion of RPA.

II. THE DIELECTRIC FUNCTION

The Hamiltonian, which describes the system of N interacting particles enclosed in a box of volume V, is written in the form

$$H=H_0+\sum_{\mathbf{q}}\frac{v(q)}{2V}[\rho(\mathbf{q})\rho(-\mathbf{q})-N]. \tag{2.1}$$

H_0 contains the kinetic energy of the particles and eventually their potential energy in an external field; $v(q)$ and $\rho(\mathbf{q})$ are the Fourier transforms of the interaction potential $v(r)$ and of the density of particles $\rho(\mathbf{r})=\sum_{i=1}^{N}\delta(\mathbf{r}-\mathbf{r}_i)$ where r_i is the vector coordinate of the ith particle. It will be assumed that the system considered is invariant under translations and space reflection.

The dynamical dielectric function is defined by[7]

$$\Delta_{\mathbf{q}}(\omega;T)=1+[2v(q)/V]\prod{}_{\mathbf{q}}(\omega;T), \tag{2.2}$$

where $\prod_{\mathbf{q}}(\omega;T)$ is $iN/\hbar$ times the one-sided Fourier transform in $\mathbf{q}$ and ω of the Van Hove's pair correlation function.[8] We write

$$\prod{}_{\mathbf{q}}(\omega;T)=\int d^3\mathbf{q}\int dt\,\exp[i(\mathbf{q}\cdot\mathbf{r}-\omega t)]\times(i/h)NG(\mathbf{r},t;T)u_\epsilon(t), \tag{2.3}$$

where

$$\begin{aligned}u_\epsilon(t)&=e^{-\epsilon t}\quad t>0\quad \epsilon\to 0\\&=0\qquad t<0,\end{aligned} \tag{2.4}$$

and

$$G(\mathbf{r},t;T)=\frac{1}{N}\left\langle\int\rho(\mathbf{r}-\mathbf{r}';0)\rho(\mathbf{r}';t)d\mathbf{r}'\right\rangle. \tag{2.5}$$

$\rho(\mathbf{r}';t)$ is the density $\rho(\mathbf{r}')$ at time t in the Heisenberg representation and the symbol $\langle\ \rangle$ means that the average value of the operator is to be taken with respect to the canonical ensemble at temperature T.

The classical dielectric function, which is equal to the inverse dielectric constant and describes the response of the medium to an external field, is given by[7,9]

$$D_{\mathbf{q}}(\omega;T)=\frac{1}{\epsilon_{\mathbf{q}}(\omega;T)}=1+\frac{2v(q)}{V}P_{\mathbf{q}}(\omega;T), \tag{2.6}$$

$$P_q(\omega;T)=T^{\mathbf{q}}T^{\omega}(i/\hbar)N\,\mathrm{Im}G(\mathbf{r},t;T)u_\epsilon(t), \tag{2.7}$$

where the symbol "Im" means that the imaginary part of the function considered is to be taken. The explicit form of $\Delta_{\mathbf{q}}(\omega;T)$ and $D_{\mathbf{q}}(\omega;T)$ is

$$\Delta_{\mathbf{q}}(\omega;T)=1+\frac{2v(q)}{\hbar V}\sum_n p_m(T)\sum_n\frac{|\langle n|\rho(\mathbf{q})|m\rangle|^2}{\omega-\omega_{nm}-i\epsilon}, \tag{2.8}$$

$$D_q(\omega;T)=1+\frac{v(q)}{\hbar V}\sum_m p_m(T)\sum_n\frac{|\langle n|\rho(\mathbf{q})|m\rangle|^2}{\omega-\omega_{nm}-i\epsilon}+\frac{|\langle n|\rho(-\mathbf{q})|m\rangle|^2}{-\omega-\omega_{nm}+i\epsilon}, \tag{2.9}$$

where $p_m(T)$ is the statistical weight at temperature T for the normalized state $|m\rangle$ of energy E_m; $\omega_{nm}=(E_n-E_m)/\hbar$ and the summation is over all the eigenstates of H. In all expressions involving summations, as those that appear in (2.8) or (2.9), it has to be understood that one has first to transform the summation into an integration by allowing $V\to\infty$ and then only let $\epsilon\to 0$.

Equations (2.8) and (2.9) show that the dielectric functions are analytic functions of ω everywhere except on the real axis, where they have poles which in the limit $V\to\infty$ become lines of discontinuities (except for possible bound states). Therefore, these functions satisfy the Kramer-Kronig dispersion relation. In addition, we have the symmetry relation

$$D_{-\mathbf{q}}^*(-\omega;T)=D_{\mathbf{q}}(\omega;T), \tag{2.10}$$

and the thermodynamic relation

$$\mathrm{Im}D_{\mathbf{q}}(\omega;T)=\mathrm{Im}\Delta_{\mathbf{q}}(\omega;T)\tfrac{1}{2}[1-\exp(-h\omega/kT)], \tag{2.11}$$

which is obtained by rearranging the second term in the right-hand side of (2.9). It follows from the assumption of reflection invariance that $G(\mathbf{r},t;T)=G(-\mathbf{r},t;T)$ and thus $D_{\mathbf{q}}(\omega;T)=D_{-\mathbf{q}}(\omega;T)$. Thus (2.10) implies that the real part of $D_{\mathbf{q}}(\omega;T)$ is an even function of ω whereas the imaginary part is odd.

