Applications of Scattering Theory to Quantum Statistical Mechanics

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A Laplace transform relation between the distribution function $\exp\{-\beta H\}$ in quantum statistical mechanics and the Green's function of the wave equation has been noted by Koppe. This relationship may be extended to the stationary-state scattering equation. General properties of the transformation are discussed. Applications to the evaluation of the virial coefficients are considered. A further application of the perturbation methods of Brueckner and his collaborators is described.

I. INTRODUCTION

THE evaluation of the thermodynamic functions in quantum statistical mechanics necessitates the evaluation of such quantities as

$$Z \equiv \mathrm{Tr}\{u(\beta)\}, \tag{1}$$

where

$$u(\beta) = \exp\{-\beta H\}. \tag{2}$$

Here H is the Hamiltonian for a system of N identical particles and $\beta \equiv \theta^{-1} \equiv (kT)^{-1}$, where T is the absolute temperature.

The Hamiltonian H can ordinarily be decomposed into the sum of a kinetic energy term K and a potential energy term V:

$$H = K + V,$$
$$K = \sum_{i=1}^{N} \frac{1}{2M} p_i^2, \tag{3}$$
$$V = \sum_{i<j=1}^{N} V_{ij}.$$

Here $\mathbf{p}_i$ is the momentum operator of the ith particle and M is its mass. The potential energy of interaction between the ith and jth particles is represented by $V_{ij} = v(\mathbf{r}_i - \mathbf{r}_j)$. It will prove convenient to express the pair (i, j) by a single index α, so

$$V = \sum_\alpha V_\alpha, \tag{4}$$

where the index α runs over all $\frac{1}{2}N(N-1)$ pairs.

A great variety of approximate methods for evaluating Eqs. (1) and (2) have of course been developed. When the "thermal" de Broglie wavelength, $\hbar/(M\theta)^{\frac{1}{2}}$, is small compared to regions over which $v(\mathbf{r}_i - \mathbf{r}_j)$ varies appreciably, the expansions of Wigner[1] and of Mayer and Band[2] in powers of $\hbar/\theta$ are useful. General methods of developing such expansions have been obtained by Goldberger and Adams[3] and by Goldberger and Gell-Mann.[4] These latter methods have made use of the fact that the differential equation satisfied by $u(\beta)$

$$\partial u/\partial\beta = -Hu, \tag{5}$$

is formally equivalent to the Schrödinger equation if β is replaced by it, permitting application of methods employed in quantum electrodynamics.

More recently, the similarity of (5) to the Schrödinger equation has been exploited by several different methods. Feynman[5] has used his path-integral technique to give a theory of liquid He. Kubo,[6] Schafroth,[7] Chester,[8] and Nakajima[9] have discussed perturbation expansions in powers of V. In these developments there is considerable similarity to quantum mechanical perturbation theory.

To our knowledge, the close relation of Eq. (5) to the stationary-state Schrödinger equation of scattering theory[10] has not been developed. Indeed, as we shall see in the next section, the Laplace transform of Eq. (5) leads directly to the stationary state scattering equation. At this point we have available the great variety of techniques for handling the scattering equation. We may, for instance, at the very outset formulate the problem in terms of the solutions to the two-body problem in quantum mechanics (which we may consider as a soluble problem, and for which there exist useful variational principles), eliminating completely any appearance of the potentials V_{ij} of Eq. (3). This involves applications of the quantum mechanical theory of multiple scattering.[11–13] In Sec. III, the evaluation of the virial coefficients with the use of variational principles will be considered.

In Sec. IV a method will be discussed for replacing the Hamiltonian H by one of the form $H = K(p) + V_C(p)$, where K and V_C are *functions* of the particle momenta rather than *matrices*. As will be seen in Sec. V, this is formally related to the problem of obtaining the index of refraction of a scattering medium (i.e.,

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[1] E. P. Wigner, Phys. Rev. **40**, 749 (1932).
[2] J. Mayer and W. Band, J. Chem. Phys. **15**, 191 (1947).
[3] M. L. Goldberger and E. N. Adams, J. Chem. Phys. **20**, 240 (1952).
[4] M. L. Goldberger and M. Gell-Mann (unpublished).
[5] R. D. Feynman, Phys. Rev. **91**, 1291 and 1301 (1953).
[6] R. Kubo, J. Chem. Phys. **20**, 770 (1952).
[7] R. Schafroth, Helv. Phys. Acta **24**, 645 (1951).
[8] G. V. Chester, Phys. Rev. **93**, 606 (1954).
[9] S. Nakajima, Phil. Mag. Suppl. **4**, 363 (1955).
[10] See, for instance, M. Gell-Mann and M. L. Goldberger, Phys. Rev. **91**, 398 (1953).
[11] K. M. Watson, Phys. Rev. **89**, 575 (1953).
[12] N. C. Francis and K. M. Watson, Phys. Rev. **92**, 291 (1953).
[13] Gyo Takeda and K. M. Watson, Phys. Rev. **97**, 1336 (1955).

the "optical model"), as was done by Francis and Watson.[12] It is even closer to the theory of nuclear binding of Brueckner and his collaborators.[14–17] By this method one does not have to expand the exponential in Eq. (2), for instance.

The use of contour integrals much like those which we shall encounter is already familiar in quantum mechanical perturbation theory[18,19] and in statistical mechanical perturbation theory.[9] Wentzel,[20] for instance, has formulated the eigenvalue problem in meson field theory in a form closely related to that which we shall use. His method has been extended to the evaluation of the quantity Z in Eq. (1) in unpublished work by Goldberger. Finally, it has been noted by Koppe[21] that a Laplace transform of $\exp\{-\beta H\}$ leads to the Green's function for the wave equation having H as its Hamiltonian. It is this latter observation which provides the starting point for our present application of stationary-state scattering theory to statistical mechanics.

II. GENERAL DEVELOPMENT

In the present section we shall discuss the properties of the Laplace transform of $u(\beta)$ and develop techniques for its evaluation.

Let us designate the eigenfunctions of H for our N particle system by $\psi_\lambda(\lambda=1, 2, 3, \cdots)$, so

$$H\psi_\lambda = E_\lambda \psi_\lambda. \tag{6}$$

To obtain a sensible statistical-mechanical problem, we must (in general) suppose that the system is enclosed in a box of finite volume $\mathcal{V}$, at the limits of which the ψ_λ satisfy appropriate boundary conditions. Under these conditions, we may suppose the states λ to be discrete and denumerable. For many calculations, however, it is convenient to let $\mathcal{V}\to\infty$ at certain stages of the calculation. This is done in order to replace sums over intermediate states by integrals. We shall henceforth refer to this as the "$\mathcal{V}(\infty)$ limit." We shall also assume (as is customarily done in quantum mechanics) that this limit is unique for any specified set of boundary conditions on the system. In particular, the set of states ψ_λ and the density of states λ are supposed to approach definite limits, the states ψ_λ remaining orthonormal in the "large" volume $\mathcal{V}$.

