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David Schleef
University of California - Berkeley

Michelle Parry
Longwood University, parryml@longwood.edu

Shu-Ju Tu
Purdue University

Brian Woodahl
Purdue University

Ephraim Fischbach
Purdue University

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Application of geometric probability techniques to the evaluation of interaction energies arising from a general radial potential

David Schleef,[a] Michelle Parry,[b] Shu-Ju Tu,
Brian Woodahl, and Ephraim Fischbach
Department of Physics, Purdue University, West Lafayette, Indiana 47907

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A formalism is developed for using geometric probability techniques to evaluate interaction energies arising from a general radial potential $V(r_{12})$, where $r_{12}=|\mathbf{r}_2-\mathbf{r}_1|$. The integrals that arise in calculating these energies can be separated into a radial piece that depends on r_{12} and a nonradial piece that describes the geometry of the system, including the density distribution. We show that all geometric information can be encoded into a ''radial density function'' $G(r_{12};\rho_1,\rho_2)$, which depends on r_{12} and the densities ρ_1 and ρ_2 of two interacting regions. $G(r_{12};\rho_1,\rho_2)$ is calculated explicitly for several geometries and is then used to evaluate interaction energies for several cases of interest. Our results find application in elementary particle, nuclear, and atomic physics. © *1999 American Institute of Physics.* [S0022-2488(99)00102-4]

I. INTRODUCTION

In many areas of physics, integrals of the form

$$U=\int d^3r_1\, d^3r_2\, \rho(\mathbf{r}_1)\rho(\mathbf{r}_2)V(|\mathbf{r}_1-\mathbf{r}_2|) \tag{1.1}$$

are encountered, which typically describe the self-energy of a system with density profile $\rho(\mathbf{r})$ in the presence of a two-body central potential $V(|\mathbf{r}_1-\mathbf{r}_2|)$. A familiar example of such an integral arises in the calculation of the electrostatic self-energy of a spherical charge distribution (e.g., a nucleus) due to the Coulomb potential $V_{\mathrm{C}}(|\mathbf{r}_1-\mathbf{r}_2|)$,

$$V_{\mathrm{C}}(|\mathbf{r}_1-\mathbf{r}_2|)=\frac{e_0^2}{|\mathbf{r}_1-\mathbf{r}_2|}, \tag{1.2}$$

where e_0 is the electric charge ($e_0^2\cong\frac{1}{137}$). For a simple potential such as $V_{\mathrm{C}}(|\mathbf{r}_1-\mathbf{r}_2|)$, the integral in Eq. (1.1) can be evaluated directly, by expanding $1/|\mathbf{r}_1-\mathbf{r}_2|$ in terms of Legendre polynomials. However, for some types of potentials, evaluating U in this way can be extremely tedious. An example of current interest[1,2] is the self-energy of a nucleus or a neutron star arising from neutrino–antineutrino ($\nu-\overline{\nu}$) exchange. In this case the analog of V_{C} in Eq. (1.2) for the neutron–neutron ($n-n$) potential in a neutron star arising from $\nu-\overline{\nu}$ exchange is[3–5]

$$V_{\nu\nu}(|\mathbf{r}_1-\mathbf{r}_2|)=\frac{G_{\mathrm{F}}^2a_n^2}{4\pi^3|\mathbf{r}_1-\mathbf{r}_2|^5}, \tag{1.3}$$

where G_{F} is the weak Fermi constant, and $a_n=-\frac{1}{2}$ the coupling constant describing the strength of the $\nu-n$ interaction. One of the difficulties that arises in evaluating U, starting from Eq. (1.3),

[a]Present address: Department of Physics, University of California—Berkeley, Berkeley, California 94720.
[b]Present address: Department of Natural Sciences, Longwood College, Farmville, Virginia 23909.

is that the integral is well defined only if the neutron–neutron hard core interaction is used to cut off the lower limit of integration when $|\mathbf{r}_1-\mathbf{r}_2|<r_c\cong 0.5\times 10^{-13}$ cm. However, since this constraint applies to $r_{21}=|\mathbf{r}_1-\mathbf{r}_2|=r_{12}$, and not to $r_1=|\mathbf{r}_1|$ or $r_2=|\mathbf{r}_2|$ separately, the integration region in Eq. (1.1) implied by this constraint is somewhat complicated. As we discuss in detail below, the evaluation of integrals involving potentials such as $V_{\nu\nu}(r_{12})$, and other potentials as well, can be greatly facilitated using geometric probability techniques. By use of these techniques the six-dimensional integral in Eq. (1.1) can be replaced by a one-dimensional integral in the variable r_{12}, which can be easily integrated in all cases of interest. The geometric probability techniques are especially useful when $\rho(\mathbf{r}_1)$ is radially varying $(\rho(\mathbf{r}_1)=\rho(|\mathbf{r}_1|))$.

