Relaxation of a Fast Ion in a Plasma

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The relationship between a simple calculation (making no use of a distribution function) due to Butler and Buckingham, and previous work on relaxation processes (based on the Boltzmann or the Fokker-Planck equations) is examined. The Butler-Buckingham calculation is shown to correspond rigorously to a specific assumption as to the nature of the distribution function of the test particle: This assumption is shown to be valid for particles of high energy which relax by many small collisions. This approximation, in conjunction with its opposite extreme (the Mott-Smith approximation), covers essentially all relaxation problems.

1. INTRODUCTION

THE behavior of a fast test particle injected into a homogeneous plasma of electrons and ions, and particularly the rate of energy loss of such a test particle by Coulomb collisions, is a problem of obvious interest. This problem has been discussed in terms of relaxation times by various authors,[1,2] who have used both the Boltzmann[3] and the Fokker-Planck[4] collision equations. Kranzer[5] has used the Fokker-Planck equation to study the rate of energy loss as a function of time; this required numerical computation which was done for a few cases.

Starting from first principles, Butler and Buckingham[6] (hereafter called BB) recently derived an equation for the rate of energy loss. Their method avoided the introduction of a distribution function. Then in the limit when the energy of the test particle is in excess of the electron and ion thermal energy in the plasma, their expression simplifies, and they got a closed expression for the mean energy of the test particle as a function of time. (We shall see below that their initial equation for the rate of energy loss is in fact only valid in this high-energy limit.)

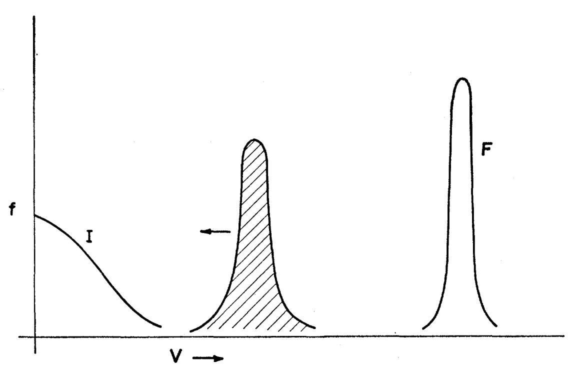

FIG. 1. The approximation (2).

The aim of this paper is to investigate the relationship between the BB calculation and the more usual treatment of the problem in terms of the Boltzmann or Fokker-Planck equations together with a distribution function $f(v,t)$ for the test particle.

We see that the BB equation corresponds to a specific approximation to $f(v,t)$. This is established in Sec. 2 where we show that the BB equation for energy loss due to Coulomb collisions,

$$\frac{d}{dt}\left(\frac{MV^2}{2}\right)=\frac{4\pi}{M}(Zze^2)^2\ln\Lambda\int F(\mathbf{w})d\mathbf{w}\times\left[\frac{(\mathbf{w}-\mathbf{V})\cdot[(\mathbf{w}-\mathbf{V})+\mathbf{V}(M+m)/m]}{|\mathbf{w}-\mathbf{V}|^3}\right], \quad (1)$$

may be derived *exactly* from the Boltzmann collision equation if the test particle distribution function is assumed to be

$$f(v,t)=\delta[v-V(t)]. \quad (2)$$

[In Eq. (1), M is test particle mass, $F(\mathbf{w})$ the distribution function for plasma particles of mass m. Although the proof is not included, it can also be shown that substitution of (2) into the Fokker-Planck equation (22) leads *exactly* to the result (1).]

The physical significance of the approximation (2) is clear: It applies when the test particle relaxes from its initial distribution function [$\delta(v-V_0)$, say] to its final thermalized distribution function by *a large number of small collisions*, such that at intermediate times it has some intermediate distribution function, in "local" equilibrium. The situation may be illuminated by considering the opposite extreme case where test particles relax in *one* collision: The approximation for this process is the well-known Mott-Smith[7] approximation

$$f(v,t)=A(t)f_I(v)+B(t)f_F(v), \quad (3)$$

where f_I is the initial distribution [$\delta(v-V_0)$ say] and f_F the final distribution when all test particles are thermalized. Here, in contrast to (2), $f(v,t)$ for intermediate times is a mixture of initial and final distributions and not some intermediate function. The situation is further displayed in Figs. 1 and 2: In both figures the

