Long-range interaction in a system of three particles

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A transcendental equation is obtained from the Faddeev equations for the action of the two heavy particles in a system consisting of two heavy and one light particles with short-range pair potentials. Simple quantization of the motion according to the Bohr–Sommerfeld formula yields the three-particle spectrum of the system, in good agreement with the direct solution of the Faddeev equations. This permits a system with a vanishingly light exchange particle to be described, whereas the direct solution of the Faddeev equations is fraught with numerical problems. In particular, one concludes that a rich spectrum can exist in A_2^- systems even when there is no bound state of the electron and an atom, i.e., A^-. The effective quasi-two-particle interaction potential is determined for the heavy particles. It is local, energy-independent, and has a long-range Coulomb-type region, which is primarily responsible for determining the spectrum of the system. © *1994 American Institute of Physics.*

1. INTRODUCTION

The three-body problem gives rise to many new and beautiful phenomena. One of these is the Efimov effect:[1] either varying as R^{-2} in terms of the hyperradius of the system[1] or as ρ^{-2} in terms of the relative coordinate[2] between one of the particles and the remaining pair. The explanation for this phenomenon is quite simple. In a three-body system the de Broglie energy of a particle in a volume of dimension ρ can go into exciting the pair and does not lead to effective repulsion as in the two-body problem. This is equivalent to the action of an effective attractive potential of the form $-\gamma/2m\rho^2$. From the uncertainty principle it is evident that γ must be larger than 1/4.[1)] This coupling constant can give rise to a series of bound states if it allows a region in which a potential of the form ρ^{-2} acts. The same range for the effective long-range interaction can be deduced from simple considerations. This mechanism for the occurrence of a long-range interaction presupposes the virtual excitation of the pair, which imposes a condition on the time the particle remains in the interaction region: this time must be much less than the time required to traverse an orbit, which is determined by the binding energy $\varepsilon=-\kappa^2/2m$ of the pair. On the other hand, this time must be much greater than the characteristic interaction times, determined by the potential energy $U\simeq -1/2mr_0^2$, where r_0 is the radius of the interaction. These two conditions yield to the familiar long-range interaction region[1,2]

$$\kappa^{-1}\gg\rho\gg r_0 \tag{1}$$

for identical particles. In this case we have $\gamma=1.26$. The effect increases as the pair interaction becomes more resonant, i.e., as the quantity κr_0 decreases.

The system consisting of two heavy particles (assumed identical for simplicity) with masses m_1 and m_3 and a light particle with mass m_2 is of particular interest. The process associated with the exchange of this particle gives rise to a long-range interaction with a large coupling constant $\gamma \propto \sqrt{m_{13}/m_2}$, but only in the narrow range of conditions[3]

$$\sqrt{\frac{m_2}{m_{13}}}\,\kappa^{-1}\gg\rho\gg 2r_0, \tag{2}$$

which approaches zero in the limit $m_2\to 0$. Consequently, there are no bound states in this potential. This stems from the fact that as the region in which the motion of the heavy particles is quantized decreases the above long-range mechanism disappears. The motion of the heavy particles becomes quasiclassical.

In order to convince ourselves of this, in what follows we will consider a system in which the potential U only acts between the light particle and the heavy ones; the heavy particles do not interact, and all interactions in the system take place through the light particle. Then when the interaction of the light and heavy particles is resonant (when the binding energy is small) its binding energy with the pair of heavy particles is in fact determined by a double potential well. Consequently, the energy scale of a heavy particle in the system is determined primarily by the half-depth of the pair interaction potential. At this energy on the length scale $\sim\kappa^{-1}$ of the system there are many wavelengths of the heavy particle. Thus, we will consider a system of three particles in which the motion of the light particle is quantized to a considerable degree, i.e., $\kappa r_0\ll 1$, while the motion of the heavy particles is quasiclassical. In this case the long-range component of the effective interaction between the heavy particles is determined not by their de Broglie energy as in the Efimov effect but by the potential energy of the interaction with the light particle. But the wave function of the latter drops off as $1/\rho$ in region (1), which gives rise to two types of long-range interaction: $1/\rho$ and $1/\rho^2$. As we will see shortly, the spectrum is determined primarily by the quasi-Coulomb interaction.