It is helpful to introduce the formalism of geometric probability by first considering the electrostatic (Coulomb) energy of a uniform spherical charge distribution of radius R. Direct evaluation of the six-dimensional integral in Eq. (1.1) yields

$$U_{\mathrm{C}}=\frac{6}{5}\frac{e_0^2}{R}. \tag{1.4}$$

For a spherically symmetric distribution containing Z charges there are $Z(Z-1)/2$ possible pairs, and hence the total Coulomb energy W_{C} of such a distribution is

$$W_{\mathrm{C}}=\frac{Z(Z-1)}{2}\,U_{\mathrm{C}}=\frac{3}{5}\,Z(Z-1)\,\frac{e_0^2}{R}, \tag{1.5}$$

which is the standard result.[6,7]

In contrast to the preceding derivation, which begins with a six-dimensional integral, the formalism of integral geometry expresses U_{C} immediately as a one-dimensional integral. For any function $g(r_{12})$, its average value $\langle g\rangle$ taken over a uniform spherical volume of radius R is

$$\langle g\rangle=\int_0^{2R} dr_{12}\,\mathcal{P}_3(r_{12})g(r_{12}), \tag{1.6}$$

where

$$\int_0^{2R} dr_{12}\,\mathcal{P}_3(r_{12})=1. \tag{1.7}$$

The function $\mathcal{P}_3(r_{12})$ denotes the normalized probability density for finding two points randomly chosen in a uniform three-dimensional sphere to be a distance r_{12} apart. The functional form of $\mathcal{P}_3(r_{12})$ has been obtained previously by a number of authors,[8–13]

$$\mathcal{P}_3(r_{12})=\frac{3r_{12}^2}{R^3}\left[1-\frac{3}{2}\left(\frac{r_{12}}{2R}\right)+\frac{1}{2}\left(\frac{r_{12}}{2R}\right)^3\right]. \tag{1.8}$$

Using Eq. (1.8), U_{C} is given by

$$U_{\mathrm{C}}=\langle e_0^2/r_{12}\rangle=\int_0^{2R} dr_{12}\left(\frac{3r_{12}^2}{R^3}\right)\left[1-\frac{3}{2}\left(\frac{r_{12}}{2R}\right)+\frac{1}{2}\left(\frac{r_{12}}{2R}\right)^3\right]\left(\frac{e_0^2}{r_{12}}\right)=\frac{6}{5}\frac{e_0^2}{R}, \tag{1.9}$$

in agreement with Eq. (1.4). The utility of the geometric probability formalism becomes more evident when one attempts to evaluate $U_{\nu\nu}=\langle V_{\nu\nu}(r_{12})\rangle$ using Eq. (1.3),

$$U_{\nu\nu}=\frac{G_{\mathrm{F}}^2a_n^2}{4\pi^3}\int_{r_c}^{2R} dr_{12}[\,\eta(r_c,R)\mathcal{P}_3(r_{12})]\,\frac{1}{r_{12}^5}. \tag{1.10}$$

In Eq. (1.10) $\eta(r_c,R)$ is a constant that ensures that $\mathcal{P}_3(r_{12})$ is appropriately normalized in the interval $2R \geqslant r_{12} \geqslant r_c$, and is given by

$$\eta(r_c,R)=(1-8s_c^3+8s_c^4-2s_c^6)^{-1}, \tag{1.11}$$

where $s_c=r_c/2R$. It follows from Eq. (1.11) that $\eta(0,R)=1$, as expected. Combining Eqs. (1.10) and (1.11) then gives immediately,

$$U_{\nu\nu}=\frac{3}{8\pi^3}\frac{G_F^2 a_n^2}{\hbar c}\frac{1}{R^3 r_c^2}\left(1-\frac{r_c}{2R}\right)^3 \eta(r_c,R). \tag{1.12}$$