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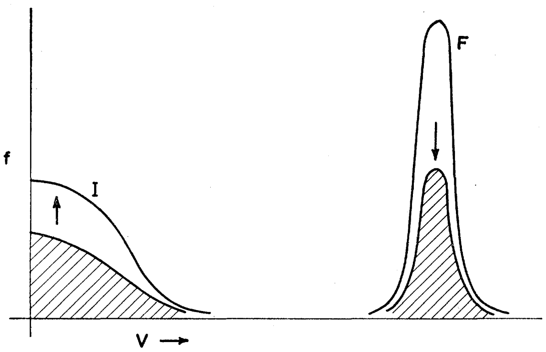

FIG. 2. The Mott-Smith approximation.

curve labeled I represents the initial distribution, F the final one, and the hatched curve a distribution for some intermediate time. (Arrows show the manner in which the intermediate distributions "move.")

In the preceding paragraph we have given a qualitative account of the validity of the approximation (2): We now formulate a precise criterion. The criterion for applicability of the Mott-Smith approximation is well known: Various velocity moments of the Boltzmann equation may be taken to find the coefficients A and B, and the approximation is good if and only if the results do not depend on which moment is chosen. Similarly, for the opposite extreme approximation (2), $V(t)$ is calculated from a moment of the Boltzmann equation, and the approximation is valid if and only if all moments give essentially the same result for $V(t)$. In Sec. 3 this criterion is applied to (2) for the case of the Boltzmann equation with Coulomb collisions. The approximation is shown to be valid when the energy of the test particle is large compared to the energy of plasma particles. This is the limit considered by BB. [Again, in this limit we could also show the approximation (2) is good in the case of the Fokker-Planck equation, by applying the above criterion.]

It is worth noting that just as the Mott-Smith approximation can be improved by writing $A_1+A_2v^2+\cdots$ in place of A and $B_1+B_2v^2+\cdots$ in place of B in Eq. (3), so the opposite approximation (2) can be improved by writing

$$f(v,t)=\left(\frac{M}{2\pi kT(t)}\right)^{3/2}\exp\left[\frac{-M[v-V(t)]^2}{2kT(t)}\right]. \quad (4)$$

Whereas one moment equation was needed to get $V(t)$, two are now required. An alternative criterion for the validity of the approximation is that the thermal velocity spread about $V(t)$ be less than $V(t)$ itself; i.e., $MV^2(t)>2kT(t)$. Equation (4) could be substituted into the Fokker-Planck equation or the Boltzmann equation with Coulomb collisions and moments taken (after the style of Sec. 2 below): The resulting calculation reproduces exactly the results in Sec. 6 of BB.

In an Appendix, we outline a calculation which is supplementary to the discussion above. We take the usual Fokker-Planck equation (as used, for example, by Kranzer[5]) and simplify the coefficients $h(v)$ and $g(v)$ by taking a test particle with energy greater than the energy of the plasma electrons and ions. The resulting partial differential equation for $f(v,t)$ may be solved analytically to get a δ-function distribution function, just as in Eq. (2).

2. DEDUCTION OF Eq. (1) FROM Eq. (2)

For a spatially homogeneous system in the absence of external fields, the Boltzmann collision equation is

$$\frac{\partial f(\mathbf{v})}{\partial t}=\int\int[f(\mathbf{v}')F_\alpha(\mathbf{w}')-f(\mathbf{v})F_\alpha(\mathbf{w})]\times\sigma(\Omega)|\mathbf{g}|d\Omega d\mathbf{w}. \quad (5)$$

$f(\mathbf{v})$ is the distribution function for the test particle (mass M), $F_\alpha(\mathbf{w})$ is the distribution of the species "α" of thermalizing particle (mass m_α). Unprimed quantities are before collisions, primed quantities after collisions: The dynamics of binary encounters gives (in center-of-mass coordinates)

$$\mathbf{v}'=\mathbf{v}+[2m_\alpha/(M+m_\alpha)](\mathbf{k}\cdot\mathbf{g})\mathbf{k}, \quad (6)$$

where $\mathbf{g}$ is the relative velocity, $\mathbf{g}=\mathbf{w}-\mathbf{v}$. $\mathbf{k}$ is a unit vector connected with the angle of scattering [$\mathbf{g}\cdot\mathbf{k}\equiv g\sin(\theta/2)$, where θ is the scattering angle]. For Coulomb collisions we can write the differential cross section as

$$\sigma(\Omega)|\mathbf{g}|d\Omega=\left(\frac{Zze^2(M+m_\alpha)}{Mm_\alpha}\right)^2\frac{\cos(\theta/2)d(\theta/2)d\phi}{(\mathbf{g}\cdot\mathbf{k})^3}. \quad (7)$$