The asymptotic behavior of the dielectric functions for large ω is obtained by expanding (2.8) and (2.9) in powers of $1/\omega$; one can show easily that

$$\Delta_{\mathbf{q}}(\omega;T)=1+\frac{2v(q)}{V\hbar}\langle|\rho(\mathbf{q})|^2\rangle\frac{1}{\omega}+O\left(\frac{1}{\omega^2}\right), \tag{2.12}$$

and

$$D_{\mathbf{q}(\omega;T)}=1+\frac{v(q)}{V\hbar}\langle\{[\rho(-\mathbf{q}),H]\rho(\mathbf{q})\}\rangle\frac{1}{\omega^2}+O\left(\frac{1}{\omega^4}\right). \tag{2.13}$$

[5] D. J. Thouless, 1959 (to be published); H. deWitt, University of California Radiation Laboratory, 1959 (to be published).
[6] E. W. Montroll and J. C. Ward, Phys. Fluids 1, 55 (1958).
[7] F. Englert, J. Phys. Chem. Solids 11, 78 (1959).
[8] L. Van Hove, Phys. Rev. 95, 249 (1954).
[9] U. Fano, Phys. Rev. 103, 1202 (1956).

The double commutator in (2.13) can be evaluated in the usual way for obtaining sum rules[10] and one obtains with $\hbar\omega_{\mathbf{q}}=\hbar^2q^2/2m$

$$D_{\mathbf{q}}(\omega;T)=1+\frac{2v(q)}{\hbar}\frac{N}{V}\frac{\omega_q}{\omega^2}+O\left(\frac{1}{\omega^4}\right). \quad (2.14)$$

This expression is independent of the temperature and is thus identical with Nozières' and Pines' asymptotic expression[4] for the dielectric constant at $T=0$; in particular for Coulomb interaction one has $v(q)=4\pi e^2/q^2$ and

$$D_q(\omega;T)=1+\left(\frac{\omega_p}{\omega}\right)^2+O\left(\frac{1}{\omega^4}\right), \quad (2.15)$$

where $\omega_p{}^2=4\pi e^2N/mV$ is the plasma frequency.

We shall now relate $1/\epsilon_{\mathbf{q}}(\omega;T)$ to $\langle|\rho(q)|^2\rangle$; according to (2.8), we may write

$$\mathrm{Im}\Delta_{\mathbf{q}}(\omega;T)=\frac{2\pi i}{\hbar V}v(q)\sum_n p_m(T)$$
$$\times\sum_n \delta(\omega-\omega_{nm})|\langle n|\rho(\mathbf{q})|n\rangle|^2, \quad (2.16)$$

so that

$$\frac{h}{4\pi i}\int_{-\infty}^{+\infty}\mathrm{Im}\Delta_{\mathbf{q}}(\omega;T)d\omega=\frac{v(q)}{2V}\langle|\rho(\mathbf{q})|^2\rangle. \quad (2.17)$$

From (2.11) and from the fact that $\mathrm{Im}D_{\mathbf{q}}(\omega;T)=\mathrm{Im}[\epsilon_{\mathbf{q}}(\omega;T)]^{-1}$ is an odd function of ω, it follows from (2.17)

$$\frac{\hbar}{4\pi i}\int_{-\infty}^{+\infty}\coth\frac{h\omega}{2kT}\,\mathrm{Im}\frac{1}{\epsilon_{\mathbf{q}}(\omega;T)}d\omega=\frac{v(q)}{2V}\langle|\rho(\mathbf{q})|^2\rangle. \quad (2.18)$$

This expression generalizes Nozières-Pines' formula[4] to finite temperature; their result is obtained by taking the limit $T\rightarrow 0$ in (2.18). Equation (2.18) is a particular case of the general fluctuation-dissipation theorem.[11]

We shall now transform (2.18) to a form which will be useful for further investigation. Due to the nonsingular nature of the integrand at $\omega=0$, we may replace the integral by its principal value. Further, the asymptotic behavior (2.19) allows us to perform the integral on the contour in the complex plane indicated in Fig. 1, after a convenient subtraction for purposes of convergence.

$$\frac{\hbar}{8\pi i}\int_c \coth\frac{\hbar\omega}{2kT}\left[\frac{1}{\epsilon_{\mathbf{q}}(\omega;T)}-1\right]d\omega=\frac{v(q)}{2V}\langle|\rho(\mathbf{q})|^2\rangle. \quad (2.19)$$

Now, the analyticity of $[1/\epsilon_{\mathbf{q}}(\omega;T)]$ implies that the only singularities of the integrand in (2.19) within the domain limited by C are the poles on the imaginary

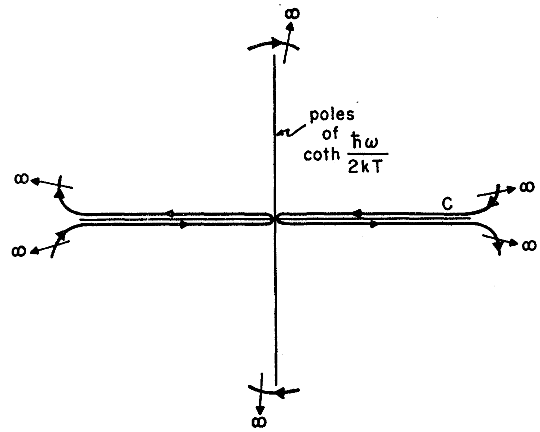

FIG. 1. Contour of integration for the evaluation of Eq. (2.19).

axis of $\coth(\hbar\omega/2kT)$; these occur at values $\omega_n=i\lambda_n$ such as

$$\lambda_n=(2\pi kT/\hbar)n, \quad (2.20)$$

where n is an integer, positive, negative or zero. Taking the residues at these poles, we find

$$\frac{kT}{2}\sum_{n=-\infty}^{+\infty}\left[1-\frac{1}{\epsilon_{\mathbf{q}}(i\lambda_n;T)}\right]=\frac{v(q)}{2V}\langle|\rho(\mathbf{q})|^2\rangle. \quad (2.21)$$

