General cusp conditions for Coulomb systems

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Cusp conditions are obtained for the coalescence of any number of particles interacting Coulombically. This is an extension of the results of Hoffmann-Ostenhof and Seiler for atoms and molecules in the infinite-nuclear-mass approximation in two aspects: (1) the center of mass is first removed, and (2) the masses and charges are all allowed to differ.

I. INTRODUCTION

The Hamiltonian for an N-particle Coulombic system in the nonrelativistic regime,

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2m_i}+\sum_{i<j}^{N}\frac{e_ie_j}{r_{ij}}, \qquad \vec{p}_j=-i\hbar\vec{\nabla}_i,\quad \vec{r}_{ij}=\vec{r}_i-\vec{r}_j, \tag{1}$$

with $\hbar$ Planck's constant, e_i the charge, and m_i the mass of particle i, has a potential which becomes singular at all points of particle coalescence. Eigenfunctions of H which do not vanish there must satisfy *cusp conditions*[1] (or *coalescence conditions*[2] in general, whether they vanish or not).

Recognition of the cusp conditions in the case of two-particle coalescences is useful, say, in the united atom perturbation theory of diatomic molecules,[3] although they have generally proven to be of little help in the construction of accurate variational wave functions (see Ref. 2 for a discussion).

Nonetheless, it is of interest to know as much as possible about the behavior of exact many-particle wave functions, including the coalescence of more than two particles. Earlier work on this problem[4-6] has been somewhat sparse, but a recent paper by Hoffmann-Ostenhof and Seiler[7] gives exact cusp conditions for the coalescence of k electrons at an atomic nucleus or elsewhere, and extensions to molecular systems, within the infinite-nuclear-mass approximation.

Pack and Byers Brown[2] have derived the two-particle cusp conditions with the removal of this approximation, and it seems reasonable to expect that such can be done for the higher-order coalescences also. It is the purpose of this paper to show that the results of Hoffmann-Ostenhof and Seiler[7] can be easily extended, as they suggest, to derive the conditions for coalescence of an arbitrary number of particles interacting Coulombically (with possibly different masses and charges). The effects of the Pauli exclusion principle have been discussed before,[2,6,7] and are not dealt with here.

In Sec. II, the center of mass (c.m.) is removed by transformation to Jacobi coordinates, which are particularly well-suited to this problem. In Sec. III, the Jacobi coordinates are used in place of, and exactly analogously to, the electronic coordinates of Ref. 7, resulting in the cusp condition as given in Eq. (28). Section IV considers more than one coalescence point.

II. SEPARATION OF THE c.m. MOTION

The part of H due to the uniform motion of the c.m. may be eliminated by an orthogonal transformation of (mass-weighted) coordinates,[8-10]

$$\vec{R}_i=\sum_{j=1}^{N}D_{ij}\vec{r}_j, \tag{2}$$

$$\vec{P}_i=\sum_{j=1}^{N}(\underline{D}^{-1T})_{ij}\vec{p}_j, \tag{3}$$

where

$$\underline{D}=\underline{\mu}^{-1/2}\,\underline{d}\,\underline{m}^{1/2}, \tag{4}$$

$\underline{m}$ and $\underline{\mu}$ are diagonal ($m_{ij}=m_i\delta_{ij}$, $\mu_{ij}=\mu_i\delta_{ij}$), and μ_N is fixed as the total mass of the system:

$$\mu_N=M=\sum_{i=1}^{N}m_i. \tag{5}$$

The remaining $N-1$ μ_i are arbitrary positive scale factors which play the role of reduced masses. The $N\times N$ orthogonal matrix $\underline{d}$ is