For a sphere containing N particles, the total energy $W_{\nu\nu}$ is then given by

$$W_{\nu\nu}=\frac{N(N-1)}{2}U_{\nu\nu}=\frac{3}{16\pi^3}N(N-1)\frac{G_F^2 a_n^2}{\hbar c}\frac{1}{R^3 r_c^2}\left(1-\frac{r_c}{2R}\right)^3 \eta(r_c,R). \tag{1.13}$$

To evaluate $\langle g\rangle$ in Eq. (1.6) for a particular geometry, one must first determine the functional form of $\mathcal{P}_3(r_{12})$ appropriate to that geometry. In practice, it would be of great value to know $\mathcal{P}(r)\equiv\mathcal{P}_3(r_{12})$ for different (nonconstant) density distributions, as well as for other geometries. In this paper we address the former problem, by developing a general framework for calculating $\mathcal{P}(r)$ for geometries with variable density. We illustrate this approach in Sec. II by first rederiving (in a much simpler way) the result for a sphere of constant density given in Eq. (1.8). We then obtain $\mathcal{P}(r)$ for a sphere with a Gaussian density distribution. In Sec. III we apply our formalism to geometries that can be used to calculate the interaction energy between microscopic objects due to a generalized two-body interaction potential. One example is the van der Waals interaction.

II. GENERAL FORMALISM

A. The radial density function

Returning to Eq. (1.1), we introduce the change of variables,

$$\begin{aligned}\mathbf{r}_{12}&=\mathbf{r}_2-\mathbf{r}_1,\\ d^3r_{12}&=d^3r_2,\end{aligned} \tag{2.1}$$

so that

$$\begin{aligned}U&=\int dr_{12}\left[r_{12}^2\int d\Omega_{12}\int d^3r_1\ \rho_1(\mathbf{r}_1)\rho_2(\mathbf{r}_{12}+\mathbf{r}_1)\right]V(r_{12}),\\ &\equiv\int dr_{12}\ G(r_{12};\rho_1,\rho_2)V(r_{12}),\end{aligned} \tag{2.2}$$

where $r_{12}=|\mathbf{r}_2-\mathbf{r}_1|$. The ''radial density function'' $G(r_{12};\rho_1,\rho_2)$ is the generalization of the probability function $\mathcal{P}_3(r_{12})$ in Eq. (1.8). $G(r_{12};\rho_1,\rho_2)$ incorporates all the geometric information about the densities $\rho_1(\mathbf{r}_1)$ and $\rho_2(\mathbf{r}_2)$ and the geometry, but is independent of $V(r_{12})$.

B. Geometry with spherical symmetry

The first case we consider is when both $\rho_1(\mathbf{r}_1)$ and $\rho_2(\mathbf{r}_2)$ exhibit spherical symmetry about a common origin, so that $\rho_1=\rho_1(|\mathbf{r}_1|)$ and $\rho_2=\rho_2(|\mathbf{r}_2|)$ about this origin. From Eq. (2.2) we can then write

$$G(r_{12};\rho_1,\rho_2)=r_{12}^2\int d^3r_1\int d\Omega_{12}\ \rho_1(r_1)\rho_2(|\mathbf{r}_{12}+\mathbf{r}_1|). \tag{2.3}$$

Since $\rho(r_1)$ and $\rho_2(|\mathbf{r}_{12}+\mathbf{r}_1|)=\rho(r_2)$ are independent of $d\Omega_1$ and $d\phi_{12}$, we can integrate over these variables immediately to give

$$G(r_{12};\rho_1,\rho_2)=r_{12}^2\int_0^\infty dr_1\ 4\pi r_1^2\rho_1(r_1)\int_0^\pi d\theta_{12}\,2\pi\ \sin\ \theta_{12}\rho_2(|\mathbf{r}_{12}+\mathbf{r}_1|). \tag{2.4}$$

