Density Matrices in the Many-Body Problem: Connection with Scattering Theory

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The energy per particle in a many-particle system, both for bosons and fermions, is discussed using a perturbation method and some results on reduced density matrices obtained previously. The theory is tested for hard-sphere, Lennard-Jones, and nonsingular potentials; it exhibits clearly the difficulties in going to higher-order approximations and gives results which correspond to those obtained by other methods.

1. PERTURBATION THEORY

DENSITY-MATRIX methods have proved a powerful tool for studying both quantitative and qualitative aspects of the many-body problem, particularly in calculations of ground-state and correlation energies.[1] Variation principles using density matrices have been recently developed and applied to several models,[2] restrictions on functions corresponding to N-representable density matrices discussed[2,3] and perturbation theories employed.[1,4]

Here we would like to exhibit the connection between energy perturbation theory and the partial-wave formalism, to apply some results of the density-matrix approach of Ref. 4, and to generalize from a solution of the two-particle problem to the calculation of the energy per particle of a many-body system.

Let us briefly recall the result of the partial-wave analysis of two-particle scattering. The phase shifts are given by[5]

$$\sin\delta_l = \frac{-m\pi K}{\hbar^2}\int_0^\infty j_l(r)R_l(r)u(r)r^2dr, \qquad (1)$$

where $\mathbf{K}=\mathbf{k}_1-\mathbf{k}_2$ is the difference of initial wave vectors, $j_l(r)$ is the Bessel function of order 1, $R_l(r)$ is the solution of the radial equation, and $u(r)$ is the scattering potential. A close relation between the partial-wave formalism and the usual energy-perturbation theory is easily established. The latter is the result of iterating the identity for the wave function

$$\psi = u_0 + \sum_{n\neq 0} u_n\langle u_n|Q|\psi\rangle|(E-E_n), \qquad (2)$$

where the operator Q is the difference in the pair and single-particle contribution to the potential energy, u_0 is the eigenfunction of the single particle, and u_n is that of the full Hamiltonian. Consider the unperturbed wave function of two particles,

$$u_0 = e^{2\pi i\mathbf{R}\cdot(\mathbf{k}_1+\mathbf{k}_2)}e^{2\pi i\mathbf{K}\cdot\mathbf{r}}.$$

Transforming away the center-of-mass motion by a Lorentz transformation, the eigenvalue is $E_0=(\hbar^2/2m)\times(2\pi k)^2$.[6] The exact wave function can be similarly factorized:

$$\psi = e^{2\pi i(\mathbf{k}_1'+\mathbf{k}_2')\cdot\mathbf{R}}\psi_{\text{relative}},$$

with

$$E = \frac{\hbar^2k^2}{m} + 4\pi\sum_{l=0}^{\infty}(2l+1) \times\frac{1}{V}\int_0^\infty j_l(\pi Kr)R_l(r)u(r)r^2dr. \qquad (3)$$

Equation (3) is derived by using

$$\psi_{\text{relative}} = \sum_{l=0}^{\infty} A_lR_l(r)P_l(\cos\theta), \qquad (4)$$

where the A_l are coefficients, together with the orthogonal property of Legendre polynomials. If the wave functions have specified symmetry properties, then $\sum(2l+1)$ is replaced by

$$\{A\sum_{l\ \text{even}} + B\sum_{l\ \text{odd}}\}(2l+1),$$

with $A+B=1$, and A and B are determined by symmetry considerations. For example $A=1$, $B=0$ for a spin-zero Bose gas, $A=\frac{1}{4}$, $B=\frac{3}{4}$ for a spin-$\frac{1}{2}$ Fermi gas, etc.

