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Effective elementarity of resonances and bound states in statistical mechanics*

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Operational criteria are presented for determining those bound states and resonances which can approximately be included in the complete set of states in the S-matrix formulation of statistical mechanics. The criteria depend only on the energy dependence of S-matrix elements, as compared to the energy scales determined by the temperature and density. They are thus expressible free of nonrelativistic potential-theory language, and are hopefully valid for relativistic hadron systems as well. As an application, it is shown that the Δ resonance can be effectively treated as an elementary species under the temperature and density conditions encountered in neutron stars, while nuclei such as the deuteron can be ignored to lowest approximation. Possible conflicts with the Pauli principle, as invoked between the "constituents" of composite resonances and bound states on the one hand and free particles on the other, are resolved.

I. INTRODUCTION

In the quantum statistical mechanics of a nonrelativistic system, the grand partition function Z is defined by

$$Z = \mathrm{Tr} e^{-\beta(H-\mu)}, \tag{1}$$

where H is the total Hamiltonian. The value of μ, the total chemical potential operator for any given state depends on all its internal quantum numbers, and the trace is taken over a complete set (say, the plane waves) of states of all possible numbers of "elementary" particles. Once Z is known, the thermodynamic behavior of the system can be deduced.

The prescription in Eq. (1) is satisfactory for most nonrelativistic systems of interest. For example, in atomic systems at $\beta^{-1} \equiv kT \simeq$ ionization energy, free states of nuclei, electrons, and photons form a satisfactory complete set, with H well defined in that basis. In the MeV energy range (nuclear physics), protons and neutrons instead of nuclei act as elementary particles. While H is not so well known here, thanks to the complicated nuclear two-body force and uncertain many-body forces, the choice of neutrons and protons as elementary particles with their respective statistics is well supported by the structure of large nuclei.

Unfortunately, in relativistic systems, particularly ones involving hadrons, there is no clear knowledge of which particles are elementary or of what the Hamiltonian should be in a basis constructed from them. Nor is it certain that either "elementarity" or the Hamiltonian operator will remain as viable concepts, if and when a fully satisfactory dynamical theory of such systems becomes available.

It is therefore better, from the point of view of extending quantum statistics to relativistic systems, to use an alternate prescription for Z in the place of (1). The S-matrix formalism of statistical mechanics[1] provides a candidate. Therein,

$$\ln Z = \sum_i \ln Z_0^{(i)} + \frac{1}{2\pi i} \sum_{\{n_i\}} \int dE\, e^{-\beta(E-\mu)} \left[\mathrm{Tr}_{\{n_i\}} A S^{-1}(E) \frac{\partial}{\partial E} S(E) \right]_c . \tag{2}$$

The label i runs over all species of *stable* particles. The trace is taken over all plane-wave states of every set $\{n_i\}$ with n_i particles from the ith stable species. The other symbols in (2) are defined in Ref. 1 and the preceding paper.[2]

Equation (2) is derived[1] from potential theory,

where it is exact. Since it involves, first, all stable particles with no distinction between elementary and composite ones, and second, the S matrix instead of H, it lends itself to extension to relativistic systems as well.

However, in practice, the exact equation (2) is too cumbersome to use in its fullness for the following reasons:

(i) The summation i goes over *all* asymptotic states, bound or elementary. Not only are free-particle terms and S matrices of protons, electrons, etc. to be included, but also those of large nuclei, the hydrogen atom, the uranium atom, large molecules, and so on. Physically, one expects that this summation over an endless number of loosely bound states should not be necessary at some given finite T.

(ii) The summation does not go over unstable particles. Even relatively long-lived particles like the neutron enter Eq. (2) only as resonances in the S-matrix contribution from stable particles. Thus, formally, a gas of noninteracting neutrons would have to be treated as an interacting system of protons, electrons, and neutrinos. Similarly, consider a gas of atoms at low enough temperature so that only a few excited states above the ground state are occupied. Because the excited atomic states are unstable, they would occur in Eq. (2) through complicated S matrices of e-p-γ, or γ–ground-state scattering, whereas we know it should be possible to treat the system as essentially a noninteracting one, provided ideal-gas terms for the ground-state *and* excited-state atoms are used.

In other words, it would be better in practice to approximate the exact sum over all stable species (asymptotic states) in Eq. (2) by a reduced sum, depending upon the temperature and density range of interest. This approximate reduced sum should exclude all "loosely" bound states (to be suitably defined), but should include certain narrow resonances. We show in this paper that such a replacement can be done and provide criteria for determining which resonances and asymptotic states are "effectively elementary," i.e., appear in the reduced sum over states.

We will present the discussion in potential-theory language, where Levinson's theorem is valid. But the criteria obtained will be solely in terms of the energy dependence of S-matrix elements. If this behavior of S matrices is available from experiment, or from any other source, it can be directly used in our results, regardless of whether the underlying mechanism was potential theory or not. The validity or the provability of Levinson's theorem will not matter as long as S matrices behave in a certain way. Finally, information about S matrices will be needed only for energies up to an energy scale determined by kT and the density, and not for all energies.

In Sec. II we develop these ideas for resonances and also apply them to examples. It will be seen that the narrowness of width is a necessary, but not sufficient condition for treating a resonance as if it were an elementary species. Not surprisingly, the additional conditions will be seen to be very well satisfied for all ranges of temperatures and density of interest, by pions, neutrons, Λ, Σ, etc. Thus the common use of these particles as elementary—even though they are unstable—is justified from our point of view for all statistical ensembles of physical interest.

More interestingly, we find that the Δ or 3-3 resonance can also be treated as a separate elementary particle for the conditions of temperature and density encountered in neutron stars. It is seen that this does *not* conflict with exclusion principle between nucleons in the medium and the nucleon "inside" the Δ resonance. Of course, the large width of the Δ necessitates large corrections, which amount to saying that interactions of the Δ with the medium may be substantial (see also Sec. IV).

In Sec. III we deal with loosely bound states, once again giving operational criteria on S-matrix elements to help weed out loosely bound states from the sum in Eq. (2). An appendix, promised in the preceding paper, is also provided. It clarifies the role of the $\partial/\partial E$ operation in Eq. (2), which should be useful not only for the full understanding of these two papers, but for all applications of the S-matrix formula for the grand partition function.

II. RESONANCES

It might seem that the preceding paper (I) has already obtained the desired result as far as resonances are concerned. It was shown that systems which interacted solely through narrow-resonance formation behaved as though there were an additional species corresponding to the quantum numbers of the resonance. The analysis there was, however, incomplete.

First, the narrow resonance in (I) behaved like an elementary particle with its own separate statistics. This is puzzling, at least in potential theory, where one would expect the resonance to be a composite object whose "wave function" should obey symmetrization constraints with its constituent species. Second, the only condition on the resonance required in (I) was that it be narrow in order that it behave like a separate elementary particle. But the narrowness of width does not

ensure elementarity. Even when the width is zero (bound states), the object could be composite so that some symmetry constraint may be expected with respect to its constituent species.

These questions are resolved by appealing to ideas that parallel Levinson's theorem, which provide an additional criterion besides narrowness of width, for treating a resonance approximately as an additional species in the sum (2).

To see this, let us return to the example in Sec. II of the preceding paper, where π^- and n interacted solely through narrow-resonance formation. By this we meant that the $\pi^- n$ amplitude consisted of just one term corresponding to a narrow elastic S-wave resonance,

$$\langle p'k' \mid T(E) \mid pk \rangle = \frac{(2\pi)^3 g^2 \delta(\vec{p}+\vec{k}-\vec{p}'-\vec{k}')}{E-[M^2+(\vec{p}+\vec{k})^2]^{1/2}+i\Gamma}, \quad (3)$$

where g^2 and Γ tend to the limit zero. Corresponding, unitarily consistent many-particle scattering matrices were also then introduced, and the virial series in Eq. (2) evaluated. Let us just look at the lowest virial term, which depends only on the two-particle $\pi^- n$ amplitude. This term just reduces to the Beth-Uhlenbeck formula,[3]

$$\ln Z - \ln Z_0 = V \int \frac{d^3P}{(2\pi)^3} e^{\beta(\mu_n+\mu_\pi)} b_2(P) + \text{higher virial terms}, \quad (4)$$

where

$$b_2(P) = \sum_l \frac{(2l+1)}{\pi} \int d\epsilon \exp[-\beta(\vec{P}^2+\epsilon^2)^{1/2}] \frac{\partial}{\partial\epsilon}[\delta_l(\epsilon)], \quad (5)$$

where ϵ and $\delta_l(\epsilon)$ are the c.m. energy and phase shift, respectively. Now, the amplitude Eq. (3) corresponds to a phase shift

$$\delta_l(\epsilon) = \delta_{l0}\pi\theta(\epsilon - M). \quad (6)$$

When Eq. (6) is substituted in Eqs. (4) and (5), one obtains an "ideal"-Boltzmann-gas term due to the resonance as though it were stable. [The higher virial terms from the many-particle S matrices convert this to a Fermi-Dirac ideal gas as seen in (I), but let us stay with the lowest virial coefficient for the moment.]

