Coulomb Forces in Quantum-Mechanical Three-Body Problems*

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A method for handling the three-body problem with two of the particles charged is presented in terms of the corresponding uncharged problem. Coulomb wave functions are used in the relative coordinate of the charged particles and the resulting expressions subjected to an approximation. The technique should be useful for He^3 calculations.

I. INTRODUCTION

ALTHOUGH a great deal of attention has been paid the triton using "exact" three-body techniques, surprisingly little work has been done on He^3. The Coulomb force, which is operative in that system, is particularly unsuited to expansion in terms of (nonlocal) separable potentials. This is a severe restriction in an area of physics where separable potentials are found to be so useful. In this paper we present an approximate method for handling this complication. Although the parameters given in examples are those of He^3, the technique is more general. Moreover, separability plays no essential role; however, we feel that in that context the approximation will find greatest use.

In Sec. II we show in detail where the approximation enters in a simple three-body problem. Much of our notation here follows that of Mitra.[1] More detailed analysis follows in Sec. III, where we try to develop a feeling for the domain of validity of the approximation and argue in favor of its usefulness in He^3. This section also has a short derivation of the result which makes its greater generality apparent. Section IV is a summary.

II. THE APPROXIMATION IN A SPECIFIC THREE-BODY CONTEXT

We start from Schrödinger's equation in momentum space. We do not symmetrize and consider (beside the Coulomb force) only a short-range two-body separable central potential.

$$\left[\frac{P_1^2}{2M}+\frac{P_2^2}{2M}+\frac{P_3^2}{2M}+V^C(2,3)-E\right]\psi(\mathbf{P}_1,\mathbf{P}_2,\mathbf{P}_3) = -V^{\text{Nuclear}}\psi, \quad (1)$$

where neutrons and protons are taken with mass M, index No. 1 refers to the neutron, Nos. 2 and 3 to the protons; $V^C(2,3)$ is the Coulomb interaction. In the center-of-mass system $\mathbf{P}_1=-\mathbf{P}_2-\mathbf{P}_3$, and taking $\mathbf{P}=\mathbf{P}_2+\mathbf{P}_3$, $\mathbf{p}=\frac{1}{2}(\mathbf{P}_2-\mathbf{P}_3)$ (1) becomes

$$\left[\frac{3}{4}\frac{P^2}{M}+\frac{p^2}{M}+V^C(2,3)-E\right]\psi(\mathbf{P},\mathbf{p})=-V^N\psi. \quad (2)$$

The V^N term is of the form

$$\int d^3P'd^3p'\langle\mathbf{Pp}|V^N|\mathbf{P'p'}\rangle\psi(\mathbf{P'},\mathbf{p'}),$$

with $V^N=V_{12}+V_{23}+V_{13}$. The $|\mathbf{Pp}\rangle$ matrix elements of each of these conserve the momentum of the non-interacting particle:

$$\begin{aligned}\langle\mathbf{Pp}|V_{23}|\mathbf{P'p'}\rangle&=\delta(\mathbf{P}-\mathbf{P'})\langle\mathbf{p}|\tilde{V}_{23}|\mathbf{p'}\rangle,\\ \langle\mathbf{Pp}|V_{13}|\mathbf{P'p'}\rangle&=\delta(\mathbf{p}+\tfrac{1}{2}\mathbf{P}-\mathbf{p'}-\tfrac{1}{2}\mathbf{P'})\\ &\quad\times\langle\tfrac{1}{2}\mathbf{p'}-\tfrac{3}{4}\mathbf{P}|\tilde{V}_{13}|\tfrac{1}{2}\mathbf{p'}-\tfrac{3}{4}\mathbf{P'}\rangle, \quad (3)\\ \langle\mathbf{Pp}|V_{12}|\mathbf{P'p'}\rangle&=\delta(-\mathbf{p}+\tfrac{1}{2}\mathbf{P}+\mathbf{p'}-\tfrac{1}{2}\mathbf{P'})\\ &\quad\times\langle-\tfrac{1}{2}\mathbf{p}-\tfrac{3}{4}\mathbf{P}|\tilde{V}_{12}|-\tfrac{1}{2}\mathbf{p'}-\tfrac{3}{4}\mathbf{P'}\rangle,\end{aligned}$$