If we take the v^2 moment of Eq. (5), we have

$$\frac{\partial}{\partial t}\int f(\mathbf{v})v^2d\mathbf{v}=\int\int\int(f'F_\alpha'-fF_\alpha)v^2\sigma|\mathbf{g}|d\Omega d\mathbf{v}d\mathbf{w}. \quad (8)$$

Finally, we use the relations (which can be proved from conservation and symmetry properties of binary collisions)

$$d\mathbf{v}d\mathbf{w}=d\mathbf{v}'d\mathbf{w}', \qquad |\mathbf{g}|\sigma(\Omega)d\Omega=|\mathbf{g}'|\sigma(\Omega')d\Omega'. \quad (9)$$

These, together with a change of variables in the first term in the collision integral in (8), lead to

$$\frac{\partial}{\partial t}\int f(\mathbf{v})v^2d\mathbf{v}=\int\int\int f(\mathbf{v})F_\alpha(\mathbf{w})\times[(v')^2-v^2]|\mathbf{g}|\sigma d\Omega d\mathbf{v}d\mathbf{w}. \quad (10)$$

This, with (6) and (7), is the energy moment of the Boltzmann equation for Coulomb collisions.

Now we take the approximate distribution function

(2): substitution into (10) gives

$$\frac{\partial V^2(t)}{\partial t}=4\left(\frac{Zze^2}{M}\right)^2\int F_\alpha(\mathbf{w})d\mathbf{w}\int\frac{\cos(\theta/2)d(\theta/2)d\phi}{(\mathbf{g}\cdot\mathbf{k})^2}\times\left[\mathbf{g}\cdot\mathbf{k}+\mathbf{V}\cdot\mathbf{k}\left(\frac{M+m_\alpha}{m_\alpha}\right)\right],\quad(11)$$

with $\mathbf{g}=\mathbf{w}-\mathbf{V}$. In the angle integration, we make the usual observation that there is a minimum angle of scattering θ_0. Doing the angle integrals (exactly), we get

$$\frac{\partial}{\partial t}V^2=8\pi\left(\frac{Zze^2}{M}\right)^2\ln\Lambda\int F_\alpha(\mathbf{w})d\mathbf{w}\times\left[\frac{g^2+\mathbf{V}\cdot\mathbf{g}(M+m_\alpha)/m_\alpha}{g^3}\right],\quad(12)$$

which is Eq. (1). $\ln\Lambda$ has been defined as usual as $\ln\Lambda=-\ln(\sin(\theta_0/2))\approx\ln(2/\theta_0)$.

This completes the derivation of (1) from the Boltzmann equation, under the assumption (2).

Starting from the Fokker-Planck equation (22), an identical procedure leads again to exactly Eq. (1).

3. VALIDITY OF THE APPROXIMATION

In Sec. 2 we assumed the distribution function (2), and used the v^2 moment of the Boltzmann equation to get an equation for $V(t)$. The approximation (2) will be a good one if and only if *any* moment of the Boltzmann equation leads to essentially the same expression for $V(t)$. In this section we examine the conditions under which the v^4 moment leads to the same results as the v^2 moment.

It is possible to use an arbitrary moment, $|\mathbf{v}|^n$, to compare with $n=2$: The end result is the same as for the comparison of $n=4$ and $n=2$ (unless n is vast), and involves more work.

