smaller), when in the initial state one normal mode is excited, equipartition of the energy is never achieved. On the contrary, in this case, when in the initial state the energy is equally distributed among the normal modes, one has in general, during the motion, a nonequipartition in time average. However, the modes with greater energy are scattered at random over the whole spectrum of the normal modes, and one has a coarse-grained equipartition. Of the many cases studied we present in Figs. 1–17 a selection which illustrates some typical behaviors discussed above.

CONCLUSIONS

The most important conclusion of this paper is that when the energy of vibration per particle is equal to or greater than 2 or 3% of depth of the potential well and the number of particles is sufficiently large, one has, in time average, equipartition of the energy among the normal modes, in spite of the fact that there is no evidence for the system to be ergodic. For lower energies one has recurrent motions if, in the initial condition, only one normal mode is excited, as found by FPU. In this respect one must remark two facts: The times over which the system is studied, i.e., some thousands of longest periods of the unperturbed system, are in effect rather short. A thousand longest periods of the system amounts to $5\times10^{-10}N$ sec, and that means that for 20–100 atoms, if the energy is sufficiently great, one reaches equipartiton in 10^{-8} sec.

The practical difficulty of keeping the numerical error small over times longer, for some order of magnitudes, than those over which the system has been studied makes it difficult to reach numerical conclusions on the equipartition of the energy for low excitation of the system. However, in such a case if the initial state is one of equal distribution of the energy, such a state is macroscopically conserved in time average, the more excited modes being distributed randomly over the whole frequency spectrum.

We may conclude by saying that, in the case of very low total energies, the relaxation mechanism towards the standard Boltzmann distribution of the normal modes might act so slowly that the coupling of the system with a thermal bath could be very important in determining the approach of the model towards such a distribution.

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Scattering Probability for Fast Test Particles in a Plasma*

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An effective total cross section is calculated for elastic scattering of a monoenergetic beam of test particles in a plasma of arbitrary velocity distribution. Closed-form solutions are obtained for the special case of Maxwellian field particles taking into account small-angle scattering. The result are compared with those obtained using the Debye cutoff technique, and it is shown that such an arbitrary cutoff can lead to erroneous results in the effective cross section and can lead to different conclusions with regard to the relative importance of plasma ions and electrons in test-particle scattering.

I. INTRODUCTION

Recent feasibility studies[1–4] of possible steady-state thermonuclear reactors have shown the need to investigate in detail the behavior of fast charged particles in energetic plasmas. Such studies are important in calculating the thermalization rates of fast test ions,[1,2] the slowing-down time necessary for these ions to transfer a major fraction of their energy to the plasma,[1] secondary fusion reactions,[3] and velocity distributions[4] which are essential in studying the dynamic behavior of fusion reactors.[5]

Several investigators have used the Rosenbluth-MacDonald-Judd[6] (RMJ) form of the Fokker-Planck equation in their studies of this problem. For example, Kranzer[7] has determined numerically the time history of the probability distribution of fast test ions in velocity space for some special cases. More recently Kuo-Petravic, Petravic, and Watson have used the RMJ equation to study the energy transfer from reaction-produced α particles to plasma electrons and ions in mirror reactors.[4] A modified approach has previously been taken by Butler and Buckingham[8] to calculate the energy-loss rate from fast test ions. In all of the above work, the classical Rutherford scattering cross section has been used. To avoid the well-known divergence in integrating over the deflection angles, scattering for angles smaller than $\chi_0^{(c)}$ is neglected where

$$\chi_0^{(c)} = \xi / v_r^2 \lambda_D \quad , \tag{1}$$

and where $\xi = (q_t q_f / 4\pi\epsilon_0 \mu)$. Here q_t and q_f are the charges of the test and field particles, respectively, μ is the reduced mass, v_r is the relative velocity, λ_D is the Debye screening length, and the rest of the notation is used in the standard manner. The validity criterion for the use of this classical cutoff limit rather than the quantum-mechanical cutoff angle[9]