Note that the upper limit of integration for r_1 can always be taken to be infinite, even for a finite spherical mass distribution, since $\rho_1(r_1)$ can be defined to be zero for $r_1>R$. Using the law of cosines, we have

$$-\cos\ \theta_{12}=\frac{r_{12}^2+r_1^2-r_2^2}{2r_1r_{12}}. \tag{2.5}$$

Since r_{12} and r_1 are the independent variables of integration in Eq. (2.3), it follows that $\cos\theta_{12}$ depends only on r_2 for fixed values of r_{12} and r_1. Thus,

$$\sin\ \theta_{12}\ d\theta_{12}=\frac{-r_2}{r_1r_{12}}\ dr_2. \tag{2.6}$$

Combining Eqs. (2.6) and (2.4) then gives

$$G(r_{12};\rho_1,\rho_2)=8\pi^2r_{12}\int_0^\infty dr_1\ r_1\rho_1(r_1)\int_{|r_{12}-r_1|}^{r_{12}+r_1}dr_2\ r_2\rho_2(r_2). \tag{2.7}$$

As an application of Eq. (2.7) we recalculate the Coulomb energy of a sphere of radius R and constant density $1/V$, where the density is normalized so that its integral over the spherical volume is unity. Since the integral in Eq. (2.7) is symmetric in the interchange of r_1 and r_2, we can write

$$G_{\text{sphere}}(r_{12};\rho_1,\rho_2)=16\pi^2r_{12}\int_{r_{12}/2}^\infty dr_1\ r_1\rho(r_1)\int_{|r_{12}-r_1|}^{r_1}dr_2\ r_2\rho(r_2). \tag{2.8}$$

The lower limit on the r_1 integration follows by noting that when $r_2=r_1$ the triangle formed by the vectors $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_{12}$ is isosceles, and hence by the triangle inequality $2r_1>r_{12}$. From Eq. (2.8) we have

$$G_{\text{sphere}}(r_{12};\rho_1,\rho_2)=\frac{16\pi^2r_{12}}{V^2}\int_{r_{12}/2}^R dr_1\ r_1\int_{|r_{12}-r_1|}^{r_1}dr_2\ r_2=\frac{3r_{12}^2}{R^3}\left[1-\frac{3}{2}\left(\frac{r_{12}}{2R}\right)+\frac{1}{2}\left(\frac{r_{12}}{2R}\right)^3\right], \tag{2.9}$$

in agreement with the expression for $\mathcal{P}_3(r_{12})$ in Eq. (1.8). The expression for the Coulomb energy of a sphere of charge then follows immediately from Eq. (1.9). Having demonstrated that the present formalism correctly reproduces the classical results for a sphere of constant density, we turn in the next section to a problem that has not been considered previously in the literature, the distribution of points in a sphere with a Gaussian density variation.

III. RADIAL DENSITY FUNCTION FOR A GAUSSIAN DISTRIBUTION

We derive in this section the radial density function for a spherically symmetric distribution of matter centered at the origin, whose density varies as

$$\rho(r)=Ae^{-r^2/R_0^2}, \tag{3.1}$$

where A and R_0 are constants, and r is measured from the origin. If we normalize $\rho(r)$ so that its integral over all space is unity, then