Next we will construct the effective potential V^{eff} for the interaction of the two heavy particles. For simplicity we take the potential U in the separable form of a Yamaguchi interaction $U_i=|v_i\rangle\langle v_i|$ ($i=1, 3$, as usual, runs over the particles present in the subsystem), or

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$$U(p,p')=-\frac{4\pi}{m_{12}}\frac{(\beta+\kappa)^2\beta}{(\beta^2+p^2)(\beta^2+p'^2)}. \quad (3)$$

Here κ is the wave number of a real ($\kappa>0$) or virtual ($\kappa<0$) state, β determines the radius of the interaction ($r_0=\beta^{-1}$), and in our case the depth of the two-particle potential; and m_{ij} is the reduced mass of particles i and j. Hence the Yamaguchi potential acts only through the S wave.

It is found that the potential can be local and energy-independent. Ordinary Bohr–Sommerfeld quantization yields the spectrum of the three-particle system. For comparison we present the spectrum of this system, calculated from the Faddeev equations for both real and virtual pair states.

It should be noted that the problem has been solved similarly, proceeding from the Bohr–Oppenheimer approximation[4] in order to analyze the Efimov long-range interaction. Our work differs in having a quasiclassical solution of the Faddeev equations, from which it is obvious that the long-range interaction of the Efimov effects as well as its spectrum differ from the long-range interaction considered here.

2. EQUATIONS AND EFFECTIVE POTENTIAL

As mentioned in the Introduction, we will treat a system of three particles (1+2+3) in which the heavy identical spinless particles 1 and 3 interact through the potential U with the light particle 2. Then, because particles 1 and 3 are identical, the pair of Faddeev equations for the three-particle wave function Ψ reduce to an equation for the projection $\psi=\langle\nu|\Psi\rangle$:

$$\psi=\frac{1}{1-A_{ii}}A_{ij}\psi, \quad (4)$$

where $A_{ij}=\langle\nu_i|G_0(Z)|\nu_j\rangle$ and G_0 is the three-particle Green's function of the free motion.

For convenience we will use quantities nondimensionalized in terms of β without changing the notation. Moreover, we introduce the dimensionless energy parameter λ through the relation $Z=-\lambda^2E_0$; $E_0=\beta^2/2m_{12}$ determines the characteristic depth of the two-particle potential. In this notation the complete form of Eq. (4) can be written as

$$\psi(\mathbf{k})=\int_0^\infty\frac{d^3k'}{\pi^2}\frac{(1+\kappa)^2(1+a)^2\psi(\mathbf{k}')}{(a-\kappa)(a+\kappa+2)(1+t^2)(1+t'^2)(\lambda^2+E)}, \quad (5)$$

$$\mathbf{t}=\mathbf{k}+\delta\mathbf{k}', \quad \mathbf{t}'=\mathbf{k}'+\delta\mathbf{k}, \quad E=k^2+k'^2+2\delta\mathbf{k}\mathbf{k}',$$

where $\delta=m_{12}/m_2$, $a=\sqrt{\lambda^2+\alpha^2k^2}$, and $\alpha^2=m_{12}/m_{1,23}$. It was by solving Eq. (5) numerically that the spectrum of the system was found.

The form of Eq. (5) shows that for $\alpha\to0$ ($\delta\to1$) its kernel contains a nonlocal interaction in configuration space. This can easily be removed from the equation by introducing the free-particle Green's function for the two-particle motion and calling the remaining part of the effective potential V^{eff}. The potential thus constructed will be local in the limit $\alpha\to0$, but it is energy-independent and on the whole does not represent the spectrum of the system very accurately. The main reason for this is that the transition to the local form of V^{eff} without treating the wave function ψ is incorrect because the wave function of the relative motion contains a factor which varies rapidly as a function of the relative coordinate.