$$\chi_0^{(q)} = \hbar / \mu v_r \lambda_D \tag{2}$$

is discussed by several authors. The use of the Rutherford cross section is limited to situations in which the orbital model for scattering can be used, and the validity criterion for the use of this has been discussed by Williams,[10] Bohr,[11] Everhart, Stone, and Carbone,[12] and Lane and Everhart.[13] In cases when the particle's wave properties must be considered, the Born approximation should be used. The present authors have treated the problem of slowing down of fast test ions in plasmas in the limit of $v_r \simeq v_t$, where v_t is the test-particle velocity.[9,14] In this case the Born approximation can be used for deflection angles from 0 to π, and no cutoff angle need be assigned to get a closed-form solu- n. For the general evaluation of energy degradation of ions released from thermonuclear reactions in a plasma, both the classical and quantum-mechanical formulas for the cross section must be used since they are valid for mutually exclusive velocity ranges. Lane and Everhart[13] have examined a similar situation in calculating the total cross section for scattering from Coulomb potentials with exponential screening for the interaction of two colliding atoms. Their technique is adopted here to include all angles of deflection in the calculations and to obtain results which are valid for the complete velocity range.

It is the purpose of this paper to calculate the effective total scattering cross section for the interaction between a test particle or a beam of monoenergetic particles in a plasma which has an arbitrary velocity distribution. The thermal motion of the field particles affects the cross section greatly if the test particle moves with a velocity less than or equal to the mean thermal velocity of the field particles. Closed-form solutions are obtained for the special case of Maxwellian field particles.

The total cross section obtained can not be measured owing to the dominant contribution of immeasurable small-angle encounters; however, its use is essential in calculating the steady-state distribution of charged fusion reaction products in a thermonuclear plasma from the transport equation.[1] In addition, the relative importance of plasma ions and electrons is found for the special case of a Maxwellian plasma. The results obtained here are compared with the results obtained using different limits for the cutoff angle.

The differential cross sections for elastic scattering by an exponentially screened Coulomb potential are taken for the different angular regions as

$$\sigma_s^{(c)}(v_r, \chi) = (\xi / 2v_r^2)^2 \sin^{-4} \tfrac{1}{2}\chi \quad , \chi_0^{(q)} < \chi \leq \pi \tag{3}$$

and the Born approximate formula

$$\sigma_s^{(q)}(v_r, \chi) = (\xi / 2v_r^2)^2 (\sin^2 \tfrac{1}{2}\chi + \tfrac{1}{4}\chi_0^2)^{-2} \quad , \quad 0 \leq \chi < \chi_0^{(q)} \tag{4}$$

There is an uncertainty about the transition region in which neither expression is valid. However, extending the range of validity of Eqs. (3) and (4) to $\chi = \chi_0^{(q)}$ leads to an uncertainty in the effective total cross section of a factor of $\frac{3}{2}$. Since the uncertainty resides within a small numerical factor, the results are qualitatively correct. Quantitatively, we have included angular regions which have previously been neglected in the cutoff technique, and thus the results are expected to be numerically more rigorous than those using the classical scattering cross section, and a comparison is made in Sec. VI.

II. BINARY ENCOUNTERS

Consider the elastic scattering of a charged test particle whose speed lies between v and $v + dv$ by a charged field particle whose speed lies between V and $V + dV$. As viewed in the c.m. frame of reference the test particle will only change its direction after an encounter, and therefore we can write its speed in the laboratory system as

$$v'^2 = v_m^2 + \left(\frac{M}{m+M}\right)^2 v_r^2 + \frac{2M}{m+M} v_r v_m \cos\chi \quad . \tag{5}$$

We use standard notation where m and M are, respectively, the masses of the test and field particles, v' is the speed of the test particle after an encounter,

χ is the deflection angle in the c. m. system, and v_m is the velocity of the center of momentum. The interaction between the two charged particles is described by a screened Coulomb potential, and the differential cross sections for such an interaction are given by Eqs. (3) and (4).