Let us denote the least of the eigenvalues E_λ by E_L:

$$E_L \leqslant E_\lambda \quad (\text{all } \lambda). \tag{7}$$

The matrix $u(\beta)$ is positive definite, having eigenvalues $e^{-\beta E_\lambda} > 0 (\lambda = 1, 2, \cdots)$, of which the greatest is $e^{-\beta E_L}$. Now let ϕ_a and ϕ_b be arbitrary, normalized state vectors (not necessarily belonging to the set ψ_λ), satisfying $(\phi_a, \phi_b)=0$. We may easily verify then the following inequalities[22]:

$$\begin{aligned} E_L &\leqslant (a|H|a), \\ e^{-\beta E_L} &\geqslant (a|u(\beta)|a) \geqslant 0, \\ |\mathrm{Re}(b|u|a)| &\leqslant e^{-\beta E_L}, \\ |\mathrm{Im}(b|u|a)| &\leqslant e^{-\beta E_L}. \end{aligned} \tag{8}$$

Conditions (8) imply the convergence of the Laplace-transform integral

$$W(E) = -\int_0^\infty e^{E\beta} u(\beta) d\beta, \tag{9}$$

where E is a complex number and

$$\mathrm{Re}[E] < E_L. \tag{10}$$

The inversion of Eq. (9) is

$$u(\beta) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{-E\beta} W(E) dE. \tag{11}$$

Here c is real and[23]

$$c < E_L.$$

For brevity, the contour in Eq. (11) will be referred to as C_1.

Applying the transform (9) to Eq. (5) and using the boundary condition that $u(0)=1$, we obtain

$$(E-K)W = 1 + VW. \tag{12}$$

Operating on this equation with $(E-K)^{-1}$, which is nonsingular on C_1,[24] we obtain

$$W = +\frac{1}{E-K} + \frac{1}{E-K} VW. \tag{12'}$$

W is evidently the Green's function for the operator $(E-H)$. Finally, the "Møller wave-matrix" $\Omega(E)$ is introduced as

$$\Omega(E) \equiv W(E)(E-K). \tag{13}$$

Since $(E-K)^{-1}$ is nonsingular on C_1, we may multiply (12') from the right by $(E-K)$ to obtain

$$\Omega = 1 + \frac{1}{E-K} V\Omega. \tag{14}$$

[14] Brueckner, Levinson, and Mahmoud, Phys. Rev. **95**, 217 (1954).
[15] K. Brueckner, Phys. Rev. **96**, 908 (1954); **97**, 1353 (1955).
[16] K. Brueckner and C. A. Levinson, Phys. Rev. **97**, 1344 (1955).
[17] R. Eden and N. Francis, Phys. Rev. **97**, 1366 (1955).
[18] S. Kato, Progr. Theoret. Phys. **5**, 95, 207 (1950).
[19] B. DeWitt, University of California Radiation Laboratory Report UCRL-2884 (unpublished).
[20] G. Wentzel, Helv. Phys. Acta **15**, 111 (1942).
[21] H. Koppe, Ann. Physik **9**, 423 (1951).

[22] These relations may be easily demonstrated by using $\chi_1^\pm = [\phi_a \pm \phi_b]/\sqrt{2}$, $\chi_2^\pm = [\phi_a \pm i\phi_b]/\sqrt{2}$, $e^{-\beta E_L} \geq (\chi_{2,2}^\pm, u\chi_{1,2}^\pm) \geq 0$, etc.
[23] Conditions (8) and the conditions that the matrix elements of $u(\beta)$ and $\partial u/\partial\beta$ be piecewise continuous are sufficient to imply the validity of Eq. (11), we recall.
[24] If $E_L > 0$ it is convenient to replace E_L by a new quantity $E_L' < 0$ so as to avoid the *apparent* singularities arising from $(E-K)^{-1}$ on the positive real axis. We may henceforth consider $E_L < 0$.

This is precisely the familar stationary state scattering equation in quantum mechanics,[25] except for our apparent use of E as an arbitrary complex variable rather than as the energy.

To solve Eq. (14) it is convenient to use a representation in which the kinetic energy K is diagonal. Such a representation will be designated by the symbol p, which includes a specification of the momenta, spins, and any internal variables for our N particles. Thus the matrix elements of Ω are labeled as

$$\langle p'|\Omega|p\rangle.$$

[Our formal arguments do not require that we specify "p" as a momentum representation. For these, then, "p" can be any representation which diagonalizes K.]

The evaluation of Eq. (1) requires only the probability distribution $\langle p|u(\beta)|p\rangle$ for which we shall need only the diagonal elements of Ω, or

$$\Omega_d\equiv\langle p|\Omega|p\rangle,$$

and

$$W_d\equiv\langle p|W|p\rangle. \tag{15}$$

Our next problem is to study the singularities of Ω and W in the complex E-plane. We shall, indeed, find that the only singularities lie on the *real* axis for $E_L\leqslant E<\infty$.[24] This will permit us to deform the contour C_1 into a new contour along the real axis. Thus E is a real "energy" in Eq. (14). It will, of course, be necessary to specify the limiting process by which E becomes real just as in conventional scattering theory.

To begin the discussion of the analytic properties of $W_d(E)$ and $\Omega_d(E)$ in the complex E-plane, we impose some conditions on the potentials V_{ij}. It is reasonable to suppose that the "range" of the potentials $V_{ij}=v(\mathbf{r}_i-\mathbf{r}_j)$ is much less than $\mathcal{V}^{\frac{1}{3}}$. This is necessary for passage to the $\mathcal{V}(\infty)$ limit discussed at the beginning of this section. It will also be supposed that the potentials $v(\mathbf{r}_i-\mathbf{r}_j)$ are everywhere finite. Whether or not this is "true" for the potentials found in nature is probably a useless question, since the very concept of a potential is expected to fail as $\mathbf{r}_i\to\mathbf{r}_j$. It would appear therefore that no loss of generality is incurred by assuming the finiteness of the V_{ij} everywhere.

It follows from Eqs. (9) and (10) that $\Omega(E)$ and $W(E)$ are analytic everywhere for $\mathrm{Re}(E)<E_L$. Also, it will appear that as $|E|\to\infty$ [$\mathrm{Im}(E)\neq 0$ and greater in magnitude than some arbitrary positive number],

$$\Omega_d(E)\to 1,\quad W_d(E)\to 1/E, \tag{16}$$

and $T_d(E)$ is bounded.