$$\underline{d}=\begin{pmatrix} \left(\frac{m_2}{M_2}\right)^{1/2} & -\left(\frac{m_1}{M_2}\right)^{1/2} & 0 & 0 & & 0 \\ \left(\frac{m_1m_3}{M_2M_3}\right)^{1/2} & \left(\frac{m_2m_3}{M_2M_3}\right)^{1/2} & -\left(\frac{M_2}{M_3}\right)^{1/2} & 0 & \cdots & 0 \\ \left(\frac{m_1m_4}{M_3M_4}\right)^{1/2} & \left(\frac{m_2m_4}{M_3M_4}\right)^{1/2} & \left(\frac{m_3m_4}{M_3M_4}\right)^{1/2} & -\left(\frac{M_3}{M_4}\right)^{1/2} & & 0 \\ & & \cdots & & & \\ \left(\frac{m_1m_N}{M_{N-1}M}\right)^{1/2} & \left(\frac{m_2m_N}{M_{N-1}M}\right)^{1/2} & \left(\frac{m_3m_N}{M_{N-1}M}\right)^{1/2} & \left(\frac{m_4m_N}{M_{N-1}M}\right)^{1/2} & & -\left(\frac{M_{N-1}}{M}\right)^{1/2} \\ & & & & \cdots & \\ \left(\frac{m_1}{M}\right)^{1/2} & \left(\frac{m_2}{M}\right)^{1/2} & \left(\frac{m_3}{M}\right)^{1/2} & \left(\frac{m_4}{M}\right)^{1/2} & & \left(\frac{m_N}{M}\right)^{1/2} \end{pmatrix}. \tag{6}$$

The intermediate mass sums in Eq. (6) are

$$M_k=\sum_{i=1}^{k} m_i\,,\quad M_N\equiv M\,. \tag{7}$$

This transformation delivers the well-known Jacobi coordinates, with $\vec{R}_N$ the c.m.:

$$\vec{R}_i=\left(\frac{m_{i+1}M_i}{\mu_i M_{i+1}}\right)^{1/2}\left(\sum_{j=1}^{i}\frac{m_j}{M_i}\vec{r}_j-\vec{r}_{i+1}\right),\quad 1\le i\le N-1$$
$$\vec{R}_N=\sum_{j=1}^{N}\frac{m_j}{M}\vec{r}_j\,. \tag{8}$$

The key use of these coordinates in the current circumstances stems from the fact that $\vec{R}_k\propto\vec{S}_k-\vec{r}_{k+1}$, where $\vec{S}_k$ is the c.m. of the first k particles. For the coalescence of the first $k+1$ particles,

$$\vec{r}_1=\vec{r}_2=\cdots=\vec{r}_{k+1}=\vec{S}_1=\vec{S}_2=\cdots=\vec{S}_{k+1}\,, \tag{9}$$

and we have $\vec{R}_i=0$ for $i\le k$. The remaining coordinates only contain the coalescent variables as a multiple of $\vec{S}_{k+1}$. The customary restrictions are made here that (i) $\vec{r}_i\neq\vec{S}_{k+1}$ and (ii) $\vec{r}_i\neq\vec{r}_j$ for i and $j>k+1$. The first, (i), is essential for the derivation of the cusp conditions,[7] although (ii) seems too strong (see Sec. IV).

The interparticle distances may be expressed in terms of the internal coordinates $\vec{R}_i$, $i<N$:

$$\vec{r}_{12}=\vec{r}_1-\vec{r}_2=\left(\frac{\mu_1M_2}{m_1m_2}\right)^{1/2}\vec{R}_1\,,$$
$$\vec{r}_{13}=\left(\frac{\mu_1m_2}{m_1M_2}\right)^{1/2}\vec{R}_1+\left(\frac{\mu_2M_3}{m_3M_2}\right)^{1/2}\vec{R}_2\,,$$
$$\vec{r}_{23}=-\left(\frac{\mu_1m_1}{m_2M_2}\right)^{1/2}\vec{R}_1+\left(\frac{\mu_2M_3}{m_3M_2}\right)^{1/2}\vec{R}_2\,, \tag{10}$$
$$\cdots\,,$$

and in fact, for $i,j\le k+1$, $\vec{r}_{ij}$ is a linear combination of no more than the first k $\vec{R}_i$'s. Different choices for the arbitrary scale factors can be made, but this is not of concern here.