The probability $g(v, v', V, \cos\theta)dv'$ that a test particle of velocity between v and $v+dv$ will emerge within a velocity interval between v' and $v'+dv'$ after an encounter with a field particle of velocity V whose direction makes an angle θ with the direction of the test particle is given by

$$g(v'; v, V, \cos\theta)dv' = -\frac{\sigma_s(v_r, \chi)d\Omega(\chi)}{\sigma_s(v_r)}, \tag{6}$$

where $d\Omega(\chi)$ is the element of solid angle and $\sigma_s(v_r)$ is the total elastic cross section integrated over all deflection angles as given in Ref. 13. By the use of Eqs. (3)–(5) the probability given in Eq. (6) can be expressed in terms of velocity as

$$g(v'; v, V, \cos\theta) = \begin{cases} 0, & v' > v_+ \\ \dfrac{2\pi\xi^2 v'(v_+^2 - v_-^2)}{v_r^4\sigma_s(v_r)[v_+^2 - v'^2 + \frac{1}{4}\chi_0^{(q)2}(v_+^2 - v_-^2)]^2}, & v_0 < v' \leq v_+ \\ \dfrac{2\pi\xi^2 v'(v_+^2 - v_-^2)}{v_r^4\sigma_s(v_r)(v_+^2 - v'^2)^2}, & v_- \leq v' < v_0 \\ 0, & v' < v_- \end{cases} \tag{7}$$

where v_+, v_0, and v_- are the values of v' at $\chi = 0$, $\chi = \chi_0$, and $\chi = \pi$, respectively.

III. TOTAL CROSS SECTION FOR ARBITRARY VELOCITY DISTRIBUTION

Consider the interaction between a charged test particle and field particles of number density n with an angular velocity distribution $N(v, \Omega(\theta))$. The encounter rate per unit volume is

$$v_r\sigma_s(v_r)nN(v, \Omega(\theta))d\Omega(\theta)dV\ , \tag{8}$$

which can also be expressed as

$$vnd\sigma_s(v, V, \Omega(\theta))\ . \tag{9}$$

Here $d\sigma_s(v, V, \Omega(\theta))$ is the microscopic cross section for a test particle to encounter a field particle whose velocity lies in a direction contained in the solid angle $\Omega(\theta)$ relative to the initial test-particle velocity. Equating both results gives an expression for the differential cross section defined by Eq. (9), i.e.,

$$d\sigma_s(v, V, \Omega(\theta)) = (v_r/v)\sigma_s(v_r)N(v, \Omega(\theta))d\Omega(\theta)dV\ . \tag{10}$$

Now the total cross section for elastic scattering between the test particle under question and the field particles is obtained by multiplying Eq. (10) by the probability given in Eq. (7) and integrating over v', V, and $\Omega(\theta)$, that is,

$$\overline{\sigma}_s(v) = \int_{v'}\int_V\int_{\Omega(\theta)} g(v'; v, V, \cos\theta)d\sigma_s(v, V, \Omega(\theta))dv'\ . \tag{11}$$

For a given distribution, Eqs. (7) and (10) can be substituted into Eq. (11) and the solution gives the desired cross section.

IV. SCATTERING CROSS SECTION IN A MAXWELLIAN MEDIUM

Consider a single-species Maxwellian plasma of energy kT where Eq. (11) can be written explicitly as

$$\overline{\sigma}_s(v) = \frac{2\pi\xi^2}{v}\left(\frac{M}{2\pi kT}\right)^{3/2}\left[\int_{v_-}^{v_0}\int_0^{\infty}\int_{-1}^{1}\frac{v'V^2(v_+^2 - v_-^2)}{v_r^3(v_+^2 - v'^2)^2}\exp\left(-\frac{MV^2}{2kT}\right)d\cos\theta\, dv'\, dV\right.$$
$$\left. + \int_{v_0}^{v_+}\int_0^{\infty}\int_{-1}^{1}\frac{v'V(v_+^2 - v_-^2)\exp(-MV^2/2kT)d\cos\theta\, dv'\, dV}{v_r^3[v_+^2 - v'^2 + \hbar^2(v_+^2 - v_-^2)/4\mu^2 v_r^2\lambda_D^2]^2}\right] \tag{12}$$

While the evaluation of this equation is tedious, it is straightforward and gives the result

$$\overline{\sigma}_s(v) = 6\pi\left(\frac{q_t q_f}{4\pi\epsilon_0}\right)^2\left(\frac{\lambda_D}{\hbar v}\right)^2 \operatorname{erf}(x)\ , \tag{13}$$

where x is the dimensionless velocity $(Mv^2/2kT)^{1/2}$. In the limit of $x > 1$, the error function asymptotically approaches unity. The expression preceeding the error function is in fact the total cross section for elastic scattering by a fixed scattering center. Since a plasma is composed of two or more species, it is more convenient to describe the medium by a total macroscopic cross section $\overline{\Sigma}_s$, that is

$$\overline{\Sigma}_s = 6\pi\left(\frac{Z_t e^2}{4\pi\epsilon_0}\right)^2\frac{\epsilon_0}{\hbar^2 v^2} \times [kT_e \operatorname{erf}(x_e) + \textstyle\sum_j kT_j \operatorname{erf}(x_j)]\ , \tag{14}$$

where the summation is over all ion species.