In the classical limit ($\hbar\rightarrow 0$), only the term $n=0$ contributes to (2.21) and the mean square fluctuation of the density is thus simply expressed in terms of the static dielectric constant,

$$\frac{kT}{2}\{1-[1/\epsilon_{\mathbf{q}}(0;T)]\}=\frac{v(q)}{2V}\langle|\rho(\mathbf{q})|^2\rangle. \quad (2.22)$$

The asymptotic formula (2.14) shows that the contribution from λ_n such that $\lambda_n{}^2\gg 2v(q)\omega_q(N/V)$ is small; in the case of Coulomb interaction this cutoff occurs when $\lambda_n\gg\omega_p$ or

$$n\gg\hbar\omega_p/2\pi kT, \quad (2.23)$$

where ω_p is the plasma frequency. The classical limit is therefore valid only if

$$2\pi kT\gg\hbar\omega_p. \quad (2.24)$$

The formula (2.22) shows also, that in the classical limit the $|\rho(\mathbf{q})|^2$ behave approximately like independent classical oscillators when $\epsilon_{\mathbf{q}}(0;T)\gg 1$, i.e., when the static polarizability is large at wave vector $\mathbf{q}$, a result to be expected on physical grounds.

III. FREE ENERGY

The free energy is given by the usual expression $F=-(1/\beta)\ln Z$, where $\beta=1/kT$ and Z is the partition function $Z=\sum_m e^{-\beta E_m}$. Introducing the coupling pa-

[10] D. Pines and P. Nozières, Phys. Rev. **109**, 741 (1958).
[11] L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon Press, Ltd., New York, 1958), p. 401.

rameter ξ, one may write

$$H(\xi)=H_0+\xi(H_{\rm int})=H_0+H_{\rm int}(\xi), \quad (3.1)$$

$$Z(\xi)=\mathrm{Tr}\exp\{-\beta[H_0+\xi H_{\rm int}]\}. \quad (3.2)$$

We then obtain

$$\frac{1}{Z(\xi)}\frac{dZ(\xi)}{d\xi}=-\beta\frac{\sum_m e^{-\beta E_m(\xi)}dE_m(\xi)/d\xi}{\sum_m e^{-\beta E_m(\xi)}}, \quad (3.3)$$

where

$$\frac{dE_m(\xi)}{d\xi}=\frac{1}{\xi}\langle m(\xi)|H_{\rm int}(\xi)|m(\xi)\rangle,$$

as a consequence of the stationary property of the expectation value of $H(\xi)$; integrating (3.3) we find

$$F(1)=F(0)+\int_0^1\frac{1}{\xi}\langle H_{\rm int}(\xi)\rangle_\xi, \quad (3.4)$$

where the average is taken at temperature T and coupling ξ.[12] For $\langle H_{\rm int}(\xi)\rangle_\xi$, one has

$$\langle H_{\rm int}(\xi)\rangle_\xi=\sum_{\mathbf{q}}\left[\xi\frac{v(q)}{2V}\langle|\rho(\mathbf{q})|^2\rangle_\xi-\xi\frac{v(q)}{2V}N\right]. \quad (3.5)$$

It then follows from (3.4), (3.5), (2.18), and (2.21) that the free energy may be expressed in terms of the dielectric constant at all coupling ξ in the two equivalent forms

$$F(1)=F(0)-\sum_{\mathbf{q}}\frac{v(q)}{2V}N+\sum_{\mathbf{q}}\frac{\hbar}{4\pi i}\int_{-\infty}^{+\infty}\coth\frac{\hbar\omega}{2kT}d\omega\times\int_0^1\frac{d\xi}{\xi}\,\mathrm{Im}\frac{1}{\epsilon_{\mathbf{q}}(\omega;T)_\xi}, \quad (3.6)$$

$$F(1)=F(0)-\sum_{\mathbf{q}}\frac{v(q)}{2V}N-\frac{1}{2\beta}\sum_{\mathbf{q}}\sum_{n=-\infty}^{+\infty}\int_0^1\left[\frac{1}{\epsilon_q(i\lambda_n,T)_\xi}-1\right]\frac{d\xi}{\xi}. \quad (3.7)$$

If the classical approximation is valid (see discussion in Sec. II) only the term $n=0$ contributes to the sum in (3.7).

Equation (3.6) or its equivalent (3.7) generalizes the Nozières-Pines formula relating the ground-state correlation energy to the imaginary part of the zero temperature dielectric constant. It may be looked upon as an alternative way of expressing the free energy in terms of the time-independent pair correlation function.

We now give an approximate evaluation of $(1/\epsilon)$ by first calculating its value by neglecting the interaction between particles. This is equivalent to a first-order approximation in ξ [as may be seen from (2.9)]. For simplicity of notation we assume that H_0 contains only the kinetic energy of the particles so that in a second quantization scheme $\rho(\mathbf{q})$ is the operator

$$\rho_{\mathbf{q}}=\sum_{\mathbf{k}}a_{\mathbf{k+q}}{}^\dagger a_{\mathbf{k}}, \quad (3.8)$$

where the summation includes spin states and the creation and annihilation operators $a_{\mathbf{k}}{}^\dagger$, $a_{\mathbf{k}}$ refer to a particle of wave vector $\mathbf{k}$ and energy $E_k=\hbar^2k^2/2m$. As the sum over n in (2.9) contains only one nonvanishing term for a given m, one may use the completeness relation $\sum_n|n\rangle\langle n|=1$ to obtain the first-order approximation,

$$\frac{1}{\epsilon_{\mathbf{q}}(\omega;T)}-1=\frac{v(q)}{V}\sum_{\mathbf{k}}\frac{\langle n_{\mathbf{k}}(1-n_{\mathbf{k+q}})\rangle_0}{\hbar\omega-(E_{\mathbf{k+q}}-E_{\mathbf{k}})-i\epsilon}+\frac{\langle n_k(1-n_{\mathbf{k+q}})\rangle_0}{-\hbar\omega-(E_{\mathbf{k+q}}-E_{\mathbf{k}})+i\epsilon}, \quad (3.9)$$