To continue, we introduce the scattering operator T as

$$\Omega=1+\frac{1}{E-K}T,\qquad T=V+V\frac{1}{E-K}T. \tag{17}$$

The second equation follows from the first and Eq. (14). These are of course familiar equations in scattering theory. The second Eq. (17) has the formal Chew-Goldberger[26] solution $T=V+V(E-K-V)^{-1}V$, which in terms of the representation "λ" of Eq. (6) may be written as

$$T_d=\langle p|T|p\rangle=\langle p|V|p\rangle+\sum_\lambda\frac{\langle p|V|\lambda\rangle\langle\lambda|V|p\rangle}{E-E_\lambda}$$
$$=\langle p|V|p\rangle+\sum_\lambda\frac{|\langle\lambda|V|p\rangle|^2}{E-E_\lambda}. \tag{18}$$

Now the sum

$$S_V\equiv\sum_\lambda|\langle\lambda|V|p\rangle|^2=\langle p|V^2|p\rangle \tag{19}$$

in absolutely convergent by our assumptions that the V_{ij} are everywhere finite and that the system is confined within the volume $\mathcal{V}$.

To show that the series in Eq. (18) is absolutely convergent for $\mathrm{Im}(E)\neq 0$, we choose some Δ ($0<\Delta<\Delta_0$), where $\Delta_0=$ least of the values $|E-E_\lambda|$ (for any λ). Then

$$\left|\frac{|\langle\lambda|V|p\rangle|^2}{E-E_\lambda}\right|<\frac{1}{\Delta}|\langle\lambda|V|p\rangle|^2.$$

From this inequality and the comparison theorem, it follows from the absolute convergence of (19) that the series (18) is absolutely convergent. Thus $T_d(E)$ exists everywhere, except on the real axis. The quantity

$$\frac{dT_d(E)}{dE}=-\sum_\lambda\frac{|\langle\lambda|V|p\rangle|^2}{(E-E_\lambda)^2}$$

also exists (by the same arguments) everywhere off the real axis. Thus $T_d(E)$ is analytic everywhere in the complex plane, except on the real axis. It is evident from Eq. (18) that T_d has just simple poles at all $E=E_\lambda$ on the real axis. Since K is diagonal in the "p" representation, it follows from Eqs. (13) and (16) that *both* Ω_d and W_d are analytic everywhere except on the real axis for $E_L\leqslant E<\infty$ and that these have simple poles for $E=E_\lambda$ ($\lambda=1, 2, \cdots$). Finally, the relations (16) follow from Eqs. (18), (19) and the argument following these.

At this point we are evidently able to deform our contour C_1 into a new contour C_2, which runs from $+\infty$ to E_L just above the real axis and returns to $+\infty$

[25] See, for instance, reference 10, for a systematic account of stationary state scattering theory in the form used in the present paper.

[26] G. F. Chew and M. L. Goldberger, Phys. Rev. **87**, 778 (1952).

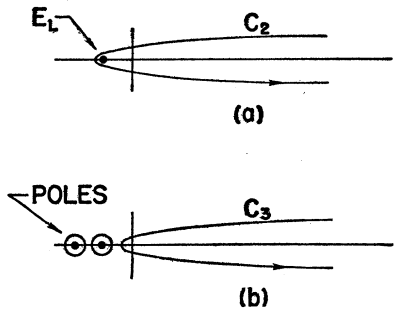

FIG. 1. Contours of integration, as described in text.

below the real axis, as is shown in Fig. 1(a). This follows from the fact that T is bounded [see Eqs. (16) and (18)] when C_2 is held a fixed distance from the real axis. Since the only singularities of $W_d(E)$ are on the real axis, we may take C_2 as close to the real axis as we please.

If some of the E_λ are negative (corresponding to "bound states"), it may be convenient to explicitly evaluate the residues at these poles and to define a new contour C_3 which runs along the *positive* real axis. This is shown in Fig. 1(b).

The integral (11) for $u(\beta)$ may now be written in several forms:

$$\langle p|u(\beta)|p\rangle=\frac{1}{2\pi i}\int_{C_2}e^{-E\beta}\left[\frac{1}{E-K}+\frac{\langle p|T(E)|p\rangle}{(E-K)^2}\right]dE$$
$$=\sum_{\lambda_b}e^{-\beta E_{\lambda b}}|\langle\lambda_b|p\rangle|^2+e^{-\beta K}$$
$$+\frac{1}{2\pi i}\int_0^\infty\left\{\frac{T_d(E-i\eta)}{(E-i\eta-K)^2}-\frac{T_d(E+i\eta)}{(E+i\eta-K)^2}\right\}e^{-E\beta}dE. \quad (20)$$

Here $K=K(p)$ and the $E_{\lambda b}$ are the negative-energy eigenvalues of H. The second integral is over real E and η is the (small) distance of the contour C_2 from the real axis.

The integral in Eq. (20) is of course independent of η. We must be careful in passing to the limit $\eta=0$, however. This is a consequence of the expected noncommutativity of this limit with the $\mathcal{V}(\infty)$ limit discussed at the beginning of the present section. To study the effect of these limits, we rewrite Eq. (18) as

$$T_d(E)=\langle p|V|p\rangle+\int dn_\lambda\frac{|\langle\lambda|V|p\rangle|^2}{E-E_\lambda}. \quad (21)$$

In this expression, $\int dn_\lambda$ represents a discrete sum over states λ before going to the $\mathcal{V}(\infty)$ limit and an integral over continuous variables (with possible discrete terms also appearing) after passage to the $\mathcal{V}(\infty)$ limit.

The expression (21) is to be inserted into the C_2-integral in Eq. (20). Because of the absolute convergence of both integrals and the boundedness of $T_d(E)$ on C_2, we may interchange orders of integration and perform the E integral before doing the n_λ integral. This integration may be carried out explicitly, since there are only simple poles at $E=E_\lambda$ (one readily verifies that there is no pole at $E=K$). Finally, the resulting expression is substituted into the expression (1) for Z:

$$Z=\int dn_p\langle p|u(\beta)|p\rangle.$$

Here the order of the sums (or integrals) over p states and λ states may be interchanged. This follows, since for large E_λ we expect $dn_\lambda\approx(E_\lambda)^{\frac{3}{2}N}dE_\lambda$ and since the p-sum is absolutely convergent. Indeed, using $\langle\lambda|V|p\rangle=(E-K)\langle\lambda|p\rangle$, we have

$$Z=\int dn_p\left\{\int dn_\lambda e^{-\beta E_\lambda}|\langle\lambda|p\rangle|^2\right\}=\int dn_\lambda e^{-\beta E_\lambda}. \quad (22)$$

Had we not taken the $\mathcal{V}(\infty)$ limit before, we could do so now. The point is that we get the same result in either case, so it is correct to take this limit either before or after doing the E-integral.