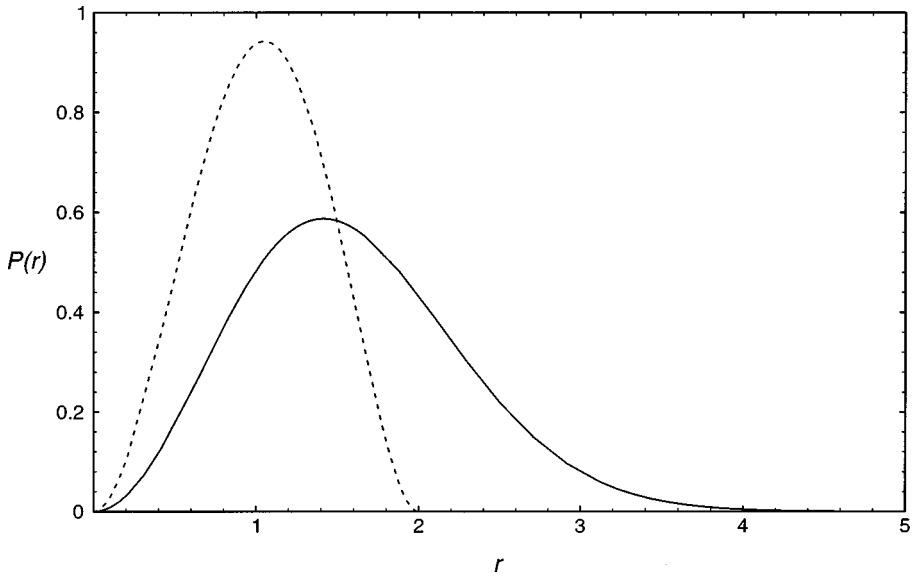

FIG. 1. The plot of $P(r)\equiv G(r;\rho)$ in Eq. (3.6) as a function of $r=r_{12}$ (solid line). For comparison the function $\mathcal{P}_3(r)$ in Eq. (1.8) is also shown (dashed line).

$$A=R_0^{-3}\pi^{-3/2}. \tag{3.2}$$

Combining Eqs. (3.1) and (2.8), we find

$$G(r_{12};\rho_1,\rho_2)\equiv G(r_{12};\rho)=8\pi^2A^2r_{12}\int_0^\infty dr_1 r_1 e^{-r_1^2/R_0^2}\int_{|r_{12}-r_1|}^{r_{12}+r_1} dr_2 r_2 e^{-r_2^2/R_0^2}. \tag{3.3}$$

Carrying out the integration with respect to r_2, we find

$$G(r_{12};\rho)=4\pi^2A^2R_0^2r_{12}e^{-r_{12}^2/R_0^2}\int_0^\infty dr_1 r_1 e^{-2r_1^2/R_0^2}[e^{-2r_{12}r_1/R_0^2}-e^{2r_{12}r_1/R_0^2}]. \tag{3.4}$$

The integration with respect to r_1 can then be performed by completing the square, which gives

$$G(r_{12};\rho)=4\pi^2A^2R_0^2r_{12}e^{-r_{12}^2/2R_0^2}\int_0^\infty dr_1\ r_1\{\exp[-2(r_1-r_{12}/2)^2/R_0^2]-\exp[-2(r_1+r_{12}/2)^2/R_0^2]\}$$

$$=4\pi^2A^2R_0^2r_{12}e^{-r_{12}/2R_0^2}\left[\frac{1}{2}\sqrt{\frac{\pi}{2}}\,r_{12}R_0\right]. \tag{3.5}$$

Combining Eqs. (3.2) and (3.5) yields the final result,

$$G(r_{12};\rho)=\sqrt{\frac{2}{\pi}}\frac{r_{12}^2}{R_0^3}\,e^{-r_{12}^2/2R_0^2}. \tag{3.6}$$

$G(r_{12};\rho)$ is shown in Fig. 1 and is normalized to unity over the interval $[0,\infty]$. When the lower limit of integration is replaced by r_c, $G(r_{12};\rho)$ must be divided by the constant $C(r_c,R_0)$ to be properly normalized, where

$$C(r_c,R_0)=\int_{r_c}^\infty dr_{12}\,G(r_{12};\rho)\cong 1-\sqrt{\frac{2}{\pi}}\frac{r_c^3}{3R_0^3}. \tag{3.7}$$

We note that for $r_{12}^2/R_0^2 \ll 1$, $G(r_{12};\rho)$ can be approximated by

$$G(r_{12};\rho) \cong \sqrt{\frac{2}{\pi}} \frac{r_{12}^2}{R_0^3}, \tag{3.8}$$

which agrees (up to an overall constant) with the results for a uniform sphere given in Eqs. (1.8) and (2.9). This agreement conforms to our intuition that when r_{12} is small compared to R_0, a spherically symmetric Gaussian distribution will look like that of a sphere with an approximately constant local density.