In potential theory, however, our initial assumption for the elastic amplitude Eqs. (3) or (6) is not permitted. This is because of Levinson's theorem, which states (where ϵ_0 is the threshold) that

$$-\pi[\delta(\infty)-\delta(\epsilon_0)] = -\pi \int_{\epsilon_0}^{\infty} d\epsilon \frac{\partial}{\partial\epsilon}\delta_l(\epsilon) = \text{number of bound states} = 0 \quad (7)$$

for a system with no bound states. Our phase shift Eq. (6) by contrast started from zero at threshold, jumped to π around $\epsilon = M$, and stayed constant thereafter. This was the cause behind the contradictory result that the resonance behaved completely like an independent elementary particle, even though it was composite.

Even if the dynamics is dominated solely by narrow-resonance formation, the phase shift in Eq. (6) is not an adequate representation of such an interaction in potential theory. Let us replace Eq. (6) by the phase-shift in Fig. 1(a), which has just enough structure besides the resonance, to satisfy Levinson's theorem.

Note that b_2 involves the function

$$\sum_l f_l(\epsilon) = \sum_l \frac{2l+1}{\pi}(\partial/\partial\epsilon)[\delta_l(\epsilon)],$$

which is nothing but the change in the density of states at c.m. energy ϵ due to the interaction.[3] The S-wave phase shift in Fig. 1(a) provides $f_0(\epsilon)$ with two pieces, a positive $f_R(\epsilon)$ due to the resonance which *adds* one extra state at $\epsilon \simeq M$ and a negative Levinson compensating piece $f_L(\epsilon)$, which effectively *removes* one state from the energy region between ϵ_1 and ϵ_L. (Such language,

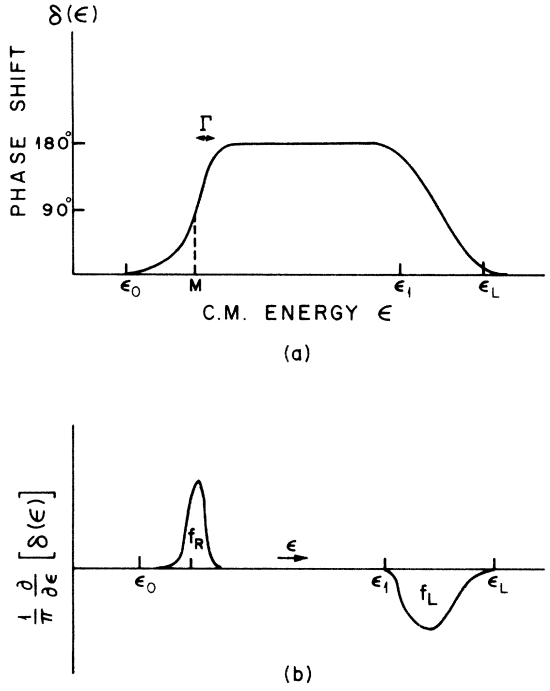

FIG. 1. (a) A prototype phase shift containing a narrow resonance at $\epsilon = M$, and minimal structure needed to satisfy Levinson's theorem in the absence of bound states, viz, $\delta(0) = \delta(\infty)$. (b) The difference in density of states in the c.m. frame produced by this interaction, related to the derivative of the phase shift in (a).

while convenient for our purposes here, must be used with care. There is no pole in the S matrix, nor a negative-norm state corresponding to the piece f_L. While f_R which is due to a resonance pole can be as narrow as it likes, the width of f_L is restricted by the inverse range of the potential, as pointed out long ago by Wigner.[4] When the phase shift in Fig. 1(a) is substituted into the Beth-Uhlenbeck formula [Eq. (5)], clearly three regions of interest emerge:

(i) $\beta^{-1}=kT\ll M$. Here $\exp[-\beta(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}]$ is very small throughout the energy region where scattering takes place and $b_2\simeq 0$. This is the trivial case when the system is not hot enough to provide energy for the particles to interact via the mechanism in Fig. 1.

(ii) $kT\gg\epsilon_L$. Here $e^{-\beta\epsilon}$ is nearly unity throughout the region where $\delta(\epsilon)$ exists. Thus

$$\begin{aligned} b_2(P)&\simeq\{\exp[-\beta(\vec{\mathbf{P}}^2+\epsilon^2)^{1/2}]\}_{\epsilon=0}\frac{1}{\pi}\int d\epsilon\,\frac{\partial}{\partial\epsilon}[\delta_0(\epsilon)]\\ &=\{\exp[-\beta(\vec{\mathbf{P}}^2+\epsilon^2)^{1/2}]\}_{\epsilon=0}\int[f_R(\epsilon)+f_L(\epsilon)]d\epsilon\\ &=\{\exp[-\beta(\vec{\mathbf{P}}^2+\epsilon^2)^{1/2}]\}_{\epsilon=0}[-\delta(\epsilon_0)+\delta(\infty)]\\ &=0. \end{aligned}\tag{8}$$

The "extra state" picked up at $\epsilon\sim M$ is wiped out by the negative contribution f_L. This is just an example of the general rule that at very high temperatures, the effect of any potential disappears.

(iii) $M\lesssim kT\ll\epsilon_L,\epsilon_1$. This is the interesting case where the Boltzmann factor $e^{-\beta\epsilon}$ is sizable near M, but vanishes near ϵ_1. Thus, the piece f_R is picked up in b_2 but the Levinson compensation f_L is not. Hence,

$$\begin{aligned} b_2(P)&\simeq\frac{1}{\pi}\int d\epsilon\,\exp[-\beta(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}]\frac{\partial}{\partial\epsilon}[\delta(\epsilon)]\\ &\simeq\exp[-\beta(M^2+\vec{\mathbf{P}}^2)^{1/2}]\int d\epsilon f_R(\epsilon)\\ &=\exp[-\beta(\vec{\mathbf{P}}^2+M^2)^{1/2}]. \end{aligned}\tag{9}$$

In this limited temperature range, we thus recover the ideal-gas term.

There is, however, no contradiction between this apparent elementarity versus the actual compositeness of the resonance in potential theory. Notice that this operational elementarity occurs only for $kT\ll\epsilon_1,\epsilon_L$. The range ϵ_1 to ϵ_L may be roughly interpreted as the range of kinetic energy of the constituents inside the resonance. This interpretation is motivated by Wigner's time-delay argument that in potential theory $\{-(\partial/\partial q)[\delta(q)]\}<a$, where a is the range of the potential and q is the c.m. relative momentum. In fact, for a square-well potential of range a, the phase shift vanishes asymptotically as

$$\delta_l(q)\underset{q\to\infty}{\sim}\frac{\text{constant}}{qa}.$$

Hence the momentum q_L (corresponding to the c.m. energy ϵ_L) at which $\delta_0(q)$ returns to zero is indicative of the inverse range of the potential, which in turn gives the typical momentum of the constituents in the resonance wave function. On the other hand, $kT\ll\epsilon_L$. Thus, the typical momenta of the π^- and the neutrons in the medium which are of the order of kT are much smaller than and do not overlap with the momenta of the constituent n and π^- "inside" the resonance. This very qualitative argument has been provided only to help understand why, in this limited range of temperature, even a composite resonance is effectively elementary. If the momenta of the constituents of the resonance and the momenta of the corresponding free particles in the medium are in different energy range, it is clear why neglect of symmetrization or antisymmetrization (the Pauli principle) between the two groups is a good approximation.

Furthermore, while we have used the language of potential theory and Levinson's theorem, operationally it is not necessary either that potential theory be valid or that Levinson's theorem be true. As long as the basic formula [Eq. (2)] for $\ln Z$ is valid, and S matrices exhibit experimentally the stated criteria, our results are valid.

