Potential Theory Calculations by the Quasiparticle Method*

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The quasiparticle method is used to find binding energies, scattering lengths, and cross sections for one particle in a strong Yukawa, Hulthen, or exponential potential. The results are excellent in the lowest approximation.

I. INTRODUCTION

 $\sum_{i=1}^{n}$ HE quasiparticle method¹⁻³ allows any nonrelativistic scattering problem to be solved, in principle, by perturbation theory. The purpose of this article is to determine by actual calculation whether this method gives rapid convergence in practice.

Our test problem is that of finding cross sections, scattering lengths, and binding energies for one particle in a strong short-range potential.⁴ The quasiparticle method is first reviewed in Sec. II, and then applied to the Yukawa potential in Secs. III—VI, and to the Hulthen and exponential potentials in Sec. VII. In most of the cases considered, the ordinary Born approximation either does badly or fails entirely. The "quasi-Born" approximation gives excellent agreement with exact results (to a few percent, and often much better) for reasons discussed in Sec. VIII. A particularly eocouraging calculation is performed in Sec. V, where we knowingly introduce the quasiparticle in a very crude way, but nevertheless find that our error drops from 19% to 5% in going from the first to the second order in the modified potential.

The authors are not skilled in the use of electronic computers, so all integrals were done in closed form in terms of tabulated functions. This has the advantage of providing analytic approximation formulas, but it prevents our being able to say whether the quasiparticle method is more or less convenient than well-established variational or direct-integration techniques. However, our chief purpose here is not to establish another approximation scheme for potential scattering, but rather to encourage use of the quasiparticle method in multiparticle problems (and, we hope, relativistic problems) by showing that it gives a rapidly converging sequence of approximations in the simpler case of potential scattering.

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II. THE QUASI-BORN APPROXIMATIONS

We shall first review the quasiparticle method⁵ and use it to derive approximate formulas for scattering amplitudes and binding energies. The Hamiltonian is taken as

$$
H = -\nabla^2 + V(r). \tag{1}
$$

(We use units with $\hbar=2m=1$.) The potentials $V(r)$ used in actual calculation will be the Yukawa, Hulthén, and exponential potentials, but the general discussion in this section applies to any $V(r)$ which is short range in the sense that

$$
\int_0^\infty |V(r)|^2 r^2 dr < \infty . \tag{2}
$$

We will attack the scattering and bound state problems by calculating the operator $T(W)$, defined by

$$
T(W) = V + VG_0(W)T(W), \qquad (3)
$$

where

$$
G_0(W) \equiv \left[W + \nabla^2\right]^{-1}.\tag{4}
$$

In coordinate space Eq. (3) is an integral equation, with

$$
\langle \mathbf{r}' | G_0(k^2) | \mathbf{r} \rangle = -\frac{\exp[ik|\mathbf{r} - \mathbf{r}'|]}{4\pi |\mathbf{r} - \mathbf{r}'|}, \qquad (5)
$$

$$
\langle \mathbf{r}' | V | \mathbf{r} \rangle = V(r) \delta(\mathbf{r} - \mathbf{r}'). \tag{6}
$$

The scattering amplitude is

$$
f(E,\theta) = -2\pi^2 \langle \mathbf{k}' | T(E+i\epsilon) | \mathbf{k} \rangle
$$

= $-\frac{1}{4\pi} \int d^3r d^3r' \langle \mathbf{r}' | T(E+i\epsilon) | \mathbf{r} \rangle$
× $\exp(i\mathbf{k} \cdot \mathbf{r} - i\mathbf{k}' \cdot \mathbf{r}')$, (7)

where

$$
E = \mathbf{k}^{2} = \mathbf{k}'^{2}
$$

$$
\cos \theta = \hat{k} \cdot \hat{k}',
$$

$$
d\sigma/d\Omega = |f|^{2}.
$$

The bound-state energies are the locations of the poles of $T(W)$ for $W<0$.

Solution of Eq. (3) by iteration gives the Born series

$$
T(W) = V\{1 + K(W) + K^2(W) + \cdots\},\tag{8}
$$

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¹ S. Weinberg, Phys. Rev. 130, 776 (1963).

S. Weinberg, Phys. Rev. 131, 440 (1963).

^s S. Weinberg, Phys. Rev. 133, B232 (1964).