The Hamiltonian is now (with $\vec{P}_N$ the total momentum)

$$H=\frac{P_N^2}{2M}+h\,, \tag{11}$$

where the internal Hamiltonian is diagonal in the kinetic energy

$$h=\sum_{i=1}^{N-1}\frac{P_i^2}{2\mu_i}+\sum_{i<j}^{N}\frac{e_ie_j}{r_{ij}}\,, \tag{12}$$

the notation r_{ij} representing functions of the internal coordinates as in Eq. (10). The reduced Schrödinger equation one would want to solve is then

$$(h-E)\psi(\vec{R}_1,\vec{R}_2,\ldots,\vec{R}_{N-1})=0\,. \tag{13}$$

The cusp conditions for coalescence of the first $k+1$ particles are now sought in precisely the same manner as in Ref. 7. The surface difference is that the potential terms appear more complicated here, but this turns out not to be any problem.

III. CUSP CONDITIONS FOR ARBITRARY MASSES AND CHARGES

The treatment of Ref. 7 uses hyperspherical coordinates in a $3k$-dimensional space, where the Cartesian coordinates of the first k electrons are converted to $3k-1$ angles and one extensive variable. In our case, the first k Jacobi coordinates are transformed into an alternative set of hyperspherical variables given by Delves[10] some 20 years ago.

First the spherical polar angles θ_i,ϕ_i of $\vec{R}_i$, $i\le k$, are taken as $2k$ variables. The radii R_i are then used to define a set of $k-1$ hyperspherical angles and one hyperradius:

$$\mu_1^{1/2}R_1 = R\sin\alpha_1\sin\alpha_2\cdots\sin\alpha_{k-1},$$
$$\mu_2^{1/2}R_2 = R\cos\alpha_1\sin\alpha_2\cdots\sin\alpha_{k-1},$$
$$\mu_3^{1/2}R_3 = R\cos\alpha_2\sin\alpha_3\cdots\sin\alpha_{k-1},$$
$$\cdots, \tag{14}$$
$$\mu_k^{1/2}R_k = R\cos\alpha_{k-1}.$$

The hyperradius R is the only extensive variable and has the significance of being related to the trace of the inertia tensor of the $k+1$ particles measured from their c.m. (Refs. 8 and 11):

$$R^2 = \sum_{i=1}^{k}\mu_i R_i^2 = \sum_{i=1}^{k+1} m_i(\vec{r}_i - \vec{S}_{k+1})^2 = \tfrac{1}{2}\sum_{i=1}^{k+1}\sum_{j=1}^{k+1}\frac{m_i m_j}{M_{k+1}}(\vec{r}_i - \vec{r}_j)^2. \tag{15}$$

If particle 1 is very heavy compared to the rest, then this reduces to

$$R^2 \cong \sum_{i=2}^{k+1} m_i(\vec{r}_i - \vec{r}_1)^2, \tag{16}$$

which is essentially the same as the definition used in Ref. 7 when all of the masses other than m_1 are equal.

The volume element in $\mathcal{R}^{3k}$ is, up to a constant,

$$d\vec{R}_1 d\vec{R}_2\cdots d\vec{R}_k = R^{3k-1}dR\,d\omega, \tag{17}$$

$$d\omega = \left(\prod_{i=1}^{k-1}\cos^2\alpha_i\sin^{3i-1}\alpha_i d\alpha_i\right)\times\left(\prod_{j=1}^{k}\sin\theta_j d\theta_j d\phi_j\right), \tag{18}$$

where $0 \le \alpha_i \le \pi/2$. Integration over all the angles gives the volume of the $3k$-dimensional unit sphere

$$\int_{S^{3k-1}} d\omega = \sigma_{3k-1} = \frac{2\pi^{3k-2}}{\Gamma(3k/2)}. \tag{19}$$

Following Hoffmann-Ostenhof and Seiler, we denote the $3k$ Cartesian coordinates by simply

$$(\vec{R}_1, \vec{R}_1, \ldots, \vec{R}_k) = R\omega, \tag{20}$$

and the remaining coordinates $\vec{R}_{k+1}, \vec{R}_{k+2}, \ldots, \vec{R}_{N-1}$ collectively by y. Equation (13) is transformed into[6,10,11]

$$\left(R^{1-3k}\frac{\partial}{\partial R}R^{3k-1}\frac{\partial}{\partial R} - W\right)\psi(R\omega, y) = 0, \tag{21}$$

where

$$W = \frac{\Lambda^2}{R^2} - \sum_{i=k+1}^{N-1}\nabla_i^2 + \frac{2}{\hbar^2}\left(\sum_{i<j}^{N}\frac{e_i e_j}{r_{ij}} - E\right), \tag{22}$$

and Λ^2 is the square of the grand angular momentum operator[11] defined on S^{3k-1}.