This is because, as far as thermodynamics at some temperature T is concerned, the behavior of $\delta(\epsilon)$ for $\epsilon\gg kT$ does not make any difference. Its effect on the partition function is damped out by the Boltzmann factor $\exp[-\beta(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}]$. Thus, in our example in Fig. 1(a), if the phase shift had not fallen back to zero by $\epsilon=\epsilon_L$, but had instead remained constant at π for $\epsilon>M$, this would make no operational difference to $\ln Z$ for $kT\ll\epsilon_L$. For instance, if the dynamics underlying the resonance had not been potential theory, then the phase shift, having jumped up to π at $\epsilon=\epsilon_R$, need never return to zero. This could mean that the resonance was "truly" elementary. In practice, one may never know this information, inasmuch as scattering data will be available only up to some finite energy. However, for a system at temperature T, this knowledge of absolute elementarity is not needed. As long as the phase shift does not return to zero at energies of the order of kT, the resonance is effectively elementary, regardless of what happens at higher energies.

Thus, at least in the context of the lowest virial coefficient b_2 and an elastic resonance-dominated two-particle scattering amplitude, an operational criterion emerges for when the resonance acts

elementary: The phase shift should not have returned to zero by energies of order kT. This requirement has nothing to do with the narrowness of the width Γ. The smallness of Γ is of course an additional condition necessary for proving elementarity, as the proof in the preceding paper shows.

So far, the discussion was restricted to b_2. At high densities, all the higher virial coefficients in (2) also contribute. The principles outlined above also apply to them, although the analysis is more complicated since many-particle S matrices are involved. The higher virial terms have the form

$$\int d^3p_1 \cdots d^3p_n \prod_i \left(\frac{1}{e^{\beta(e_i-\mu_i)}\pm 1}\right) \left\langle p_1 \cdots p_n \left| \left[AS^{-1}(E)\frac{\partial}{\partial E}S(E)\right]_c \right| p_1 \cdots p_n \right\rangle \tag{10}$$

due to n interacting particles. Exchanges with noninteracting lines have already been included[2] in converting the Boltzmann factor $e^{-\beta(e_i-\mu_i)}$ into Bose or Fermi occupation members $\{\exp[\beta(e_i-\mu_i)] \pm 1\}^{-1}$.

As a result, the energy cutoff is determined by these occupation probabilities. For low-temperature systems involving degenerate fermions (as in the case of a neutron-star interior), the Fermi energy E_F takes on the role that kT did in our earlier discussion. Given the phase shift of Fig. 1(a), if $M < E_F < \epsilon_1$, the resonance will contribute as an additional species. Assuming that Levinson compensation does take place by some energy ϵ_L, we see that the resonance will be canceled away at high enough densities when $E_F > \epsilon_L$.

It is worth mentioning that in neutron-star interiors, the density is in the range of 10^{15}–10^{16} g/cm^3, which corresponds to E_F in the range of hundreds of MeV. The 3-3 phase shift[5] in πN scattering (see Fig. 2) rises from zero to π at the Δ resonance energy $E_R = m_\Delta - m_\pi - m_n \simeq 150$ MeV. After that, the phase shift remains essentially constant near 180° for several hundred MeV, before inelasticity sets in strongly, making the phase shift hard to extract. Therefore at neutron-star densities Levinson compensation does *not* take place and the Δ can be considered as a separate species. Of course, in reality the Δ is not narrow. Corrections for this and for nonresonant π-N interactions will have to be added on as pointed out in (I) and in the Conclusion.

In discussing higher virial terms, this criterion on the 2-body phase shift must also hold as extended to the many-body S matrices. In potential theory, Levinson's theorem can be extended[1] to many-particle S matrices. For a set of conserved quantum numbers μ,

$$\frac{1}{2\pi i}\int_0^\infty d\epsilon \left[\mathrm{Tr}_\mu AS^{-1}(\epsilon)\frac{\partial}{\partial\epsilon}S(\epsilon)\right]_c = -[\text{number of bound states}]_\mu, \tag{11}$$

where ϵ is the c.m. energy and the trace is taken in the c.m. frame. The right-hand side is zero if we assume no bound states, as in our example here. Now, in (I) we showed that the resonance behaves like an elementary particle with its correct statistics, provided the many-particle S matrices are as defined in (I). They were defined as all possible graphs made of stable particle and resonance propagators. This choice will not satisfy Levinson's theorem [Eq. (11)], as the two-particle example [which could be written simply in terms of the phase shift in Eq. 6] showed. Therefore, in addition to the piece $S_R^{(n)}$ defined in (I), the n-particle S matrix must contain, in potential theory, some Levinson-compensating piece $S_L^{(n)}$, so that Eq. (11) may be satisfied. However, if $[S_L^{(n)}]^{-1}(\partial/\partial\epsilon)[S_L^{(n)}]$ exists only at much higher energies than $[S_R^{(n)}]^{-1}(\partial/\partial\epsilon)[S_R^{(n)}]$, *and* if kT (or E_F, in the case of degenerate fermions) lies in between these two energy regions, then, and only then, will the result of (I) survive. In principle, this will have to be verified operationally for every n-particle S matrix—clearly impossible in practice. However, it is reasonable to expect that if the elastic 2-particle phase shift satisfies the stated criteria at some kT and E_F, the many-particle S matrices, governed by the same dynamics, will do the same.

We have already applied these ideas to the Δ

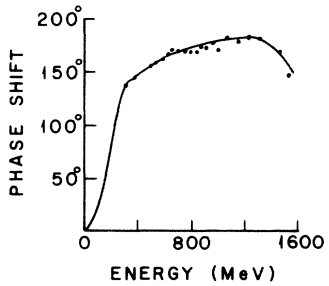

FIG. 2. The πN phase shift in the 3-3 channel as a function of lab energy in MeV. Note that the phase shift rises rapidly due to the Δ resonance, and does not begin to fall until 1,000 MeV or so. Strong inelasticity makes measurement of $\delta(\epsilon)$ harder at higher energies. The graph indicates qualitatively that Δ is effectively elementary until kT or the Fermi energy approaches 1 GeV.

resonance in neutron states. We found that the elastic πN phase shift indicates that the treatment of Δ as a separate species is valid at neutron-star densities. As another example, consider the treatment of pions, muons, neutrons, etc., as elementary although they are unstable. Strictly speaking, the pion, for instance, will first enter the virial series [Eq. (2)] formally as a ν-e resonance. Now, the ν-e scattering amplitude is expected to be very small (of the order G_{weak}) except at total c.m. energy $\epsilon = M_\pi$. At this energy, the ν-e system will resonate as a pion, with a large amplitude of order unity. The phase shift, essentially zero for $\epsilon < M_\pi$, will jump up to π at this energy. For $\epsilon > M_\pi$, it is again expected to vary slowly. Levinson compensation, if it takes place at all, will require energies of order $1/\sqrt{G}$, which is about 300 GeV. No system of interest has either a temperature or Fermi energy of that magnitude. Thus, the pion, to an excellent approximation, can be treated as a separate elementary species in statistical ensembles of interest—as one has always done in practice.

III. LOOSELY BOUND STATES

We now apply the ideas of the previous section to discard loosely bound states, as defined below, from the virial sum in Eq. (2). At the technical level there is a difference between the way resonances enter the problem as distinct from stable states. The original formula [Eq. (2)] contains no resonances in the sum over states. Resonances enter solely through the S matrices. The technically involved analyses of the preceding paper were needed to show that narrow-resonance-dominated S matrices, when substituted in the interacting terms in [Eq. (2)], lead to what looks like an additional ideal-gas term with appropriate statistics. This part of the work is not needed for bound states in that Eq. (2) already involves all bound and elementary states, both in the ideal-gas term $\ln Z_0$, as well as the trace in the $S^{-1}(\partial/\partial E)S$ term.

Instead, our purpose here is to show that the effect of loosely bound states in both the ideal-gas contribution $\ln Z_0$ and in $\mathrm{Tr}[S^{-1}(\partial/\partial\epsilon)S]$ are canceled off by the low-energy structure of the S matrices. The physical motivation for anticipating such a result is evident. For a thermodynamic system where the temperature and density set up some energy scale, one does not expect phenomena operating at a much lower energy range to be significant. For instance, in a gas with $kT \simeq 1$ keV, one does not expect molecules or the hydrogen atom to be present in sizable quantities. One customarily ignores such loosely bound species and their interactions with other particles in calculating the equation of state. A less clear-cut illustration arises higher up in the energy scale. Nuclei, as, for instance, the deuteron or α particles are not usually included in the set of states considered in dealing with phenomena where kT or the Fermi energy are in the hundreds of MeV. Calculations of neutron-star interiors or thermodynamic models of elementary particle physics are examples of such phenomena.