where $n_{\mathbf{k}}$ is the number operator $a_{\mathbf{k}}{}^\dagger a_{\mathbf{k}}$. Rearrangement of the second term in (3.9) by writing $\mathbf{k}'=\mathbf{k}-\mathbf{q}$ gives

$$\frac{1}{\epsilon_{\mathbf{q}}(\omega;T)}-1=-\frac{v(q)}{V}\sum_{\mathbf{k}}\frac{\langle n_{\mathbf{k}}\rangle_0-\langle n_{\mathbf{k+q}}\rangle_0}{-\hbar\omega+(E_{\mathbf{k+q}}-E_{\mathbf{k}})+i\epsilon}. \quad (3.10)$$

The right-hand side of (3.10) may be interpreted as a generalized temperature-dependent polarizability (13); we write then

$$4\pi\alpha_{\mathbf{q}}(\omega;T)=\frac{v(q)}{V}\sum_{\mathbf{k}}\frac{\langle n_{\mathbf{k}}\rangle_0-\langle n_{\mathbf{k+q}}\rangle_0}{-\hbar\omega+(E_{\mathbf{k+q}}-E_{\mathbf{k}})+i\epsilon}. \quad (3.11)$$

Comparing (3.10) and (2.21) we obtain the following sum rule

$$\sum_{n=-\infty}^{+\infty}4\pi\alpha_{\mathbf{q}}(i\lambda_n;T)=\beta\frac{v(q)}{V}\sum_{\mathbf{k}}\langle n_{\mathbf{k}}(1-n_{\mathbf{k+q}})\rangle_0. \quad (3.12)$$

In the classical limit this becomes simply

$$4\pi\alpha_{\mathbf{q}}(0;T)=\beta\frac{v(q)}{V}N, \quad (3.13)$$

which may be checked directly from (3.10). It is possible to use the approximation (3.10) to calculate (3.7). This leads of course to the first-order exchange energy. However, it is well known that neglecting local field corrections in the calculation of the dielectric constant is equivalent to writing[13] $\epsilon=1+4\pi\alpha$; so that we put

$$\epsilon_{\mathbf{q}}(\omega;T)=1+4\pi\alpha_{\mathbf{q}}(\omega;T), \quad (3.14)$$

where $4\pi\alpha_{\mathbf{q}}(\omega;T)$ is given by (3.11). Formula (3.14) is the same as that derived by Ehrenreich and Cohen[14] by the self-consistent field approach so that we have

[12] This formula may also be derived by using the cyclic invariance of the trace. See M. L. Goldberger and E. N. Adams, J. Chem. Phys. **20**, 240 (1952).

[13] For a detailed discussion of this point, see work cited in footnote 4.

[14] H. Ehrenreich and M. H. Cohen, Phys. Rev. **115**, 786 (1959).

shown the equivalence between this approach and the neglect of local field effects.

Using (3.14) we obtain by direct substitution in (3.7) and integration over the coupling constant

$$F(1)=F(0)-\sum_{\mathbf{q}}\frac{v(q)}{2V}N+\frac{1}{2\beta}\sum_{\mathbf{q}}\sum_{n=-\infty}^{+\infty}\ln|1+4\pi\alpha_{\mathbf{q}}(i\lambda_n;T)|. \quad (3.15)$$

This may be written in a slightly different way by using the sum rule (3.12)

$$F(1)=F(0)+\frac{1}{2\beta}\sum_{\mathbf{q}}\sum_{n=-\infty}^{+\infty}\ln|1+4\pi\alpha_{\mathbf{q}}(i\lambda_n;T)|-4\pi\alpha_{\mathbf{q}}(i\lambda_n;T)-\sum_{\mathbf{q}}\frac{v(q)}{2V}\sum_{\mathbf{k}}\langle n_{\mathbf{k}}n_{\mathbf{k+q}}\rangle_0. \quad (3.16)$$

This result is similar (except for the first order exchange term) to that obtained by Thouless[5] and Montroll and Ward[6] by perturbation theory, summing over ring diagrams.

We notice, however, that (3.16) has been established in the petit canonical ensemble and that these authors have evaluated the ring diagrams in the grand ensemble. This leads to the conclusion that in RPA the perturbed Fermi level should not be taken different from the unperturbed one in the evaluation of each term of the perturbation series. Indeed, one has the general thermodynamic relation

$$F=E-TS,\quad \Omega=E-TS-\mu N, \quad (3.18)$$

where $e^{-\beta\Omega(\mu,V,T)}$ is the grand partition function; by differentiation of (3.18), one has the well-known relation

$$\left(\frac{\partial\Omega(\mu,V,T)}{\partial T}\right)_{\mu,V}=\left(\frac{\partial F(N,V,T)}{\partial T}\right)_{N,V}=-S. \quad (3.19)$$

As comparison of (3.16) with previous work implies by (3.19) that $S(\mu,V,T)=S(\mu_0,V,T)$ in RPA, we are forced to put $\mu=\mu_0$ in this approximation. In another publication, it will be shown that this results directly from comparison between perturbation expansion of F and Ω, the essential feature being that in RPA the cluster expansion is the same in both grand and petit canonical ensembles.

The classical limit of (3.10) is immediately obtained with the help of (3.13)

$$F(1)=F(0)+\frac{1}{2\beta}\sum_{\mathbf{q}}\ln\left|1+\beta v(q)\frac{N}{V}\right|-\beta v(q)\frac{N}{V}, \quad (3.17)$$

which is the Debye-Hückel theory.