In line with the statement after Eq. (9), the terms in the potential which become singular at the coalescence point of the $k+1$ particles are

$$V_k = \sum_{i<j}^{k+1}\frac{e_i e_j}{r_{ij}} = V_k(\vec{R}_1, \vec{R}_2, \ldots, \vec{R}_k). \tag{23}$$

It can be proven as in Ref. 7 that

$$\left.\frac{\partial\psi_{av}(R,y)}{\partial R}\right|_{R=0} = \frac{2}{\hbar^2}[(3k-1)\sigma_{3k-1}]^{-1}\times\int_{S^{3k-1}} RV_k\,d\omega\,\psi(0,y), \tag{24}$$

where

$$\psi_{av}(R,y) = \frac{1}{\sigma_{3k-1}}\int_{S^{3k-1}}\psi(R\omega, y)d\omega, \tag{25}$$

and $\psi(0,y)$ is independent of ω.

The simplest term of the integral on the right-hand side of Eq. (24) is the r_{12} term, which, by using Eqs. (10), (14), and (18) is evaluated as

$$\int_{S^{3k-1}} R\frac{e_1 e_2}{r_{12}}d\omega = e_1 e_2\left(\frac{m_1 m_2}{M_2}\right)^{1/2}\times\int_{S^{3k-1}}\frac{d\omega}{\sin\alpha_1\sin\alpha_2\cdots\sin\alpha_{k-1}} = e_1 e_2\left(\frac{m_1 m_2}{M_2}\right)^{1/2}4\pi^{(3k-1)/2}\Big/\Gamma\left(\frac{3k-1}{2}\right). \tag{26}$$

While all of the other terms appear to be more complicated, it is known that any desired reordering of the $k+1$ particles can be accomplished by a kinematic rotation,[11,12] an orthogonal rotation of the angular variables. This means that by a redefinition of the angles, each of the r_{ij} terms can be brought into a form analogous to Eq. (26), except that the charges and masses are changed accordingly.[13] Consequently,

$$\int_{S^{3k-1}} RV_k\,d\omega = 4\frac{\pi^{(3k-1)/2}}{\Gamma((3k-1)/2)}\sum_{i<j}^{k+1} e_i e_j\left(\frac{m_i m_j}{m_i + m_j}\right)^{1/2}, \tag{27}$$

and Eq. (24) reduces to

$$\left.\frac{\partial\psi_{av}(R,y)}{\partial R}\right|_{R=0} = C\sum_{i<j}^{k+1} e_i e_j\left(\frac{m_i m_j}{m_i + m_j}\right)^{1/2}\psi(0,y), \tag{28}$$

$$C = \frac{2}{\hbar^2}\pi^{-1/2}\frac{\Gamma(3k/2)}{\Gamma((3k+1)/2)}. \tag{29}$$

This is the completely general set of cusp conditions alluded to by Hoffmann-Ostenhof and Seiler (ignoring statistics since the charges and masses may not be the same at all) for the eigenfunctions of the reduced Hamiltonian h. There is no restriction on the number of particles coalescing, nor of the species involved. If we take particle 1 as a nucleus (charge Ze) and the remaining k as

electrons (charge $-e$, mass m), Eq. (28) becomes

$$\left.\frac{\partial\psi_{\rm av}(R,y)}{\partial R}\right|_{R=0} = C\left[-kZ\left(\frac{m_1}{m_1+m}\right)^{1/2} + 2^{-1/2}\frac{k(k-1)}{2}\right] \times e^2 m^{1/2}\psi(0,y)\,, \tag{30}$$

which reduces to Theorem 1 of Ref. 7 when $m_1/m \to \infty$.