But the S-matrix formula for the partition function in Eq. (2) involves both ideal-gas terms and scattering contributions from all stable species, including all bound states, however loosely they may be bound. This is because Eq. (2) is meant to be valid at all temperatures and densities. For a given temperature and density range however, it should be possible to show that comparatively low-energy phenomena including loosely bound states can be neglected in Eq. (2). We show this and present criteria stated entirely in S-matrix language for determining what constitutes a loosely bound state and when it can be neglected.

The results of this section will be analogous to what we did for resonances in Sec. II, where the effective elementarity of a resonance proved in the preceding paper could be canceled by a Levinson compensation piece of the S matrix, provided the latter existed and occurred at energies less than kT and Fermi energies.

As before, we will work in potential-theory language, but evolve criteria that depend only on the observable behavior of S-matrix elements. We start with two particles "a" and "b" which scatter through a weak long-range S-wave potential V. Let the potential lead to one bound state B_{ab} of mass M and a phase shift $\delta(\epsilon)$. Generalization to several bound states and all partial waves is straightforward, but omitted here for simplicity.

To lowest order in fugacity (i.e., the coefficient of $e^{(\mu_a+\mu_b)\beta}$) there are two contributions to $\ln Z$. One is the ideal-gas term due to the bound state giving

$$V e^{\beta(\mu_a+\mu_b)} \int_0^\infty \frac{d^3P}{(2\pi)^3} \exp[-\beta(\vec{\mathbf{P}}^2 + M^2)^{1/2}]. \tag{12}$$

The other comes from the scattering of a with b giving

$$V e^{\beta(\mu_a+\mu_b)} \int_0^\infty \frac{d^3P}{(2\pi)^3} \int_{\epsilon_0}^\infty d\epsilon \exp[-\beta(\vec{\mathbf{P}}^2 + \epsilon^2)^{1/2}] \times \frac{1}{\pi}\frac{\partial}{\partial\epsilon}[\delta(\epsilon)]. \tag{13}$$

In potential theory, Levinson's theorem for this example implies that

$$[\delta(\infty) - \delta(\epsilon_0)] = -\pi. \tag{14}$$

[We ignore Castillejo-Dalitz-Dyson (CDD) poles. If present, they would effectively add more elementary particles.] Equation (14) tells us that the phase shift will begin at π at threshold and go to zero as $\epsilon \to \infty$. Let us suppose that the phase shift is negligible beyond $\epsilon = \epsilon_L$. If the temperature is high enough, i.e., $kT \gg \epsilon_L$, then $\exp[-\beta(\vec{P}^2 + M^2)^{1/2}]$ and $\exp[-\beta(\vec{P}^2 + \epsilon^2)^{1/2}]$ are not significantly different from each other for all $\epsilon < \epsilon_L$. Thus, given Eq. (14), the contributions Eqs. (12) and (13) cancel each other. The situation is identical to the previous discussion of resonances, except that the ideal-gas term [Eq. (12)] is already present in Eq. (2) for a bound state, whereas the corresponding term for the resonance arose out of the resonance pole in the S matrix. Generalization of this to higher virial coefficients follows along similar lines as in Sec. II, and it is clear that for degenerate fermions, the Fermi energy ϵ_F must be much larger than ϵ_L for the bound state to be canceled away by the phase shift. It is also clear that our definition of a "weak long-range" potential V giving a "loosely bound" state is a temperature- and density-dependent definition, stated precisely by the condition $kT \gg \epsilon_L$, or for low temperature degenerate fermions, $\epsilon_F \gg \epsilon_L$. Note that the energy ϵ_L is defined here independently of potential theory, as the point beyond which $\delta(\epsilon)$ is nearly zero. Assuming that experiment does yield such an ϵ_L, we see that the corresponding bound state in that channel is canceled away by the scattering for kT (or ϵ_F) $\gg \epsilon_L$.

Before proceeding further, note that the D function is defined in S-matrix theory by[6]

$$D(\epsilon + i\eta) = \left(1 - \frac{M}{\epsilon}\right) \exp\left[-\frac{1}{\pi}\int_0^\infty \frac{\delta(\epsilon')}{\epsilon' - \epsilon - i\eta} d\epsilon'\right], \quad (15)$$

where, in our case there is one bound state at $\epsilon = M$. It obeys

$$\lim_{\eta \to 0} \frac{D(\epsilon + i\eta)}{D(\epsilon - i\eta)} = S^{-1}(\epsilon) = e^{-2i\delta(\epsilon)}, \quad (16)$$

where for simplicity we continue to work with only one partial (S) wave. Now, if $\delta(\epsilon) \cong 0$ for $\epsilon > \epsilon_L$, then

$$D(\epsilon) \cong 1 + \frac{\text{constant}}{\epsilon} \text{ for } \epsilon \gg \epsilon_L. \quad (17)$$

Further, if $\psi_\epsilon(r)$ is the scattering solution in the presence of the potential V, and $\psi^0_\epsilon(r)$ is the free-particle solution then

$$\left|\frac{\psi_\epsilon(r=0)}{\psi^0_\epsilon(r=0)}\right| = \frac{1}{|D(\epsilon)|} \to 1 \text{ for } \epsilon \gg \epsilon_L. \quad (18)$$

Finally, the density of states in the c.m. frame $\rho(\epsilon)$ in the presence of the interaction V and $\rho_0(\epsilon)$ in the absence of V are related by

$$\rho(\epsilon) - \rho_0(\epsilon) = \frac{1}{\pi}\frac{\partial}{\partial \epsilon}[\delta(\epsilon)] \quad (19)$$

so that for $\epsilon > \epsilon_L$, $\rho_0(\epsilon) = \rho(\epsilon)$. In other words, the extra (bound) state created by the potential V at $\epsilon = M$ is compensated by an effective loss of a state in the region between threshold and ϵ_L.

Keeping these assorted facts in mind, we proceed to a more interesting case, where there is a strong short-range force operating, in addition to the weak long-range force V that resulted in the loosely bound state. If the only interaction had been V, it is reasonable to assume that for $kT \gg \epsilon_L$ the higher virial terms in the expansion would also add up to zero along with possible (if any) many-particle bound states bound by V. But if there is a strong short-range potential U in addition, its effects on $\mathrm{Tr}[S^{-1}(\partial/\partial\epsilon)S]$ will survive even for $kT \gg \epsilon_L$, where ϵ_L corresponds to V. Nevertheless, if our assertion that loosely bound states do not matter at high kT is valid, then the scattering of the bound state B_{ab} with other particles due to the strong potential U should be canceled away by some pieces of the many-body scattering of the constituents a and b with these other particles. We demonstrate this for the three-particle case.

Consider two particles a and b as before, interacting through V_{ab} and producing the bound state B_{ab}, along with scattering states. Consider another particle c, which scatters with a and b, and with B_{ab} through a strong short-range potential U. Let the scattering due to U take place only when the particles are at a short distance from one another (short, as compared with the range of V_{ab} which is of the order of $1/\epsilon_L$).

Let us then collect contributions to the virial series (2) proportional to $\exp[\beta(\mu_a + \mu_b + \mu_c)]$. These clearly involve the scattering processes $(abc \to abc)$, $(B_{ab}, c \to B_{ab}, c)$, $(B_{ab}, c \to abc)$, and $(abc \to B_{ab}, c)$. The resulting contributions to $\mathrm{Tr}[S^{-1}(\partial/\partial\epsilon)S]_c$ are schematically shown in Fig. 3. Since, for simplicity, we have designed V_{ab} to act only between a and b, there will be no connected three-particle diagrams involving V_{ab} alone.