(where $\tilde{V}_{ij}$ is the two-body operator corresponding to V_{ij}). For convenience we assume

$$\langle\mathbf{q}|\tilde{V}_{ij}|\mathbf{q'}\rangle=\frac{-\lambda}{M}g(\mathbf{q})g(\mathbf{q'}) \quad \text{for all} \quad i,j.$$

Schrödinger's equation is then

$$\begin{aligned}&M\left(\frac{3}{4}\frac{P^2}{M}+\frac{p^2}{M}+V^C(2,3)-E\right)\psi(\mathbf{P},\mathbf{p})\\ &=\lambda g(\mathbf{p})\int d^3p'g(\mathbf{p'})\psi(\mathbf{P},\mathbf{p'})+\lambda\left\{g(\tfrac{1}{2}\mathbf{p}-\tfrac{3}{4}\mathbf{P})\int d^3\xi g(\xi)\right.\\ &\left.\times\psi\left(-\xi+\tfrac{1}{2}(\mathbf{p}+\tfrac{1}{2}\mathbf{P}),\frac{\xi}{2}+\tfrac{3}{4}(\mathbf{p}+\tfrac{1}{2}\mathbf{P})\right)+(\mathbf{p}\to-\mathbf{p})\right\}. \quad (4)\end{aligned}$$

The Coulomb potential, of course, is not diagonal in this representation. However, we can diagonalize the left-hand side of Eq. (4) by transforming to momentum-Coulomb space, i.e., the representation whose basis vectors are plane waves in $\mathbf{P}$ and repulsive Coulomb waves in the relative momentum of the two protons, $\mathbf{p}$. Let U be the unitary operator which accomplishes this. Then $U[(p^2/M)+V^C]U^{-1}=k^2/M$ and $U\psi(\mathbf{P},\mathbf{p})=\psi_C(\mathbf{P},\mathbf{k})$, with $\mathbf{k}$ interpreted as the asymptotic relative momentum of the Coulomb wave.

In non-Coulombic problems, $e=0$, one usually defines $D(\mathbf{P},\mathbf{p},E)=M[(3P^2/4M)+(p^2/M)-E]$, and the left-hand side of the equation corresponding to (4) is $D(\mathbf{P},\mathbf{p},E)\psi(\mathbf{P},\mathbf{p})$. For $e\neq0$, we see that after U is

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[1] A. N. Mitra, Nucl. Phys. 32, 529 (1962).

applied, the left-hand side of (4) is $D(\mathbf{P},\mathbf{k},E)\psi_C(\mathbf{P},\mathbf{k})$, with the *same function D*.

Now consider the right-hand side of (4). The action of U on the first term (p-p potential) is relatively simple and parallels the two-body results of Harrington.[2]

$$g(\mathbf{p})\int d^3p'g(\mathbf{p}')\psi(\mathbf{p}')\rightarrow\int d^3p\ U(\mathbf{k},\mathbf{p})g(\mathbf{p})\times\int d^3k'\int d^3p'g(\mathbf{p}')U^*(\mathbf{p}',\mathbf{k}')\psi_C(\mathbf{k}')$$
$$=\left[\int d^3p\ U(\mathbf{k},\mathbf{p})g(\mathbf{p})\right]\times\int d^3k'\left[\int d^3p'g(\mathbf{p}')U^*(\mathbf{p}',\mathbf{k}')\right]\psi_C(\mathbf{k}'). \quad (5)$$