To see this we can represent the classical action in the form

$$S=s/\alpha, \quad s=\int\sqrt{u^2-\lambda^2}d\rho. \quad (6)$$

Here u^2 is the dimensionless effective potential of the relative motion, i.e., $V^{\text{eff}}=-u^2E_0$ (we will refer to u as the wave number of this potential). As can readily be seen, the quantity s does not depend on α, since its scale is determined by the binding energy of the light particle with the pair of heavy ones. For the Yamaguchi potential these elementary ideas yield an equation for the limiting value u_{lim}:

$$(1+u_{\text{lim}})^2=2(1+\kappa)^2, \quad (7)$$

from which we obtain $u_{\text{lim}}=\sqrt{2}-1+\sqrt{2}\kappa$. Hence the quantity S in the limit $\alpha\to0$ becomes large and the wave function ψ will have a rapidly oscillating factor $\exp(is/\alpha)$.

In order to simultaneously take into account the rapidly varying part of both the kernel of the integral equation and the wave function, it is convenient to represent Eq. (4) in the form $\psi=(A_{ii}+A_{ij})\psi$, which can be written in configuration space in the limit $\alpha\to0$ in the form

$$\psi(\boldsymbol{\rho})=8\pi\int\left(I\left(\frac{r_-}{\alpha},0\right)+I\left(\frac{r_+}{\alpha},\rho'\right)\right)\psi(\rho')d^3\rho',$$

$$\mathbf{r}_+=\boldsymbol{\rho}+\boldsymbol{\rho}', \quad \mathbf{r}_-=\boldsymbol{\rho}-\boldsymbol{\rho}',$$

$$I(x,y)=\frac{(1+\kappa)^2}{4\pi\alpha^3x}\int\frac{d^3q}{(2\pi)^3}\frac{\exp(-i\mathbf{q}\mathbf{y}-\sqrt{\lambda^2+q^2}x)}{(1+q^2)^2}.$$

The technique for carrying out this limiting process is as follows: the integrand $I(r_+/\alpha,\rho')\psi(\rho')d^3\rho'$ is rewritten through the change of variables $\mathbf{x}=\mathbf{r}_+/\alpha$ and becomes $\alpha^3I(x,|\alpha\mathbf{x}-\boldsymbol{\rho}|)\psi(\alpha\mathbf{x}-\boldsymbol{\rho})d^3x$, which is finite in the limit $\alpha\to0$. In order to include the finite part of the oscillatory factor in ψ we must take into account the first term in the expansion in S as well. Retaining nonvanishing terms in α and performing the trivial integration with respect to $\mathbf{x}$ and $\mathbf{q}$, we find a transcendental equation for the gradient of the action, which in the notation $(\nabla s)^2+\lambda^2=u^2$ [cf. Eq. (6)] can be written as

$$1-\left(\frac{1+\kappa}{1+u}\right)^2=2\left(\frac{1+\kappa}{1-u^2}\right)^2\left(\frac{\exp(-u\rho)-\exp(-\rho)}{\rho}-\frac{1-u^2}{2}\exp(-\rho)\right). \quad (8)$$

Having thus determined the action, we can determine the spectrum of the system according to the usual quasiclassical formula

$$s(\rho_{\max})-s(0)=\pi\alpha(n+3/4).$$

TABLE I. Binding energy of a three-particle system in eV for real and virtual two-particle pair wise binding energy $\epsilon=-0.002$ eV; (a) solutions of the Faddeev equations; b) quasiclassical spectrum

N	Real level		Virtual level	
	a	b	a	b
0	$-0.4614\cdot10^{-1}$	$-0.4557\cdot10^{-1}$	$-0.7265\cdot10^{-2}$	$-0.7009\cdot10^{-2}$
1	$-0.2975\cdot10^{-1}$	$-0.2940\cdot10^{-1}$	$-0.1448\cdot10^{-2}$	$-0.1379\cdot10^{-2}$
2	$-0.1896\cdot10^{-1}$	$-0.1871\cdot10^{-1}$		
3	$-0.1185\cdot10^{-1}$	$-0.1180\cdot10^{-1}$		
4	$-0.7583\cdot10^{-2}$	$-0.7510\cdot10^{-2}$		
5	$-0.5056\cdot10^{-2}$	$-0.4988\cdot10^{-2}$		
6	$-0.3613\cdot10^{-2}$	$-0.3565\cdot10^{-2}$		
7	$-0.2799\cdot10^{-2}$	$-0.2776\cdot10^{-2}$		
8	$-0.2354\cdot10^{-2}$	$-0.2344\cdot10^{-2}$		
9	$-0.2123\cdot10^{-2}$	$-0.2118\cdot10^{-2}$		
10	$-0.2021\cdot10^{-2}$	$-0.2019\cdot10^{-2}$		