Following the method used in Ref. 1 for deriving our Eq. (2), we note that the diagrams in Fig. 3 arise from

$$C_{abc} \equiv \frac{1}{\pi}\int_0^\infty d\epsilon\, e^{-\beta\epsilon}\, \mathrm{Tr}\left(\frac{1}{E - H_0 - U} - \frac{1}{E - H_0}\right)_c, \quad (20)$$

where $H_0 = K + V_{ab}$ and $K = K_a + K_b + K_c$ = total kinetic energy operator. Note that since V_{ab} by itself cannot lead to three-particle-connected diagrams for the particles a, b, and c, H_0 instead of K can be

used in Eq. (20) as the unperturbed Hamiltonian. Following the methods of Ref. 1, Eq. (20) can be related to

$$C_{abc} \equiv \frac{V}{4\pi i}\int \frac{d^3P}{(2\pi)^3}\sum_{\Phi_\alpha} \exp[-\beta(\vec{\mathrm{P}}^2+\omega^2)^{1/2}] \times\left\langle \Phi_\alpha \left| S^{-1}(\omega)\frac{\vec{\partial}}{\partial\omega}S(\omega)\right| \Phi_\alpha\right\rangle_c , \tag{21}$$

where

$$\Phi_\alpha \equiv \Phi(\epsilon, i, \vec{\mathrm{p}}) = \begin{cases} \psi_{\epsilon,i}(\vec{\mathrm{r}}_{ab})e^{-i\vec{\mathrm{p}}\cdot\vec{\mathrm{R}}_{ab}}e^{i\vec{\mathrm{p}}\cdot\vec{\mathrm{r}}_c}, & \text{for } \epsilon > \epsilon_0 \\ \psi^B(\vec{\mathrm{r}}_{ab})e^{-i\vec{\mathrm{p}}\cdot\vec{\mathrm{R}}_{ab}}e^{i\vec{\mathrm{p}}\cdot\vec{\mathrm{r}}_c}, & \text{for } \epsilon = M \end{cases} \tag{22a}$$

and

$$\omega^2 = (\vec{\mathrm{p}}^2+m_c^2)+(\vec{\mathrm{p}}^2+\epsilon^2). \tag{22b}$$

In Eq. (22), $\psi_{\epsilon,i}(\vec{\mathrm{r}})$ are the scattering solutions in the relative coordinate of the pair (ab), with ϵ the c.m. energy and i denoting angular momentum quantum numbers. $\psi^B(\vec{\mathrm{r}})$ is the bound-state solution. Clearly, Φ_α are the complete eigenfunctions of zero total momentum of $H_0 = K + V$, including states composed of the bound pair B_{ab} and the free particle c. In Eq. (21), $S(\omega)$ is defined by[7]

$$S(\omega) = 1 - 2\pi i(\omega - H_0)T(\omega), \qquad T(\omega) = U + \frac{1}{\omega - H_0 + i\epsilon}T(\omega), \tag{23}$$

where H_0 is in the over-all c.m. frame. Now, since U is a short-range strong potential compared to V, one can use the impulse approximation on the $T(\omega)$ in Eq. (23) to write

$$T(\omega) \simeq U + \frac{1}{\omega - K + i\epsilon}T(\omega). \tag{24}$$

In this approximation, $T(\omega)$ is approximated by the scattering matrix due to U alone. The presence of V is of course felt by the fact that the states Φ_α are eigenstates of $K+V$. In other words, our approximation consists of saying that V gives rise only to "final-state interactions," changing the plane waves of the pair (ab) before and after scattering into scattering states (and the bound state) of the potential V. Such approximations are frequently used, for instance, in the high-energy scattering of hadrons with nuclei.

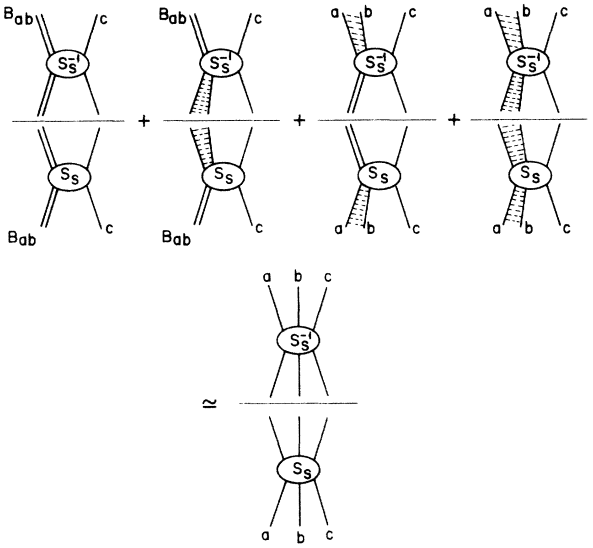

FIG. 3. The four contributions from $\mathrm{Tr}[S^{-1}(\partial/\partial\epsilon)S]$ giving the coefficient of $\exp[\beta(\mu_a+\mu_b+\mu_c)]$ in the strong short-range force U, while the dashed lines are final-state interactions due to the long-range force V, which also binds the bound state B_{ab} (double line). At high temperatures (see text), the four terms add up to just the short-range S-matrix effect, taken between plane-wave states of a, b, and c.

On substituting Eq. (23) into (21), there are as usual the linear terms $(\partial/\partial\omega)T$ and $(\partial/\partial\omega)T^\dagger$ and the bilinear term $T^\dagger(\partial/\partial\omega)T$. We will use off-energy-shell T matrices as defined by Eq. (23) and the off-energy-shell derivative $\partial/\partial\omega$. The equivalence of this to using on-energy-shell T matrices and derivatives has been discussed in Ref. 1 and in the Appendix of this paper. Consider the linear term in Eq. (21), given by

$$\frac{V(-2\pi i)}{4\pi i}\int\frac{d^3P}{(2\pi)^3}\int\frac{d^3p}{(2\pi)^3}\int d\epsilon\sum_i \exp[-\beta(\vec{\mathrm{P}}^2+\omega^2)^{1/2}]\rho_i(\epsilon)\frac{\partial}{\partial\omega}[\langle\psi_{\epsilon,i},\vec{\mathrm{p}}|\,T(\omega)+T^\dagger(\omega)|\,\psi_{\epsilon,i},\vec{\mathrm{p}}\rangle]_c . \tag{25}$$

Here $\rho_i(\epsilon)$ is the density of scattering (plus bound) states in the c.m. frame of the ab channel. We have included for notational simplicity, the bound state $\psi^B(\epsilon = M)$ as well in the set $\{\psi_{\epsilon,i}\}$ in Eq. (25). Thus, $\rho_i(\epsilon)$ contains a δ function at $\epsilon = M$ for the appropriate angular momentum index i.

Now, we note the following facts:

(a) The subspace of fixed $\vec{\mathrm{P}}$ and $\vec{\mathrm{p}}$ remains invariant under the action of the potential V_{ab}. Therefore for any operator Q,

$$\int d\epsilon\sum_i\langle\psi_{\epsilon,i}\vec{\mathrm{p}}|\,Q\,|\psi_{\epsilon,i}\vec{\mathrm{p}}\rangle\rho_i(\epsilon) = \int d\epsilon\sum_i\langle\psi^0_{\epsilon,i},\vec{\mathrm{p}}|\,Q\,|\psi^0_{\epsilon,i},\vec{\mathrm{p}}\rangle\rho^0_i(\epsilon), \tag{26}$$

where $\rho^0_i(\epsilon)$ and $\psi^0_{\epsilon,i}$ refer to the free system (ab)

in the absence of any potential.

(b) The expression in Eq. (25) is not quite the same as in Eq. (26) when we set $Q \equiv (\partial/\partial\omega)[T(\omega) + T^\dagger(\omega)]$ because of the Boltzmann factor $\exp[-\beta(\vec{P}^2 + \omega^2)^{1/2}]$ which depends on ϵ through Eq. (22b). However, we are working at high temperatures, where $\beta\epsilon_L \ll 1$, ϵ_L being as defined earlier for the ab system. Thus for $\epsilon < \epsilon_L$, the factor $\exp[-\beta(\vec{P}^2 + \omega^2)^{1/2}]$ is insensitive to ϵ and can be pulled out of the integral.

(c) This cannot be done for $\epsilon \gtrsim \beta \gg \epsilon_L$, but in this region, the short-distance behavior of $|\psi_{\epsilon,i}(r)|$ approaches that of the free solution $|\psi^0_{\epsilon,i}(r)|$, as shown in Eq. (18). Since T is a short-range effect (arising in the impulse approximation solely due to U), its matrix elements thus do not distinguish between ψ_ϵ and ψ^0_ϵ for large ϵ. Thus, for $\epsilon \gg \epsilon_L$,

$$\left\langle \psi_{\epsilon,i}, \vec{p} \left| \frac{\partial}{\partial\omega}(T + T^\dagger) \right| \psi_{\epsilon,i}, \vec{p} \right\rangle \simeq \left\langle \psi^0_{\epsilon,i}, \vec{p} \left| \frac{\partial}{\partial\omega}(T + T^\dagger) \right| \psi^0_{\epsilon,i}, \vec{p} \right\rangle . \quad (27)$$

(d) Finally, for $\epsilon \gg \epsilon_L$, the density of states equal, i.e., $\rho_i(\epsilon) \simeq \rho^0_i(\epsilon)$ [see Eq.(19)].

