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Statistical mechanics of the nonrelativistic Zachariasen model

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The statistical mechanics of the nonrelativistic Zachariasen model is studied for the purpose of clarifying a mechanism proposed some years ago by Omnès to effect a phase transition in hot, dense matter with zero net baryon number from a homogeneous thermodynamic state to one with local inhomogenities in the baryon number density. The model contains B and $\bar{B}$ particles, which play the role of baryons and antibaryons, respectively, and A particles, which play the role of mesons. The A particles are coupled in the Hamiltonian to $B\bar{B}$ pairs through *virtual* annihilation and creation. The Helmholtz free energy is calculated in a virial expansion for the cases in which *real* $B\bar{B}$ pair annihilation and creation is (1) important enough to achieve full thermodynamic equilibrium, and (2) unimportant enough so that over an appropriate time scale the A particles and $B\bar{B}$ pairs are independent of one another. To analyze case (2) a unitary transformation is made on the original Hamiltonian which completely renormalizes the A-particle rest energy and transforms the original interaction into an infinite sum of potentials that act within groups containing increasing numbers of particles. We then study case (2) by dropping potentials that involve *real* creation and annihilation. Within the context of the virial expansion we conclude that no Omnès transition occurs for case (1), while such a transition is possible for case (2).

I. INTRODUCTION

Several years ago Omnès[1,2] proposed a cosmology with the attractive feature that there is macroscopic symmetry between matter and antimatter, i.e., the universe as a whole contains equal amounts of matter and antimatter. The present universe is assumed to have evolved from a singularity in a manner analogous to the usual asymmetric "big bang" cosmology, although the details of the expansion entail new physical considerations due to the presence of both matter and antimatter. In the early ($t < 10^{-5}$ sec) stage of expansion, matter (including leptons and hadrons) and antimatter (including antileptons and antihadrons) will be in equilibrium with radiation. Specifically, the excess of baryons over antibaryons in a macroscopic but small region will vanish. The difficulty with such a model is that as the universe expands, the matter and antimatter annihilate with such great efficiency that the present observed matter density of the universe could not have survived.[3,4] Omnès has suggested the possibility that the statistical mechanics of strongly interacting particles presents a mechanism by which matter and antimatter effectively repel each other at short distances. At a sufficiently high temperature this repulsion then leads to a phase separation of the matter from the antimatter which, according to Omnès,[2,5] can be amplified by coalescence during later stages of expansion. In this way the evolved universe consists of islands (of galactic size or larger) of matter and similar islands of antimatter. Such a cosmology, while extremely interesting and appealing, has been criticized[6] for reasons which involve the post-separation aspects of the theory.

The essential point of the separation mechanism proposed by Omnès is that mesons are bound states of baryon-antibaryon systems. A virial expansion of the Helmholtz free energy then involves a term related to the baryon-antibaryon interaction which, according to the Beth-Uhlenbeck formula, consists of two parts: (1) a bound-state contribution related to mesons and (2) a continuum contribution related to scattering in the appropriate baryon-antibaryon channel. Omnès hypothesizes that the bound states enter into the Helmholtz free energy as an independent entity and that the free-nu-

cleon–free-antinucleon part of the Helmholtz free energy involves the strong interactions only through the continuum contribution (2) referred to above. The justification for this hypothesis is founded in the work of Dashen, Ma, and Bernstein[7] (DMB) on the S-matrix formulation of statistical mechanics. In point of fact, the DMB work refers to the structure of the thermodynamic potential in which the system's volume, temperature, and certain chemical potentials are the appropriate thermodynamic variables. For the discussion of the possibility of a phase transition, the Helmholtz free energy is more useful and, although not stated so explicitly, this is the reason for Omnès's emphasis on the Helmholtz free energy. Omnès shows that the retained continuum part of the baryon-antibaryon virial coefficient has, due to Levinson's theorem,[8] the same sign as would be produced by a repulsive interaction. Subsequent analysis then suggests that the minimum of the modified Helmholtz free energy will occur for local (but macroscopic) inhomogeneities in baryon number. One difficulty with the Omnès hypothesis concerning the nature of the Helmholtz free energy is that it is never clearly spelled out how this free energy is extracted from the underlying thermodynamic potential which is the basis of the DMB work.

The purpose of the present work is to examine systematically the role of bound states in statistical mechanics within the context of a well-defined model field theory which contains those ingredients of the physical world which seem essential to the Omnès theory: baryons, antibaryons, and mesons which are in some general sense bound states of baryon-antibaryon pairs. The model is referred to as the nonrelativistic Zachariasen model because of its similarity to a relativistic model proposed some years ago by Zachariasen[9] as an example of a soluble relativistic field theory. Unlike the present model, however, the original Zachariasen model did not possess a canonical formalism and was described in terms of dispersion relations. In Sec. II we introduce the model and determine some of the low-lying states. In Sec. III we determine the thermodynamic potential and subsequently the Helmholtz free energy (which is more useful for the discussion of phase transitions) under the assumption of *complete* thermodynamic equilibrium consistent with the totality of quantities that are additively conserved with respect to the model Hamiltonian. In this case it is found that the Helmholtz free energy, which is a function of the system volume, temperature, and eigenvalues of the conserved quantities referred to above, does not suggest the possibility of an Omnès transition. In Sec. IV a unitary transformation is performed on the model Hamiltonian which separates real from virtual pair creation and annihilation effects. The transformed Hamiltonian contains a modified kinetic energy with renormalized A-particle rest energy and a modified interaction part made up of an infinite number of "potentials." Of particular importance is the appearance of a repulsive $B\bar{B}$ interaction in the form of a finite sum of separable potentials and a dissociation potential which couples $B\bar{B}$ pairs to the renormalized A particle through real $B\bar{B}$-pair production and annihilation. When the dissociation part of the transformed Hamiltonian is neglected, the resulting reduced Hamiltonian possesses an additional constant of the motion. The Helmholtz free energy for this reduced Hamiltonian then has a negative second virial coefficient (related to the $B\bar{B}$ interaction) as is necessary for the Omnès transition. In this simple model the reduced Hamiltonian is unable, however, to give adequate $B\bar{B}$ repulsion to satisfy the necessary condition for the Omnès transition. In an appendix we give the generalization of the model to include internal degrees of freedom for the various particles. The reduced Hamiltonian for this generalized model then contains sufficient repulsion to give the Omnès transition. A summary of the present analysis is given in Sec. V.

II. THE NONRELATIVISTIC ZACHARIASEN MODEL

The nonrelativistic Zachariasen model is defined by the Hamiltonian $H = H_0 + H_1$, where

$$H_0 = \sum_p (a_p^\dagger a_p \omega_p^0 + b_p^\dagger b_p E_p + \bar{b}_p^\dagger \bar{b}_p E_p) \tag{2.1}$$

and

$$H_1 = \frac{g}{V^{1/2}} \sum_{p\,q} F_q (a_p b_{p/2-q}^\dagger \bar{b}_{p/2-q}^\dagger + a_p^\dagger b_{p/2-q} \bar{b}_{p/2-q}), \tag{2.2}$$

where V is the volume of the system. In Eqs. (2.1) and (2.2) a_p, b_p, and $\bar{b}_p$ are the destruction operators for the relevant species, which for simplicity we take as spinless bosons since the type of quantum statistics plays no essential role in the ensuing theory. In Eq. (2.1) the single-particle energies are taken as quadratic in momentum, with

$$\omega_p^0 = W_A^0 + \frac{p^2}{4M}, \quad E_p = W_B + \frac{p^2}{2M}, \tag{2.3}$$

while in Eq. (2.2) the quantity g is a coupling constant which sets the strength of the basic interaction and F_q is an arbitrary form factor which equals unity for $q = 0$ and vanishes sufficiently rapidly for $q \to \infty$. The model described by the above Hamiltonian is actually a variant of the (nonrelativistic) Lee model in which all recoil effects are

included. Since the A-particle's inertial mass is twice that of a B or $\bar{B}$, inertial mass is conserved in the elementary virtual transformation described by H_1,

$$B+\bar{B} \rightleftharpoons A, \tag{2.4}$$

and the interaction H_1 will modify the A-particle energy-momentum relation ω_p^0 simply by renormalizing the rest energy W_A^0. The B and $\bar{B}$ rest energies, on the other hand, are not renormalized by the interaction. In the following we will assume that the coupling constant g and the unrenormalized rest energy W_A^0 are such that the renormalized rest energy $W_A < 2W_B$. This constraint will ensure that the renormalized A particle is stable. A sufficient (but not necessary) condition for this constraint to hold is that $W_A^0 < 2W_B$ since the interaction lowers the rest energy. It should be noted that the model is not to be thought of as a low-velocity limit of a relativistic model since in that case $W_A^0 = 2Mc^2$ and $W_B = Mc^2$. Since we want to examine the case in which both g and W_A^0 become infinite (for fixed W_A and W_B) we purposely retain more flexibility in the choice for the bare A-particle rest energy.