If we follow the procedure of Sec. 2, but take the v^4 moment, we are led to an equation similar to (10):

$$\frac{\partial}{\partial t}\int f(\mathbf{v})v^4d\mathbf{v}=\int\int\int f(\mathbf{v})F_\alpha(\mathbf{w})\times[(v')^4-v^4]|\mathbf{g}|\sigma d\Omega d\mathbf{v}d\mathbf{w}.\quad(13)$$

On using the approximation (2) for f, Eq. (13) along with (6) and (7) leads to

$$\frac{\partial}{\partial t}V^2(n=4)=4\left(\frac{Zze^2}{M}\right)^2\int F_\alpha(\mathbf{w})d\mathbf{w}\times\int\frac{\cos(\theta/2)d(\theta/2)d\phi}{(\mathbf{g}\cdot\mathbf{k})^2}(\mathbf{g}\cdot\mathbf{k}+\mathbf{V}\cdot\mathbf{k}/x)\times\left[1+\frac{2x}{V^2}(\mathbf{V}\cdot\mathbf{k})(\mathbf{g}\cdot\mathbf{k})+\frac{2x^2}{V^2}(\mathbf{g}\cdot\mathbf{k})^2\right].\quad(14)$$

Again $\mathbf{g}=\mathbf{w}-\mathbf{V}$, and x is defined for convenience as $x=m_\alpha/(M+m_\alpha)<1$. The difference between Eq. (11) (from the moment $n=2$) and Eq. (14) (from $n=4$) lies in the last factor in the integrand in (14). Performing the angle integrals as before we get

$$\frac{\partial V^2(n=4)}{\partial t}=8\pi\left(\frac{Zze^2}{M}\right)^2\int F_\alpha(\mathbf{w})\frac{d\mathbf{w}}{g^3}\times\{\ln\Lambda[2g^2-(\mathbf{V}\cdot\mathbf{g})^2/V^2+\mathbf{g}\cdot\mathbf{V}/x]+(1/2V^2)\times[3(\mathbf{V}\cdot\mathbf{g})^2-V^2g^2+4x(\mathbf{V}\cdot\mathbf{g})g^2+2x^2g^4]\}.\quad(15)$$

It is possible to see that for all values of x (<1 by its definition) and V, the second term in the curly brackets in (15) is less than the first term by at least $1/\ln\Lambda$. We shall thus neglect the second term, which is negligible when the minimum angle of scattering θ_0 is small. This corresponds to the remark that in a low-density medium, Coulomb scattering takes place predominantly from many small scatterings rather than from large ones. (This is illustrated by the fact that in all derivations of the Fokker-Planck equation for Coulomb collisions terms of order $1/\ln\Lambda$ are discarded.) Returning to compare Eqs. (12) and (15) we see that they can be written

$$\frac{\partial}{\partial t}V^2(n=4)-\frac{\partial}{\partial t}V^2(n=2)=8\pi\left(\frac{Zze^2}{M}\right)^2\ln\Lambda\times\int F_\alpha(\mathbf{w})d\mathbf{w}\left[\frac{g^2-(\mathbf{g}\cdot\mathbf{V})^2/V^2}{g^3}\right].\quad(16)$$

The difference between $V(t)$ from the v^4 moment and $V(t)$ from the v^2 moment will thus be small [and the approximation (2) therefore valid] when the right-hand side of (16) is small compared to that of (12). It is a straightforward matter to perform the integrals in (12) and (16), using the Maxwellian distribution for the scattering particles of type α

$$F_\alpha(w)=N_\alpha(\pi\bar{w}_\alpha)^{-3/2}\exp[-(w/\bar{w}_\alpha)^2],\quad(17)$$

and then make a rigorous comparison of the two results. ($\bar{w}_\alpha$ is the thermal speed, $m_\alpha\bar{w}_\alpha^2=2kT_\alpha$.) The same results may be found, without going into detail, by the following observations:

(a) For a fast test ion colliding with plasma ions (here $\alpha\equiv i$), that is for $M\sim m_i$, $V\gg\bar{w}_i$, we put $\mathbf{g}\sim\bar{\mathbf{w}}_i-\mathbf{V}$ in Eq. (12) to get

$$\frac{1}{4\pi}\int d\Omega\left[\frac{g^2+\mathbf{V}\cdot\mathbf{g}(M+m_\alpha)/m_\alpha}{g^3}\right]\approx\frac{-MV^2}{m_i(V^3)}.\quad(18)$$

In Eq. (16)

$$\frac{1}{4\pi}\int d\Omega\left[\frac{g^2-(\mathbf{V}\cdot\mathbf{g})^2/V^2}{g^3}\right]\approx\frac{2}{3}\cdot\frac{\bar{w}_i^2}{(V^3)}.\quad(19)$$