In spite of this, the *form* of the integrand in Eq. (20) changes appreciably on passage to the $\mathcal{V}(\infty)$ limit. In scattering theory three separate classes of limits appear most frequently:

$$T^{(+)}=\lim_{\mathrm{Im}(E)\to(0+)}\left[\lim_{\mathcal{V}\to\infty}T(E)\right]$$
$$=\text{"outgoing scattered wave" solution,}$$
$$T^{(-)}=\lim_{\mathrm{Im}(E)\to(0-)}\left[\lim_{\mathcal{V}\to\infty}T(E)\right]$$
$$=\text{"incoming scattered wave" solution,}$$
$$T^{(0)}=\lim_{\mathcal{V}\to\infty}\left[\lim_{\substack{\mathrm{Im}(E)\to(0\pm)\\(E\neq E_\lambda)}}T(E)\right]$$
$$=\text{"standing wave" solutions.} \quad (23)$$

We shall have opportunity later to demonstrate applications of each of these limits. It is worth noting that $T_d^{(0)}(E)$ is real, whereas $T_d^{(+)}$ and $T_d^{(-)}$ are complex, with $T_d^{(+)}=[T_d^{(-)}]^*$. For example, passing to the limit $\eta=0$, after taking the $\mathcal{V}(\infty)$ limit in Eq. (20), we obtain[27]

$$\langle p|u(\beta)|p\rangle=\sum_b e^{-\beta E_b}|\langle\lambda_b|p\rangle|^2+e^{-\beta K}+\lim_{\eta\to0}\frac{1}{2\pi i}$$
$$\times\int_0^\infty e^{-E\beta}dE\left\{\frac{T_d^{(-)}(E)}{(E-i\eta-K)^2}-\frac{T_d^{(+)}(E)}{(E+i\eta-K)^2}\right\}. \quad (24)$$

[27] Strictly speaking, we have shown only that Eq. (20) is correct for finite η [with a trivial correction of $O(\eta)$ at the lower limit of the integral] and is indeed independent of η. There is no reason to expect that a limit does not exist as $\eta\to0$. In specific calculations, it will of course be possible to check this.

It must be emphasized that we have given an incomplete discussion of the $\mathcal{V}(\infty)$ limit. That is, we have assumed that this limit is unique and is equivalent to replacing the sum in Eq. (21) by the corresponding integral over continuous λ's. This assumption is, of course, also made in scattering theory.[25] Evidently, some care is required in taking this limit properly.

As a preliminary to our subsequent discussion, we shall express Ω in terms of the two-body scattering operators t_α:

$$t_\alpha = V_\alpha + V_\alpha \frac{1}{E-K} t_\alpha. \tag{25}$$

This is the integral equation for solving the two-body scattering problem. In terms of the t_α's, an exact expression for Ω is[28]

$$\begin{aligned} \Omega &= 1 + \frac{1}{E-K} \sum_\alpha t_\alpha \Omega_\alpha, \\ \Omega_\alpha &= 1 + \frac{1}{E-K} \sum_{\beta \neq \alpha} t_\beta \Omega_\beta. \end{aligned} \tag{26}$$

We may consider Eqs. (26) as representing a starting point for the evaluation of Ω_d and W_d—that is, a starting point after the two-body problem has been solved. Actually, these equations represent only the simplest example of an extensive class of equations involving two-body scattering operators, of which more will be said in Sec. V.

We observe also that Eqs. (26) are formally valid for either Bose-Einstein (B-E) or Fermi-Dirac (F-D) statistics. It is convenient, however, to consider the t_α's as properly symmetrized amplitudes in the equations. In Sec. V more will be said concerning this point also.

A simple perturbation expansion of Eqs. (26) leads to

$$\Omega = 1 + \frac{1}{E-K} \sum_\alpha t_\alpha + \frac{1}{E-K} \sum_\alpha t_\alpha \frac{1}{E-K} \sum_{\beta \neq \alpha} t_\beta + \cdots. \tag{27}$$

This has a structure similar to the corresponding perturbation expansion of Eq. (14)—but differs in that exact two-body t_α's rather than "Born-approximation" V_α's appear.

III. THE SECOND VIRIAL COEFFICIENT

Equations (26) permit one to calculate Z in terms of two-body scattering operators, although it is rather cumbersome in the form given if N is large [a different approach is adopted in Sec. V for large N]. For evaluation of the second virial coefficient, $N=2$ and the sum over pairs has just one term:

$$\Omega = 1 + \frac{1}{E-K} t. \tag{28}$$

[28] This is readily verified by substitution into Eq. (14), using Eq. (25). A derivation was given in reference 11.

The second virial coefficient[29] in the equation of state,

$$p\mathcal{V} = N\theta[1 + (B/\mathcal{V}) + (C/\mathcal{V}^2) + \cdots],$$

is B. On defining

$$\tau \equiv 2\sqrt{2} N [2\pi\hbar^2/M\theta]^{\frac{3}{2}}, \tag{29}$$

we have

$$\begin{aligned} B &= -\tau \int \{\langle p|u(\beta)|p\rangle - \exp(-\beta p^2/M)\} \frac{\mathcal{V} d^3p}{(2\pi\hbar)^3} \\ &= -\frac{\tau}{2\pi i} \int \frac{\mathcal{V} d^3p}{(2\pi\hbar)^3} \int_{C_2} dE e^{-E\beta} \frac{\langle p|t|p\rangle}{(E-K)^2} \\ &= -\frac{\tau}{2\pi i} \int d^3p \int_{C_2} dE e^{-\beta E} \frac{\langle p|\mathbf{t}|p\rangle}{(E-K)^2}. \end{aligned} \tag{30}$$

We have taken the $\mathcal{V}(\infty)$ limit here, and in doing so have set

$$\langle p|\mathbf{t}|p\rangle = \mathcal{V}/(2\pi\hbar)^3 \langle p|t|p\rangle, \tag{31}$$

in accordance with the accepted convention for normalization in the continuum.

There exist, for instance, variational principles which may often lead to practical means for the evaluation of $\mathbf{t}$. As an example, we quote the familiar Schwinger variational form

$$\langle p'|t^{(+)}|p\rangle = \frac{(\psi_{p'}^{(-)}, v\chi_p)(\chi_{p'}, v\psi_p^{(+)})}{\left(\psi_{p'}^{(-)}, \left[v - v\frac{1}{E_R + i\eta - K} v\right]\psi_p^{(+)}\right)}, \tag{32}$$

which is stationary with respect to independent variations of $\psi^{(-)}$ and $\psi^{(+)}$ about their correct values

$$\psi_p^{(\pm)} = \chi_p + \frac{1}{E_R \pm i\eta - K} v\psi_p^{(\pm)}. \tag{33}$$

Here we have written the E of Eq. (30) in terms of its real and imaginary parts as $E = E_R \pm i\eta$.

An alternative approach is to assume that the two-body potential in momentum space is factorable. Let

$$(\mathbf{k}|v|\mathbf{k}') = G\phi(k)\phi(k'), \tag{34}$$

for example, where $\mathbf{k}$ is the relative momentum of the two particles, G is a constant, and $\phi(k)$ is a function of k subject to the existence of the integral (36). The integral equation for t,

$$t = v + v\frac{1}{E-K} t,$$

is satisfied by

$$\langle \mathbf{k}|\mathbf{t}|\mathbf{k}'\rangle = \phi(k)\phi(k')/(1-I), \tag{35}$$

[29] See, for instance, D. ter Haar, *Statistical Mechanics* (Rinehart and Company, New York, 1954), p. 171.

where

$$I=G\int\frac{\phi^2(k)d^3k}{E-(k^2/M)}. \tag{36}$$

If there exist points E on the negative real E-axis for which $I=1$, there are bound states, according to the general remarks made in Sec. II.