⁴ We will be mostly concerned with attractive potentials, because the Born series for a repulsive interaction can always be made to converge rapidly by merely rearranging its terms. See M. Rotenberg, Ann. Phys. (N. Y.) 21, 579 (1963) and S. Weinber
(to be published).

⁵ Much of the material in this section is to be found in greater detail in Sec. II and Sec. X of Ref. 2.

where $K(W)$ is the scattering kernel

$$
K(W) = G_0(W)V.
$$
 (9)

But this series is useless in the presence of composite particles, because it starts to diverge when any eigenvalue of $K(W)$ leaves the unit circle. In particular, the truncation of the series (8) at any finite order can never yield bound states, because none of its terms have poles in W . Any such approximation is also grossly inaccurate for low energies and low angular momentum, if V is strong enough to have bound states, virtual states, or resonances, because the scattering is then controlled by the pole or the near-pole.

The quasiparticle method rests on the replacement of V by a reduced potential

$$
V_1 \equiv V - V | \Gamma \rangle \langle \bar{\Gamma} | V. \qquad (10)
$$

It is easy to show that

$$
T(W) = T_1(W) + \{1 + T_1(W)G_0(W)\} V | \Gamma \rangle
$$

$$
\times \Delta(W) \langle \overline{\Gamma} | V \{1 + G_0(W)T_1(W)\}, (11) \rangle
$$

where $T_1(W)$ is that $T(W)$ would be if the potential were V_1 :

$$
T_1(W) = V_1 + V_1 G_0(W) T_1(W) \tag{12}
$$

and $\Delta(W)$ is the "propagator"

$$
\Delta(W) = [1 - J(W)]^{-1},
$$

\n
$$
J(W) = \langle \overline{\Gamma} | V G_0(W) V | \Gamma \rangle
$$
\n(13)

$$
+\langle \bar{\Gamma} | V G_0(W) T_1(W) G_0(W) V | \Gamma \rangle. \quad (14)
$$

The reduced T-operator is then calculated from (12) by iteration:

$$
T_1(W) = V_1\{1 + K_1(W) + K_1^2(W) + \cdots\},\qquad(15)
$$

where $K_1(W)$ is the "reduced kernel"

$$
K_1(W) = G_0(W)V_1.
$$
 (16)

If $K(W)$ has at most one eigenvalue outside the unit circle, then $|\Gamma\rangle$ and $\langle\bar{\Gamma}|$ can always be chosen so that the eigenvalues of $K_1(W)$ are all drawn into the unit circle, and therefore so that the series (15) converges. The condition (2) ensures that $K(W)$ can have at most a finite number of eigenvalues outside the unit circle, so (15) can always be made to converge by a finite number of subtractions of the form (10) . [Equation (11) can be interpreted as resulting from the introduction of a fictitious elementary particle,⁶ but this aspect need not concern us here.

If (15) converges, then a bound-state pole can arise only in the propagator $\Delta(W)$, and therefore the binding energy B is to be calculated as the root of

$$
J(-B)=1.\t(17)
$$

and

where

The first "quasi-Born" approximation to $J(W)$ is given

by neglecting T_1 in (14):

$$
J(W) \cong J_{(1)}(W) \equiv \langle \overline{\Gamma} \, | \, V G_0(W) V | \, \Gamma \rangle. \tag{18}
$$

In the second approximation we approximate $T_1 \cong V_1$, so (14) gives

$$
J(W) \cong \langle \overline{\Gamma} | V G_0(W) V | \Gamma \rangle + \langle \overline{\Gamma} | V G_0(W) V_1 G_0(W) V | \Gamma \rangle
$$

= $J_{(1)}(W) - J_{(1)}^2(W) + J_{(2)}(W)$, (19)

where
$$
J_{(2)}(W) \equiv \langle \Gamma | V G_0(W) V G_0(W) V | \Gamma \rangle.
$$

The first quasi-Born approximation to the T -operator (11) is

$$
T(W) \cong T_1(W) + V|\Gamma\rangle \Delta(W)\langle \overline{\Gamma}| V
$$

= $V + V|\Gamma\rangle [J(W)/1 - J(W)]\langle \overline{\Gamma}| V.$ (20)