The only effect of U is to modify g ($\mathbf{P}$ dependencies suppressed). However, V_{13} and V_{12} are less tractable. V_{13}, for example, depends on $\mathbf{P}_1-\mathbf{P}_3$. Although $\mathbf{P}_1$ is still diagonal ($=-\mathbf{P}$), $\mathbf{P}_3$ is not. One sees this by explicitly writing out the transformation

$$\langle\mathbf{P}\mathbf{p}|\mathbf{P}'\mathbf{k}'\rangle=\delta(\mathbf{P}-\mathbf{P}')\langle\mathbf{p}|\mathbf{k}'\rangle=\delta(\mathbf{P}-\mathbf{P}')\phi_{\mathbf{k}'}(\mathbf{p}), \quad (6)$$
$$(V_{13})_C\psi_C\equiv UV_{13}U^{-1}\psi_C=\int d^3p_1d^3p_2d^3k'd^3p'\phi_k{}^*(\mathbf{p}_1)\times\langle\mathbf{P}\mathbf{p}_1|V_{13}|\mathbf{P}'\mathbf{p}_2\rangle\phi_{\mathbf{k}'}(\mathbf{p}_2)\psi_C(\mathbf{P}',\mathbf{k}'),$$

where ϕ is the Coulomb wave function in momentum space. Here the advantages arising from the separable nature of the potential are lost, since there is no breakup of the integral.

To deal with this complication—a complication intrinsic to the use of local potentials in a three-body problem—we use an approximation suggested by Guth and Mullin.[3] In coordinate space, Coulomb wave functions are locally very similar to plane waves. In momentum space this is reflected in a sharp peaking of $\phi_{\mathbf{k}}(\mathbf{p})$ near $\mathbf{k}=\mathbf{p}$. This is also evident from the expansion of $\phi_{\mathbf{k}}(\mathbf{p})$ in powers of e^2:

$$\phi_{\mathbf{k}}(\mathbf{p})=\delta(\mathbf{k}-\mathbf{p})-\frac{Me^2}{2\pi^2}\frac{1}{(k^2+i\epsilon-p^2)(\mathbf{k}-\mathbf{p})^2}+\cdots. \quad (7)$$

Thus, presented with an integral of the form $\int d^3p\ f(\mathbf{p})\phi_{\mathbf{k}}(\mathbf{p})$, we approximate f by its value at $\mathbf{p}=\mathbf{k}$ and remove it from the integral

$$\int d^3p\ f(\mathbf{p})\phi_{\mathbf{k}}(\mathbf{p})\approx f(\mathbf{k})\int d^3p\ \phi_{\mathbf{k}}(\mathbf{p})=f(\mathbf{k})\tilde{\phi}_{\mathbf{k}}(0)\equiv f(\mathbf{k})C(k), \quad (8)$$

where $\tilde{\phi}_{\mathbf{k}}(0)$ is the value of the configuration space Coulomb wave function at $\mathbf{r}=0$, and $C(k)$ is related to the barrier penetration factor. We will later, in a particular case, compare (8) with the exact integral.

This approximation effects a tremendous simplification of the problem; the action of the operator U on V_{13} becomes simply multiplication by $C(k)$ and the replacement of $\mathbf{p}$ by $\mathbf{k}$. Thus

$$((V_{13})_C\psi_C)(\mathbf{P},\mathbf{k})=\int d^3k'd^3P'C^*(k)\times\langle P\mathbf{k}|V_{13}|P'\mathbf{k}'\rangle C(k')\psi_C(\mathbf{P}',\mathbf{k}'). \quad (9)$$

[The matrix element of V_{13} in (9) is the momentum-space matrix element with the six numbers $\mathbf{k}$, $\mathbf{k}'$ replacing $\mathbf{p}$, $\mathbf{p}'$ of, e.g., Eq. (3).] We can now write Schrödinger's equation as

$$D(\mathbf{P},\mathbf{k},E)\psi_C(\mathbf{P},\mathbf{k})=-\int d^3P'd^3k'C(k)^*\times V^N(\mathbf{P},\mathbf{k},\mathbf{P}'\mathbf{k}')C(k')\psi_C(\mathbf{P}',\mathbf{k}'), \quad (10)$$

where V^N again has the same functional form as in the $e=0$ case, but $\mathbf{k}$ is given a different interpretation. Finally, we define $\psi'(\mathbf{P},\mathbf{k})$ as $\psi'(\mathbf{P},\mathbf{k})=C(k)\psi_C(\mathbf{P},\mathbf{k})$. The equation satisfied by ψ' is

$$\frac{D(\mathbf{P},\mathbf{k},E)}{|C(k)|^2}\psi'(\mathbf{P},\mathbf{k})=-\int d^3P'd^3k'\times V^N(\mathbf{P},\mathbf{k},\mathbf{P}',\mathbf{k}')\psi'(\mathbf{P}',\mathbf{k}'). \quad (11)$$

The equation for the corresponding uncharged problem differs from this only in not having the $|C(k)|^2$ term. Thus the solution of a charged problem proceeds exactly as in the uncharged case with only the replacement of $D(\mathbf{P},\mathbf{p},E)$ by $D(\mathbf{P},\mathbf{k},E)/|C(k)|^2$.