The Hamiltonian in Eqs. (2.1) and (2.2) has the property that it is left invariant under the interchange of b_p and $\bar{b}_p$. We shall refer to this exchange invariance as "charge conjugation" symmetry. Formally, we can construct a charge-conjugation operator C which has the property that

$$Cb_pC^{-1} = \bar{b}_p, \quad C\bar{b}_pC^{-1} = b_p \tag{2.5}$$

and which commutes with the Hamiltonian. We further note that there are two additional constants of the motion given by

$$\nu_+ = N + \bar{N} + 2N_A, \quad \nu_- = N - \bar{N}, \tag{2.6}$$

where $N = \sum_p b_p^\dagger b_p$, $\bar{N} = \sum_p \bar{b}_p^\dagger \bar{b}_p$, and $N_A = \sum_p a_p^\dagger a_p$. We will sometimes refer to ν_- as the baryon number operator. It is also useful to consider linear combinations of these two constants of the motion in the form of

$$\begin{aligned} \nu &\equiv \tfrac{1}{2}(\nu_+ + \nu_-) = N + N_A, \\ \bar{\nu} &\equiv \tfrac{1}{2}(\nu_+ - \nu_-) = \bar{N} + N_A. \end{aligned} \tag{2.7}$$

We now determine some of the eigenstates of H with low values of the eigenvalues of ν and $\bar{\nu}$.

(i) States of $\nu = 0$, $\bar{\nu} = 0$. There is only one such state, which is the bare vacuum with

$$H|0\rangle = 0|0\rangle. \tag{2.8}$$

(ii) States of $\nu = 1$, $\bar{\nu} = 0$. These are bare single B-particle states with

$$Hb_p^\dagger|0\rangle = E_p b_p^\dagger|0\rangle. \tag{2.9}$$

(iii) States of $\nu = 0$, $\bar{\nu} = 1$. These states are bare single $\bar{B}$-particle states with

$$H\bar{b}_p^\dagger|0\rangle = E_p \bar{b}_p^\dagger|0\rangle. \tag{2.10}$$

(iv) States of $\nu = 1$, $\bar{\nu} = 1$ $(E < 2W_B + p^2/4M)$. For a given total momentum $\vec{p}$ there is one such state, which can be written as a linear combination of a bare A state and a bare $B\bar{B}$-pair state:

$$|\Phi_p\rangle = \sum_q \phi_q b_{p/2+q}^\dagger \bar{b}_{p/2-q}^\dagger|0\rangle + Z^{1/2}a_p^\dagger|0\rangle. \tag{2.11}$$

It then follows from the Schrödinger equation $H|\Phi_p\rangle = E|\Phi_p\rangle$ that

$$\begin{aligned} &\phi_q(2W_B + p^2/4M + q^2/M - E) + Z^{1/2}\frac{g}{V^{1/2}}F_q = 0, \\ &\frac{g}{V^{1/2}}\sum_k F_k\phi_k + (\omega_p^0 - E)Z^{1/2} = 0, \end{aligned} \tag{2.12}$$

from which we obtain in the infinite-volume limit (with units in which $\hbar = 1$)

$$\begin{aligned} E &= \omega_p = W_A + p^2/4M, \\ W_A &= W_A^0 + g^2\int \frac{d^3q}{(2\pi)^3}\frac{F_q^2}{W_A - 2W_B - q^2/M}. \end{aligned} \tag{2.13}$$

We note that as previously stated we assume g and W_A^0 are such that $W_A < 2W_B$. Hence, the integral in Eq. (2.13) is negative, and we conclude $W_A < W_A^0$; the interaction lowers the rest energy of the bare A particle. The normalized eigenstate components for the value of E given in Eq. (2.13) can be determined from Eq. (2.12) together with the normalization condition $Z + \sum_q \phi_q^2 = 1$ to give

$$Z^{-1} = 1 + g^2\int \frac{d^3q}{(2\pi)^3}\frac{F_q^2}{(W_A - 2W_B - q^2/M)^2}$$

and (2.14)

$$\phi_q = g\left(\frac{Z}{V}\right)^{1/2}F_q(W_A - 2W_B - q^2/M)^{-1}.$$

(v) States of $\nu = 1$, $\bar{\nu} = 1$ $(E > 2W_B + p^2/4M)$. These states are scattering states and rather than follow the analysis that was carried out for $E < 2W_B + p^2/4M$, it is more instructive to deal directly with the scattering T matrix which satisfies the Lippmann-Schwinger equation

$$T(E) = H_1 + H_1\frac{1}{E + i\eta - H_0}T(E), \quad \eta \to 0^+. \tag{2.15}$$

By iterating Eq. (2.15) once and then taking matrix elements between plane-wave $B\bar{B}$-pair states, we obtain

$$\begin{aligned} T_{q',q}(p,E) = {} & \frac{g^2}{V}\frac{F_qF_{q'}}{E + i\eta - \omega_p^0} \\ & + \frac{g^2}{V}\frac{F_{q'}}{E + i\eta - \omega_p^0} \\ & \times\sum_k \frac{F_kT_{kq}(p,E)}{E + i\eta - 2W_B - p^2/4M - k^2/M}, \end{aligned} \tag{2.16}$$

where

$$T_{q',q}(p,E) = \langle 0|b_{p/2+q'}\bar{b}_{p/2-q'}T(E)b_{p/2+q}^\dagger\bar{b}_{p/2-q}^\dagger|0\rangle. \tag{2.17}$$

Equation (2.16) can be readily solved to obtain

$$T_{q'q}(p,E)=\frac{g^2F_qF_{q'}/V}{E+i\eta-\omega_p^0-g^2\int\frac{d^3k}{(2\pi)^3}\frac{F_k^{\,2}}{E+i\eta-2W_B-p^2/4M-k^2/M}}, \tag{2.18}$$

which possesses a pole at $E=\omega_p$, where ω_p is defined in Eq. (2.13). It will be convenient for future purposes to rewrite Eq. (2.18) in terms of the renormalized rest energy W_A rather than the bare rest energy W_A^0. From Eq. (2.13) we then obtain

$$T_{q'q}(p,E)=\frac{g^2F_{q'}F_q/V}{(E+i\eta-\omega_p)\left(1+g^2\int\frac{d^3k}{(2\pi)^3}\frac{F_k^{\,2}}{(W_A-2W_B-k^2/M)}\frac{1}{(E+i\eta-2W_B-p^2/4M-k^2/M)}\right)}. \tag{2.19}$$

When the T-matrix element $T_{q'q}(p,E)$ is put completely on-shell, with $q=q'$ and $E=2W_B+p^2/4M+q^2/M$, we obtain the scattering phase shift (S wave only in the present case) from the correspondence

$$T(q)\equiv T_{qq}(p,2W_B+p^2/4M+q^2/M)=-\frac{4\pi}{VMq}e^{i\delta(q)}\sin\delta(q), \tag{2.20}$$

from which we deduce

$$\tan\delta(q)=\frac{Mg^2}{4\pi}\frac{qF_q^{\,2}}{W_A-2W_B-q^2/M}D^{-1}(q), \tag{2.21}$$

$$D(q)=1+g^2\int\frac{d^3k}{(2\pi)^3}\frac{F_k^{\,2}M}{(W_A-2W_B-k^2/M)(q^2-k^2)},$$

where the slash on the integral sign indicates that a principal value is to be taken.