Combining these arguments, it is clear the contribution in Eq. (25) equals to a good approximation, when $\beta\epsilon_L \ll 1$,

$$\frac{V(-2\pi i)}{(4\pi i)} \int \frac{d^3P}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} \int d\epsilon \exp[-\beta(\vec{P}^2 + \omega^2)^{1/2}] \left\langle \psi^0_{\epsilon,i}, \vec{p} \left| \frac{\partial}{\partial\omega}(T + T^\dagger) \right| \psi^0_{\epsilon,i}, \vec{p} \right\rangle_c \rho^0_i(\epsilon) . \quad (28)$$

Clearly, Eq. (28) is the result one would have obtained had there been only the short-range interaction U and no long-range V, or the bound state B_{ab}. Both the matrix element and the sum over states in Eq. (28) involve only free-particle states of a, b, and c. The presence of the bound state in the initial (final) state has been canceled by the presence of low-energy final-state interactions in the initial (final) "abc" state.

This effect can be stated in purely S-matrix language. Consider the scattering process $abc \to abc$, whose scattering amplitude $\tau(\omega, \epsilon, \epsilon')$ will be a function of the total c.m. energy ω and the initial (final) subenergy ϵ (ϵ') of the pair (ab) in their own c.m. frame, apart from other variables. If there is a loosely bound state in the ab channel, then the amplitude $\tau(\omega, \epsilon, \epsilon')$ will have a pole at $\epsilon = M$ and $\epsilon' = M$ and significant structure for ϵ', $\epsilon > \epsilon_0$, the threshold. But beyond ϵ', $\epsilon = \epsilon_L$, where ϵ_L is as defined before, $\tau(\omega, \epsilon, \epsilon')$ will become smooth but continue to grow and be sizable due to the short-range interaction. Now the function $\bar{\tau}(\omega, \epsilon, \epsilon') \equiv D(\epsilon)\tau(\omega, \epsilon, \epsilon')D^*(\epsilon')$ with $D(\epsilon)$ as in Eq. (15) will be smooth even in the low $\epsilon < \epsilon_L$ region. The pole at $\epsilon = M$ in $\tau(\omega, \epsilon, \epsilon')$ will be canceled by the zero of $D(\epsilon)$, as will the low-energy structure and the pole at $\epsilon' = M$.

Operationally, if the three-particle (abc) amplitude $\tau(\omega, \epsilon, \epsilon')$ and the two-particle D function obtained from the phase shift exhibit these properties, viz.,

(i) $D(\epsilon)$ is nearly unity for $\epsilon >$ some ϵ_L, and is zero at $\epsilon = M$,

(ii) $\tau(\omega, \epsilon, \epsilon')$ has a pole at $\epsilon = M$ and considerable low-energy structure up to $\epsilon = \epsilon_L$, which, however, smoothens out for some range of $\epsilon > \epsilon_L$, and

(iii) the product $D(\epsilon)\tau(\omega, \epsilon, \epsilon')D^*(\epsilon')$ is free of the pole at $\epsilon, \epsilon' = M$ and is smooth starting from threshold,

then the situation is identical to what we described earlier in the language of potentials and wave functions. Under these circumstances our analysis indicates that the bound state can be ignored for $kT \gg \epsilon_L$. Only the scattering of $abc \to abc$ need be considered, and that too with a reduced amplitude $\bar{\tau}(\omega, \epsilon, \epsilon') = D(\epsilon)\tau(\omega, \epsilon, \epsilon')D^*(\epsilon')$. Note that $\bar{\tau}(\omega, \epsilon, \epsilon')$ will just be the extrapolation of the observed amplitude $\tau(\omega, \epsilon, \epsilon')$ from high values of ϵ and ϵ' smoothly to low values. The consequent neglect of low-energy structure is canceled by the neglect of the bound state and its scattering.

So far we dealt with terms linear in T and $T^\dagger$ since the effect in question is easiest to demonstrate there. A similar analysis is possible on the bilinear $T^\dagger(\partial/\partial\omega)T$ term as well, as we briefly sketch below. It has the form

$$\frac{V(2\pi)^2}{4\pi i} \int \frac{d^3P}{(2\pi)^3} \int \frac{d^3p d^3p'}{(2\pi)^6} \int d\epsilon\, d\epsilon' \exp[-\beta(\vec{P}^2 + \omega^2)^{1/2}] \times \sum_{ij} \rho_i(\epsilon)\rho_j(\epsilon') \left[\langle \psi_{\epsilon,i}, \vec{p} | T^\dagger(\omega) | \psi_{\epsilon',j}, \vec{p}' \rangle \delta(\omega - \omega') \left\langle \psi_{\epsilon',j}, \vec{p}' \left| \frac{\partial}{\partial\omega} T(\omega) \right| \psi_{\epsilon,i}, \vec{p} \right\rangle - \text{H.c.} \right] . \quad (29)$$

Much of the argument works in the same way as for the linear term. Once again, for large ϵ (or ϵ'), the free and interacting wave functions $\psi^0_{\epsilon,i}$ and $\psi_{\epsilon,i}$ have the same short-distance behavior which is all that matters for the T generated by the short-range U. Similarly $\rho_i(\epsilon)$ and $\rho_i(\epsilon')$ approach the free density of state functions $\rho^0_i(\epsilon)$ for $\epsilon > \epsilon_L$. Thus, for large ϵ and ϵ', the effect of the interaction V disappears from Eq. (29) for each ϵ and ϵ'. For small ϵ, since $\beta\epsilon_L \ll 1$, the Boltzmann factor is insensitive to ϵ. So is the energy-conserving function $\delta(\omega - \omega')$, as long as ω and ω' (which are the over-all c.m. energies of all three particles together) are large compared with ϵ_L. Apart from the low-ω region then, all the arguments used for the linear term are applicable here. The scattering and bound states due to V_{ab} can be replaced by plane waves.

Even for low ω, the error due to the neglect of the bound state and the final-state V interaction should tend to cancel. We content ourselves instead by observing that for high temperatures, the low-ω (order ϵ_L) region is a small part of the effective phase space. Further, $T^\dagger(\bar{\partial}/\partial\omega)T$ is expected to be small in this region. This is because T is due to a short-range force. It will be smooth in ω for low ω, and $T^\dagger(\bar{\partial}/\partial\omega)T$ involving the derivative of the imaginary part of T will be even smaller than $(\partial/\partial\omega)(\mathrm{Re}T)$ occurring in the linear term. Therefore residual effects due to the neglect of V in the low-ω region will not affect the contribution in Eq. (21) much.

More complicated examples, where more than three particles scatter and with bound states in more than one pair, can be similarly treated in principle, although the analysis will be more complicated.

We conclude with one example—the deuteron. The corresponding phase shift in the $I=0$, $J=1$ S-wave n-p scattering is shown in Fig. 4. The phase shift starts at 180° and falls off to zero by about 300 MeV. One can therefore certainly neglect the deuteron together with the triplet S-wave n-p scattering for $kT \gg 300$ MeV, or more interestingly for $\epsilon_F > 300$ MeV for cold degenerate nucleons. One might have expected the deuteron to be canceled out at lower temperatures or density, viz., of the order of 10 MeV which characterizes nuclear binding. This is partly a question of how Fig. 4 is interpreted and how much is retained as residual "strong short-range" n-p interaction. The phase shift in Fig. 4 initially falls very rapidly, a trend which if extrapolated would give $\delta(\epsilon)=0$ well before 100 MeV. Thus, the interaction can be considered as due to two parts—one which is relatively weak and long ranged and is responsible for nuclear physics and another which leads to the non-zero phase shift beyond, say, 50 MeV. The former, along with deuteron, may be neglected for kT or ϵ_F larger than tens of MeV, but the residual n-p scattering at higher energy must be retained in evaluating the partition function.

This at least qualitatively justifies the customary neglect of the deuteron and other nuclei as independent species in evaluating equations of state of neutron-star interiors.