We note incidentally that $|C(k)|^2$ is the barrier penetration factor, specifically

$$|C(k)|^2=(Me^2/k)/(e^{\pi Me^2/k}-1).$$

III. ANALYSIS OF THE APPROXIMATION

Aside from well-known three-body techniques, the results of Sec. II depend on two steps:

(A) Rather than relative plane-wave states of two protons, relative Coulomb wave functions are used.

(B) The approximation in Eq. (8) gives the prescription for treating the expressions obtained from (A).

If $\mathbf{P}$ is the total momentum of the two protons and $\mathbf{p}$ is their relative momentum, let U be the (unitary) operator diagonalizing the Coulomb part of potential, but which, of course, leaves $\mathbf{P}$ unchanged. This achieves objective (A) and introduces a coordinate $\mathbf{k}$, the relative "Coulomb momentum", satisfying

$$U[p^2/M+V^C]U^{-1}=k^2/M.$$

[2] D. R. Harrington, Phys. Rev. **139**, B691 (1965).
[3] E. Guth and C. J. Mullin, Phys. Rev. **83**, 667 (1951).

U, however, is not diagonal; and while it is tailored to simplify the kinetic and Coulomb parts of the Hamiltonian, it only complicates the nuclear potentials existing between the protons and the neutron. U can be represented by $\delta(\mathbf{P}-\mathbf{P})\langle\mathbf{p}|\mathbf{k}\rangle^*$, where $\langle\mathbf{p}|\mathbf{k}\rangle=\phi_k(\mathbf{p})$, the momentum-space Coulomb wave function. One then takes advantage of the concentration of ϕ near $\mathbf{p}=\mathbf{k}$ and introduces the approximation

$$\langle\mathbf{p}|\mathbf{k}\rangle\approx\delta(\mathbf{p}-\mathbf{k})C(k), \tag{12}$$

where $|C(k)|^2=$(barrier penetration factor). That $\langle\mathbf{p}|\mathbf{k}\rangle$ is sharply peaked is evident from, e.g., the Born approximation [Eq. (7)], where not only the first term (a δ function) exhibits this singularity, but all subsequent terms are infinite at $\mathbf{p}=\mathbf{k}$ (magnitude and direction) as well.

One can also derive easily the result of Sec. II in another way. The Schrödinger equation for He^3 is

$$[T(\mathbf{P},\mathbf{p})+V^C]\psi=-V^N\psi+E\psi. \tag{13}$$

$T=$kinetic energy, $V^C=$Coulomb potential, $V^N=$nuclear potential. Let U be as above. Then $U(T+V^C)U^{-1}=T(\mathbf{P},\mathbf{k})$, i.e., the same functional form for T, except that $\mathbf{p}$ is replaced by $\mathbf{k}$. To UV^NU^{-1} apply Eq. (12) to obtain $UV^NU^{-1}\approx C(k)^*V^N(\mathbf{P},\mathbf{k},\mathbf{P}\mathbf{k}')C(k')$. Let $\psi'=C(k)U\psi$, and (13) becomes

$$\left[\frac{T(\mathbf{P},\mathbf{k})-E}{|C(k)|^2}\right]\psi'(\mathbf{P},\mathbf{k})$$

$$=-\int V^N(\mathbf{P},\mathbf{k},\mathbf{P}'\mathbf{k}')\psi'(\mathbf{P}',\mathbf{k}')d^3P'd^3k'=-V^N\psi'. \tag{14}$$

It should be clear that the separability or other special properties of V^N play no role other than to put the approximation in an otherwise solvable framework.