That is to say the v^2 and v^4 moments give the same expression for $V(t)$ up to corrections of the order

$$m_i\bar{w}_i^2/MV^2.$$

(b) For a test ion with speed less than the electron thermal speed (here $\alpha\equiv e$), that is for $M\gg m_e$, $V\lesssim\bar{w}_e$, in Eq. (12) we get

$$\int d\Omega\left[\frac{g^2+\mathbf{V}\cdot\mathbf{g}(M+m_\alpha)/m_\alpha}{g^3}\right]\sim\frac{MV^2}{m_e(\bar{w}_e^3)} \tag{20}$$

and in (16)

$$\int d\Omega\left[\frac{g^2-(\mathbf{V}\cdot\mathbf{g})^2/V^2}{g^3}\right]\sim\frac{1}{\bar{w}_e}. \tag{21}$$

So that here the v^2 and v^4 moments give the same equation for $V(t)$ up to corrections of relative order

$$m_e\bar{w}_e^2/MV^2.$$

The above results are borne out by an explicit evaluation of the integrals in (12) and (16). We conclude that the approximate distribution function (2) is valid [and the consequent energy loss equation (1) is also valid] provided that the energy of the test particle is greater than the thermal energies of the various plasma particles.

A calculation similar to that above leads to the same conclusion for the Fokker-Planck equation. The only difference is that terms of order $1/\ln\Lambda$ [cf. Eq. (15)] never appear, as all such terms have been dropped in the derivation of the Fokker-Planck equation.

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APPENDIX

In this appendix we write down the Fokker-Planck equation for the distribution function, make those simplifications in the coefficients h and g which are applicable to the limit when the test particle energy is greater than that of the plasma particles, and solve the resulting equation exactly to get a solution of the form of (2). (In view of the discussion above, it would be surprising if we did not get such an answer.)

The Fokker-Planck equation for a test particle relaxing by Coulomb collisions is[4]

$$\frac{1}{\Gamma}\frac{\partial f}{\partial t}=-\frac{\partial}{\partial v_j}\left(f\frac{\partial h}{\partial v_j}\right)+\tfrac{1}{2}\frac{\partial^2}{\partial v_j\partial v_k}\left(f\frac{\partial^2 g}{\partial v_j\partial v_k}\right) \tag{22}$$

with the friction coefficient

$$h(v)=\sum_\alpha(1+M/m_\alpha)\int F_\alpha(\mathbf{w})\frac{d\mathbf{w}}{|\mathbf{v}-\mathbf{w}|} \tag{23}$$

and the convection coefficient

$$g(v)=\sum_\alpha\int F_\alpha(\mathbf{w})|\mathbf{v}-\mathbf{w}|d\mathbf{w}. \tag{24}$$

All other quantities are as defined previously, and Γ is

$$\Gamma=4\pi\left(\frac{Zze^2}{M}\right)^2\ln\Lambda. \tag{25}$$

We now consider the limit where the test particle is an ion with energy in excess of the thermal energy of the plasma ions and electrons. For plasma electrons it can then be seen that the friction term dominates the convection term:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{els}}\to-\Gamma\frac{\partial h_e}{\partial v}\frac{\partial f}{\partial v}-\Gamma f\nabla^2 h_e, \tag{26}$$

with

$$h_e=(MN_e/m_ev)\,\mathrm{erf}(v/\bar{w}_e). \tag{27}$$

For plasma ions ($m_i\sim M$) in this limit we must have that $\mathbf{v}\gg\mathbf{w}$ on the average, and thus simplifying h_i and g_i we get

$$\left(\frac{\partial f}{\partial t}\right)_{\text{ions}}\to\frac{MN_i}{m_iv^2}\left[\frac{\partial f}{\partial v}+\mathcal{O}\left(\frac{m_i\bar{w}_i^2}{Mv}\frac{\partial^2 f}{\partial v^2}\right)\right]. \tag{28}$$

If we take the Laplace transform in time in the above limit, we have

$$\sigma f(\sigma)-f(t=0)=a(v)f(\sigma)+b(v)[\partial f(\sigma)/\partial v], \tag{29}$$

where we have introduced the definitions

$$a(v)=-\Gamma\nabla^2 h_e, \tag{30}$$

$$b(v)=\frac{\Gamma MN_i}{m_iv^2}-\frac{\Gamma MN_e}{m_e}\frac{d}{dv}\left[\frac{1}{v}\,\mathrm{erf}(v/\bar{w}_e)\right]. \tag{31}$$