The result in Eq. (3.6) can be applied immediately to calculate both the Coulomb energy and the neutrino-exchange energy of a matter distribution with the Gaussian density profile given in Eq. (3.1). The Coulomb energy W_C is then given by

$$W_C = \frac{Z(Z-1)}{2} \left\langle \frac{e^2}{r_{12}} \right\rangle = \frac{Z(Z-1)}{2} \int_0^\infty dr_{12} \left(\frac{e^2}{r_{12}} \right) \times \frac{r_{12}^2}{R_0^3} \sqrt{\frac{2}{\pi}} e^{-r_{12}^2/2R_0^2} = \frac{1}{\sqrt{2\pi}} \frac{Z(Z-1)e^2}{R_0}. \tag{3.9}$$

As noted in the Introduction, geometric probability techniques are particularly useful when evaluating expressions where the nucleon–nucleon hard core radius r_c appears, as in the integral for $U_{\nu\nu}$ in Eq. (1.10). From Eq. (3.6) we have, for a Gaussian density distribution of N neutrons,

$$W_{\nu\nu} = \frac{N(N-1)}{2} \left\langle \frac{G_F^2 a_n^2}{4\pi^3 r_{12}^5} \right\rangle = \frac{N(N-1)}{2C(r_c,R_0)} \int_{r_c}^\infty dr_{12} \left(\frac{G_F^2 a_n^2}{4\pi^3 r_{12}^5} \right) \frac{r_{12}^2}{R_0^3} \sqrt{\frac{2}{\pi}} e^{-r_{12}^2/2R_0^2}. \tag{3.10}$$

Evaluation of the integral in Eq. (3.10) yields

$$W_{\nu\nu} = \frac{G_F^2 a_n^2}{8\pi^3} \frac{N(N-1)}{C(r_c,R_0)} \left\{ \frac{1}{\sqrt{2\pi}} \frac{e^{-r_c^2/R_0^2}}{r_c^2 R_0^3} + \frac{1}{2} \sqrt{\frac{\pi}{2}} \frac{1}{R_0^5} \left[-i + \frac{1}{\pi} Ei\left(\frac{-r_c^2}{2R_0^5} \right) \right] \right\},$$
$$Ei(z) = P \int_{-z}^\infty \frac{(-1)}{te^t} dt, \tag{3.11}$$

where P denotes the principal value integration. We note that the quantity in square brackets in Eq. (3.11) is real, as hence $W_{\nu\nu}$ is real as well. As can be seen from Eq. (3.11), by using $G(r_{12};\rho)$ in Eq. (3.6) we obtain an exact closed-form expression for $W_{\nu\nu}$ for the case of a Gaussian density distribution. By way of contrast, the conventional approach would lead to an infinite series expression for $W_{\nu\nu}$. We complete this discussion by noting that for $r_c/R_0 \ll 1$ we can write

$$\int_{r_c}^\infty dr \frac{G(r;\rho)}{r^5} \cong \frac{2}{\sqrt{\pi}} \frac{1}{r_c^2 R_0^3}, \tag{3.12}$$

and, hence,

$$W_{\nu\nu} \cong \frac{G_F^2 a_n^2 N(N-1)}{8\sqrt{2}\pi^{7/2}} \frac{1}{r_c^2 R_0^3}. \tag{3.13}$$

As expected from Eq. (1.13), $W_{\nu\nu} \sim 1/r_c^2$ when $r_c/R_0 \ll 1$ for the Gaussian distribution, just as in the case of the uniform sphere.

IV. INTERACTION BETWEEN SOURCES

A. General formalism

In the previous section we have focused on calculating the radial density function $G(r_{12};\rho_1,\rho_2)$ needed to evaluate the self-energy of a spherically symmetric matter distribution. In this section we calculate the analogous expressions for $G(r_{12};\rho_1,\rho_2)$, which characterize the interaction of two different matter distributions in volumes ω_1 and ω_2, respectively. In particular, we generalize the calculations of Israelachvili[14] to allow any two-body radial potential. These results are of interest in the field of tribology, specifically in calculating interaction forces and energies due to van der Waals-type forces. This technique has been used to study the force of interaction between an Atomic Force Microscopy (AFM) probe tip and a flat sample.[15]

Returning to Eq. (2.3), we can rewrite the expression for $G(r_{12};\rho_1,\rho_2)$ in the form

$$G(r_{12};\rho_1,\rho_2)=r_{12}^2\int d\Omega_{12}\int d^3r_1\ \rho_1(\mathbf{r}_1)\rho_2(\mathbf{r}_{12}+\mathbf{r}_1)$$
$$=\int d^3r_1\ \rho_1(\mathbf{r}_1)\left\{r_{12}^2\int d\Omega_{12}\ \rho_2(\mathbf{r}_2)\right\}. \tag{4.1}$$