V. SCATTERING PROBABILITIES IN A THERMONUCLEAR PLASMA

The probability per unit time that a charged test particle will undergo scattering is related to the total cross section by the relation

$$p_s(v) = v\Sigma_s(v) \quad . \tag{15}$$

Consider the interaction of an energetic ion produced through a fusion reaction with the background thermonuclear plasma. In this case, $x_e < 1$ and $x_i > 1$, and the scattering probability is approximately given by

$$p_s(v) \simeq \frac{3Z_t^2 e^4}{8\pi\epsilon_0 \hbar^2 v}\left[2\left(\frac{m_e E k T_e}{\pi m}\right)^{1/2} + \sum_j kT_j\right] \tag{16}$$

because we approximate

$$\mathrm{erf}(x) \simeq \begin{cases}(2/\sqrt{\pi})x, & x<1\\ 1, & x>1\ .\end{cases}$$

More terms can be included for greater accuracy, but here we are only interested in the investigation of the relative probability of scattering by different species. The values of the dimensionless velocity x for charged fusion reaction products in plasmas of thermonuclear interest are always greater than unity for ions and less than unity for electrons so long as $T_e \gtrsim 10$ keV.

For all cases considered here the probability that an ion produced from the fusion reaction will scatter via plasma ions is larger than the probability that it will scatter via electrons. Because the reaction-produced particle is degraded in energy due to collisions and therefore eventually $x_i \leq 1$ and $x_e \ll 1$, thus Eq. (16) is not valid for the whole thermalization range. At these lower test-particle speeds the scattering probabilities become

$$p_s(v) \simeq \frac{3Z_t^2 e^4}{4\sqrt{2}\ \pi^{3/2}\epsilon_0 \hbar^2} \times\left[\sqrt{m_e kT_e} + \sum_j \sqrt{m_j kT_j}\left(1 - \frac{m_j v^2}{6kT_j}\right)\right]. \tag{17}$$

In practice the plasma gains energy from the hotter charged reaction products, and consequently the plasma temperature increases. However, in the steady state, energy losses may balance energy gains and the plasma temperature may be fairly constant. As long as $T_j \sim T_e$ the second term dominates the first and the probability of scattering via hydrogen ions is 30–45 times larger than that via electrons. The same conclusion can be reached by investigating the probability distribution function given by Eq. (7). The probability per unit speed that a test particle emerges after an encounter with a speed v_+ is

$$g(v_+; v, V, \cos\theta)dv_+ \simeq \frac{4\mu m v_r \lambda_D^2 v_+ dv_+}{3v_m \hbar^2} \quad . \tag{18}$$

The probability per unit speed that the velocity of a test particle is reduced to v_- is

$$g(v_-; v, V, \cos\theta)dv_- \simeq \frac{m\hbar^2 v_- dv_-}{12\mu^3 v_r^3 \lambda_D^2 v_m} \quad , \tag{19}$$

and this corresponds to a head-on collision.

Comparison of Eqs. (18) and (19) reveals that the probability per unit velocity of a small change in the velocity of the test particle is much much larger than the corresponding probability for large changes. As a matter of fact if $v \gg V$, test particle may lose all its energy in one encounter with an ion of equal mass. However, the probability that a 1-MeV reaction triton loses its energy in a single encounter with 10-keV plasma triton is of the order of 10^{-7} per J, while the probability that the test triton loses a very small fraction of its energy in a single encounter is about 10^{32} per J. In addition, Eq. (18) indicates that the velocity of the test particle is more likely to be reduced by an encounter with an ion than with an electron while Eq. (19) shows that electrons are more likely to reduce v to v_- rather than the ions.