Note. a—solutions of the Faddeev; b—quasiclassical spectrum.

Below we present a table in which the spectra calculated from the exact equation and in the quasiclassical approximation are compared for the real and virtual pair states with $\alpha=0.1$. The mass of the heavy particles was taken to be equal to two nucleon masses, i.e., the mass of the light particle was equal to 0.01 nucleon masses; we took $\beta=1$ Å and the two-particle binding energy was -0.002 eV, which yielded $\kappa\simeq\pm0.1$ respectively for the real and virtual states.

3. LONG RANGE OF THE EFFECTIVE POTENTIAL

It is evident that the quantity u determined by Eq. (8) is the wave number of the potential introduced above. Equation (8) can be regarded as the equation for the effective potential. To within differences in notation this equation is the same as the expression for the interaction energy of two particles found previously by A. S. Fonseki *et al.*[4] in their analysis of the long-range Efimov effect. Here, in contrast, we show that the main contribution to the spectrum comes not from the Efimov long-range interaction but from the quasi-Coulomb interaction.

Let us discuss Eq. (8) in more detail. In the limit $\rho\to0$ the quantity u satisfies Eq. (7), which confirms our elementary discussion. Hence it follows that the attractive potential V^{eff} exists even for virtual binding ($\kappa<0$) for $\kappa>\sqrt{2}/2-1$. For the virtual two-particle interaction the potential V^{eff} is restricted to a region $\sim1/\kappa$. For the real state the asymptotic value is $u=\kappa$, and so we must call the effective interaction potential $V^{\text{eff}}=-(u^2-\kappa^2)E_0$, which corresponds to measuring the binding energy from the two-particle threshold.

In this case the effective potential contains two terms:

$$V_1^{\text{eff}}=-(u-\kappa)^2E_0,\quad V_2^{\text{eff}}=-2\kappa(u-\kappa)E_0,$$

which have different asymptotic forms in the region (1): $V_1^{\text{eff}}\propto\rho^{-2}$, while V_2^{eff} falls off only as ρ^{-1}. In fact, in this case in region (1) we can legitimately simplify Eq. (8):

$$u-\kappa=\exp(-\rho u)/\rho, \tag{9}$$

the main term of whose solution has the long-range component

$$u=c/\rho+\kappa,$$

where the constant $c=0.5671\ldots$ is the solution of $c=\exp(-c)$.

To be sure, the potential V_2^{eff} has a factor that vanishes in the limit $\kappa\to0$. It is therefore necessary to estimate separately the contribution of this potential to the spectrum of the system. That it can be substantial is clear from simple considerations. Since this potential is Coulomb-like in region (1) with a "Bohr radius" $\tilde a=\alpha^2/c\kappa$ and states with index n bound in this field correspond to average radii $\tilde an^2$, from the requirement that they must be localized within a region $\sim1/\kappa$ it follows that the number of Coulomb-like states is

$$n\approx\sqrt{c/\alpha},$$

which does not depend on κ (of course, we are considering the case $\kappa\ll1$) and can be large when the exchange particle is light.