When $k=1$ (a two-particle overlap),

$$\left.\frac{\partial\psi_{\rm av}(R,y)}{\partial R}\right|_{R=0} = \frac{e_1e_2}{\hbar^2}\left(\frac{m_1m_2}{m_1+m_2}\right)^{1/2}\psi(0,y)\,. \tag{31}$$

Recognizing from Eq. (15) that $R=[m_1m_2/(m_1+m_2)]^{1/2}r_{12}$ brings Eq. (31) into agreement with Pack and Byers Brown.[14]

Finally, again borrowing from Hoffman-Ostenhof and Seiler,[7] we may obtain similar results for the bound-state reduced densities[15]

$$\rho_k(\vec{R}_1,\vec{R}_2,\ldots,\vec{R}_k) = \int_{\mathbb{R}^{3(N-k-1)}} |\psi(\vec{R}_1,\vec{R}_2,\ldots,\vec{R}_{N-1})^2| \times d\vec{R}_{k+1}\cdots d\vec{R}_{N-1}\,. \tag{32}$$

With $\tilde{\rho}_k$ being given by ρ_k averaged over S^{3k-1}, then

$$\left.\frac{d}{dR}\tilde{\rho}_k(R)\right|_{R=0} = 2C\sum_{i<j}^{k+1} e_ie_j\left(\frac{m_im_j}{m_i+m_j}\right)^{1/2}\rho_k(0)\,. \tag{33}$$

Note, however, that this is not precisely the same definition of particle density as given in Ref. 7. A definition closer to that can be formulated, but we will not do so here.

IV. MULTIPLE COALESCENCE POINTS

As general as the preceding results may be, it seems conceivable that there is more information to be gleaned from such an approach. The usual conditions that no more coincidences of particles take place appears to be unreasonably restrictive. Certainly the manifolds in configuration space for which the many-particle Coulomb potential becomes singular are much broader than those considered here (a single coalescence of $k+1$ particles).

For instance, consider the next simplest possibility, two coalescences in distinct separated clusters of particles. Internal coordinates[9] (and hyperspherical coordinates[12]) can certainly be defined so that each coalescence is described by the vanishing of a different set of independent variables. We describe the wave function (with c.m. removed) by $\psi(R_a\omega_a,R_b\omega_b,y)$, where a and b correspond to the two separate clusters and y denotes any remaining internal coordinates. There are now two separate averagings: $\psi_a(R_a,R_b\omega_b,y)$ is obtained from an average over ω_a, $\psi_b(R_a\omega_a,R_b,y)$ from an average over ω_b, and $\psi_{ab}(R_a,R_b,y)$ from an average over both. We then have two separate equations of the form of Eq. (28):

$$\left.\frac{\partial}{\partial R_a}\psi_a(R_a,R_b\omega_b,y)\right|_{R_a=0} = Q_a\psi(0,R_b\omega_b,y)\,, \tag{34}$$

$$\left.\frac{\partial}{\partial R_b}\psi_b(R_a\omega_a,R_b,y)\right|_{R_b=0} = Q_b\psi(R_a\omega_a,0,y)\,, \tag{35}$$

the constants Q_a and Q_b being appropriate to the two separate clusters. Differentiating Eq. (34) with respect to R_b, averaging over ω_b, and then using Eq. (35) with $R_a=0$ leads to

$$\left.\frac{\partial^2}{\partial R_a\partial R_b}\psi_{ab}(R_a,R_b,y)\right|_{R_a=R_b=0} = Q_aQ_b\psi(0,0,y)\,, \tag{36}$$

which can also be obtained starting from Eq. (35). Similar results would then occur for any number of independent coalescences.

This is obviously not a rigorous proof (which would be welcome); the normal restrictions preclude those regions of configuration space where both coalescences take place. The point is that the two singularities are *independent* of each other and involve different independent coordinates.