It only remains to describe how we choose the state vectors $|\Gamma\rangle$ and $\langle \overline{\Gamma} |$. We have considerable freedom here, because the only requirement that must be met is that $K_1(W)$ have no eigenvalues outside the unit circle. But there is one choice that may be called ideal. Let $\eta_1(W)$ be the largest eigenvalue of $K(W)$, and assume that all the other eigenvalues lie within the unit circle. Then choose $|\Gamma\rangle$ and $\langle \bar{\Gamma}|\$ as the energy-dependent normalizable eigenvectors

$$
K(W) |\Gamma\rangle = \eta_1(W) |\Gamma\rangle, \qquad (21)
$$

$$
\langle \bar{\Gamma} | K^{\dagger} (W^*) = \langle \bar{\Gamma} | \eta_1 (W) , \qquad (22)
$$

normalized so that

$$
\langle \bar{\Gamma} | V | \Gamma \rangle = 1. \tag{23}
$$

With this choice, the reduced kernel $K_1(W)$ will have precisely the same eigenvalues as $K(W)$, except that $\eta_1(W)$ is replaced by the eigenvalue zero. If the original Born series diverged (because $|\eta_1| \ge 1$), then this cures the divergence. If it converged then this accelerates the rate of convergence.

We cannot usually hope to find exact solutions to (21) and (22), but this need not worry us. As long as our guess at $\ket{\Gamma}$ and $\bra{\bar{\Gamma}}$ is not too bad, we can still carry our calculations to unlimited accuracy by using more and more terms in (15). In practice, we guess $|\Gamma\rangle$ and $\langle \overline{\Gamma} |$ by requiring that they match the properties of the ideal choice defined by (21) – (23) . These properties can be determined by noting that (21) is just Schrodinger's equation for a fictitious energy eigenvalue W and a fictitious potential $V/\eta_1(W)$. The largest eigenvalue η_1 will usually correspond to an s state, so

$$
\langle \mathbf{r} | \Gamma \rangle = C(k) \Gamma(r, k) / r(4\pi)^{1/2}, \qquad (24)
$$

$$
\langle \bar{\Gamma} | \mathbf{r} \rangle = \bar{C}(k) \Gamma^*(r, -k^*)/r(4\pi)^{1/2}, \qquad (25)
$$

$$
\Gamma(r,k) \propto e^{ikr} \quad (r \to \infty), \tag{26}
$$

$$
\Gamma(r,k) \propto r \qquad (r \to 0) \tag{27}
$$

$$
k \equiv (W)^{1/2}; \quad \text{Im} k > 0. \tag{28}
$$

Note that $-k^*$ also has positive imaginary part, so both (24) and (25) are normalizable wave functions. The

³ Reference 1. In this connection, see also S. Tani, Phys. Rev. 121, 346 (1961).

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normalization condition (23) gives the constants as

where $f^{\text{B}}(W,\theta)$ is the Born term

$$
C(k)\overline{C}(k) = \left[\int_0^\infty \Gamma^*(r, -k^*) \Gamma(r, k) V(r) dr\right]^{-1}.
$$
 (29) $f^B(E, \theta) = -\frac{1}{4\pi} \int d^3r V(r) \exp[i\mathbf{r} \cdot (\mathbf{k} - \mathbf{k}')]$

Once we guess a $\Gamma(r,k)$ satisfying (26) and (27), we can use Eqs. (7), (20), (24), (25), and (29) to calculate the scattering amplitude as

less a
$$
\Gamma(r,k)
$$
 satisfying (26) and (27), we
\n7), (20), (24), (25), and (29) to calculate
\namplitude as
\n
$$
f(E,\theta) = f^{B}(E,\theta) + g(E),
$$
\n(30) and $g(E)$ is an isotropic correction

$$
g(E) = -k^{-2} \frac{J(E+i\epsilon)}{1 - J(E+i\epsilon)} \frac{\left[\int_0^\infty V(r)\Gamma(r,k)\sinkr dr\right] \left[\int_0^\infty V(r)\Gamma^*(r,-k)\sinkr dr\right]}{\left[\int_0^\infty \Gamma^*(r,-k)V(r)\Gamma(r,k)dr\right]}.
$$
\n(32)

Setting $W = E + i\epsilon$ with $\epsilon \to +0$ in (28) shows that k must now be taken as the positive value of $E^{1/2}$.