In Eq. (4.1) we have interchanged the order of the integrations, and have used Eq. (2.1) to replace $\mathbf{r}_{12}+\mathbf{r}_1$ by $\mathbf{r}_2$. In this section we deal with the situation in which $\rho_i(\mathbf{r}_i)$ are given by

$$\rho_i(\mathbf{r}_i)=\begin{cases}\rho_i, & \text{when } \mathbf{r}_i\in\omega_i,\\ 0, & \text{otherwise.}\end{cases} \tag{4.2}$$

For illustrative purposes we take ρ_1 and ρ_2 to be constants, so that

$$G(r_{12};\rho_1,\rho_2)=\rho_1\rho_2\int_{\omega_1}d^3r_1\left\{r_{12}^2\int_{4\pi}d\Omega_{12}\right\}\equiv\rho_1\rho_2\int_{\omega_1}d^3r_1\ S(r_{12},\mathbf{r}_1). \tag{4.3}$$

$S(r_{12},\mathbf{r}_1)$ can be viewed as the surface area formed by the intersection of a sphere centered at $\mathbf{r}_1=0$ (in the volume ω_1) and having radius r_{12}, with the second volume ω_2. Several examples will serve to clarify the application of Eq. (4.3).

B. Point to sphere

Here ω_1 is a point having an infinitesimal volume $d\tau$, so that Eq. (4.3) becomes

$$G(r_{12};\rho_1,\rho_2)=(\rho_1\ d\tau)\rho_2 S(r_{12},\mathbf{r}_1). \tag{4.4}$$

If ω_2 is a sphere of radius R, then, from Fig. 2,

$$R^2=r_{12}^2+r^2-2rr_{12}\cos\ \theta_0, \tag{4.5}$$

where r is the distance from the point to the center of the spherical distribution ω_2. It follows that

$$S(r_{12},\mathbf{r}_1)=2\pi r_{12}^2\int_0^{\theta_0}\sin\ \theta_{12}\,d\theta_{12}=\pi\,\frac{r_{12}}{r}\,[R^2-(r-r_{12})^2]. \tag{4.6}$$

Combining Eqs. (4.4) and (4.6) then gives

$$G(r_{12};\rho_1,\rho_2)=(\rho_1 d\tau)\rho_2\left\{\pi\,\frac{r_{12}}{r}\,[R^2-(r-r_{12})^2]\right\}. \tag{4.7}$$

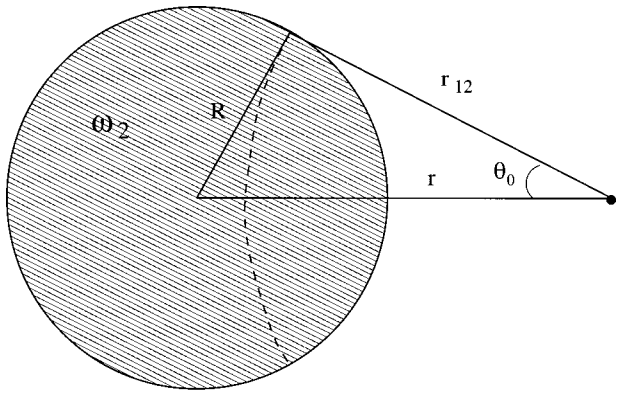

FIG. 2. The representation of the point-to-sphere geometry. R is the radius of the sphere, whose center is a distance r from the external point. $G(r_{12};\rho_1,\rho_2)$ is calculated as a function of the distance r_{12} between the external point and a point in the sphere.

Equation (4.7) can be checked by noting that when $r=R$, $G(r_{12};\rho_1,\rho_2)$ describes the distribution of distances between two points in a sphere, given that one of these points lies on the surface of the sphere. The latter distribution has been derived by Parry,[16] and it is straightforward to show that Eq. (4.7) agrees with this result when $r=R$. When combined with Eq. (2.3), Eq. (4.7) allows the interaction energy U to be calculated for an arbitrary two-body potential $V(r_{12})$ (e.g., Coulomb, Yukawa, van der Waals, etc.).