On the other hand, in the limit $T\rightarrow 0$ the sum over discrete indices $\sum_{n=-\infty}^{+\infty}$ is to be replaced by

$$\frac{h}{2\pi}\beta\int_{-\infty}^{+\infty}d\lambda,$$

and it is immediately verified by comparing with reference 3 that (3.16) goes into the Gell-Mann Brueckner formula for the ground state, including first-order exchange corrections.

IV. GREEN'S FUNCTION FORMALISM

We define a Green's Function very similar to that used by several authors[15]:

$$G_{\mathbf{q}}(\beta_2;\beta_1)=\langle\tau\rho_{\mathbf{q}}(\beta_2)\rho_{\mathbf{q}}^{\dagger}(\beta_1)\rangle \quad \begin{array}{l}\beta\geq\beta_1\geq 0\\ \beta\geq\beta_2\geq 0.\end{array} \quad (4.1)$$

$\beta=1/kT$ defines the temperature at which the average is taken, τ is the ordering operator which orders operators in a sequence such that operators labeled by $(\beta_j>\beta_i)$ always appear at the left of operators labeled by β_i. The $\rho_{\mathbf{q}}(\beta_2)$ and $\rho_{\mathbf{q}}^{\dagger}(\beta_1)$ are

$$\begin{aligned}\rho_{\mathbf{q}}(\beta_2)&=e^{\beta_2 H}\rho(\mathbf{q})e^{-\beta_2 H},\\ \rho_{\mathbf{q}}^{\dagger}(\beta_1)&=e^{\beta_1 H}\rho(-\mathbf{q})e^{-\beta_1 H}.\end{aligned} \quad (4.2)$$

The function $G_{\mathbf{q}}(\beta_2;\beta_1)$ has the following properties:

(A) $\quad G_{\mathbf{q}}(\beta_2;\beta_1)=G_q(\beta_2-\beta_1;0)=G_q(0;\beta_1-\beta_2). \quad (4.3)$

This is an immediate consequence of the cyclic invariance of the trace. We shall thus write the function $G_{\mathbf{q}}(\beta_2;\beta_1)=G_{\mathbf{q}}(\beta_2-\beta_1)=G_{\mathbf{q}}(\beta')$ where $+\beta\geq\beta'\geq-\beta$.

(B) $\quad G_q(\beta')=G_q^{*}(\beta'). \quad (4.4)$

For $\beta'>0$ we have

$$\begin{aligned}G_{\mathbf{q}}^{*}(\beta')&=(1/Z)[\mathrm{Tr}e^{-\beta H}e^{\beta' H}\rho(\mathbf{q})e^{-\beta' H}\rho(-\mathbf{q})]^{*}\\&=(1/Z)\,\mathrm{Tr}[\rho(\mathbf{q})e^{-\beta' H}\rho(-\mathbf{q})e^{\beta' H}e^{-\beta H}]\\&=G_{\mathbf{q}}(0;-\beta')=G_{\mathbf{q}}(\beta').\end{aligned}$$

The demonstration is the same for $\beta'<0$

(C) $\quad G_{\mathbf{q}}(\beta)=G_{\mathbf{q}}(-\beta)=G_{\mathbf{q}}(0). \quad (4.5)$

We have

$$\begin{aligned}G_{\mathbf{q}}(\beta)=\langle\rho_{\mathbf{q}}(\beta)\rho_{\mathbf{q}}^{*}(0)\rangle&=(1/Z)\,\mathrm{Tr}[e^{-\beta H}e^{\beta H}\rho(\mathbf{q})e^{-\beta H}\rho(\mathbf{q})]\\&=(1/Z)\,\mathrm{Tr}[e^{-\beta H}\rho(-\mathbf{q})\rho(\mathbf{q})]\\&=(1/Z)\,\mathrm{Tr}[e^{-\beta H}\rho(\mathbf{q})\rho(-q)]=G_{\mathbf{q}}(0).\end{aligned}$$

The same for $G_{\mathbf{q}}(-\beta)$.

(D) $$\begin{aligned}G_{\mathbf{q}}(\beta'-\beta)&=G_{\mathbf{q}}(\beta') \quad \beta>\beta'>0,\\ G_{\mathbf{q}}(\beta'+\beta)&=G_{\mathbf{q}}(\beta') \quad -\beta<\beta'<0.\end{aligned} \quad (4.6)$$

---

[15] T. Matsubara, Progr. Theoret. Phys. (Kyoto) **14**, 351 (1955); S. Fujita, Phys. Rev. **115**, 1335 (1959); P. C. Martin and J. Schwinger, Phys. Rev. **115**, 1342 (1959). Many other references on this subject and related topics may be found in this article.

The first identity follows from

$$\begin{aligned}G_{\mathbf{q}}(\beta'-\beta)&\\ &=\langle\rho_{\mathbf{q}}{}^*(0)\rho_{\mathbf{q}}(\beta'-\beta)\rangle\\ &=(1/Z)\,\mathrm{Tr}[e^{-\beta H}\rho(-\mathbf{q})e^{\beta' H}e^{-\beta H}\rho(\mathbf{q})e^{\beta' H}e^{\beta H}]\\ &=(1/Z)\,\mathrm{Tr}[e^{-\beta H}e^{\beta' H}\rho(\mathbf{q})e^{-\beta' H}\rho(-\mathbf{q})]=G_{\mathbf{q}}(\beta').\end{aligned}$$

The second identity follows in the same manner as a consequence of cyclic invariance and of the occurrence of the ordering symbol τ.