An example was given in Ref. 7 of cusp conditions for two electrons situated at different (fixed) nuclei.[16] To obtain the analog for the a and b systems (with k_a+1 and k_b+1 particles, respectively), we change variables from R_a and R_b to R and a new hyperangle β $(0\le\beta\le\pi/2)$:

$$R_a = R\cos\beta\,,\quad R_b = R\sin\beta. \tag{37}$$

The change in the volume element is

$$\begin{aligned} &R_a^{3k_a-1}R_b^{3k_b-1}dR_a dR_b \\ &= R^{3(k_a+k_b)-1}dR\cos^{3k_a-1}\beta\sin^{3k_b-1}\beta\,d\beta \\ &= R^{3(k_a+k_b)-1}dR\,d\mu(\beta)\,, \end{aligned} \tag{38}$$

allowing an additional averaging of the wave function over β as well as ω_a and ω_b. Then, using

$$\frac{\partial}{\partial R} = \frac{R_a}{(R_a^2+R_b^2)^{1/2}}\frac{\partial}{\partial R_a} + \frac{R_b}{(R_a^2+R_b^2)^{1/2}}\frac{\partial}{\partial R_b}, \tag{39}$$

Eqs. (34) and (35), and the fact that

$$\psi_a(0,0,y) = \psi_b(0,0,y) = \psi(0,0,y)\,, \tag{40}$$

we obtain

$$\begin{aligned} \left.\frac{\partial}{\partial R}\psi_{ab\beta}\right|_{R=0} &= \left(\int d\mu(\beta)\right)^{-1}\int d\mu(\beta)\left[\cos\beta\left(\frac{\partial}{\partial R_a}\psi_{ab}\right)_{R=0} + \sin\beta\left(\frac{\partial}{\partial R_b}\psi_{ab}\right)_{R=0}\right] \\ &= \left(\int d\mu(\beta)\right)^{-1}\int d\mu(\beta)(Q_a\cos\beta + Q_b\sin\beta)\psi(0,0,y) = Q_{ab}\psi(0,0,y)\,. \end{aligned} \tag{41}$$

Here Q_{ab} is given by

$$Q_{ab}=2\pi^{-1/2}\hbar^{-2}\frac{\Gamma(3(k_a+k_b)/2)}{\Gamma([3(k_a+k_b)+1]/2)}\left[\sum_{i<j}^{k_a+1} e_{ai}e_{aj}\left(\frac{m_{ai}m_{aj}}{m_{ai}+m_{aj}}\right)^{1/2}+\sum_{i<j}^{k_b+1} e_{bi}e_{bj}\left(\frac{m_{bi}m_{bj}}{m_{bi}+m_{bj}}\right)^{1/2}\right], \tag{42}$$

where the subscript a or b denotes the appropriate cluster. This result reduces to Eq. (25) of Ref. 7 when a and b each contain one electron and one infinitely heavy nucleus.

Equations (36) and (41) are in accord with the general idea of attributing individual prefactors for each two-particle interaction to the wave function,[2,17] used to remove the singularities from the Schrödinger equation. The explicit form for the higher-order cusp conditions may serve as useful restrictions on *Ansätze* for such prefactors, or for expansions around the singularities which remove the angular averaging.[18]

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[13]There is only one type of integral to evaluate here, as opposed to two when the nucleus is taken as the origin of coordinates in the infinite-nuclear-mass approximation. Note that the integrals in Eqs. (15) and (16) of Ref. 7 differ only by a factor of $\sqrt{2}$. This stems from the mass factor in the present work, as is seen from Eq. (26).

[14]Pack and Byers Brown (Ref. 2) did not separate the total c.m. from the problem, but this makes no difference. A plane wave $\exp(i\vec{k}\cdot\vec{R}_N)$ can be incorporated into the definition of $\psi(R\omega,y)$ or not, depending upon choice.

[15]As mentioned after Eq. (10), the choice of the scale factors μ_i is not important in this paper. Nonetheless, these factors do enter into the Jacobian of the transformation of Sec. II, and certain choices may be more convenient than others in defining these many-particle densities. The definition $\mu_i=m_{i+1}M_i/M_{i+1}$ in particular ensures that $\int \rho_k d\,\mathrm{R}_1\cdots d\,\mathrm{R}_k=1$ for any k.

[16]The hyperradius R in Eq. (25) of Ref. 7 appears to be (in their notation) $R=[(x_1-Y_1)^2+(x_2-Y_2)^2]^{1/2}$.

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