Of particular interest is the case in which $g^2\to\infty$ for fixed W_A. This limit implies, of course, that

$$W_A^0=W_A-g^2\int\frac{d^3q}{(2\pi)^3}\frac{F_q^{\,2}}{W_A-2W_B-q^2/M} \tag{2.22}$$

also approaches $+\infty$. In this limit we obtain from Eq. (2.19) the T-matrix element

$$T_{q'q}(p,E)\to\frac{1}{V}\frac{F_qF_{q'}}{(E+i\eta-\omega_p)}\left[\int\frac{d^3k}{(2\pi)^3}\frac{F_k^{\,2}}{(W_A-2W_B-k^2/M)(E+i\eta-2W_B-p^2/4M-k^2/M)}\right]^{-1} \tag{2.23}$$

and from Eq. (2.21) the scattering phase shift

$$\tan\delta(q)\to\frac{q}{4\pi}\frac{F_q^{\,2}}{(W_A-2W_B-q^2/M)}\left[\int\frac{d^3k}{(2\pi)^3}\frac{F_k^{\,2}}{(W_A-2W_B-k^2/M)(q^2-k^2)}\right]^{-1}. \tag{2.24}$$

It is of interest to note that such a T matrix and phase shift would result from an attractive separable potential

$$V_{q'q}=-\lambda F_qF_{q'}/V, \tag{2.25}$$

where the potential strength λ is given by

$$\lambda^{-1}=\int\frac{d^3k}{(2\pi)^3}\frac{F_k^{\,2}}{2W_B+k^2/M-W_A}. \tag{2.26}$$

Thus, in the limit of infinite coupling constant (fixed W_A) the Zachariasen model is equivalent to an attractive separable $B\bar{B}$-potential model in which the renormalized A particle appears as a bound state of the attractive potential. In field-theoretic language this composite nature of the A particle is signaled by the vanishing of the quantity Z given in Eq. (2.14), which is the probability of finding a bare A particle in the renormalized A particle. Finally, the composite nature of the renormalized A particle in the infinite-coupling limit can be seen from the behavior of the phase shift as a function of q. In Fig. 1 we have indicated the qualitative behavior of $\delta(q)$ for various strengths of coupling. For finite g the phase shift is zero at $q=0$, goes negative for $q>0$ and reaches a minimum before returning to zero as $q\to\infty$. For infinite g the phase shift also vanishes at $q=0$ and goes negative for $q>0$, but approaches $-\pi$ as $q\to\infty$. This difference in behavior can be summarized by

$$\begin{aligned}&\delta(0)-\delta(\infty)=0\quad(\text{finite } g),\\&\delta(0)-\delta(\infty)=\pi\quad(\text{infinite } g).\end{aligned} \tag{2.27}$$

In terms of Levinson's theorem,[8] the renormalized A particle is an elementary particle for finite coupling constant, but is a composite bound state of the $B\bar{B}$ system in the infinite coupling limit.

The off-shell T matrix is closely related to the A particle vacuum propagator, which is defined by

$$D_p^v(t-t')=-i\theta(t-t')\langle 0|a_p(t)a_p^\dagger(t')|0\rangle, \tag{2.28}$$

where $\theta(t-t')=1$ for $t>t'$ and vanishes for $t<t'$, and $a_p(t)=e^{iHt}a_p e^{-iHt}$. Since this propagator will turn out to play an essential part in the approximate calculation of the thermodynamic potential, we will now establish the relationship between it and the T-matrix element. It is evident that

$$\left(i\frac{\partial}{\partial t}-\omega_p^0\right)D_p^\nu(t-t')=\delta(t-t')-i\theta(t-t')\frac{g}{V^{1/2}}\sum_q F_q\langle 0|b_{p/2+q}(t)\bar{b}_{p/2-q}(t)a_p^\dagger(t')|0\rangle, \tag{2.29}$$

where we have used the equation of motion for the Heisenberg destruction operator $a_p(t)$. We may then write an equation of motion for the term on the right-hand side of Eq. (2.29). Again using the Heisenberg equation of motion for $b_p(t)$ and $\bar{b}_p(t)$ we obtain

$$\left(i\frac{\partial}{\partial t}-2W_B-p^2/4M-q^2/M\right)[\theta(t-t')\langle 0|b_{p/2+q}(t)\bar{b}_{p/2-q}(t)a_p^\dagger(t')|0\rangle]=\theta(t-t')\frac{g}{V^{1/2}}F_q\langle 0|a_p(t)a_p^\dagger(t')|0\rangle. \tag{2.30}$$

With the aid of the Green's function $G(t-t';E)$ defined by

$$\left(i\frac{\partial}{\partial t}-E\right)G(t-t';E)=\delta(t-t')$$

$$[G(t-t';E)=0,\quad t<t'], \tag{2.31}$$

Eq. (2.30) can be integrated and Eq. (2.29) converted to an integral equation for $D_p^\nu(t-t')$. By introducing the Fourier transform

$$D_p^\nu(\omega)=\int_{-\infty}^{\infty}dt\,D_p^\nu(t)e^{i\omega t} \tag{2.32}$$

we obtain

$$D_p^\nu(\omega)=\frac{1}{\omega+i\eta-\omega_p^0-\pi_p^\nu(\omega)}, \tag{2.33}$$

where

$$\pi_p^\nu(\omega)=g^2\int\frac{d^3k}{(2\pi)^3}\frac{F_k{}^2}{\omega+i\eta-2W_B-p^2/4M-k^2/M}. \tag{2.34}$$

By comparison with Eq. (2.18) we then obtain

$$T_{q'q}(p,\omega)=g^2F_qF_{q'}D_p^\nu(\omega)/V. \tag{2.35}$$

For future purposes it is convenient to write $D_p^\nu(\omega)$ in spectral form. Because $D_p^\nu(t-t')$ is a retarded propagator, $D_p^\nu(\omega)$ is analytic in the upper-half complex ω plane and can be written as

$$D_p^\nu(\omega)=\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}\frac{A_p^\nu(\omega')}{\omega+i\eta-\omega'}\quad(\omega\text{ real}), \tag{2.36}$$

where the real spectral weight $A_p^\nu(\omega)$ can be found from Eq. (2.33) by

$$A_p^\nu(\omega)=-2\,\mathrm{Im}\,D_p^\nu(\omega)$$

$$=2\pi Z\delta(\omega-\omega_p)+\frac{\rho_p(\omega)}{[\omega-\omega_p^0-\Delta_p(\omega)]^2+\frac{1}{4}\rho_p{}^2(\omega)}, \tag{2.37}$$

$D_p^\nu(t-t')$ can be calculated directly from the definition Eq. (2.28) by inserting a complete set of intermediate states with the quantum number $\nu=\bar{\nu}=1$ and total momentum $\vec{p}$. We shall obtain $D_p^\nu(t-t')$, however, by the standard equation-of-motion technique with

where ω_p and Z are given in Eqs. (2.13) and (2.14), respectively, and

$$\rho_p(\omega)=g^2\int\frac{d^3k}{(2\pi)^3}2\pi\delta(\omega-2W_B-p^2/4M-k^2/M)\,F_k{}^2,$$

$$\Delta_p(\omega)=g^2\int\frac{d^3k}{(2\pi)^3}\frac{F_k{}^2}{\omega-2W_B-p^2/4M-k^2/M}. \tag{2.38}$$

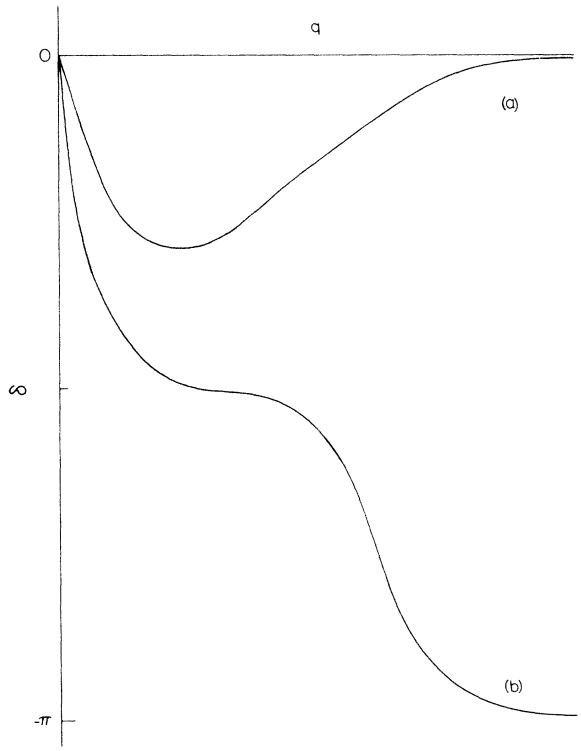

FIG. 1. Qualitative dependence of the $B\bar{B}$-scattering phase shift δ as a function of relative momentum q for the cases of (a) a typical finite value of coupling constant and (b) infinite coupling constant but finite renormalized A-particle rest energy.

It is evident from Eq. (2.38) that $\rho_p(\omega) = 0$ for $\omega < 2W_B + p^2/4M$.

In principle, we can determine states with quantum numbers ν and $\bar{\nu}$ other than those given above. However, to go further would require the solution of coupled integral equations which cannot be carried out in closed form. In fact, the above explicit content of the model is sufficient for a discussion of the Omnès transition. We now turn to a discussion of the statistical mechanics of the model.