The potential (34) describes scattering in the S-state only. It is easily generalized to describe scattering in all angular momentum states:

$$(\mathbf{k}|v|\mathbf{k}')=\sum_l\sum_{\nu=1}^{n_l}G_{\nu,l}\phi_{\nu,l}(k)\phi_{\nu,l}(k')\sum_m Y_l^m(\hat{k})Y_l^m(\hat{k}'),$$

where $\hat{k}$ is a unit vector in the direction of $\mathbf{k}$. The $G_{\nu,l}$ are constants and n_l is some positive integer dependent on l. Spin dependence may also be included. The integral equation for $\mathbf{t}$ may still be solved explicitly.

As a specific example, let us take

$$\phi(k)=(k^2+\alpha^2)^{-\frac{1}{2}},\quad \alpha>0. \tag{37}$$

The integral (36) for I is readily evaluated to give

$$I=q\{(1+iZ)/(Z^2+1)\}, \tag{38}$$

where

$$q=-(2\pi)^2GM/2\alpha,$$

and

$$Z^2=(ME/\alpha^2)(0<\arg(Z)<\pi). \tag{39}$$

There is evidently a single bound state when

$$q>1$$

at

$$E_b=-(\alpha^2/M)[q-1]^2.$$

We interpret q as giving a measure of the strength of the potential, being positive for an attractive potential and negative for a repulsive potential.

Substituting into Eq. (30) and doing the $\mathbf{p}$-integral, we obtain

$$B=-\tau\left\{e^{-\beta E_b}+\frac{q}{\pi}\int_0^\infty dz\right.$$
$$\left.\times\exp[-(\beta\alpha^2/M)Z^2]\frac{[1-q-Z^2]}{\{q^2Z^2+[q-1-Z^2]^2\}}\right\}. \tag{40}$$

The $e^{-\beta E_b}$ term is missing when there is no bound state. In the low-temperature limit this becomes

$$B=-\tau\left\{e^{-\beta E_b}+\tfrac{1}{2}\left(\frac{q}{1-q}\right)\left(\frac{M\theta}{\pi\alpha^2}\right)^{\frac{1}{2}}\right\}. \tag{41}$$

It is beyond our present scope to develop further applications. We observe, however, that a great variety of potentials may be approximated by "factorable potentials" such as we have discussed.

A third possibility for at least approximate calculation of the second virial coefficient lies in the use of *dispersion relations*[30] for the evaluation of the amplitude $\langle p|t|p\rangle$.

IV. A GENERAL PERTURBATION METHOD

In the present section we seek a perturbation method for labeling the states E_λ in terms of the "unperturbed" states $|p\rangle$. That is, we seek a correspondence between λ and p. This means that we shall have "untangled" the operators K and V in H and may write

$$\langle p|u(\beta)|p\rangle=e^{-\beta[K(p)+V_L(p)]},$$

where V_L is a function of p. The task of accomplishing this bears great similarity to the problem of calculating the refractive index of a scattering medium[12] and to the theory of muclear saturation of Brueckner *et al.*[14–17]

By an appeal to the adiabatic theorem, we may for instance imagine that we gradually turn the potential V on or off [the energy levels are all discrete, since the system is confined to a box]. The transition of the system from λ to p levels (or vice versa) may then be observed. In the presence of unresolved degeneracies, however, this transition is not unique. Furthermore, in systems as complex as those which we are considering, the problem of resolving these degeneracies is in general unmanageable. The quantum mechanical perturbation problem is thus quite difficult in most cases, unless the perturbation is very weak or unless simple symmetries obtain.

The corresponding statistical problem is in some respects much simpler. Let us suppose that we have an ensemble of identical systems for which the "coarse-grained volume-elements"

$$\delta\tau_i=\int_i dn_p(i=1,2,\cdots) \tag{42}$$

are each uniformly populated, and suppose also that $V=0$. We now "turn on" V very slowly and follow the members of the ensemble which started, say in $\delta\tau_{i0}$. To accomplish this change in V, we replace it by gV, where g is a dimensionless parameter confined to the range of values $0\leqslant g\leqslant 1$. Because the ensemble is uniform in $\delta\tau_{i0}$, the initial degeneracy is immaterial for its subsequent behavior. When g has reached the value $g=1$, the members of the ensemble coming from $\delta\tau_{i0}$ will occupy some "volume element"

$$\int_{i0}dn_\lambda$$

of λ states. Their energies will lie in some range

$$\bar{E}_{i0}-\tfrac{1}{2}\delta E_{i0}\leqslant E_\lambda\leqslant\bar{E}_{i0}+\tfrac{1}{2}\delta E_{i0}. \tag{43}$$

As long as the range δE_{i0} is small enough to be unimport-

[30] Goldberger, Gell-Mann, and Thirring, Phys. Rev. **95**, 1612 (1954); M. L. Goldberger, Phys. Rev. **99**, 979 (1955); R. Karplus and M. A. Ruderman, Phys. Rev. **98**, 771 (1955).

ant for *macroscopic* considerations, we need never have worried about the degenerate states.[31] We may go even further in the application of "coarse-grained" distributions. Having chosen a given range of energies as defining our approximation, we need say only that most of the states in $\delta\tau_{i0}$ go into the range δE_{i0}. In other words, the calculation of individual energy levels is not required—it is only necessary to follow some mean of the energy of the set of states originally in $\delta\tau_{i0}$ into the range δE_{i0}. The statistical problem may thus be much simpler than the corresponding dynamical one, and this simplification of course results from the limited dynamical information required to obtain thermodynamic properties of a system. (The arguments of this paragraph will be given more formally at the end of this section.)

To develop the formal perturbation technique, we shall follow an argument similar to that of Eden and Francis.[17,32] The quantity W of Eq. (12) may be used to define a quantity $M_0|p\rangle$ as follows:

$$W|p\rangle=M_0|p\rangle W_d, \tag{44}$$

with

$$\langle p|M_0|p\rangle=1, \tag{45}$$

of course, W_d is defined in Eq. (15). Equation (12) for $W|p\rangle$ is then

$$(E-K)M_0|p\rangle W_d=|p\rangle+VM_0|p\rangle W_d. \tag{46}$$

If we define

$$V_C=\langle p|VM_0|p\rangle, \tag{47}$$

and operate on $\langle p|$ by Eq. (46), we obtain

$$[E-K(p)]W_d=1+V_C(p)W_d, \tag{48}$$

using Eq. (45).