Equation (3) may now be iterated in two different ways. One can approximate $R_l(r)$ in Eq. (3) by $j_l(r)$, which is similar to the Born approximation. This in fact is the first step in ordinary perturbation theory and suffers from divergence difficulties when the interaction is singular at the origin $u(r)\gtrsim r^{-3-2l}$ as $r\to 0$. The second method, which avoids divergencies, consists of taking the faster-converging Taylor expansion for R_l,

$$R_l(K',r) = R_l(K,r) + [(\partial/\partial K)R_l(K',r)](K'-K)+\cdots, \qquad (5)$$

[1] T. Shibuya and O. Sinanoglu, J. Math. Phys. **10**, 1032 (1969). This reference contains many earlier ones, e.g., J. E. Mayer, Phys. Rev. **100**, 1574 (1955).
[2] C. Garrod and J. K. Percus, J. Math. Phys. **5**, 1756 (1964); L. J. Kijewski and J. K. Percus, Phys. Rev. **164**, 228 (1967).
[3] R. V. Ayres, Phys. Rev. **111**, 1453 (1958).
[4] P. Gluck, Phys. Rev. **176**, 1534 (1968); hereafter referred to as I.
[5] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Co., New York, 1955).
[6] If the reduced mass $\mu=\frac{1}{2}m$ is used, then $E_0=(\hbar^2/2\mu)(\pi K)^2$, with $K^2=4k^2$.

where $K'=K+\cdots$. Such an iteration, based on the unperturbed energy given by K, is an improvement over the perturbation of the unperturbed wave function $j_l(r)$. For a two-particle system the procedure is tautological since it relies on knowing R_l explicitly, but once the latter is known the problem is solved. Before generalizing to a many-particle system, we note that the potential energy of the two-particle system can be given explicitly in terms of the δ_l,

$$E_p=-\frac{4\hbar^2}{mKV}(A\sum_{l\text{ even}}+B\sum_{l\text{ odd}})(2l+1)\sin\delta_l+O(K'-K). \quad (6)$$

In the many-particle generalization of Eq. (6), the sum over the products j_lR_l will clearly become the pair distribution function $\rho_2(r)$. We shall return to this later.

Equation (6) is one of many possible formal approximate solutions to the two-body problem. How will the introduction of an extra $(N-2)$ particle affect the picture? For extremely dilute systems the changes are small (cf. Mayer gas theory), while for dense systems the two-particle picture is qualitatively wrong. Regardless of the density one may proceed as follows:

(i) Suppose the remaining particles are uncorrelated and constitute a uniform "field" of uniform probability density. Since the original pair could be any pair, one need then only average over all possible pairs using correct weighting factors for different possible values of K.

(ii) Suppose a third particle is detached from the uncorrelated field. One would then have to solve a three-body problem exactly and average in the same way as above.

(iii) Suppose a fourth particle is detached. It would then be necessary to solve a four-body problem. And so forth.

Clearly, we can only discuss stage (i). The weighting function is $\rho_2(\tau)$, the Fourier-transformed diagonal two-particle density matrix. Before averaging, one must be certain that there is no correlation in momentum space affecting the probability of two particles having relative momentum K. As long as the interaction is momentum-independent, one can make this assumption (for spin-dependent forces and magnetic forces, in general, one cannot argue thus). In the absence of such an interaction, only the change in kinetic energy due to correlation will affect $\rho_2(K)$.

The pair distribution for an interacting gas will clearly be defined in a way analogous to the noninteracting case ρ_{20}:

$$\int\rho_{20}(K)|\psi_{\text{relative}}|^2d^3K\Big/\int\rho_{20}(K)d^3K=1\pm\rho_{10}^2(r),$$
$$V\int\rho_{20}d^3K=\tfrac{1}{2}N(N-1)+\tfrac{1}{2}[\rho_1^2(0)-\rho_1(0)]. \quad (7)$$