III. STATISTICAL MECHANICS

We now consider a macroscopic subvolume V containing B, $\bar{B}$, and A particles at temperature T. This subvolume is assumed to be imbedded in a much larger volume also containing B, $\bar{B}$, and A particles at temperature T. This larger volume serves as an energy and particle reservoir for the subvolume. The thermodynamic state of the subvolume is thus described by a grand canonical ensemble in which constraints due to conservation laws for the additively conserved quantities ν and $\bar{\nu}$ in Eq. (2.7) are taken into account with Lagrange multipliers μ and $\bar{\mu}$, which can be interpreted physically as chemical potentials. The density matrix for such a system is then given by

$$\rho = e^{-\beta(H-\mu\nu-\bar{\mu}\bar{\nu})} . \tag{3.1}$$

We note here that a density matrix of the form

$$\rho = e^{-\beta(H-\mu N-\bar{\mu}\bar{N}-\mu_A N_A)} \tag{3.2}$$

does not describe an equilibrium ensemble since

$$\frac{\partial\rho}{\partial t} = \frac{1}{i}[H, \rho] \neq 0 \tag{3.3}$$

unless $\mu_A = \mu + \bar{\mu}$. We next assume that our system, described by the density matrix of Eq. (3.1), together with the surrounding reservoir contains no net baryon number. For a uniform system we will then have $\langle\nu\rangle = \langle\bar{\nu}\rangle$, where

$$\langle\nu\rangle = \mathrm{Tr}(\rho\nu)/\mathrm{Tr}\rho, \qquad \langle\bar{\nu}\rangle = \mathrm{Tr}(\rho\bar{\nu})/\mathrm{Tr}\rho . \tag{3.4}$$

Such a "charge-symmetric" system is described by a density matrix which is invariant under charge conjugation. Formally, we have

$$C\rho C^{-1} = \rho \tag{3.5}$$

from which it follows that $\mu = \bar{\mu}$. What we would like to determine is whether a macroscopically charge-conjugate-invariant density matrix allows any thermodynamic states other than $\langle\nu\rangle = \langle\bar{\nu}\rangle$. In particular, thermodynamic states for which $\langle\nu\rangle \neq \langle\bar{\nu}\rangle$ can be interpreted as describing a nonuniform system in which the baryon number excess in the system subvolume is balanced by a net baryon number of the opposite sign in the reservoir.[2] Thus, the system develops an inhomogeneity in baryon number.

The starting point for the thermodynamic analysis of the system is the calculation, in some approximation, of the thermodynamic potential which is related to the grand canonical density matrix of Eq. (3.1) by

$$\Omega(g) = -kT\ln(\mathrm{Tr}\rho) , \tag{3.6}$$

where we have indicated explicitly the dependence on the coupling constant. Our ultimate aim is to obtain a virial expansion of the Helmholtz free energy which is a function of the volume V, temperature T, and quantities η and $\bar{\eta}$, which are conjugate to the chemical potentials μ and $\bar{\mu}$ in the sense that

$$\frac{\partial F}{\partial\eta} = \mu , \quad \frac{\partial F}{\partial\bar{\eta}} = \bar{\mu} , \tag{3.7}$$

where the Helmholtz free energy is obtained from the thermodynamic potential by the Legendre transformation

$$F = \Omega(g) + \mu\eta + \bar{\mu}\bar{\eta} . \tag{3.8}$$

The quantities η and $\bar{\eta}$ are simply system eigenvalues of the operators ν and $\bar{\nu}$. From Eqs. (3.7) and (3.8) together with the thermodynamic relations

$$\langle\nu\rangle = -\frac{\partial\Omega}{\partial\mu} , \quad \langle\bar{\nu}\rangle = -\frac{\partial\Omega}{\partial\bar{\mu}} \tag{3.9}$$

it follows that the conjugate variables η and $\bar{\eta}$ are numerically equal to the grand-ensemble average values $\langle\nu\rangle$ and $\langle\bar{\nu}\rangle$, respectively. The symmetry condition $\mu = \bar{\mu}$ and Eq. (3.7) then give self-consistent equations for $\langle\nu\rangle$ and $\langle\bar{\nu}\rangle$ as functions of V, T, and μ. The special ("blackbody") case of $\mu = 0$ is the physical condition under which Omnès carries out his analysis. The value $\mu = 0$ arises in that work because mesons and pairs can be created and destroyed in elementary processes, and there is no analog of ν_+ as a conserved quantity. The analysis here is more general and contains the blackbody condition as a special case.

The thermodynamic potential itself is calculated by using the standard device[10] of differentiation of $\ln(\mathrm{Tr}\rho)$ with respect to the coupling constant g,

$$\frac{\partial\Omega(g)}{\partial g} = \frac{\mathrm{Tr}(\rho\,\partial H_1/\partial g)}{\mathrm{Tr}\rho} \equiv \left\langle\frac{\partial H_1}{\partial g}\right\rangle , \tag{3.10}$$

followed by integration from $g = 0$ to the full coupling strength,

$$\Omega(g) - \Omega(0) = \int_0^g \frac{dg}{g}\langle H_1\rangle , \tag{3.11}$$

where $\Omega(0)$ is the thermodynamic potential for the

noninteracting system of bosons and is given by[10]

$$\Omega(0)=kTV\int\frac{d^3p}{(2\pi)^3}[\ln(1-e^{\beta(\mu+\bar{\mu}-\omega_p^0)})+\ln(1-e^{\beta(\mu-E_p)})+\ln(1-e^{\beta(\bar{\mu}-E_p)})]. \tag{3.12}$$

We note that the *bare* A-particle rest energy appears in $\Omega(0)$. By inserting the explicit form of H_1 into Eq. (3.11), we obtain

$$\Omega(g)=\Omega(0)+\frac{2}{V^{1/2}}\mathrm{Re}\int_0^g dg\sum_{pq}F_q\langle b_{p/2+q}\bar{b}_{p/2-q}a_p^\dagger\rangle\,. \tag{3.13}$$

To evaluate the required ensemble average in Eq. (3.13) we introduce the A-particle propagator[10] defined by

$$D_p(t-t')=\theta(t-t')D_p^>(t-t')+\theta(t'-t)D_p^<(t-t')\,, \tag{3.14}$$

where

$$\begin{aligned}D_p^>(t-t')&=-i\langle a_p(t)a_p^\dagger(t')\rangle\\&=-i\sum_{mn}P_m|\langle m|a_p|n\rangle|^2\times e^{i(E_m-E_n)(t-t')}\,,\\D_p^<(t-t')&=-i\langle a_p^\dagger(t')a_p(t)\rangle\\&=-i\sum_{mn}P_n|\langle m|a_p|n\rangle|^2\times e^{i(E_m-E_n)(t-t')}\,,\end{aligned} \tag{3.15}$$

and $P_m=e^{-\beta(E_m-\mu\nu_m-\bar{\mu}\bar{\nu}_m)}/\mathrm{Tr}\rho$. In Eq. (3.15) the states $|m\rangle$ are eigenstates of H, ν, and $\bar{\nu}$, with respective eigenvalues E_m, ν_m, and $\bar{\nu}_m$. The functions defined in Eq. (3.15) are not independent. This can easily be seen by taking the Fourier transforms defined by

$$\begin{aligned}D_p^<(\omega)&=i\int_{-\infty}^{\infty}dt\,e^{i\omega t}D_p^<(t)\\&=2\pi\sum_{mn}P_m\delta(E_m-E_n+\omega)|\langle m|a_p|n\rangle|^2\end{aligned} \tag{3.16}$$

and

$$\begin{aligned}D_p^>(\omega)&=i\int_{-\infty}^{\infty}dt\,e^{i\omega t}D_p^>(t)\\&=2\pi\sum_{mn}P_n\delta(E_m-E_n+\omega)|\langle m|a_p|n\rangle|^2\,.\end{aligned} \tag{3.17}$$

Since $E_n-E_m=\omega$, $\nu_n-\nu_m=1$, and $\bar{\nu}_n-\bar{\nu}_m=1$ in the above sums, it is evident that

$$D_p^>(\omega)=e^{\beta(\omega-\mu-\bar{\mu})}D_p^<(\omega)\,. \tag{3.18}$$

If we define an A-particle spectral function $A_p(\omega)$ by

$$D_p^>(\omega)-D_p^<(\omega)=A_p(\omega)\,, \tag{3.19}$$

then Eq. (3.18) enables us to write

$$\begin{aligned}D_p^<(\omega)&=f(\omega)A_p(\omega)\,,\\D_p^>(\omega)&=[1+f(\omega)]A_p(\omega)\,,\end{aligned} \tag{3.20}$$

where $f(\omega)=(e^{\beta(\omega-\mu-\bar{\mu})}-1)^{-1}$. As we will see below, the thermodynamic potential can be expressed in a simple formal manner in terms of the A-particle spectral function. As we will be interested in the simplest of approximations for $A_p(\omega)$ which will enable us to investigate the possibility of an Omnès transition, we will not go into details of a general scheme by which $A_p(\omega)$ can be determined. We simply note in passing that the spectral function satisfies several sum rules which can be easily proven and which take the form