IV. CONCLUSION

Our principal aim in this paper and the preceding one was to show how, in a purely S-matrix formalism of statistical mechanics, certain narrow resonances and stable states are effectively elementary, depending upon the temperature and the density. The main conclusion—that certain narrow resonances can be included, while all loosely bound states can be excluded from the complete set of states—should come as no surprise. Physicists have customarily been using such a restricted set of species, both stable and unstable, for any given situation. But the justification for this, particularly for unstable objects (resonances), has been vague. We hope our work makes it less so. We have also offered operational criteria, based only on S-matrix elements which are in principle measurable, for determining the elementarity of a given resonance or stable state. For resonances, this gave us a condition not so widely appreciated hitherto, viz. that narrowness of width alone does not ensure elementarity which requires a further condition on the S matrix in that channel. Even when the resonance was narrow and satisfied

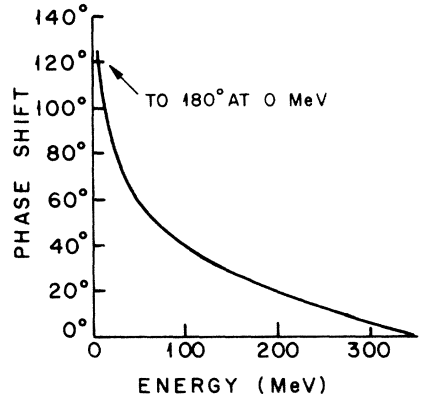

FIG. 4. The n-p phase shift (see Ref. 8) in the deuteron channel, which starts at 180° and falls to zero around 350 MeV. Note the steep fall at low energies, which, if extrapolated would have given a zero phase shift at nuclear-physics-type energies (well below 100 MeV).

the conditions of Sec. II, we saw that all the work of the preceding paper was needed to show that the S matrices implied by such a resonance result, to all orders in the virial series, in an ideal-gas term with the correct statistics.

An interesting question remains, which has nothing to do with elementarity or compositeness. Once all the resonances in the dynamics (satisfying the criteria of Sec. II) have been pulled out as additional ideal gases, one might ask how much residual interaction remains. Ideally it would be nice if "elementary" resonances saturated the dynamics, in which case the system would be effectively a sum of ideal gases. For a gas of hydrogen and photons at a temperature of an eV, if one includes apart from photons and the H ground state, also the H excited states (which are actually resonances) in the set of species, one finds the dynamics very well described by the resulting "ideal gases." Whether this is even nearly true for hadronic systems is not clear, although dual models and thermodynamic models of particle physics work on that assumption. In neutron-star interior calculations, the use of Δ as a separate species (which we have justified) certainly absorbs a great deal of the π-N interaction. However, considerable amounts of π-N and NN interactions still exist besides Δ formation, not to mention the interaction of the Δ with itself and with other particles. For a dense system, the effect of such nonresonant interactions continues to be a difficult problem to solve.

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APPENDIX

We make some remarks here on different ways of using the basic equation (2). Some of what follows is contained in Ref. 1, but in a somewhat compact form. A little elaboration may be helpful to anyone wishing to use Eq. (2) in practice, and to readers of this paper.

Since the S matrix has no dependence on the total space momentum, except through the δ function conserving it, Eq. (2) may be rewritten as[1]

$$\ln Z - \ln Z_0 = V \int \frac{d^3P}{(2\pi)^3} \sum_n e^{+\beta\mu_n} a_n(P) , \tag{A1}$$

where

$$a_n(P) = \frac{1}{4\pi i} \int d\omega \exp[-\beta(\omega^2 + \vec{P}^2)^{1/2}] \times \left[\mathrm{Tr}_n A S^{-1}(\omega) \frac{\vec{\partial}}{\partial \omega} S(\omega) \right]_c , \tag{A2}$$

$$S(\omega) = 1 - 2\pi i \delta(\omega - H_0) T(\omega) . \tag{A3}$$

The sum $\sum_n$ is over channels, each containing a given number of free stable particles with total chemical potential μ_n. The trace Tr_n in Eq. (A2) is to be taken in the c.m. frame, i.e., over a complete set of states with zero total space momentum in the channel n.

Customarily, one takes this trace in the momentum basis

$$\mathrm{Tr}_n \to \int \prod_{j=1}^{n} \frac{d^3 p_j}{(2\pi)^3 e_j} \delta^3 \left(\sum \vec{p}_j \right) . \tag{A4}$$

We will start here with a different description of states, in order to resolve unambiguously the operators $\partial/\partial\omega$ and $\delta(\omega - H_0)$ in $a_n(P)$. Let us describe each state in the channel in the c.m. frame by variables (ϵ, ξ), where ϵ is the total energy in the c.m. frame and $\{\xi\}$ stands for all the remaining variables needed. Since all subenergies in the c.m. frame can be scaled by ϵ, the set $\{\xi\}$ can be dimensionless. For example, a two-particle state in the c.m. frame can be described by (ϵ, θ, ϕ), where ϕ and θ denote the direction of the relative momentum $\vec{k}$. Such a choice for $\{\xi\}$ is not unique, nor need it be dimensionless. One could have labeled the two-particle state, for instance, by $(\epsilon, \epsilon\theta, \epsilon\phi)$ or (ϵ, k_x, k_y).

It is true that the energy derivative of the on-shell amplitude

$$[(\partial/\partial\epsilon) \langle \epsilon\xi_1 | T(\epsilon) | \epsilon\xi_2 \rangle]_{\xi_1, \xi_2 \text{ fixed}}$$

depends on the choice of the set $\{\xi\}$. But we will see that the final answer Eq. (A2) does not.

For a given choice (ϵ, ξ), let $\rho(\epsilon, \xi)$ denote the density of states. We include in $\rho(\epsilon, \xi)$ appropriate step functions to specify, if necessary, the finite range of any ξ variables. Thus,

$$\mathrm{Tr}_n \to \int_0^\infty d\epsilon \int_{-\infty}^{\infty} d\xi \, \rho(\epsilon, \xi) . \tag{A5}$$

ξ stands for several variables $\xi^{(1)}\xi^{(2)} \cdots \xi^{(s)}$ ($s = 2$ for the two-particle example), but in Eq. (A5) and below, we denote it by one variable ξ to save space.

Now, Eq. (A2) can be rewritten in a variety of ways, for instance,

$$a_n(P)=\frac{1}{2\pi}\int d\omega\exp[-\beta(\omega^2+\vec{\mathbf{P}}^2)^{1/2}]\frac{\partial}{\partial\omega}\{\mathrm{Im}[\mathrm{Tr}_n A\ln S(\omega)]_c\}$$

$$=\frac{-\beta}{2\pi}\int d\omega\exp[-\beta(\omega^2+\vec{\mathbf{P}}^2)^{1/2}]\frac{\omega}{(\omega^2+\vec{\mathbf{P}}^2)^{1/2}}\,\mathrm{Im}\left[\mathrm{Tr}_n A\sum_{r=1}^{\infty}[2\pi i\delta(\omega-H_0)T(\omega)]^r\frac{1}{r}\right]_c$$

$$=-\beta\sum_{r=1}^{\infty}\frac{1}{r}\int d\epsilon\int d\xi\exp[-\beta(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}]\left(\frac{\epsilon}{(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}}\right)\rho(\epsilon,\xi)\,\mathrm{Re}\langle\epsilon\xi|AT(\epsilon)[2\pi i\delta(\epsilon-H_0)T(\epsilon)]^{r-1}|\epsilon\xi\rangle_c\,. \tag{A6}$$

This form shows clearly how $a_n(P)$ is to be evaluated. Only on-shell T matrices $T(\epsilon)$ occur and can be inserted from a theoretical model, or directly from experiment. The energy derivative has been removed by integration by parts. The choice (ϵ,ξ) for state labels is not necessary in this form. If the T matrix were more naturally available in terms of, say, the momenta of all the particles, then $\int d\epsilon\,d\xi\,\rho(\epsilon,\xi)$ in Eq. (A6) would be merely replaced by Eq. (A4), with $\epsilon=\sum_j\epsilon_j$.

Equation (A6), however, involves an infinite series, which can be quite complicated to evaluate and sum. In some cases (as with the preceding paper I), it might be easier to revert to Eq. (A2), which is at most bilinear in T.

The linear term in T (and $T^\dagger$) in Eq. (A2) is simple. Upon inserting Eq. (A3) into Eq. (A2), we see that this linear term is

$$\frac{-2\pi i}{4\pi i}\int d\omega\exp[-\beta(\omega^2+\vec{\mathbf{P}}^2)^{1/2}]\frac{\partial}{\partial\omega}\{\mathrm{Tr}_n A\delta(\omega-H_0)[T(\omega)+T^\dagger(\omega)]\}_c$$

$$=\frac{-\beta}{2}\int d\epsilon\,d\xi\exp[-\beta(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}]\rho(\epsilon,\xi)\left(\frac{\epsilon}{(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}}\right)\langle\epsilon,\xi|A[T(\epsilon)+T^\dagger(\epsilon)]|\epsilon,\xi\rangle_c\,. \tag{A7}$$

The energy derivative again does not appear in Eq. (A7), and any on-shell T matrix can be substituted into it. In fact Eq. (A7) is just the first term in the series in Eq. (A6).