Since W_d, V_C, and K are all functions of p (and not matrices), Eq. (48) may be solved algebraically for W_d:

$$W_d(p)=\frac{1}{E-K(p)-V_C(p)}. \tag{49}$$

We repeat that all quantities appearing in Eq. (49) are numbers and not operators. Thus the "untangling" of noncommuting operators mentioned at the beginning of this section has been formally accomplished. Equation (11) is now

$$(p|u(\beta)|p)=\frac{1}{2\pi i}\int_{C_2}\frac{e^{-E\beta}dE}{E-K(p)-V_C(p)}. \tag{50}$$

W_d has, as we have seen, only simple poles [before going to the $\mathcal{V}(\infty)$ limit]. These occur at

$$E=K(p)+V_C(p), \tag{51}$$

which is the Brueckner-Levinson[16] and Eden-Francis[17] form of the eigenvalue problem. Unfortunately, Eq. (51) is somewhat misleading, since it has solutions for *all* E_λ quite independently of the momentum state p. (This point was perhaps not sufficiently emphasized by the above authors.[17]) To see this, we observe that

$$\begin{aligned}\langle p'|W|p\rangle&=\sum_\lambda\frac{\psi_\lambda(p')\psi_\lambda^*(p)}{E-E_\lambda},\\ W_d&=\sum_\lambda\frac{|\psi_\lambda(p)|^2}{E-E^\lambda},\end{aligned} \tag{52}$$

where $\psi_\lambda(p)$ is the eigenfunction ψ_λ in a p-representation. Comparison of Eqs. (49) and (52) makes it quite evident that $E=E_\lambda$ (any λ) is a solution of Eq. (51).

Equation (51) then establishes no connection between a given state $|p\rangle$ and a particular ψ_λ. On the other hand, if a convergent perturbation procedure can be found, leading from a state p_0 to a state λ_0, Eq. (51) will certainly be satisfied for $E=E_{\lambda 0}$, $p=p_0$ (since it is true for any E_λ and any p). Defining

$$\mathcal{V}_C=V_C\mathcal{I}, \tag{53}$$

where $\mathcal{I}$ is the unit matrix, we rewrite Eq. (46) as

$$\begin{aligned}(E-K-\mathcal{V}_C)M_0|p\rangle=(E-K-\mathcal{V}_C)|p\rangle\\ +[V-\mathcal{V}_C]M_0|p\rangle.\end{aligned} \tag{54}$$

It is evidently verified that

$$\langle p|[V-\mathcal{V}_C]M_0|p\rangle=0, \tag{55}$$

so Eq. (54) may be put into the form

$$M_0|p\rangle=|p\rangle+\frac{1}{E-K-\mathcal{V}_C}[1-\Lambda_p][V-\mathcal{V}_C]M_0|p\rangle. \tag{56}$$

Here Λ_p is the projection operator onto the state $|p\rangle$.[33]

In the next section, methods of solving the perturbation problem will be considered. For the moment, let us suppose it has been completely solved. By this, we imply that we have started from a state $|\mathbf{p}_0\rangle$, belonging to the set for which[34]

$$K|p_0\rangle=K(p_0)|p_0\rangle, \tag{57}$$

and obtained a unique eigenstate of H with eigenvalue $E_{\lambda 0}$, the states $|\mathbf{p}_0\rangle$ and λ_0 being paired. We have therefore found a transformation $T_{\mathbf{p}_0}(p)$ of the p-representation onto the $\mathbf{p}$-representation such that

$$\textstyle\sum_p T_{\mathbf{p}_0}(p)\psi_\lambda(p)=\delta(\lambda-\lambda_0). \tag{58}$$

[31] That difficulties from singular energy denominators do not occur has been observed, for instance, in references 8 and 9.

[32] A more comprehensive formulation of the method of Eden and Francis has been given in the review by DeWitt (reference 19), which contains a survey of perturbation methods in quantum mechanics.

[33] Equation (56) is just Eq. (117) of Eden and Francis (reference 17). In contrast to these authors, we still consider E to be a complex variable which is made to approach its desired eigenvalue as a limit. This simplifies the handling of singularities associated with the degeneracy of those states $|p\rangle$ having eigenvalue $K(p)$.

[34] The state $|\mathbf{p}_0\rangle$ will in general be a linear combination of the degenerate states $|p_0\rangle$.

The corresponding transformation on W is

$$(\mathbf{p}_0'|W|\mathbf{p}_0)=\sum_{p',p} T_{\mathbf{p}_0}(p')\langle p'|W|p\rangle T_{\mathbf{p}_0}{}^*(p)$$
$$=\frac{\delta(\lambda_0-\lambda_0')}{E-E_{\lambda_0}}=\frac{\delta(\mathbf{p}_0-\mathbf{p}_0')}{E-E_{\lambda_0}}, \quad (59)$$

because of the one-to-one correspondence $\mathbf{p}_0\leftrightarrow\lambda_0$. [We have used Eqs. (52) and (58) here.]

We now transform back to the p_0-states of Eq. (57). Let the transformation function be $S_{\mathbf{p}_0}(\mathbf{p}_0)$ so

$$(p_0|W|p_0)=\sum_{\mathbf{p}_0',\mathbf{p}_0} S_{p_0}(\mathbf{p}_0')(\mathbf{p}_0'|W|\mathbf{p}_0)S_{p_0}{}^*(\mathbf{p}_0)$$
$$=\sum_{\mathbf{p}_0}\frac{|S_{p_0}(\mathbf{p}_0)|^2}{E-E_{\lambda_0}}. \quad (60)$$

In accordance with the remarks made at the beginning of this section, we suppose the eigenenergies E_{λ_0} in the sum (60) to lie within a small range of values, δE_{λ_0}. We also suppose that we made no effort to find the set of states $\mathbf{p}_0$, but began with the state p_0, and that the perturbation procedure led to a limit $V_L(p_0)$ for V_C: that is,

$$V_C\rightarrow V_L(p_0). \quad (61)$$

The energy $K(p_0)+V_L(p_0)$ cannot be identified with any one of the E_{λ_0}, but may be supposed to lie within the range δE_{λ_0} if our perturbation procedure is a correct one. If δE_{λ_0} is small enough to be neglected, we may set

$$E_{\lambda_0}\simeq K(p_0)+V_L(p_0) \quad (62)$$

in Eq. (60) to obtain

$$(p_0|W|p_0)=\frac{1}{E-K(p_0)-V_L(p_0)}\sum_{\mathbf{p}_0}|S_{p_0}(\mathbf{p}_0)|^2$$
$$=\frac{1}{E-K(p_0)-V_L(p_0)}. \quad (63)$$

Finally, we return to the "coarse-grained" volume elements, $\delta\tau_{p_0}$ mentioned earlier. Let us suppose that "most of the states" in $\delta\tau_{p_0}$ go into a range "δE_{λ_0}" about some limit

$$K(p_0)+V_C\rightarrow K(p_0)+V_L(p_0).$$

[$V_L(p_0)$ is not necessarily the same as the V_L in Eq. (61), since we are considering a cruder approximational technique.] If this approximation method has been a valid one, we may suppose that we have found an "approximate wave function" $\mathcal{T}_{p_0}(p)$ such that

$$\begin{aligned}&\textstyle\sum_p \mathcal{T}_{p_0}(p)\psi_\lambda(p)=\Delta(\lambda-\lambda_0),\\ &\textstyle\sum_\lambda|\Delta(\lambda-\lambda_0)|^2=1,\end{aligned} \quad (63a)$$

where $\Delta\simeq 0$ except for E_λ within the range "δE_{λ_0}" of $K(p_0)+V_L(p_0)$.