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}A_p(\omega)&=1\,,\\\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega-\omega_p^0)A_p(\omega)&=0\,.\end{aligned} \tag{3.21}$$

We now return to the expression for the thermodynamic potential, Eq. (3.13), to determine how it can be written in terms of the spectral function. To see this, we write an equation of motion for $D_p^<(t-t')$:

$$\left(i\frac{\partial}{\partial t}-\omega_p^0\right)D_p^<(t-t')=-i\frac{g}{V^{1/2}}\sum_q F_q\langle a_p^\dagger(t')b_{p/2+q}(t)\bar{b}_{p/2-q}(t)\rangle\,. \tag{3.22}$$

The right-hand side of Eq. (3.22) with $t'=t$ appears in $\Omega(g)-\Omega(0)$, while the left-hand side can be evaluated with the aid of Eq. (3.20) to give

$$\Omega(g)=\Omega(0)+2\int_0^g\frac{dg}{g}\sum_p\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}(\omega-\omega_p^0)f(\omega)\,A_p(\omega)\,, \tag{3.23}$$

which is the analog of a similar result in potential scattering.

As a first approximation to $\Omega(g)$ we now replace $A_p(\omega)$ by its vacuum value. We note that the vacuum case can be obtained by setting $\mu=\bar{\mu}=0$ and letting $\beta\to\infty$. In this limit

$$\begin{aligned}D_p(t-t')&\to-i\theta(t-t')\langle 0|a_p(t)a_p^\dagger(t')|0\rangle\\&=D_p^v(t-t')\,,\end{aligned} \tag{3.24}$$

which has been determined in Sec. II. In this approximation all dependence on the thermodynam-

ic parameters T, μ, and $\bar{\mu}$ is contained in the Bose function $f(\omega)$, while all the dynamical information is contained in the vacuum spectral function $A_p^v(\omega)$. Fortunately, the dependence of $A_p^v(\omega)$ on the coupling constant is sufficiently simple so that the integration over coupling constant can be carried out explicitly. The contribution from the δ-function part of $A_p^v(\omega)$ in Eq. (2.37) to the interaction part of the thermodynamic potential is given by

$$[\Omega^{\text{int}}(g)]_{\text{pole}} = VkT \int \frac{d^3p}{(2\pi)^3} \ln\left[\frac{1-e^{\beta(\mu+\bar{\mu}-\omega_p)}}{1-e^{\beta(\mu+\bar{\mu}-\omega_p^0)}}\right]. \quad (3.25)$$

When added to $\Omega(0)$ this contribution simply replaces the unrenormalized A-particle rest energy in $\Omega(0)$ by the renormalized A-particle rest energy. This renormalization of $\Omega(0)$ is in agreement with the general S-matrix formulation of statistical mechanics given by DMB. The contribution from the continuum part of $A_p^v(\omega)$ in Eq. (2.37) to the interaction part of the thermodynamic potential can also be calculated explicitly and, when compared with the expression for the scattering phase shift in Eq. (2.21), we obtain

$$[\Omega^{\text{int}}(g)]_{\text{cont}} = -V\frac{4\pi}{M}\int \frac{d^3p}{(2\pi)^3}\int \frac{d^3k}{(2\pi)^3} f(2W_B + p^2/4M + k^2/M) \times \delta(k)/k\,. \quad (3.26)$$

For temperatures such that $W_B \gg kT$ we may approximate the Bose distribution function in Eq. (3.26) by its Maxwellian limit. We then obtain the final approximate form for the thermodynamic potential,

$$\Omega(g) = \Omega^{\text{ren}}(0) - Ve^{\beta(\mu+\bar{\mu})}\Lambda_c\,, \quad (3.27)$$

where Λ_c is the virial coefficient given by

$$\Lambda_c = +e^{-2\beta W_B}\lambda_{\text{th}}^{-3}\int_0^\infty \frac{d\epsilon}{\pi}\,\delta(k(\epsilon))e^{-\beta\epsilon}\,, \quad (3.28)$$

with $\lambda_{\text{th}}^{-1} = (MkT/\pi)^{1/2}$. By partial integration Eq. (3.28) can be converted into the standard Beth-Uhlenbeck[11] formula for the second virial coefficient. In Eq. (3.27) the quantity $\Omega^{\text{ren}}(0)$ is the noninteracting thermodynamic potential defined in Eq. (3.12) but with the unrenormalized A-particle rest energy W_A^0 replaced by the renormalized rest energy W_A.

For purposes of discussing the possibility of an Omnès transition we now use the above approximate thermodynamic potential as the basis for a virial expansion of the Helmholtz free energy in terms of the densities $\langle\nu\rangle/V$ and $\langle\bar{\nu}\rangle/V$. As stated previously, the Helmholtz free energy is obtained from Eq. (3.8), while use of Eq. (3.9) is made in the form

$$\eta = \langle\nu\rangle = -\beta z\frac{\partial\Omega(g)}{\partial z}\,, \quad \bar{\eta} = \langle\bar{\nu}\rangle = -\beta\bar{z}\frac{\partial\Omega(g)}{\partial\bar{z}}\,, \quad (3.29)$$

where $z = e^{\beta\mu}$ and $\bar{z} = e^{\beta\bar{\mu}}$. The approximate thermodynamic potential in Eq. (3.27) is now regarded as giving the first few terms in an infinite double series in z and $\bar{z}$:

$$\Omega(g) = -kTV[C_1(z+\bar{z}) + C_2 z\bar{z} + \cdots]\,, \quad (3.30)$$

where

$$C_1 = \lambda_{\text{th}}^{-3}e^{-\beta W_B}\tfrac{1}{4}\sqrt{2}\,, \quad C_2 = \lambda_{\text{th}}^{-3}e^{-\beta W_A} + \Lambda_c/kT\,. \quad (3.31)$$

In the standard manner the double series in z and $\bar{z}$ obtain for η and $\bar{\eta}$ from Eqs. (3.29) and (3.30) can be inverted, and the Helmholtz free energy can be expressed as a double power series in $\xi = \eta/V$ and $\bar{\xi} = \bar{\eta}/V$, with the result

$$F = kTV[\xi\ln(\xi/eC_1) + \bar{\xi}\ln(\bar{\xi}/eC_1) - C_2\xi\bar{\xi}/C_1^2 + \cdots]\,. \quad (3.32)$$

We emphasize that the Helmholtz free energy is a function of the system eigenvalues of the additively conserved quantities ν and $\bar{\nu}$. The condition of macroscopic charge-conjugation invariance is now set by imposing Eq. (3.7) with $\mu = \bar{\mu}$. From these relations we then obtain the basic equations for the self-consistent determination of ξ and $\bar{\xi}$,

$$\xi = C_1\exp(C_2\bar{\xi}/C_1^2)e^{\beta\mu}\,, \quad \bar{\xi} = C_1\exp(C_2\xi/C_1^2)e^{\beta\mu}\,. \quad (3.33)$$

From an analysis similar to that used by Omnès[1,2] it can be seen that the solution $\xi = \bar{\xi}$ (and thus $\langle N-\bar{N}\rangle = 0$) is the *only* solution for $C_2 > 0$. Rather than use Eqs. (3.28) and (3.31) as the definition of C_2, it is convenient at this point to go back and write C_2 in the alternate form [from which Eqs. (3.31) and (3.28) can be obtained]

$$C_2 = \int \frac{d^3p}{(2\pi)^3}\,e^{-\beta\omega_p^0}[1+\beta\chi_p(\beta)]\,, \quad (3.34)$$

where

$$\chi_p(\beta) = -2\int_0^g \frac{dg}{g}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-\beta(\omega-\omega_p^0)}(\omega-\omega_p^0)A_p^v(\omega). \quad (3.35)$$

From the second sum rule in Eq. (3.21) we conclude that $\chi_p(0) = 0$. Furthermore, from the explicit expressions for $A_p^v(\omega)$ in Eqs. (2.37) and (2.38) it is clear that $d\chi_p(\beta)/d\beta > 0$ for all β. Hence, we conclude that $\chi(\beta) \geq 0$ and thus $C_2 > 0$. Thus, within the context of the present approximations, the only possibility is the homogeneous (symmetric) solution $\langle N\rangle = \langle\bar{N}\rangle$.