It follows from (B), (C), (D) that $G_{\mathbf{q}}(\beta')$ may be expressed on a Fourier series with real coefficients in the periodicity interval β; the development is valid in the interval $+\beta\geq\beta'\geq-\beta$. We thus write:

$$G_{\mathbf{q}}(\beta')=\sum_{j=-\infty}^{+\infty}G_{\mathbf{q}}(\lambda_j)e^{i\hbar\lambda_j\beta'},\tag{4.7}$$

where

$$\lambda_j=(2\pi/\hbar\beta)j.\tag{4.8}$$

j is any integer positive, negative or zero. We now evaluate

$$G_{\mathbf{q}}(\lambda_j)=\frac{1}{\beta}\int_0^\beta G_{\mathbf{q}}(\beta')e^{-i\hbar\lambda_j\beta'}d\beta',\tag{4.9}$$

or

$$G_{\mathbf{q}}(\lambda_j)=\frac{1}{\beta}\sum_m p_m(T)\sum_n\frac{\langle m|\rho(\mathbf{q})|n\rangle\langle n|\rho(-\mathbf{q})|m\rangle}{(-\hbar\omega_{nm}-i\hbar\lambda_j)}\times(e^{\beta\hbar\omega_{mn}}-1).\tag{4.10}$$

Using

$$p_m(T)=p_n(T)e^{\hbar\omega_{mn}\beta},\tag{4.11}$$

one may rearrange expression (4.10) to obtain

$$G_{\mathbf{q}}(\lambda_j)=-\frac{2}{\beta}\frac{1}{2\hbar}\sum_m p_m(T)\sum_n\frac{|\langle n|\rho(-\mathbf{q})|m\rangle|^2}{-i\lambda_j-\omega_{nm}}+\frac{|\langle n|\rho(\mathbf{q})|m\rangle|^2}{i\lambda_j-\omega_{nm}}.\tag{4.12}$$

Comparing this expression with (2.9) we see that

$$G_q(\beta')=\frac{V}{\beta v(q)}\sum_{j=-\infty}^{+\infty}\left[1-\frac{1}{\epsilon_q(i\lambda_j;T)}\right]e^{i\hbar\lambda_j\beta'}\qquad+\beta\geq\beta'\geq-\beta;\tag{4.13}$$

putting $\beta'=0$ in (4.13) we immediately obtain (2.23) from which (3.7) follows.

We can now express $G_{\mathbf{q}}(\beta')$ in terms of a power series of the interaction; in complete analogy with the usual field theoretic derivation,[16] we show easily that:

$$G_{\mathbf{q}}(\beta')=\frac{\mathrm{Tr}[e^{-\beta H_0}\tau U(\beta,0)\bar{\rho}_{\mathbf{q}}(\beta')\rho_{\mathbf{q}}{}^\dagger(0)]}{\mathrm{Tr}e^{-\beta H_0}U(\beta,0)},\tag{4.14}$$

where $\bar{\rho}_{\mathbf{q}}(\beta')$ is the value of $\rho(\mathbf{q})$ in the "interaction representation"

$$\bar{\rho}_{\mathbf{q}}(\beta')=e^{\beta_1 H_0}\rho(\mathbf{q})e^{-\beta_1 H_0},\tag{4.15}$$

and the "evolution operator" in β space is defined by

$$U(\beta_1,\beta_2)=e^{\beta_1 H_0}e^{-(\beta_1-\beta_2)H}e^{-\beta_2 H_0},\tag{4.16}$$

so that $U(\beta,0)$ is the analog of the S matrix. The perturbation expansion of (4.15) is

$$U(\beta_1,\beta_2)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_{\beta_2}^{\beta_1}\cdots\int_{\beta_2}^{\beta_1}d\beta_n'\cdots\times d\beta_1'\tau\{\bar{H}_{\mathrm{int}}(\beta_n')\cdots\bar{H}_{\mathrm{int}}(\beta_1')\},\tag{4.17}$$

and its substitution in (4.14) yields a perturbation expansion of $G_{\mathbf{q}}(\beta')$ and hence of the free energy. This expansion (which corresponds to the Bloch-De Dominicis[17] expansion in the grand ensemble) will be discussed in detail in a forthcoming paper. We notice that, if expressed in the grand ensemble (4.14) is the expression of a linked cluster expression which allows a perturbation calculation of the dielectric constant at imaginary frequencies $i\lambda$ and at temperature T. It may be supposed that it is possible, by analytic continuation to determine from $\epsilon_q(i\lambda;T)$ the complex dielectric constant at real frequency ω. In the next section such determination of the dielectric constant (and conductivity) at arbitrary temperature is given in RPA. In the Appendix it will be demonstrated that relation (4.13) relating the correlation function in β space to the dielectric constant is a particular case of a general relation valid for all admittance tensors.

We conclude this section by noting that the unperturbed Green's function, which will be useful for perturbation calculations, is obtained immediately from (3.10) so that

$$G_{\mathbf{q}}{}^0(\beta')=\langle\tau\bar{\rho}_{\mathbf{q}}(\beta')\bar{\rho}_{\mathbf{q}}{}^\dagger(0)\rangle_0=\frac{V}{\beta v(q)}\sum_{j=-\infty}^{+\infty}4\pi\alpha_{\mathbf{q}}(i\lambda_j;T)e^{i\hbar\lambda_j\beta'}\qquad+\beta\geq\beta'\geq-\beta.\tag{4.18}$$

V. THE RANDOM-PHASE APPROXIMATION

It has been established in Sec. III that evaluation of the free energy with help of the dielectric constant (3.14) is equivalent to a formal summation over ring diagrams as obtained by Thouless[5] and Montroll and Ward.[6] We shall now show that such a selection of diagrams is equivalent to a very simple dynamical condition, namely,

$$[\bar{\rho}_{\mathbf{q}}(\beta),\bar{\rho}_{\mathbf{q}'}{}^\dagger(\beta')]=0,\tag{5.1}$$

which is the random-phase approximation. The proof of (5.1) is obtained directly from evaluation of ring diagrams. Condition (5.1) will then be utilized to evaluate by perturbation theory the dielectric function,

[16] S. S. Schweber, H. A. Bethe, and F. de Hoffmann, *Mesons and Fields* (Row, Peterson and Company, Evanston, Illinois, 1955), Vol. 1, p. 384.