Recall the connection between the Born approximation for (5) and the usual first-order perturbation theory. If $R_l\to j_l$, we would have for a many-body system the usual result, making use of the identity

$$2\sum_l(2l+1)j_l^2(\pi Kr)=1\pm\frac{\sin(2\pi Kr)}{2\pi Kr}. \quad (8)$$

Thus, averaging over $\rho_{20}(K)$ as in (7), we get for an ideal Fermi gas,

$$\rho_{20}(r)=1-\tfrac{1}{2}\rho_{10}^2(r). \quad (9)$$

The Hartree-Fock potential energy per particle is obtained from the usual formula

$$E_p=\frac{N}{2V}\int\rho_2(r)u(r)d^3r, \quad (10)$$

so we define, following (6),

$$\tfrac{1}{2}(N-1)\rho_2(r)=2(A\sum_{l\text{ even}}+B\sum_{l\text{ odd}})(2l+1)\times\frac{V}{N}\int_0^\infty j_l(\pi Kr)R_l(K,r)\rho_2(K)K^2dK. \quad (11)$$

For practical calculations we note that $\rho_1(K)$ and $\rho_2(K)$ also have a perturbation expansion for interacting systems (cf. I), and that Eq. (11) is defined in the same iterative sense as Eqs. (3) and (5).

In the next section the method for various kinds of interaction potential is illustrated.

2. ENERGY PER PARTICLE

A. Hard-Sphere Gas

The hard-sphere system is a useful test of the formulas of the approach outlined above since the phase shifts can be easily calculated exactly. Thus assuming

$$u(r)=\infty, \quad r<a$$
$$=0, \quad r>a$$

the phase shifts are[5]

$$\tan\delta_l=j_l(\pi Ka)/n_l(\pi Ka), \quad (12)$$

with j_l, n_l being spherical Bessel and Neumann functions. In the limit $\pi Ka\ll1$ it is easy to verify that

$$\tan\delta_l\approx\sin\delta_l\approx\delta_l\approx(\pi Ka)^{2l+1}/(2l+1)!!, \quad (13)$$

so that the only contribution to terms of order a and a^2 are due to S-wave scattering $\delta_0=-\pi Ka+O(a^3)$. We observe that the linear term in K will just cancel the $1/K$ dependence in (5), so that the average over all K states is trivial. The only step necessary to obtain the first-order energy per particle of the many-body system is to match the normalization constant, which means multiplying Eq. (5) by $\frac{1}{2}N$. This can be verified by comparing Eqs. (5) and (2) with the usual formula for the

potential energy. The result, at low density, is

$$E_p=(2\pi\hbar^2N/mV)aA+\cdots, \tag{14}$$

where $A=1$ for bosons and $\frac{1}{4}$ for fermions. These results are well known (originally found by Lenz[7]).

We make some remarks concerning higher-order calculations. It is clear that P, D, and higher-order partial waves do not contribute until at least the order a^3, for both bosons and fermions. If a term of order a^2 exists, it must arise from a modification to the approximate function $R_l(K,r)$ due to the correction just calculated, i.e.,

$$K'^2=K^2+4aA/\pi V+\cdots. \tag{15}$$

Hence, although the first-order correction can be found without calculating $R_l(r)$ at all, higher-order corrections need a more detailed approach.[8,9] However, it can be seen that in the Bose case there will not be corrections from the ground-state distributions $\rho_{20}(K)$ or $\rho_0(k)$ since these vanish identically except at $K=0$, $k=0$. Hence all corrections to (14) for bosons (for all partial waves) must also involve the expansion parameter W_0 (cf. I), $\propto(a^3N/V)^{1/2}$. Hence we expect an extra term in (14),

$$E_{p\ \mathrm{Bose}}=(2\pi\hbar^2Na/mV)[1+\alpha(a^3N/V)^{1/2}+\cdots]. \tag{16}$$

In the Fermi case, the ground-state distribution has a different form and one would expect the next contribution beyond (14) to contain only the Fermi parameter k_F, i.e.,

$$E_{p\ \mathrm{Fermi}}=(\pi\hbar^2Na/2mV)(1+\beta k_Fa+\cdots). \tag{17}$$

The expansion (16) is interesting in that it predicts the failure of any attempt to expand the wave function, for example, in simple powers of a. The correct parameter arises from the convergent expansion of the momentum distribution functions $\rho(k)$ and $\rho_2(K)$. The deviations from the ground-state contributions represent zero-point oscillations (phonons). Thus W_0 refers to phonon interactions and aW_0 to phonon-particle interactions, while a term of order W_0^2 represents phonon-phonon interactions.