Applying the transformation $\mathcal{T}$ to W, we have [again, not the same W as in Eq. (63)]

$$(p_0'|W|p_0)=\sum_{p',p}\mathcal{T}_{p_0'}(p')\langle p'|W|p\rangle\mathcal{T}_{p_0}{}^*(p)$$
$$=\sum_\lambda\frac{\Delta(\lambda-\lambda_0')\Delta(\lambda-\lambda_0)}{E-E_\lambda}. \quad (64)$$

In the "coarse-grained" sense, this is diagonal. If the range "δE_{λ_0}" is negligible, we may again set

$$E_\lambda=K(p_0)+V_L(p_0). \quad (65)$$

In view of the normalization (63), we obtain from Eq. (64)

$$(p_0|W|p_0)=\frac{1}{E-K(p_0)-V_L(p_0)}. \quad (66)$$

Evaluating the integral (50), we have

$$(p_0|u(\beta)|p_0)=\exp\{-\beta[K(p_0)+V_L(p_0)]\}. \quad (67)$$

The use of a "coarse-grained" density has many advantages for providing simple physical interpretations of methods employed for approximation. For instance, "wave packets" may be used to approximately diagonalize matrices (this was, of course, done in Eq. (64) by means of physical rather than mathematical arguments). As an example, the degeneracy associated with the position of "liquid droplets" in the gas may be resolved by the use of wave packets. Again, the "potential" V_L may be given a physical interpretation which can be of help in estimating the position and density of large groups of energy levels.[35]

V. AN EXPRESSION FOR $\mathcal{U}_C$

In the present section we propose to develop an expression for $\mathcal{U}_C$ in terms of two-body scattering operators. To do this we shall make use of the fact that evaluation of $\langle p|\Omega|p\rangle$ is formally identical with the problem of calculating the index of refraction of an extended, homogeneous medium, as was done by Francis and Watson.[12] The final result provides just the Brueckner-Levinson-Eden-Francis[14–17] formulation of the eigenvalue problem.

Let Λ be a projection operator onto the appropriately symmetrized Bose-Einstein or Fermi-Dirac subspace of the states $|p\rangle$, which will be called $|\bar{p}\rangle$.[36] Then

$$\mathbf{\Omega}=\Omega\Lambda \quad (68)$$

is the required solution to Eq. (14) (being a linear combination of unsymmetrized solutions).[13] The equation obtained by letting Eq. (14) operate on Λ is

$$\mathbf{\Omega}=\bar{I}+\frac{1}{E-K}V\mathbf{\Omega}, \quad (69)$$

[35] Applications and more detailed development will be published separately by W. B. Riesenfeld and K. M. Watson.

[36] That is, $|\bar{p}\rangle=\Lambda|p\rangle$, if properly normalized.

where $\bar{I}=\Lambda$ is the unit operator on the symmetrized states. It is easily seen that Eq. (69) is equivalent to

$$\mathbf{\Omega}=\bar{I}+\frac{1}{E-K}\bar{V}\mathbf{\Omega}. \tag{70}$$

Here

$$\bar{V}=\sum_{i<j}\bar{V}_{ij}=\sum_{\alpha}\bar{V}_{\alpha},$$

$$\bar{V}_{ij}=\tfrac{1}{2}[(p_i'p_j'|V|p_ip_j)\pm(p_i'p_j'|V|p_jp_i)], \tag{71}$$

the + or − sign referring to B-E or F-D statistics, respectively. Now consider the solutions to

$$\Omega_0=1+\frac{1}{E-K}\bar{V}\Omega_0. \tag{72}$$

Evidently, we obtain

$$\mathbf{\Omega}=\Omega_0\Lambda. \tag{73}$$

The two-body scattering amplitudes are introduced by ["α" refers to the pair "(i, j)"]

$$t_\alpha=\bar{V}_\alpha+\bar{V}_\alpha(1/e)I_\alpha,$$

$$(p_i'p_j'|t_C|p_ip_j)=(p_ip_j|t|p_ip_j)[\delta_{p_i'p_i}\delta_{p_j'p_j}\pm\delta_{p_i'p_j}\delta_{p_j'p_i}],$$

$$t_\alpha=I_\alpha+t_{C\alpha},$$
$$e=E-K-Q, \tag{74}$$
$$Q=\textstyle\sum_\alpha t_{C\alpha}.$$

The set of equations (74) defining t_α is not identical with Eq. (26). To understand this difference, we must consider the magnitude of the matrix elements of t_α:

$$t_\alpha=[\text{an "interaction energy"}]\times\frac{(4\pi/3)r_0^3}{\mathcal{V}}\approx O(\bar{V}_\alpha). \tag{75}$$

Here r_0 is the "range of the interaction." By the assumptions made in Sec. II, we consider $[(4\pi/3)r_0^3]\mathcal{V}^{-1}$ to be a very small number.

Factors such as $\bar{V}_\alpha(1/e)\bar{I}_\alpha$ are of course of the order of (75), because the sum over states involves $\int dn=\int\mathcal{V}d^3p/(2\pi\hbar)^3$, which cancels one factor of $(4\pi/3)r_0^3\times\mathcal{V}^{-1}$. On the other hand,

$$\frac{1}{e}\bar{V}_\alpha t_\alpha-\frac{1}{e}\bar{V}_\alpha I_\alpha=\frac{1}{e}\bar{V}_\alpha t_{C\alpha}, \tag{76}$$

does not contain a sum over states since $t_{C\alpha}$ is diagonal. It is thus of $O[(4\pi/3)r_0^3\mathcal{V}^{-1}]^2$ and negligible.

However, the difference between e and $(E-K)$ is not negligible for very strong interactions.[37] The physical interpretation of the use of e in Eqs. (74) is that the two-body scattering must be calculated in a self-consistent manner for a pair of particles moving in the medium of the other particles.

It is important for what follows that the I_α's have *no* diagonal matrix elements with respect to the complete set of symmetrized states $|\bar{p}\rangle$.