[17] C. Bloch and C. De Dominicis, Nuclear Phys. **7**, 459 (1958).

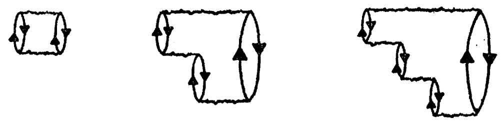

FIG. 2. Sample ring diagrams in RPA.

yielding a result identical to (3.14). This then completes the analysis of RPA in its various forms and interconnections which may be set forth schematically in a logical triangle.

summation over ring diagrams

$\nearrow\swarrow$ $\searrow\nwarrow$

self-consistent field approach or neglect of local field corrections. $\rightarrow$ $\leftarrow$ RPA in form (5.1)

The free energy Ω (or F) may be put in the following form easily accessible to perturbation expansion

$$\ln\frac{\operatorname{Tr} e^{-\beta H_0'}\tau \exp\left[-\int_0^\beta d\beta' \bar{H}_{\rm int}(\beta')\right]}{\operatorname{Tr} e^{-\beta H_0'}} \equiv \ln\left\langle \tau \exp\left[-\int_0^\beta d\beta' \bar{H}_{\rm int}(\beta')\right]\right\rangle_0, \quad (5.2)$$

where

$$H_0' = H_0 - \mu N \text{ (or } H_0).$$

Among the diagrams that appear in this expansion, are the ring diagrams.[18] We use the notation of Goldstone[19]; a line going up is a "particle" line and carries with it a factor $\langle 1-n_{\mathbf{p}}\rangle_0$ and a line going down is a "hole," carrying with it a factor of $\langle n_{\mathbf{p}}\rangle_0$. In Fig. 2, we give the first few cycle graphs. These cycles appear in all orders, i.e., in nth order the cycles involving the particle lines $\mathbf{p}_1, \mathbf{p}_2\cdots\mathbf{p}_n$ are arranged in their $(n-1)!$ different orders in time. Further, it is evident from their structure that if a given ring in nth order starts with an interaction that the same value of $\mathbf{q}$ characterizes each and every interaction, by conservation of momentum. In this way it is seen that all ring diagrams of nth order are contained in the expression:

$$\left[\frac{v(q)}{V}\right]^n \int_0^\beta \cdots \int_0^\beta d\beta_n \cdots \times d\beta_1 \langle \tau \bar{\rho}_{\mathbf{q}}^\dagger(\beta_n)\bar{\rho}_{\mathbf{q}}(\beta_n)\cdots\bar{\rho}_{\mathbf{q}}^\dagger(\beta_1)\bar{\rho}_{q}(\beta_1)\rangle_0, \quad (5.3)$$

since the various contractions (mean value of the $\rho_{\mathbf{q}}$ with $\rho_{\mathbf{q}}^\dagger$) give all the possible orderings of the graphs. Finally, resummation over n and final summation over $\mathbf{q}$ gives instead of (5.2)

$$\tfrac{1}{2}\sum_q \ln\left\langle \tau \exp\left[-\int_0^\beta \frac{v(q)}{V}\bar{\rho}_{\mathbf{q}}^\dagger(\beta)\bar{\rho}_{\mathbf{q}}(\beta)\right]\right\rangle_0, \quad (5.4)$$

where the first-order exchange energy is also included. The appearance of the factor $\frac{1}{2}$ comes about because in the restriction to ring diagrams q and $-q$ must be taken together. The result is a sum on $q>0$ which restriction is then removed by summing on all q with a factor of $\frac{1}{2}$. Finally, we remark that since $H_{\rm int}=\sum_{\mathbf{q}} = \sum_{\mathbf{q}} v(q)/2V[|\rho(\mathbf{q})|^2 - N]$, the same result could have been obtained directly from (5.2) under the simple assumption of commutation (5.1) since in this case the exponential factorizes automatically. It is thus the essential nature of the ring diagram approximation to select only those terms which are correctly evaluated under (5.1).

Dielectric Constant

We divide both numerator and denominator of (4.14) by $\operatorname{Tr}[e^{-\beta H_0}]$ and we simplify the resulting expression by using (5.1) to obtain:

$$G_{\mathbf{q}}(\beta_1) = \frac{\displaystyle\sum_{n=0}^\infty (-1)^n \frac{1}{n!}\left(\frac{v(q)}{V}\right)^n \left\langle \tau \int_0^\beta \cdots \int^\beta d\beta_{n+1}\cdots d\beta_2 \bar{\rho}_{\mathbf{q}}^\dagger(\beta_{n+1})\cdots\bar{\rho}_{\mathbf{q}}(\beta_1)\bar{\rho}_{\mathbf{q}}^\dagger(0)\right\rangle_0}{\displaystyle\sum_{n=0}^\infty (-1)^n \frac{1}{n!}\left(\frac{v(q)}{V}\right)^n \left\langle \tau \int_0^\beta \cdots \int_0^\beta d\beta_{n+1}\cdots d\beta_2 \bar{\rho}_{\mathbf{q}}^\dagger(\beta_{n+1})\cdots\bar{\rho}_{\mathbf{q}}(\beta_2)\right\rangle_0},$$

where we recall that $\langle\ \rangle_0$ is the average in the petit canonical ensemble. We thus may write, in analogy with field theory,

$$G_{\mathbf{q}}(\beta_1) = \sum_{n=0}^\infty (-1)^n \frac{1}{n!}\left(\frac{v(q)}{V}\right)^n \left\langle \tau \int_0^\beta \cdots \int_0^\beta d\beta_{n+1}\cdots \times d\beta_2 \bar{\rho}_{\mathbf{q}}^\dagger(\beta_{n+1})\cdots\rho_{\mathbf{q}}(0)\right\rangle_{0;L},$$