B. Lennard-Jones Potential

Consider the potential[9]

$$u(r)=u_0[(a/r)^{10}-(a/r)^6].$$

In the case of zero-energy scattering, the radial equation is

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_0}{dr}\right)-\frac{2\mu}{\hbar^2}u(r)R_0(r)=0, \tag{18}$$

with Whittaker's function as solution,

$$R_0(r)=[\Gamma(\tfrac{5}{8}-\eta)/\Gamma(\tfrac{1}{4})](\tfrac{1}{2}\lambda^{1/2})^{-3/8}\times r^{3/2}W_{\eta,1/8}(\tfrac{1}{2}\lambda^{1/2}r^{-4}), \tag{19}$$

and with the asymptotic form

$$R_0(r)=1+\frac{\Gamma(-\frac{1}{4})\Gamma(\frac{5}{8}-\eta)}{\Gamma(\frac{1}{4})\Gamma(\frac{3}{8}-\eta)}(\tfrac{1}{2}\lambda^{1/2})^{1/4}\frac{1}{r}+O(1/r^4). \tag{20}$$

Here λ and η are defined as

$$\lambda=m\mu_0a^{10}/\hbar^2,\quad \eta^2=m\mu_0a^2/64\hbar^2.$$

Since we are taking $K=0$, only $\delta_0\neq0$, and the first-order Bose-gas energy is

$$E_p^{(0)}=4\pi2^{3/4}\frac{\Gamma(\frac{3}{4})\Gamma(\frac{5}{8}-\eta)}{\Gamma(\frac{1}{4})\Gamma(\frac{3}{8}-\eta)}u_0^{1/8}a^{5/4}\frac{\hbar^{7/4}}{m^{7/8}}\frac{N}{V}, \tag{21}$$

which is exactly Abe's result.[9] It is not defined when $\eta=\frac{5}{8}$, the case of resonant scattering, when a bound state is about to be formed.[10] Then

$$R_0(r)=\frac{1}{r}\exp\left[-\frac{5}{4}\left(\frac{a}{r}\right)^4\right]\rightarrow\frac{1}{r}+O\left(\frac{1}{r^5}\right)\quad\text{as}\quad r\rightarrow\infty. \tag{22}$$

This form is quite different from Eq. (19). This is connected with the fact that for resonance scattering we have $\delta_l\neq0$ ($l>0$) and the scattering is not momentum-independent. The form $1/r$ indicates that the S-wave function is pulled in by the attractive potential and higher waves contribute to the asymptotic form of the total wave function.

For a Fermi gas, the first-order energy can be calculated as in (20) but here, since it is not reasonable to assume $K=0$, a better perturbation treatment of the *full* radial equation is needed in which (20) may be taken as the first approximation. This is under study, is quite complicated, and will be reported later.

C. Nonsingular Potentials

Though not of great physical interest, nonsingular potentials allow the derivation of simple results as illustration of the method. Consider

$$u_1(r)=\begin{cases}-d, & r<a\\ 0, & r>a\end{cases} \tag{23a}$$

and

$$u_2(r)=\begin{cases}d, & r<a\\ 0, & r>a.\end{cases} \tag{23b}$$

As usual, at low density, we focus on S-wave scattering and do not consider bound states or resonant scattering

[7] W. Lenz, Z. Physik **56**, 778 (1929).
[8] K. Huang and C. N. Yang, Phys. Rev. **105**, 767 (1957).
[9] R. Abe, Progr. Theoret. Phys. (Kyoto) **19**, 1 (1958); **19**, 699 (1958); **19**, 713 (1958).