In the Omnès modification of the present anal-

ysis, the bound-state contribution to C_2 is dropped. The additional assumptions needed to justify this modification are a main concern of the present work, and in Sec. IV we introduce a method of analysis whereby the modification can be introduced in a systematic manner. We note here that if the bound-state contribution to C_2 is dropped from Eq. (3.28), C_2 is simply given by Λ_c/kT defined in Eq. (3.28). Since Λ_c is negative, the possibility arises that Eq. (3.30) will possess solutions for which $\xi \neq \bar{\xi}$, i.e., for which $\langle N\rangle \neq \langle \bar{N}\rangle$. Such solutions break the macroscopic charge-conjugation symmetry noted prior to Eq. (3.2). These solutions thus indicate the possibility of an inhomogeneity in the baryon number density.

IV. THE UNITARY TRANSFORMATION

The interaction Hamiltonian of Eq. (2.2) explictly couples the A particle to a $B\bar{B}$ pair in a virtual process. In Sec. III we have seen how a density matrix, when parametrized with respect to thermodynamic variables conjugate to each of the conserved quantities dictated by the nature of the Hamiltonian, does not lead (in the given approximation) to asymmetric solutions that indicate a local baryon-number-density inhomogeneity. The purpose of the present section is to make a unitary transformation on the original Hamiltonian in order to separate the effects of the original interaction into two parts. The first of these parts is the renormalization of the A-particle rest energy, while the second part leads to scattering among various of the system's constituents. This second part takes the form of an infinite sum of potential-like interactions between various groupings of particles. The procedure is then to retain only a certain portion of the transformed Hamiltonian and, in particular, to neglect those potentials which describe the *real* process of $B\bar{B}$-pair annihilation and creation. Physically, the neglect of real-pair annihilation and creation allows the renormalized A particles on the one hand and B and $\bar{B}$ particles on the other hand to appear as independent components of the system. Such a situation then leads to the possibility of an Omnès transition. Thus the state of incomplete thermodynamic equilibrium[12] brought about by the inefficiency of real-pair creation and annihilation seems to be a necessary condition for an Omnès transition.

We now consider the unitary transformation $U = e^{\Psi}$, where Ψ is chosen so that the transformed Hamiltonian takes the form

$$H' = e^{\Psi} H e^{-\Psi} = H_0' + H_{\rm int}' , \tag{4.1}$$

where

$$H_0' = \sum_p (a_p^\dagger a_p \omega_p + b_p^\dagger b_p E_p + \bar{b}_p^\dagger \bar{b}_p E_p) \tag{4.2}$$

and

$$H_{\rm int}' = V^{(1)} + V^{(2)} + V^{(3)} + \cdots , \tag{4.3}$$

with

$$V^{(1)} = \frac{1}{V} \sum_{pqq'} b^\dagger_{p/2+q}, \bar{b}^\dagger_{p/2-q'}, \bar{b}_{p/2-q} b_{p/2+q} V^{(1)}_{qq'} ,$$

$$V^{(2)} = \frac{1}{2V} \sum_{pp'p''} a^\dagger_{p-p'}, a_{p-p''} (b^\dagger_{p'}, b_{p''} + \bar{b}^\dagger_{p'}, \bar{b}_{p''}) V^{(2)}_{p'p''} , \tag{4.4}$$

$$V^{(3)} = \frac{1}{V^{3/2}} \sum_{pp'p''q} a^\dagger_{p-p'} (b^\dagger_{p'}, b_{p''} + \bar{b}^\dagger_{p'}, \bar{b}_{p''}) \times b_{(p-p'')/2-q}\, \bar{b}_{(p-p'')/2+q} V^{(3)}_{p''p'q} + \text{H.c.} ,$$

$$\cdots .$$

In Eq. (4.4) $V^{(1)}$, $V^{(2)}$, and $V^{(3)}$ are potentials that describe $B\bar{B}$ scattering, AB and $A\bar{B}$ scattering, and $B\bar{B}$-pair production and annihilation, respectively. Additional potentials also arise which involve ever-increasing numbers of particles. The invariance of $V^{(i)}$ under charge conjugation follows from the invariance of the untransformed Hamiltonian H, together with a charge-conjugation-invariant operator Ψ. To yield the transformed Hamiltonian indicated in Eqs. (4.1)–(4.4), we take Ψ of the form

$$\Psi = \sum_{pq} \Psi_q (a_p b^\dagger_{p/2+q} \bar{b}^\dagger_{p/2-q} - a_p^\dagger b_{p/2+q} \bar{b}_{p/2-q}) , \tag{4.5}$$

with $\Psi_q = \Psi_{-q}$. The task now is to determine both Ψ_q and the various potentials. In particular, we will determine only $V^{(1)}_{qq}$ explicitly in the present work since it exhibits the essential feature necessary for the Omnès transition.

Since the operators ν and $\bar{\nu}$ commute with Ψ, the eigenstates of H' can be simultaneously labeled by the eigenvalues of ν and $\bar{\nu}$. In particular, $a_p^\dagger|0\rangle$ is an eigenstate of H' with eigenvalue ω_p and eigenvalues $\nu = \bar{\nu} = 1$. We note that ω_p is the renormalized A-particle energy. It then follows that

$$H e^{-\Psi} a_p^\dagger |0\rangle = \omega_p e^{-\Psi} a_p^\dagger |0\rangle , \tag{4.6}$$

from which we conclude by reference to Eq. (2.11) that

$$e^{-\Psi} a_p^\dagger |0\rangle = Z^{1/2} \left(a_p^\dagger |0\rangle - \frac{g}{V^{1/2}} \sum_q \frac{F_q}{\epsilon_q} b^\dagger_{p/2+q} \bar{b}^\dagger_{p/2-q} |0\rangle \right) , \tag{4.7}$$

where $\epsilon_q = 2W_B + q^2/M - W_A$. On the other hand, the

potential $V^{(1)}_{q'q}$ can be calculated by taking matrix elements of H' between bare pair states since

$$\langle 0|b_{p/2+q'}\,\bar{b}_{p/2-q'}\,e^{\Psi}He^{-\Psi}b^{\dagger}_{p/2+q}\,\bar{b}^{\dagger}_{p/2-q}|0\rangle = \left(\frac{p^2}{4M}+\frac{q^2}{M}+2W_B\right)\delta_{q'q}+V^{(1)}_{q'q}\,. \quad (4.8)$$

Thus, the determination of $e^{-\Psi}a^{\dagger}_p|0\rangle$ in terms of the Ψ_q will enable a determination of that parameter through Eq. (4.7), whereas the determination of $e^{-\Psi}b^{\dagger}_{p/2+q}\,\bar{b}^{\dagger}_{p/2-q}|0\rangle$ in terms of the now known Ψ_q will enable a determination of $V^{(1)}_{q'q}$ through Eq. (4.8). To this end we introduce two state vectors,

$$|\Phi_p(\lambda)\rangle = e^{-\lambda\Psi}a^{\dagger}_p|0\rangle$$

and (4.9)

$$|\Phi_{pq}(\lambda)\rangle = e^{-\lambda\Psi}b^{\dagger}_{p/2+q}\,\bar{b}^{\dagger}_{p/2-q}|0\rangle\,,$$

which satisfy "equations of motion"

$$\frac{d}{d\lambda}|\Phi_p(\lambda)\rangle = -\sum_q \Psi_q|\Phi_{pq}(\lambda)\rangle$$

and (4.10)

$$\frac{d}{d\lambda}|\Phi_{pq}(\lambda)\rangle = \Psi_q|\Phi_p(\lambda)\rangle\,,$$

as can be easily verified by direct differentiation of Eq. (4.9) together with the definition of Ψ in Eq. (4.5). These coupled first-order differential equations, together with the boundary condition at $\lambda=0$ obtained from Eq. (4.9), can be easily solved to give

$$|\Phi_p(1)\rangle \equiv e^{-\Psi}a^{\dagger}_p|0\rangle = \cos X\; a^{\dagger}_p|0\rangle - \frac{\sin X}{X}\sum_q \Psi_q b^{\dagger}_{p/2+q}\,\bar{b}^{\dagger}_{p/2-q}|0\rangle$$

and

$$|\Phi_{pq}(1)\rangle \equiv e^{-\Psi}b^{\dagger}_{p/2+q}\,\bar{b}^{\dagger}_{p/2-q}|0\rangle = b^{\dagger}_{p/2+q}\,\bar{b}^{\dagger}_{p/2-q}|0\rangle + \Psi_q\left(\frac{\cos X-1}{X^2}\sum_{q'}\Psi_{q'}\,b^{\dagger}_{p/2+q'}\,\bar{b}^{\dagger}_{p/2-q'}|0\rangle + \frac{\sin X}{X}a^{\dagger}_p|0\rangle\right), \quad (4.11)$$

where $X^2=\sum_q \Psi_q{}^2$. From Eqs. (4.7) and (4.11) we then determine

$$\Psi_q = \frac{g}{V^{1/2}}\,\frac{F_q}{\epsilon_q}\left(\frac{Z}{1-Z}\right)^{1/2}\cos^{-1}(Z^{1/2})\,. \quad (4.12)$$

It is evident that Ψ_q is independent of the total momentum p. Finally, the potential $V^{(1)}_{q'q}$, as computed from Eqs. (4.8) and (4.11), is given by

$$V^{(1)}_{q'q} = g^2\,\frac{F_q F_{q'}}{\epsilon_q\epsilon_{q'}}\,\frac{Z^{1/2}}{1+Z^{1/2}} \times\left[\frac{Z^{1/2}}{1+Z^{1/2}}\,(W^0_A-W_A)+\epsilon_q+\epsilon_{q'}\right], \quad (4.13)$$

which is a sum of separable repulsive potentials.