C. Point to half-space

This geometry is very similar to the point-to-sphere case, except that ω_2 is now an infinite half-space separated by a distance r from an external point. For this geometry, $\cos\,\theta_0$ is given by

$$\cos\,\theta_0=\frac{r}{r_{12}}, \tag{4.8}$$

and hence

$$S(r_{12},\mathbf{r}_1)=2\pi r_{12}^2(1-\cos\,\theta_0)=2\pi r_{12}(r_{12}-r). \tag{4.9}$$

Combining Eqs. (4.4) and (4.9), the radial density function is given by

$$G(r_{12};\rho_1,\rho_2)=(\rho_1\,d\tau)\rho_2\{2\pi r_{12}(r_{12}-r)\}. \tag{4.10}$$

As in the previous case, the expression in Eq. (4.10) can be checked by noting that when $r=0$, $G(r_{12};\rho_1,\rho_2)$ becomes proportional to r_{12}^2, which is the expected result for an infinite half-space.[16]

D. Arbitrary volume to half-space

We can apply the previous result to compute the radial density function for an arbitrary volume ω_1, in the presence of an infinite half-space. From Eq. (4.9) we see that $S(r_{12},\mathbf{r}_1)$ depends only on the distance x of a volume element from the boundary, and hence we need only specify the expression for the cross section $A(x)$ of ω_1 as a function of x. Then, from Eq. (4.10) we have

$$G(r_{12};\rho_1,\rho_2)=2\pi\rho_1\rho_2\int_0^{r_{12}}dx(r_{12}-x)A(x). \tag{4.11}$$

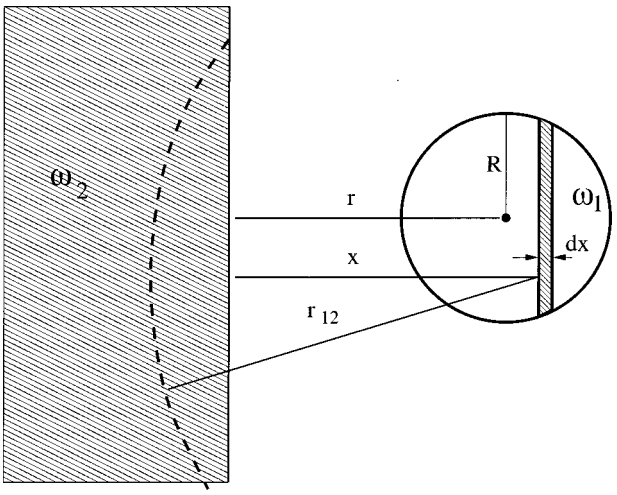

FIG. 3. Representation of the sphere-to-half-space geometry. See the text and the caption to Fig. 2 for details.

If ω_1 is a sphere of radius R whose center is a distance r from the boundary of the half-space, then, from Fig. 3,

$$A(x)=\begin{cases} 0, & x\leqslant r-R, \\ \pi[R^2-(r-x)^2], & r-R\leqslant x\leqslant r+R, \\ 0, & x\geqslant r+R. \end{cases} \tag{4.12}$$

Correspondingly, the density function is divided into three regions: $G(r_{12};\rho_1,\rho_2)=0$ if $r_{12}\leqslant(r-R)$, and

$$G(r_{12};\rho_1,\rho_2)=\begin{cases} \dfrac{\pi^2}{6}\,\rho_1\rho_2 r_{12}(r-R-r_{12})^3(r_{12}-r-3R), & r-R\leqslant r_{12}\leqslant r+R, \\ \dfrac{8\pi^2}{3}\,\rho_1\rho_2 r_{12}R^3(r_{12}-r), & r+R\leqslant r_{12}. \end{cases} \tag{4.13}$$

The results in Eq. (4.13) are useful in Atomic Force Microscopy since they can be used to analyze the interaction of a general AFM probe tip interacting with a flat sample.

V. CONCLUSIONS

The discussion in the Introduction illustrates the power of geometric probability techniques by demonstrating how a six-dimensional integral can be immediately reduced to a straightforward one-dimensional problem. In practice, this facilitates the evaluation of interaction energies such as $U_{\nu\nu}$ in Eq. (1.10), which would be extremely difficult to treat otherwise, due to the presence of r_c. We have extended the classical results of Refs. 8–13 to calculate for the first time the radial density functions for a Gaussian density profile, and for two regions of different shapes interacting with each other. These results can be applied to a wide variety of physical systems, as we will discuss elsewhere.

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