Thus we can conclude that the probability of scattering per unit time of test particles by ions exceeds the scattering rate by electrons. In addition the probability that the test particles transfer their energy in small increments to the ions is significantly more probable than transferring energy in large increments to the electrons.

Although Eq. (11) has been applied to a Maxwellian plasma, other velocity distributions can be considered as well. For example, one could consider the loss-cone distribution found in mirror machines. The evaluation of the total scattering cross section and the scattering rates using such distributions is straightforward, although it is complicated by the fact that velocity distribution of the plasma in the mirror machine is not isotropic. The degree of anisotropy depends on the mirror ratio and so does the scalar velocity distribution.

It should be emphasized that we have restricted our examples to the case where $T_e \sim T_i$; however, the result in Eq. (14) is not so restricted.

VI. COMPARISON WITH DEBYE CUTOFF TECHNIQUE

To calculate the total cross section for elastic scattering between two particles it is rather conventional to integrate the Rutherford differential cross section over all angles above some cutoff angle and thereby neglect small-angle encounters. The cutoff procedure is only meaningful if the Debye sphere contains many plasma particles of the species under consideration.[15] This condition is well satisfied in a thermonuclear plasma; however, the choice of the limiting cutoff angle is a crucial problem. The rule is to choose the classical cutoff angle $\chi_0^{(c)}$ as the lower limit of the integration if $q_t q_f / 4\pi\epsilon_0 \hbar v_r \gg 1$. If such is not the case the quantum-mechanical cutoff angle $\chi_0^{(q)}$ must be chosen, and both angles are given in Eqs. (1) and (2). For energetic test particles or interactions with electrons and a low-Z plasma, the quantum-mechanical angle is the proper angle. However, in following the degradation of energy of a test particle in a plasma there will be an energy at which $\chi_0^{(q)} \simeq \chi_0^{(c)}$ below which the cutoff angle has to be $\chi_0^{(c)}$. In studying the total cross section for binary interactions such a choice is not critical, but if the field particles constitute a plasma of a specific velocity distribution, the results will be sensitive to such choices.

If it is applicable to use $\chi_0^{(c)}$, the integrated total cross section for elastic scattering of a test particle by Maxwellian single-species field particles is

$$\overline{\sigma}_s(v)^{(c)} = \sigma_s^{(c)} (1/\sqrt{\pi}\, x^2)[x e^{-x^2} + \tfrac{1}{2}\sqrt{\pi}\,(2x^2+1)\,\mathrm{erf}(x)] \quad , \tag{20}$$

and $\sigma_s^{(c)}$ is given by the classical scattering cross section in the limit of $v \gg V$, i.e.,

$$\sigma_s^{(c)} = 4\pi\lambda_D^2 \quad . \tag{21}$$

Equation (20) is derived from Eq. (11) with the proper choice of $g(v'; v, V, \cos\theta)$.

The scattering probability per unit time for the interaction of a test particle with a plasma composed of electrons of $x_e < 1$ and ions of $x_i \gg 1$ is

$$p_s(v) = \frac{4\pi\epsilon_0 v}{e^2}\left[\frac{2}{\sqrt{\pi}}\left(\frac{m k^3 T_e^3}{m_e E}\right)^{1/2} + \frac{kT_i}{Z_i^2}\right] \quad . \tag{22}$$

If $T_e \sim T_i$, scattering by electrons is seen to dominate that by ions. The apparent contradiction between this result and that found in Sec. V is due to the fact that within the velocity range in which Eq. (22) is valid, the cutoff angle is less than that determined by the uncertainty principle. Consequently, we have included energy ranges for which classical results are strictly invalid. The use of the proper cross section given in Eq. (4) for angles larger than $\chi_0^{(q)}$ leads to results which agree with those of Eq. (16) within a numerical factor of order 1.