We now compare the result of the approximation given by Eq. (8) with a sample exact integration. The function to be integrated is a very practical one, the Yamaguchi two-body potential $g(\mathbf{p})=1/(p^2+\beta^2)$. This integral of g arises in the expression for the p-p potential either in the present context or in the two-body work of Harrington. Let

$$I=\int d^3p\,\frac{1}{p^2+\beta^2}\langle\mathbf{p}|\mathbf{k}\rangle.$$

This can be evaluated exactly, giving $I=g(\mathbf{k})C(k)\exp[2\gamma\tan^{-1}(|k|/\beta)]$; where $\gamma=\mu e^2/|k|$, μ is the reduced mass of the particles giving rise to the Coulomb wave $\langle\mathbf{p}|\mathbf{k}\rangle$ and

$$|C(k)|=C_0(\gamma)=[2\pi\gamma/(e^{2\pi\gamma}-1)]^{1/2}.$$

The result of the approximation in Eq. (8), denoted here by I', is $I'=g(\mathbf{k})C(k)$.

While comparing I and I' will certainly not guarantee the validity of the approximation in a wide variety of cases, it will indicate where the approximation is bad and will give a feeling for its validity—although we point out that this example does not have the angular dependence that would appear in the general situation.

$$(I/I')=\exp[2\gamma\tan^{-1}(|k|/\beta)]$$
$$\equiv f(k)\lesssim e^{2\mu e^2/\beta}\approx 1.023 \quad \text{for } He^3 \text{ parameters},$$
$$\mu=\tfrac{1}{2}M_P=\tfrac{1}{2}\times 4.75\ \mathrm{F}^{-1},\quad e^2=1/137,\quad \beta=1.5\ \mathrm{F}^{-1}.$$

The approximation is thus good to about 2% for He^3 parameters. But this, however, is not yet sufficient. Coulomb effects are small to begin with and not only do we desire terms deleted by approximations to be small but they should be smaller than the effects we are seeking.

It is then of interest to compare $C(k)$ with $f(k)$ for various values of k. When $C(k)$ differs from unity by a good deal more than 2% we can be sure that our calculation accounts for the bulk of the Coulomb effects. If $f(k)$ and $C(k)$ are expanded about $k=0$ and $k=\infty$, it is seen that for small k, $C(k)$ dominates, and for large k they differ from unity by about the same amount (with opposite sign). Table I gives k, $f(k)$, $C(k)$ and the kinetic energy in MeV in the proton relative coordinate system for the given k. $\beta=1.5\ \mathrm{F}^{-1}$ is approximately the value obtained from two-body data.

Below 1.6 MeV $C(k)$ is quite adequate. From 1.6 to 10 MeV $(1-C(k))$ is from 6 to 2 times as large as the $f(k)$ correction. Between 10 to 40 MeV using $C(k)$ alone tends to overestimate the Coulomb effects $(f(k)\geq 1)$; i.e., the product $C(k)f(k)$ (exact result) is closer to unity than the use of $C(k)$ by itself (present approximation) would indicate.

In general, larger β brings $f(k)$ closer to unity, so that $C(k)$ alone provides a reliable measure of the Coulomb effects for higher values k. Greater reliability of the approximation for larger β is quite reasonable: $C(k)^2$ is the barrier penetration factor, i.e., the probability of the protons being in contact (in coordinate space). If the potential is of very short range then it is this factor that cuts down the interaction energy. On the other hand, for $\beta<\infty$, the protons can interact at a finite distance and the interaction is closer to what it would be without charge effects. Hence the finite range of the potential tends to counteract the Coulomb-induced unlikelihood of proximity.