In order to determine the incomplete thermodynamic equilibrium state of a system of B, $\bar{B}$, and A particles in the absence of real $B\bar{B}$-pair creation and annihilation, we assume that this equilibrium state is determined by that portion of the Hamiltonian H' given by

$$H'_{\rm eff} = H'_0 + V^{(1)}\,. \quad (4.14)$$

We note that $H'_{\rm eff}$ possesses three conserved quanti ties, N, $\bar{N}$, and N_A, rather than the previous two conserved quantities $N+N_A$ and $\bar{N}+N_A$. The reason for the enlarged number of conserved quantities is simply that by neglecting all interactions except $V^{(1)}$ we are neglecting the *real* transformations between $B\bar{B}$ pairs and A particles. The virtual transformations lead, of course, to the A-particle rest-energy renormalization and have been taken into account by the unitary transformation. To construct a grand ensemble for the equilibrium state of a system described by $H'_{\rm eff}$, we use a density matrix defined by

$$\rho_{\rm eff} = e^{-\beta(H'_{\rm eff}-\mu N-\bar{\mu}\bar{N}-\mu_A N_A)}\,. \quad (4.15)$$

As in the case of the density matrix for full thermodynamic equilibrium discussed in Sec. III, macroscopic charge-conjugation invariance implies that $\mu=\bar{\mu}$. As before, the properties of the incomplete equilibrium state can be determined by a virial expansion of the effective Helmholtz free energy in powers of the conjugate variables η', $\bar{\eta}'$, and η_A which are related to the grand canonical ensemble averages of N, $\bar{N}$, and N_A by the numerical equalities

$$\eta' = \langle N\rangle_{\rm eff}\,,\quad \bar{\eta}' = \langle\bar{N}\rangle_{\rm eff}\,,\quad \eta_A = \langle N_A\rangle_{\rm eff}, \quad (4.16)$$

where

$$\langle X\rangle_{\rm eff} = {\rm Tr}(\rho_{\rm eff}X)/{\rm Tr}\rho_{\rm eff} \quad (4.17)$$

The conditions for incomplete equilibrium are then determined by

$$\frac{\partial F_{\rm eff}}{\partial\eta'} = \frac{\partial F_{\rm eff}}{\partial\bar{\eta}'} = \mu$$

and (4.18)

$$\frac{\partial F_{\rm eff}}{\partial\eta_A} = \mu_A\,,$$

where the chemical potentials μ and μ_A are presumed given. Explicitly, the free energy can be obtained, as before, from the thermodynamic potential and is given by

$$F_{\text{eff}} = kTV[\xi' \ln(\xi'/eC_1) + \bar{\xi}' \ln(\bar{\xi}'/eC_1) + \xi_A \ln(\xi_A/eC_A) - C_2' \xi' \bar{\xi}'/C_1^2 + \cdots], \tag{4.19}$$

where $\xi' = \eta'/V$, $\bar{\xi}' = \bar{\eta}'/V$, $\xi_A = \eta_A/V$, and C_1 is given, as before, in Eq. (3.31). The quantity C_A is given by

$$C_A = \lambda_{\text{th}}^{-3} e^{-\beta W_A}, \tag{4.20}$$

while C_2' can be computed in a manner similar to what was done in the case of full thermodynamic equilibrium, or, alternatively, we may use the Beth-Uhlenbeck formula, from which we obtain

$$\frac{C_2'}{C_1^2} = 8\lambda_{\text{th}}^3 e^{-\beta 2W_B} \int_0^\infty \frac{dq}{\pi} \frac{d\delta'(q)}{dq} e^{-\beta q^2/M}, \tag{4.21}$$

where $\delta'(q)$ is the scattering phase shift for the potential $V_{q'q}^{(1)}$.

To obtain an expression for the phase shift $\delta'(q)$, we must first calculate the T matrix for the $B\bar{B}$ interaction $V_{q'q}^{(1)}$, which can be done by solving the Lippmann-Schwinger equation for $T'(E)$ in Eq. (2.15) and using $V_{q'q}^{(1)}$ as the potential. Since $V_{q'q}^{(1)}$ is a sum of separable potentials, the Lippmann-Schwinger equation can be solved in closed form to give

$$T'_{q'q}(p,E) = \frac{g^2}{V} \frac{F_q F_{q'}}{\epsilon_q \epsilon_{q'}} \frac{\gamma(\epsilon_q + \epsilon_{q'}) + \gamma^2 (g^2/V) \sum_k (F_k^2/\epsilon_k^2 E_{p,k})[\epsilon_k E_{p,k} + (\epsilon_k - \epsilon_q)(\epsilon_k - \epsilon_{q'})]}{1 - (g^2/V) \sum_{k'} F_{k'}^2/\epsilon_{k'} E_{p,k'}}, \tag{4.22}$$

where $\gamma = Z^{1/2}/(1+Z^{1/2})$ and $E_{p,k} = E + i\eta - E_{p/2+k} - E_{p/2-k}$. This T' matrix has no poles on the real E axis which confirms the fact that there are now *no* bound states arising from our approximate Hamiltonian. When the T' matrix is placed on the energy shell, the expression in Eq. (4.22) and thus the scattering phase shift $\delta'(q)$ reduce to the expressions in Eqs. (2.20) and (2.21), respectively. Hence, the expression for C_2' becomes equal to that for Λ_c/kT, defined by Eq. (3.28), as can be seen by partial integration of Eq. (4.21). Since $\delta'(q) = \delta(q)$ is negative for all q and since, by partial integration, C_2' is proportional to $\int_0^\infty dq\, q\delta(q) \times e^{-\beta q^2/M}$, then C_2' is less than zero.

We now apply the equilibrium condition (4.18) and obtain

$$\xi' = C_1 \exp(C_2' \bar{\xi}'/C_1^2) e^{\beta\mu}, \tag{4.23}$$

$$\bar{\xi}' = C_1 \exp(C_2' \xi'/C_1^2) e^{\beta\mu},$$

and

$$\xi_A = 2\sqrt{2}\, C_1 e^{\beta\mu_A}. \tag{4.24}$$

There exist asymmetric solutions to these two equations such that $\xi' \neq \bar{\xi}'$ when

$$-\frac{C_2'}{C_1} e^{\beta\mu} > e. \tag{4.25}$$

In the model we have been considering we have seen that $C_2' < 0$ and that therefore the possibility for B-$\bar{B}$ separation exists, but numerical calculations indicate condition (4.25) cannot be satisfied at any temperature with this simple model. It is shown in the Appendix, however, that if sufficient degeneracy due to internal degrees of freedom is added to the model, the condition for asymmetric solutions (4.25) can be satisfied and such solutions arise above a certain critical temperature. As Omnès has pointed out and as is true in this approximation in our model, these asymmetric solutions correspond to a minimum in the Helmholtz free energy, while the symmetric solutions correspond to a maximum for temperatures above the critical temperature. Thus we see how essential the assumption of incomplete thermodynamic equilibrium is to the possibility of an Omnès transition in this model. This independence of the A particles and the B and $\bar{B}$ particles had its analog in the realistic problem of mesons, nucleons, and antinucleons in the original work of Omnès,[1] but the connection between this independence and a state of incomplete thermodynamic equilibrium is not clear in subsequent work.[2,13]