[10] It can be shown that for $0\leq\eta<\frac{5}{8}$ there are no bound states, while for $\eta>\frac{5}{8}$ there is at least one bound state.

with u_1. The exterior and interior solutions of the radial equation are matched by the logarithmic derivative across a. Letting

$$\pi K=(2\mu E/\hbar^2)^{1/2},\quad \pi K_1=(2\mu d/\hbar^2)^{1/2},\quad K_0^2=K^2\pm K_1^2, \tag{24}$$

where $\pm$ refers to u_1 and u_2, one gets

$$\delta_0=\tan^{-1}[(K/K_0)\tan\pi K_0 a]-\pi K a. \tag{25}$$

More detailed analysis shows[11] that the phase shift δ_0 approaches a positive integral multiple of π, the integer being the number of $l=0$ bound states. Here $\delta_0\to 0^+$ or 0^- for u_1 or u_2. The no-bound-state restriction is fulfilled if $K_1a<1$ and $K_1a\neq\frac{1}{2}$, i.e.,

$$2\mu da^2/\hbar^2<1,\quad 2\mu da^2/\hbar^2\neq\tfrac{1}{4}.$$

When either of these becomes an equality, one has resonance scattering.

The potential energy is obtained, to first order in powers of a, by noting that for bosons $A=1$ only the asymptotic value of δ_0/K is significant, since other K's do not contribute to $\rho_0(k)$ and $\rho_{20}(K)$. Thus from (25), for $Ka\ll 1$, one gets

$$E_p=\frac{2\pi\hbar^2N}{mV}\left(a-\frac{\tan\pi K_1a}{\pi K_1}\right)A+\cdots \quad \text{for } u_1, \tag{26a}$$

$$E_p=\frac{2\pi\hbar^2N}{mV}\left(a-\frac{\tanh\pi K_1a}{\pi K_1}\right)A+\cdots \quad \text{for } u_2. \tag{26b}$$

In the limit of very weak interaction, $K_1a\ll 1$, the power series for tan and tanh converge, and terms of $O(a)$ cancel for both u_1 and u_2. On the other hand, for a finite and $K_1\to\infty$, (26b) reduces correctly to the hard-sphere expression (14).

[11] N. F. Mott and W. Massey, *Theory of Atomic Collisions* (Oxford University Press, New York, 1949).

The Fermi case is superficially similar in the limit $K_1a<\frac{1}{2}$ to the above, when terms linear in a cancel. But if $K_1^2\gg K^2$, so that $K_0^2\sim K_1$ or iK_1, δ_0 again contains only a term linear in K so that the average over $\rho_2(K)$ is trivial. The first-order results are as in (26), with $A=\frac{1}{4}$ and the additional condition $K_1^2\gg K^2$. This makes (26a) worthless for fermions except near resonance, while (26b) is valid at low density $Ka\ll 1$ with a moderately "soft" repulsion or at higher densities with consequently "harder" repulsions. To calculate the energy where the above limiting conditions do not hold true involves an exceedingly complex integration which has not yet been carried out.

3. DISCUSSION

A combination of the partial-wave formalism of scattering and the reduced-density-matrix formulation of the many-body problem has been used to calculate the energy per particle of Fermi and Bose systems with various interactions and well-defined limits on the density, and some well-known results have been obtained. It would have been interesting to include a discussion of repulsive screened Coulomb and attractive Yukawa interactions, but the phase shifts cannot be obtained by analytical methods except in the Born approximation. For progress one clearly must be prepared to use numerical computing of the integrals that arise, but especially to use the many improvements over the Born approximation that are available, as well as, in the formulation of Sec. 1(ii), the recent analyses of the three-body problem.[12]

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[12] P. Resibois, Physica **31**, 645 (1965); **32**, 1473 (1966).