An important consideration in using this approximation is the location, in k space, of the principal

TABLE I. Comparison of $C(k)$ with $f(k)\equiv\exp(2\gamma\tan^{-1}(|k|/\beta))$ for various values of k. $\beta=1.5\ \mathrm{F}^{-1}$.

k in F^{-1}	0.0	0.01	0.05	0.1	0.2	0.5	1.0
$C(k)$	0.0	0.014	0.526	0.743	0.867	0.949	0.974
$f(k)$	1.023	1.023	1.023	1.023	1.023	1.022	1.020
(k^2/M_p) in MeV	0.0	0.004	0.104	0.415	1.6	10.4	41.6

contributions to various charge-induced effects, such as the Coulomb energy difference between H^3 and He^3. The regions where $|f(k)-1|\approx C(k)-1$ are regions where electrostatic effects are not very important altogether (both numbers are small) for reasonable β. Thus where charge effects are important $C(k)$ dominates. Of course, one must also examine the wave function ψ (obtained perhaps from the uncharged problem) since in special cases this argument may be false.

An analysis of the approximation for the V_{13} term shows a similar favor for short range. The exact expression from Eqs. (6) and (3) and using the Yamaguchi form for V_{13} is

$$\langle \mathbf{Pk}|\,(V_{13})_C\,|\mathbf{P'k'}\rangle$$
$$=\int d^3p_1 d^3p_2 \phi_k^*(\mathbf{p}_1)\delta(\mathbf{p}_1+\tfrac{1}{2}\mathbf{P}-\mathbf{p}_2-\tfrac{1}{2}\mathbf{P}')$$
$$\times g(\tfrac{1}{2}\mathbf{p}_1-\tfrac{3}{4}\mathbf{P})g(\tfrac{1}{2}\mathbf{p}_2-\tfrac{3}{4}\mathbf{P}')\phi_{k'}(\mathbf{p}_2)\,. \quad (15)$$

If g is very "short range" (β large) its characteristic feature is its flatness in momentum space. This flatness will be unaffected by the presence of additional vectors ($\mathbf{P}$) in the argument of g. It should be noted that the peaking of $\phi_k(\mathbf{p})$ is not only in magnitude, but in direction also. Since, however, there are additional integrations inextricably tied in here (V_{13} appears $V_{13}\psi$) there is an additional, though less stringent, requirement on the smoothness of ψ (less stringent, since there are several vectors in its argument). This is expected to have roughly the shape of g, although it probably decreases more rapidly in k (consider the size of the He^3 nucleus).

IV. SUMMARY AND CONCLUSION

Starting with the momentum-space Schrödinger equation for a three-body system, where all of the particles have a short-range force and two of them have a Coulomb interaction, we diagonalize exactly the Coulomb and kinetic parts with a unitary operator U. Although U is not diagonal in momentum space, our approximation takes advantage of its being nearly so in order to replace it by a diagonal matrix with "effective" values of U along the diagonal. This simplifies its action on the short-range potentials.

We have tried to obtain a feeling for the validity of this approximation and have found that it is likely to be better for shorter-range (in coordinate space) forces. Specifically, if the range is $(1/\beta)$ and the mass of the particles 2μ ($\hbar=c=1$), then the smaller μ/β is, the better the approximation. For $(2\mu e^2/\beta)\approx 0.02$ (He^3 case), we expect the present approximation to account for the bulk of Coulomb effects.

Perhaps the most useful aspect of the suggestion put forward in this paper is that separable potentials retain their simple form in the face of local—and therefore nonseparable—interactions. It is the peculiar nature of the Coulomb interaction that lends itself to this treatment.[4]

It is likely that there are other three-body systems for which a similar combination of range, charge, and mass parameters would indicate a useful role for the present approximation. Clearly, the method could be applied to the scattering of protons and deuterons at low energies.

The chief disadvantage of this approximation is its fuzziness. Even if in a given case it is good, one does not know how good—and if it is bad, how bad. It is, however, quite convenient and provides the solver of non-Coulombic three-body problems with a quick entry to the effect of charge.

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[4] In a sense this approximation is best for $1/r$ potentials. Consider the identical problem but with $V(r)=A\,e^{-\gamma r}/r$ replacing $1/r$, and consider the corresponding U_γ. Then the Born approximation to the off-diagonal matrix elements of U_γ in momentum (relative coordinate of particles No. 2 and No. 3) space are proportional to $A/((p^2-k^2-i\epsilon)[\gamma^2+(\mathbf{p}-\mathbf{k})^2])$. As $\gamma\to 0$, the peaking near $\mathbf{k}=\mathbf{p}$ becomes more pronounced.