V. SUMMARY AND CONCLUSION

In this paper we consider the implications of both full and partial thermodynamic equilibrium for the nonrelativistic Zachariasen model within the approximation scheme of an appropriate virial expansion of the Helmholtz free energy. For full thermodynamic equilibrium we construct a grand canonical ensemble which is parametrized by two chemical potentials that are introduced to take into account constraints on the two conserved number operators which exist in the model. The thermodynamic potential, which is the natural potential for the grand ensemble, is approximated by retaining only two body dynamics and is then used to compute the Helmholtz free energy, which is more useful for the analysis of phase transitions. The Helmholtz free energy is then a function of volume, temperature, and the system eigenvalues of the two conserved quantities. The imposition of the condition for macroscopic charge-conjuga-

tion invariance then results in two coupled equations which must be solved self-consistently for the equilibrium system eigenvalues as a function of temperature and a common chemical potential. We find only thermodynamic states of zero baryon number as solutions to these coupled equations and thus there is no Omnès transition. We next make a unitary transformation on the original Hamiltonian which separates the virtual from the real $B\overline{B}$-pair creations and annihilations. If we neglect all such real-pair creations and annihilations and retain only the two-body $B\overline{B}$ interaction we are left with an approximate Hamiltonian for which there are now three conserved number operators. In this approximation the A particles decouple completely from the B and $\overline{B}$ particles, and the Helmholtz free energy takes on the *form* assumed by Omnès in his analysis of the realistic problem involving mesons, nucleons, and antinucleons, and for which thermodynamic states of nonzero baryon number are possible.

We conclude that within the context of a virial expansion of the Helmholtz free energy, a state of incomplete thermodynamic equilibrium is necessary for an Omnès transition to be possible. Thus the conditions under which the Omnès mechanism is operational require that the effects of real-pair production and annihilation are negligible in the sense that the time scale over which the thermodynamic state of the system is being established is short compared to the relaxation time for complete thermodynamic equilibrium. We have not calculated the relaxation time for approach to complete thermodynamic equilibrium under the influence of real-pair creation and annihilation in the nonrelativistic Zachariasen model. However, it has been indicated by Schatzman[14] that for the realistic meson-nucleon-antinucleon problem full thermodynamic equilibrium is easily attained at temperatures pertinent to the environment of the Omnès transition. Hence it seems doubtful that matter-antimatter separation can take place through the Omnès mechanism. This doubt has been expressed qualitatively by Steigman.[6] In the present work we have explicitly examined the possibility of an Omnès transition in the two cases of complete and partial thermodynamic equilibrium for the purpose of clarification of the mechanism.

APPENDIX A: THE ADDITION OF AN INTERNAL DEGREE OF FREEDOM TO THE MODEL

We consider here the inclusion of an internal degree of freedom which, for simplicity, we refer to as isospin. It will be convenient to adopt the following notation:

$a_p(I,M)$ is the destruction operator for A particles with total isospin I and z component M.

$b_p(m)$ [$\overline{b}_p(m)$] is the destruction operator for B [$\overline{B}$] particles with total isospin i and z component m.

We constrain the total isospin of the B and $\overline{B}$ particles to some fixed value i, but we allow the total isospin of the A particles to range from $I=0$ to $I=2i$.

We first construct the untransformed Hamiltonian for the model with isospin included. In order that the untransformed Hamiltonian behave like a scalar under isospin rotation, it must have the form $H=H_0+H_{\rm int}$, where

$$H_0=\sum_{p,m}[b_p^\dagger(m)\,b_p(m)+\overline{b}_p^\dagger(m)\,\overline{b}_p(m)]E_p + \sum_{p,I,M} a_p^\dagger(I,M)\,a_p(I,M)\,\omega_p^0 \tag{A1}$$

and

$$H_{\rm int}=\frac{g}{\sqrt{V}}\sum_{p,q}\sum_{I,m_1m_2} F_q\langle im_1\, im_2|\, i\,i\,I m_1+m_2\rangle \times[a_p^\dagger(I,m_1+m_2)\,b_{p/2+q}(m_1)\,\overline{b}_{p/2-q}(m_2)+b_{p/2+q}^\dagger(m_1)\,\overline{b}_{p/2-q}^\dagger(m_2)\,a_p(I,m_1+m_2)]\,. \tag{A2}$$

If the unitary transformation preserves the scalar behavior of the Hamiltonian under isospin rotation, the transformed Hamiltonian $H'=e^{\Psi}He^{-\Psi}$ must have the form

$$H'=\sum_{p,m}[b_p^\dagger(m)\,b_p(m)+\overline{b}_p^\dagger(m)\,\overline{b}_p(m)]E_p+\sum_{p,I,M}a_p^\dagger(I,M)\,a_p(I,M)\,\omega_p + \frac{1}{V}\sum_{p,q,q'}\sum_{m_1,m_2} b_{p/2+q}^\dagger(m_1)\,\overline{b}_{p/2-q}^\dagger(m_2)\,\overline{b}_{p/2-q'}(m_2)\,b_{p/2+q'}(m_1)\,V_{qq}^{(1)}+\cdots\,. \tag{A3}$$

In (A3) we have written explicitly only those terms that contribute to $H'_{\rm eff}$.

In order that the unitary transformation preserve the scalar behavior of the Hamiltonian, Ψ must have the form

$$\Psi=\sum_{pq}\sum_{I,m_1,m_2}\Psi_q\langle im_1\, im_2|\, iiIm_1+m_2\rangle[b_{p/2+q}^\dagger(m_1)\,\overline{b}_{p/2-q}^\dagger(m_2)\,a_p(I,m_1+m_2)-a_p^\dagger(I,m_1+m_2)\,b_{p/2+q}(m_1)\,\overline{b}_{p/2-q}(m_2)]\,. \tag{A4}$$

The development proceeds straightforwardly in the manner of Sec. IV with appropriate inclusions of the Clebsch-Gordan coefficients. If we invoke the orthogonality and the completeness properties of the Clebsch-Gordan coefficients in the proper places, we easily find that Ψ_q and $V_{qq}^{(1)}$ are given by the same expressions obtained in the isospinless model, Eqs. (4.12) and (4.13), respectively. We have already seen in Sec. IV that $V_{qq}^{(1)}$ leads to the T matrix given in Eq. (4.22) and that, on-shell, this T matrix yields the $B\bar{B}$-scattering phase shift of Eq. (2.21).

To obtain the condition for the occurrence of the phase transition and to see how the inclusion of isospin degeneracy alters this condition by effectively replacing C_2' with $(2i+1)C_2'$ in Eq. (4.25), we make a virial expansion of the Helmholtz free energy. In making this expansion we make use of the fact that in this model the average number of B or $\bar{B}$ particles with isospin z-component m will be independent of m, and the average number of A particles of isospin I and z-component M will be independent of I and M. Thus, we can write

$$F_{\text{eff}} = F_0 - kTC_2' V\xi'\bar{\xi}'/C_1^2, \tag{A5}$$

where F_0 is the contribution to F from the free particles of all species and is given by

$$F_0 = kTV\left\{\xi'\ln\left[\frac{\xi'}{eC_1(2i+1)}\right] + \bar{\xi}'\ln\left[\frac{\bar{\xi}'}{eC_1(2i+1)}\right] + \xi_A\ln\left[\frac{\xi_A}{e2\sqrt{2}\,C_1(2i+1)^2}\right]\right\}. \tag{A6}$$

The coefficients C_1 and C_2' have been previously defined in Eq. (3.31) and (4.21), respectively. Applying the incomplete thermodynamic equilibrium conditions

$$\frac{\partial F_{\text{eff}}}{\partial \eta'} = \frac{\partial F_{\text{eff}}}{\partial \bar{\eta}'} = \mu$$

and

$$\frac{\partial F_{\text{eff}}}{\partial \eta_A} = \mu_A,$$

we obtain

$$\xi' = (2i+1)C_1 e^{\beta\mu}\exp(C_2'\bar{\xi}'/C_1^2),$$
$$\bar{\xi}' = (2i+1)C_1 e^{\beta\mu}\exp(C_2'\xi'/C_1^2), \tag{A7}$$

and

$$\xi_A = (2i+1)^2 2\sqrt{2}\, C_1 e^{\beta\mu_A}. \tag{A8}$$

From the coupled equation (A7), we find that the condition for the occurrence of solutions asymmetric in ξ' and $\bar{\xi}'$ is

$$-(2i+1)e^{\beta\mu}C_2'/C_1 > e. \tag{A9}$$

Thus, in the context of an assumption of incomplete thermodynamic equilibrium, the addition of an internal degree of freedom to the model has so weakened the condition for the existence of asymmetric solutions that the condition can now be satisfied at some temperature. Since $C_2' < 0$, for any product $-C_2' e^{\beta\mu}/C_1$ we can choose i large enough to satisfy the condition (A9).

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