In the limit of $x_e < x_i < 1$ we obtain

$$p_s(v) \simeq \frac{8\pi^{3/2}\epsilon_0 v}{e^2}\left(\frac{kT_e}{x_e} + \frac{kT_i}{Z_i^2 x_i} + \frac{kT_i x_i}{3Z_i^2}\right) \quad . \tag{23}$$

From Eq. (23) the scattering probability by electrons is larger than that by ions. The apparent contradiction between the implication of Eqs. (17) and (23) is attributed to the fact that in the derivation of Eq. (23) the classical cutoff angle is much larger than $\chi_0^{(q)}$. The choice of the larger cutoff angle does not affect the large-angle scattering cross section; however, the scattering probability and many other results are sensitive to such a choice. This is because the extremely gentle encounters leading to small-angle scattering make up a large part of the total scattering probability. Thus the main difference between Eq. (17) and Eq. (23) is that the former takes into account important scattering events which are neglected by the latter. If the contribution of these events is added to Eq. (23) we will get scattering probabilities similar to Eq. (17) within a small numerical factor. In addition, the cutoff angle $\chi_0^{(c)}$ in the limit of $x \ll 1$ is inversely proportional to the square of the thermal velocity of the field particles under consideration times the reduced mass of the test and field particles. Thus for $T_e \sim T_i$ the cutoff angle for electrons is likely to be lower than that for plasma ions and more small-angle scattering events will be included in the calculation of the scattering probability via electrons than that via ions.

Generally speaking, extreme caution must be exercised in using the cutoff technique. In the study of test-particle interactions with thermonuclear plasmas we are dealing with a broad energy spectrum and there is always a danger of cutting off dominant contributions to the results. In some cases the de Broglie wavelength is much less than the impact parameter of closest approach and consequently the scattering distribution is extremely rare for angles less than the limit given by $\chi_0^{(c)}$. Consequently, the error in the use of the cutoff technique is not significant. On the other hand if we are dealing with weak interactions, the small-angle scattering becomes more frequent than large-angle scattering and an improper choice of the low limit may lead to erroneous results. In addition, the particular composition of the plasma affects the cutoff angle. Both classical and quantum-mechanical cutoff angles depend on the reduced mass and the relative velocity. Consequently the limit on the scattering angles for small-mass electrons is different from that for ions. Furthermore, the roles of ions and electrons cannot simply be compared to each other since the neglected small-angle events may be more significant for one than for the other.

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Diagrammatic Analysis of the Method of Correlated Basis Functions. I. Jastrow Correlating Factor for a Weakly Interacting Bose Gas*

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The method of correlated basis functions (CBF) is examined for the special case of a weakly interacting Bose gas. Using the Hugenholtz-Pines theory, we compute the ground-state energy exactly to fourth order in the interaction strength. The resulting expression is compared term by term with the unperturbed ground-state energy computed in the CBF using a Jastrow function as the correlating factor. We find that the three leading orders are all accounted for by the Jastrow function, while beginning in the fourth order only selected terms are included. The use of a correlated wave function in effect corresponds to summations of selected diagrams to all orders. In particular, the ring diagrams and the ladder diagrams are most susceptible to these summations. In a separate paper we shall examine effects of perturbation in the CBF.

I. INTRODUCTION

We consider a system of N particles, contained in a volume Ω and interacting pairwise via a potential $v(r)$. N and Ω both approach infinity while the number density $n \equiv N/\Omega$ remains constant. Such a system is described by the Hamiltonian

$$H = \sum_{i=1}^{N} -\frac{\hbar^2}{2m_i}\nabla_i^2 + \sum_{\substack{i<j\\=1}}^{N} v(r_{ij}) , \tag{1}$$

and by the statistics of the particles.

A complete quantum-mechanical solution of the problem consists of determining all properly symmetrized eigenfunctions of this Hamiltonian and the corresponding spectrum of energy eigenvalues. For all realistic problems, however, we do not entertain the hope of obtaining such a complete solution; nor do we desire such a detailed description. In particular, for understanding properties of matter at low temperatures, we need only information concerning the ground state and the low-lying excitations. If the interaction $v(r)$ is weak, good approximation to these states can be found by applying low-order perturbative corrections to free-particle states.

For quantum liquids and solids, which include liquid and solid helium, Coulomb gases, and nuclear systems, the effects of $v(r)$ are far from insignificant. In fact, the interparticle correlations *dominate* the properties of these systems. Under these circumstances, the ordinary low-order perturbation theory fails. We have on our hands a many-body problem.

We distinguish in this paper two approaches toward treating the many-body problem: the independent-particle representation and the correlated representation. By the independent-particle representation we mean all field-theoretic methods which employ an independent-particle basis. When divergences arise in the matrix elements of $v(r)$, or in the perturbative expansion, one turns toward