The desired solution to Eq. (72) is

$$\Omega_0=F\Omega_C,$$

$$F=1+\frac{1}{e}\sum_\alpha I_\alpha F_\alpha,$$

$$F_\alpha=1+\frac{1}{e}\sum_{\beta\neq\alpha} I_\beta F_\beta, \tag{77}$$

$$\Omega_C=1+\frac{1}{E-K}Q\Omega_C.$$

To show that these provide a solution to Eq. (72), we substitute them into the right-hand side of Eq. (72) to obtain (after a little simplification)

$$\Omega_0=\Omega_C+\sum_\alpha\left[1-\frac{1}{E-K}t_{C\alpha}\right]\frac{1}{e}I_\alpha F_\alpha\Omega_C. \tag{78}$$

By the same argument which was used in connection with Eq. (76),

$$\left[1-\frac{1}{E-K}t_{C\alpha}\right]=1,$$

to relative order $[(4\pi/3)r_0^3\mathcal{V}^{-1}]$. In this approximation, which we may consider to be "almost exact," Eq. (78) reduces to

$$\Omega_0=F\Omega_C,$$

and the proof is complete.[38]

To proceed, we must calculate the diagonal matrix element

$$\langle\bar{p}|\Omega|\bar{p}\rangle=\langle\bar{p}|\Omega_0|\bar{p}\rangle, \tag{79}$$

where $|\bar{p}\rangle$ is a properly symmetrized state of the system. It is evident that Q and Ω_C are both diagonal in this representation, so

$$\langle\bar{p}|\Omega_0|\bar{p}\rangle=\langle\bar{p}|F|\bar{p}\rangle\langle\bar{p}|\Omega_C|\bar{p}\rangle. \tag{80}$$

The last equation (77) for Ω_C is evidently only a simple algebraic equation.

From this point, we follow in detail the method of Francis and Watson.[12] Define

$$L\equiv\langle\bar{p}|\textstyle\sum_\alpha I_\alpha F_\alpha|\bar{p}\rangle, \tag{81}$$

[37] Some calculations of this effect have been made by Brueckner *et al.* (references 14–17) and by Frank, Gammel, and Watson, Phys. Rev. **101**, 891 (1956). For nuclear forces the "self-consistency correction" seems important for quantitative calculation, but not for qualitative studies. For "weaker forces" the correction is negligible—but for much stronger forces, even the qualitative features are changed. A more careful study of the propagators is given in reference 35.

[38] This result, in the form of Eqs. (77) was first obtained in reference (11). The terms dropped were stated to be of relative order $(1/N)$, where N is the number of particles. For a uniform medium such as was there considered, this is equivalent to our present criterion that $(4\pi/3)r_0^3\,\mathcal{V}^{-1}$ be small.

so

$$\langle\bar{p}|F|\bar{p}\rangle=1+\frac{1}{e}L. \tag{82}$$

Here $e=e(p)$ is also, of course, diagonal in the p-representation. Let $\Lambda(\bar{p})$ be a projection operator onto the state $|\bar{p}\rangle$. From the third of Eqs. (77), we obtain

$$F_\alpha|\bar{p}\rangle=|\bar{p}\rangle+\frac{1}{e}\sum_{\beta\neq\alpha} I_\beta F_\beta|\bar{p}\rangle.$$

Operating on this with $[1-\Lambda(\bar{p})]$, we obtain

$$[1-\Lambda(\bar{p})]F_\alpha|\bar{p}\rangle=\frac{1}{e}\sum_{\beta\neq\alpha}[1-\Lambda(\bar{p})]$$
$$\times I_\beta[1-\Lambda(\bar{p})]F_\beta|\bar{p}\rangle+\frac{1}{e}\sum_{\beta\neq\alpha}$$
$$\times[1-\Lambda(\bar{p})]I_\beta|\bar{p}\rangle\langle\bar{p}|F_\beta|\bar{p}\rangle. \tag{83}$$

We verify that $\langle\bar{p}|F_\beta|\bar{p}\rangle$ is independent of the index β, and so define

$$F_C\equiv\langle\bar{p}|F_\beta|\bar{p}\rangle. \tag{84}$$

Now a new set of operators G_α is introduced by the relation

$$[1-\Lambda(\bar{p})]F_\alpha|\bar{p}\rangle\equiv[G_\alpha-1]|\bar{p}\rangle F_C. \tag{85}$$

Substituting Eqs. (84) and (85) into (83), we obtain for the G_α's the set of equations

$$G_\alpha=1+\frac{1}{e}\sum_{\beta\neq\alpha}\{[1-\Lambda(\bar{p})]I_\beta\}G_\beta. \tag{86}$$

To continue, we may write Eq. (81) as

$$L=\langle\bar{p}|\textstyle\sum_\alpha t_\alpha(1-\Lambda(\bar{p}))F_\alpha|\bar{p}\rangle \tag{87}$$
$$=[V_C-\langle\bar{p}|Q|\bar{p}\rangle]F_C, \tag{88}$$

where the quantity V_C is [from Eq. (85)]

$$V_C=\langle\bar{p}|\textstyle\sum_\alpha t_\alpha G_\alpha|\bar{p}\rangle. \tag{89}$$

To obtain an equation for F_C, we form the diagonal matrix elements of Eq. (77) for F_α:

$$F_C=\langle\bar{p}|F_\alpha|\bar{p}\rangle=1+\frac{1}{e}\langle\bar{p}|\sum_{\beta\neq\alpha} I_\beta F_\beta|\bar{p}\rangle. \tag{90}$$

Now to $O[(4\pi/3)r_0^3\mathcal{V}^{-1}]$, we have

$$\langle\bar{p}|\sum_{\beta\neq\alpha} I_\beta F_\beta|\bar{p}\rangle=L,$$

and

$$F_C=\langle\bar{p}|F|\bar{p}\rangle. \tag{91}$$

{We are not considering $[N(4\pi/3)r_0^3\mathcal{V}^{-1}]$ as small.}

Equations (88), (90), and (91) lead to

$$F_C=1+\frac{1}{E-K(p)-V_C}[V_C-\langle\bar{p}|Q|\bar{p}\rangle]. \tag{92}$$

To complete the evaluation of

$$\Omega_d=\langle\bar{p}|\Omega|\bar{p}\rangle=F_C\langle\bar{p}|\Omega_C|\bar{p}\rangle,$$

we write

$$\langle\bar{p}|\Omega_C|\bar{p}\rangle=1+\frac{1}{E-K(p)-\langle\bar{p}|Q|\bar{p}\rangle}\langle\bar{p}|Q|\bar{p}\rangle,$$

and use Eq. (92) to obtain

$$\Omega_d=1+\frac{1}{E-K(p)-V_C(p)}V_C(p). \tag{93}$$

Finally,

$$W_d=\langle\bar{p}|\boldsymbol{\Omega}|\bar{p}\rangle\frac{1}{E-K(p)}=\frac{1}{E-K(p)-V_C(p)}. \tag{94}$$

This is of the form of Eq. (49).

Equation (89) represents one of a variety of forms for V_C, which involve t_α's. Applications of these methods will be published separately.[35]

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