where the symbol L means restriction to linked graphs, or, equivalently, to contraction between $\bar{\rho}_{\mathbf{q}}(\beta')$ taken at different β'. Now the contraction between the ordered operators $\bar{\rho}_{\mathbf{q}}(\beta_1)$ and $\bar{\rho}_q^\dagger(\beta_2)$ which we denote by $\{\rho_q(\beta_1)\rho_q^\dagger(\beta_2)\}$ is (taking into account the time ordering),

$$\{\rho_{\mathbf{q}}(\beta_1)\rho_q^\dagger(\beta_2)\} = G_q^0(\beta_1-\beta_2), \quad (5.7)$$

where the interval of definition of the unperturbed $G_q^0(\beta_1-\beta_2)$ coincides with the integration interval in (5.6). We may then write, taking a particular set of

[18] For a discussion of the importance of these diagrams see Gell-Mann and Brueckner (reference 1), and R. Brout, Phys. Rev. **118**, 1009 (1960).

[19] J. Goldstone, Proc. Roy. Soc. (London) **A239**, 267 (1957).

the $n!$ equivalent set of contractions,

$$G_{\mathbf{q}}(\beta_1)=\sum_{n=0}^{\infty}(-1)^n\left(\frac{v(q)}{V}\right)^n\int^{\beta}\cdots\int_0^{\beta}d\beta_{n+1}\cdots$$
$$\times d\beta_2 G_{\mathbf{q}}{}^0(\beta_{n+1}-\beta_n)G_{\mathbf{q}}{}^0(\beta_n-\beta_{n-1})\cdots$$
$$\times G_{\mathbf{q}}{}^0(\beta_3-\beta_2)G_{\mathbf{q}}{}^0(\beta_2-\beta_1)G_{\mathbf{q}}{}^0(\beta_1-\beta_{n+1}). \quad (5.8)$$

Using the Fourier expansion (4.18), we have

$$\int_0^{\beta}G_{\mathbf{q}}{}^0(\beta_j-\beta_{j-1})G_{\mathbf{q}}{}^0(\beta_{j-1}-\beta_{j-2})d\beta_{j-1}$$
$$=\beta\left(\frac{V}{\beta v(q)}\right)^2\sum_{k=-\infty}^{+\infty}[4\pi\alpha_{\mathbf{q}}(i\lambda_k;T)]^2$$
$$\times\exp[i\hbar\lambda_k(\beta_j-\beta_{j-2})] \quad (5.9)$$

so that (5.8) may be written as

$$G_{\mathbf{q}}(\beta_1)=\sum_{k=-\infty}^{+\infty}\frac{V}{\beta v(q)}4\pi\alpha_{\mathbf{q}}(i\lambda_k;T)$$
$$\times\sum_{n=0}^{\infty}[-4\pi\alpha_{\mathbf{q}}(i\lambda_k;T)]^n\exp(i\hbar\lambda_k\beta_1), \quad (5.10)$$

which is formally summed to yield

$$G_{\mathbf{q}}(\beta_1)=\frac{V}{\beta v(q)}\sum_{k=-\infty}^{+\infty}\frac{4\pi\alpha_{\mathbf{q}}(i\lambda_k;T)}{1+4\pi\alpha_{\mathbf{q}}(i\lambda_k;T)}e^{i\hbar\lambda_k\beta_1}. \quad (5.11)$$

Comparison of (5.11) and (4.13) shows immediately that in RPA

$$\epsilon_{\mathbf{q}}(i\lambda_k;T)=1+4\pi\alpha_{\mathbf{q}}(i\lambda_k;T), \quad (5.12)$$

from which formula (3.14) is immediately obtained by analytic continuation, closing the proof of equivalence. We may notice that the method used here may be applied directly to the evaluation of the partition function, (5.4) resulting in formula (3.16).

Finally, it should be pointed out that calculations may be facilitated by converting summations into integrations through (3.6) and (3.7). The important point is $\epsilon_{\mathbf{q}}$ is given by (5.12) all over the complex plane.

Note added in proof. It has been pointed out by Dr. D. S. DuBois that he has used procedures similar to those in this paper for the 0 temperature electron gas [D. S. DuBois, Ann. phys. **8**, 24 (1959)].

APPENDIX

Relation (4.13) may be generalized to all admittance tensors in the following manner. The response of $V_p{}^\dagger$ to an external force to V_q is described by the admittance tensor[20]

$$f_{qp}(\omega;T)=\lim_{\epsilon\to+0}\frac{1}{i\hbar}\int_0^{\infty}e^{-(i\omega+\epsilon)t}\langle[V_q(0)V_p{}^\dagger(t)]\rangle, \quad (A.1)$$

or after explicit evaluation

$$f_{qp}(\omega;T)=\frac{1}{h}\sum_m p_m(T)\sum_n\left[\frac{\langle m|V_q|n\rangle\langle n|V_p{}^\dagger|m\rangle}{\omega_{nm}-\omega+i\epsilon}+\frac{\langle m|V_p{}^\dagger|n\rangle\langle n|V_q|m\rangle}{\omega_{nm}+\omega-i\epsilon}\right]. \quad (A.2)$$

Repeating the argument leading to (4.13), one finds easily in the interval $\beta>\beta'>0$

$$\langle V_p!(\beta')V_q(0)\rangle=\sum_{k=-\infty}^{+\infty}f_{qp}(i\omega_k;T)e^{-i\hbar\omega_k\beta'}. \quad (A.3)$$

[20] R. Kubo, J. Phys. Soc. Japan **12**, 570 (1957).