In the remaining term in Eq. (A2), energy derivative of the T matrix is unavoidable and cannot be integrated away by parts. Two possibilities arise. One may wish to use a theoretical model for $T(\omega)$, which gives an explicit off-energy-shell behavior of $T(\omega)$ with respect to ω. This was the case in the preceding paper. Since ω in such a case has nothing to do with state labels, the operation $(\partial/\partial\omega)T(\omega)$ and the result for $a_n(P)$ are trivially independent of the choice of state labels.

However, if one wished to use on-shell T matrices only, the

$$[\delta(\omega-H_0)T^\dagger(\omega)](\vec{\partial}/\partial\omega)[\delta(\omega-H_0)T(\omega)]$$

term in Eq. (A2) must be rewritten in terms of $T(\epsilon)$. This has been done in Eq. (3.40) of Ref. 1 (see also their erratum). That equation when written more fully in terms of state labels (ϵ,ξ) can be shown to be

$$a_n(P)-(\mathrm{A7})=\frac{4\pi^2}{4\pi i}\int d\epsilon\exp[-\beta(\epsilon^2+\vec{\mathbf{P}}^2)^{1/2}]$$
$$\times\int d\xi_1\int d\xi_2\left\{A[\rho(\epsilon,\xi_1)\langle\epsilon\xi_1|T^\dagger(\epsilon)|\epsilon\xi_2\rangle]\frac{\vec{\partial}}{\partial\epsilon}[\rho(\epsilon,\xi_2)\langle\epsilon\xi_2|T(\epsilon)|\epsilon\xi_1\rangle]\right\}_c\,. \tag{A8}$$

Note that in Eq. (A8), $\partial/\partial\epsilon$ acts on the full energy dependence of $\langle\epsilon\xi_2|T(\epsilon)|\epsilon\xi_1\rangle$ or $\langle\epsilon\xi_1|T^\dagger(\epsilon)|\epsilon\xi_2\rangle$, not distinguishing between the energy dependence of the operator $T(\epsilon)$ and that of the states. A phenomenological expression $T(\epsilon,\xi_1\xi_2)$ extracted from data can therefore be substituted for $\langle\epsilon\xi_2|T(\epsilon)|\epsilon\xi_1\rangle$ in Eq. (A8), if one so wished.

It is understood that the derivative $\partial/\partial\epsilon$ is taken keeping the other variables ξ_1 and ξ_2 fixed. If one had used some different set of variables, this partial derivative in general would be different. But we will show that this difference cancels out in the result for $a_n(P)$.

First, the derivatives of the density $\rho(\epsilon,\xi)$ will cancel out from Eq. (A7). Such terms have the form, in self-evident notation,

$$\int d\xi_1 d\xi_2 \left[\rho_1 T^\dagger{}_{12}\left(\frac{\partial}{\partial\epsilon}\rho_2\right)T_{21} - \left(\frac{\partial}{\partial\epsilon}\rho_1\right)T^\dagger{}_{12}\rho_2 T_{21}\right]$$
$$= \int d\xi_2 \frac{\partial\rho_2}{\partial\epsilon}\frac{(T^\dagger{}_{22}-T_{22})}{2\pi i} - \int d\xi_1 \frac{\partial\rho_1}{\partial\epsilon}\frac{(T^\dagger{}_{11}-T_{11})}{2\pi i}$$
$$= 0 \qquad \text{(A9)}$$

upon using the unitarity relation

$$T_{ij} - T^\dagger{}_{ij} = -2\pi i \int d\xi_k T_{ik}\rho_k T^\dagger{}_{kj}$$
$$= -2\pi i \int d\xi_k T^\dagger{}_{ik}\rho_k T_{kj}\,. \qquad \text{(A10)}$$

The term bilinear in T thus reduces from Eq. (A8) to

$$\frac{4\pi^2}{4\pi i}\int d\epsilon\, d\xi_1 d\xi_2 \exp[-\beta(\epsilon^2+\vec{P}^2)^{1/2}]\rho(\epsilon,\xi_1)\rho(\epsilon,\xi_2)$$
$$\times\left[A\langle\epsilon\xi_1|\,T^\dagger(\epsilon)|\epsilon\xi_2\rangle\frac{\vec{\partial}}{\partial\epsilon}\langle\epsilon\xi_2|\,T(\epsilon)|\,\epsilon\xi_1\rangle\right]_c . \qquad \text{(A11)}$$

Now suppose we had used a different set, say $(\epsilon, \bar{\xi}_2)$ for the labels of the intermediate state. As long as the transformation $\xi_2 \to \bar{\xi}_2$ did not depend on ϵ, $\partial/\partial\epsilon|_{\xi_2} = \partial/\partial\epsilon|_{\bar{\xi}_2}$ and the transformation will leave Eq. (A11) unchanged. Otherwise,

$$\left.\frac{\partial}{\partial\epsilon}\right|_{\bar{\xi}_2} = \left.\frac{\partial}{\partial\epsilon}\right|_{\xi_2} + \alpha\left.\frac{\partial}{\partial\xi_2}\right|_{\epsilon}, \qquad \text{(A12)}$$

where α is some function of ϵ and ξ_2. Then the change in Eq. (A11) is proportional to

$$\int d\xi_1 d\xi_2 \rho(\epsilon,\xi_1)\rho(\epsilon\xi_2)\alpha\left[T^\dagger{}_{12}\left(\frac{\partial}{\partial\xi_2}T_{21}\right)_\epsilon - \left(\frac{\partial}{\partial\xi_2}T^\dagger{}_{12}\right)_\epsilon T_{21}\right]$$
$$= \int d\xi_1 d\xi_2 \alpha\rho(\epsilon\xi_2)\left\{\left[\frac{\partial}{\partial\xi_2}T_{21}\rho(\epsilon,\xi_1)T^\dagger{}_{1n}\right]_{n=2,\epsilon\text{ fixed}} - \left[\frac{\partial}{\partial\xi_2}T_{n1}\rho(\epsilon,\xi_1)T^\dagger{}_{12}\right]_{n=2,\epsilon\text{ fixed}}\right\}$$
$$= \int d\xi_1 d\xi_2 \alpha\rho(\epsilon\xi_2)\frac{1}{(2\pi i)}\frac{\partial}{\partial\xi_2}(T^\dagger{}_{2n} - T_{2n} - T^\dagger{}_{n2} + T_{n2})_{n=2}$$
$$= 0$$

using the time-reversal-invariance property $T_{2n} = T_{n2}$. Therefore, even an ϵ-dependent change of variables from $(\epsilon\xi_2)$ to $\{\epsilon, \bar{\xi}_2(\xi_2,\epsilon)\}$ will not affect Eq. (A11).

To illustrate, consider a two-particle amplitude, usually written in terms of c.m. energy ϵ and momentum transfer Δ as $T(\epsilon,\Delta)$. This should first be rewritten in terms of separate initial- and final-state labels. For these we could choose, for instance, $(\epsilon, \theta_1, \phi_1)$ and $(\epsilon, \theta_2, \phi_2)$ or $(\epsilon, \epsilon\theta_1, \epsilon\phi_1)$ and $(\epsilon, \epsilon\theta_2, \epsilon\phi_2)$. Correspondingly, the amplitude will have different functional forms related by

$$T(\epsilon,\theta_1,\phi_1,\theta_2,\phi_2) = \bar{T}(\epsilon,\epsilon\theta_1,\epsilon\phi_1,\epsilon\theta_2,\epsilon\phi_2);$$

clearly,

$$\left.\frac{\partial}{\partial\epsilon}T\right|_{\substack{\theta_1\phi_1\\ \theta_2\phi_2}} \neq \left.\frac{\partial}{\partial\epsilon}\bar{T}\right|_{\substack{\epsilon\theta_1,\epsilon\phi_1\\ \epsilon\theta_2,\epsilon\phi_2}}.$$

Nevertheless, if T is unitary, either set of variables can be used in Eq. (A11) to give the same result. Along with the linear term Eq. (A7), the prescription for obtaining the virial series using on-shell amplitudes is thus unambiguous.

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