Now we estimate which of the potentials V_1^{eff} and V_2^{eff} makes the larger contribution. For the analytical dependence we use the estimate of Calogero (see, e.g., Ref. 5) for the number of states in an S wave resulting from some asymptotic region $\rho>\rho_0$ for $\rho_0\gg1$, which is equivalent to turning on an additional repulsive potential in the form of a hard sphere of radius ρ_0 between the heavy particles. On the other hand, we compare these estimates with the quasiclassical calculations of the system spectrum for both V_1^{eff} and V_2^{eff} separately and for the total effective potential, which, as we saw above, yields a spectrum that differs from the actual one (from the Faddeev equations) by a few percent. Thus, the Calogero estimate

$$n_i^c<\frac{2}{\pi}\int_{\rho_0}^{\infty}\sqrt{-2m_{13}V_i^{\text{eff}}}\,d\rho\quad(i=1,2)$$

TABLE II. Contribution to the spectrum of different parts of the effective potential (see text).

$\rho_0\kappa$	0.0	0.1	0.5	1.0	1.5	2.0	2.5	3.0	3.6	3.7
I	1.1	1.0	0.6	0.4	0.30	0.2	0.1	0.1	0.1	0.0
I_1	0.6	0.4	0.2	0.1	0.0	0.0	0.0	0.0	0.0	0.0
I_2	0.9	0.8	0.5	0.4	0.30	0.2	0.1	0.1	0.1	0.0
I_1^c		0.76	0.27	0.12	0.06	0.03	0.02	0.01	0.00	0.00
I_2^c		1.47	0.98	0.67	0.48	0.35	0.25	0.19	0.13	0.12

for the number of bound states n_1^c and n_2^c resulting respectively from the potentials V_1^{eff} and V_2^{eff} leads to the restrictions

$$n_i^c < \frac{1}{\alpha} I_i^c, \quad (i=1,2),$$

in which the quantities I_i^c depend on κ only through the lower limit of integration and are shown in Table II as a function of this limit of integration $\rho_0\kappa$. The actual number of bound states in the table is given by the quantities

$$I=\alpha n, \quad I_1=\alpha n_1, \quad I_2=\alpha n_2.$$

All parameters of the system are the same as in Table I, i.e., $\alpha=0.1$. The repulsive radii in the table have been chosen so as to illustrate the following results. The number of levels resulting from the potential V_2^{eff} is always greater than the number of levels resulting from V_1^{eff}. The Calogero estimates using the asymptotic values of the potentials are not shown in the first column. The range of validity of these estimates starts with the second column, which shows that the Coulomb-like interaction yields twice as many states as does the potential V_1^{eff}. As the repulsive radius increases the contribution of the potential V_2^{eff} dominates and it is what determines the number of levels in the system beginning with the repulsive radii, which are larger than the characteristic size of the light-particle wave function, i.e., for $\rho_0\kappa \geqslant 1$. The last columns show where the levels vanish (for $\alpha=0.1$).

If we estimate the size of a pair consisting of a light and heavy particle from the quantity $\sim 1/\kappa$, which is permissible for $\kappa \ll 1$, then the last level vanishes when the repulsive radius between the heavy particles exceeds the size of a pair by a factor of 3.7. The large size of this quantity gives an estimate of the maximum repulsive radius for a negative molecular ion. We consider a system of the form Li_2^-, with $\alpha \simeq 0.01$ and binding energy in the Li^- subsystem of about 0.6 eV (Ref. 6). Then we find $\kappa \simeq 0.4$ Å^{-1}, and the maximum value of $\kappa\rho_0$ is ~ 6 from the Calogero estimate, yielding a maximum radius $\rho_0 \sim 15$ Å, which is much greater than the interatomic repulsive radii. We can therefore expect that the quasiclassical part of the spectrum (including the higher orbital angular momenta) in actual molecular ions will have a small binding energy in atomic ions.

Note that for a system consisting of a meson and two nucleons, for which $\alpha \simeq 0.5$ holds, the maximum repulsive radius will be approximately 1 Fm.

4. CONCLUSION

This effective potential agrees well with exact calculations even for $\alpha = 0.1$. This allows us to conclude that the region in which the long-range interaction has the form $1/\rho$ is highly extended, coinciding with the region where particles of zero mass are exchanged. Consequently, the most interesting areas of application may be to the physics of two-atom negative ions, the physics of quasimolecular nuclear processes, and the physics of meson-nucleon systems, which constitute special cases of processes with exchange particles of negligible mass.

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[1)] In this work we take the Planck constant to be $\hbar=1$.

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