Solving the simple differential Eq. (29) for $f(\sigma,v)$ and inverting the Laplace transform we have

$$f(t,v)=-\frac{1}{2\pi i}\int_C e^{\sigma t}d\sigma\int^v dv'\frac{f(t=0,v')}{b(v')}\times\exp\left[\int_v^{v'}\frac{a(v'')-\sigma}{b(v'')}dv''\right]. \tag{32}$$

The exponential is the integrating factor of (29), and the contour C is the usual Bromwich contour. We now assume the initial condition

$$f(t=0, v)=\delta(v-V_0) \tag{33}$$

and thus can write

$$f(t,v)=\frac{A(v,V_0)}{2\pi i}\int_C d\sigma \exp\left\{\sigma\left[t-\int_v^{V_0} dv'/b(v')\right]\right\} \tag{34}$$

$$=A(v,V_0)\delta\left[t-\int_v^{V_0} dv'/b(v')\right]. \tag{35}$$

$A(v,V_0)$ is some (normalizing) function of v.

This is just the form of the approximate distribution function (2). Furthermore, if we include terms of next-highest order, the second derivative of f appears in (29) but it is still possible to solve and invert the Laplace transform, by making use of the fact that the coefficient of $\partial^2 f/\partial v^2$ is small. The result is a distribution function of the kind (4), where the Gaussian shape arises from use of saddle-point techniques in inverting the Laplace transform.

Finally, we remark that in the case where $\bar{w}_e > v$ on the average, we can put

$$b(v)=\frac{4\Gamma M N_e}{3\pi^{1/2} m_e \bar{w}_e^3}\left(v+\frac{3\pi^{1/2} m_e N_i \bar{w}_e^3}{4 m_i N_e v^2}\right) \tag{36}$$

$$\equiv\frac{1}{3\tau}\left(v+\frac{u^3}{v^2}\right) \tag{37}$$

and then the δ function in (35) can be replaced by

$$\delta\left(t+\tau \ln\frac{v^3+u^3}{V_0^3+u^3}\right). \tag{38}$$

This is exactly the result (16) in Butler and Buckingham's paper.

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Perturbation Correction to the Radial Distribution Function*

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The effect on the radial distribution function $g(r)$ of adding a small, long-range interaction to a short-range potential is investigated. Two equations are obtained for the corrected g, corresponding to approximations similar to those used in obtaining the Percus-Yevick and convolution hypernetted chain integral equations. The equations relate the "short-range" g (assumed known) and the long-range perturbing potential to the g corresponding to the complete potential. These equations and equations previously obtained by Broyles, Sahlin, and Carley and Hemmer have been tested numerically for a model having a negative Gaussian-Mayer f function, for which near-exact solutions are available from the work of Helfand and Kornegay.

I. INTRODUCTION

The thermodynamic behavior of a classical, one-component, monatomic fluid is completely characterized by the radial distribution function $g(r)$ when the potential energy of the system can be written as the sum of pair potentials. For an N-particle system in a volume V, $g(r)$ is defined as

$$g(r)=\frac{V^2\int\cdots_V\int \exp-\beta\sum_{i<j}\phi_{ij}d\mathbf{r}_3\cdots d\mathbf{r}_N}{\int\cdots_V\int \exp-\beta\sum_{i<j}\phi_{ij}d\mathbf{r}_1\cdots d\mathbf{r}_N}, \tag{1}$$

when the limits $N\to\infty$, $V\to\infty$ are taken such that $\rho\equiv N/V$ remains constant; $\phi_{ij}\equiv\phi(|\mathbf{r}_i-\mathbf{r}_j|)$ is the pair potential and $\beta=1/kT$.

This paper is concerned with the effect on $g(r)$, and hence on the thermodynamic quantities, of a small change in the potential $\phi(r)$. A solution to this problem could be used in a variety of applications. The need for a method to correct $g(r)$ arises, for example, in Monte Carlo calculations of the radial distribution function, where the long-range tail of a potential such as the Coulomb potential must necessarily be truncated at some finite distance. The effect of the neglected part of the potential must be found for a complete solution.[1] Furthermore, if the function $g(r)$ is known for some temperature T, $g(r)$ for some slightly different temperature T' may be easily found by considering $\beta'\phi(r)$, $\beta'=1/kT'$, to be a perturbation of $\beta\phi(r)$ at T and applying the corresponding correction. This obviates

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