The scattering length in this "quasi-Born" approximation is

$$
a_s^{\text{QB}} = -f(0,\theta) = a_s^{\text{B}} + b\,,\tag{33}
$$

where a_s ^B is the Born approximation value

$$
a_s^{\mathbf{B}} = \int_0^\infty r^2 V(r) dr \tag{34}
$$

and b is the correction

$$
b = \frac{J(0)}{1 - J(0)} \frac{\int_0^{\infty} V(r) \Gamma(r, 0) r dr}{\int_0^{\infty} V(r) |\Gamma(r, 0)|^2 dr}.
$$
 (35)

The function $J(W)$ which determines the bound state energy and which appears in (32) and (35) is given in the lowest approximation (18) as

$$
J(W) = \frac{C(k)\bar{C}(k)}{4\pi} \int \frac{d^3r d^3r' \Gamma^*(r', -k^*)V(\mathbf{r}')\langle \mathbf{r}'|G_0(W)|\mathbf{r}\rangle V(\mathbf{r})\Gamma(\mathbf{r},k)}{r'r}.
$$

Only the s-wave part of $G_0(W)$ contributes, so this is

$$
J(W) = \frac{i}{2k} \frac{\int_0^\infty \Gamma^*(r', -k^*) V(r') dr' \int_0^\infty \Gamma(r, k) V(r) dr [\exp(ik|r + r'|) - \exp(ik|r - r'|)]}{\int_0^\infty \Gamma^*(r, -k^*) \Gamma(r, k) V(r) dr}.
$$
 (36)

At zero energy it becomes

$$
J(0) = -\frac{\int_0^\infty \Gamma^*(r',0)V(r')dr'\int_0^\infty \Gamma(r,0)V(r)dr\min(r,r')}{\int_0^\infty |\Gamma(r,0)|^2 V(r)dr}.
$$
 (37)

In the bound-state region W is negative, so we must take k in (36) as

$$
k = i\kappa; \quad \kappa = (-W)^{1/2} > 0. \tag{38}
$$

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III. YUKAWA POTENTIAL: BOUND STATES

The next four sections will apply the results of Sec. II to the Yukawa potential

$$
V(r) = -\lambda e^{-r}/r. \tag{39}
$$

We are using units in which the range a of the potential is taken as the unit of length, so that the unit of energy is $\hbar^2/2ma^2$. The vertex function will be chosen as the simplest function satisfying (26) and (27), i.e.,

$$
\Gamma(r,k) = e^{ikr} \left[1 - e^{-r}\right].\tag{40}
$$

[Several advantages of this $\Gamma(r,k)$ are listed in Sec. X of Ref. 2.] With this choice the normalization integral (29) is

$$
[C(k)\bar{C}(k)]^{-1} = \int_0^\infty \Gamma(r,k)\Gamma^*(r,-k^*)V(r) = \lambda \ln\left\{\frac{(1-2ik)(3-2ik)}{(2-2ik)^2}\right\}.
$$
 (41)

The function $J(W)$ is given by (36) as⁷

$$
J(W) = \frac{\frac{i\lambda}{k} \left[\frac{1}{2} \ln^2 \left(\frac{2 - 2ik}{1 - 2ik} \right) + Li_2 \left(\frac{-2}{1 - 2ik} \right) + Li_2 \left(\frac{-1}{2 - 2ik} \right) - Li_2 \left(\frac{-1}{1 - 2ik} \right) \right]}{\ln \left\{ \frac{(1 - 2ik)(3 - 2ik)}{(2 - 2ik)^2} \right\}},
$$
(42)

where $Li₂$ is the dilogarithm

$$
Li_2(-z) \equiv -\int_0^z x^{-1} \ln(1+x) dx.
$$
 (43)

Thus, the coupling constant λ required for a state with binding energy B is given by (17) as

$$
\lambda(\kappa) = \frac{\kappa \ln \left\{ \frac{(1+2\kappa)(3+2\kappa)}{(2+2\kappa)^2} \right\}}{\frac{1}{2} \ln^2 \left(\frac{2+2\kappa}{1+2\kappa} \right) + Li_2 \left(\frac{-2}{1+2\kappa} \right) + Li_2 \left(\frac{-1}{2+2\kappa} \right) - Li_2 \left(\frac{-1}{1+\kappa} \right) - Li_2 \left(\frac{-1}{1+\kappa} \right)},
$$
(44)

where $\kappa = B^{1/2}$. These dilogarithms have been tabulated by Lewin.⁸ The best "exact" numerical results in the literature to compare with (44) seem to be given by the interpolation formula of Blatt and Jackson⁹:

$$
\lambda(\kappa) = 1.683[1.000 + 1.349\kappa - 0.153\kappa^2 + 0.064\kappa^3 + 0.281\kappa^4 \cdots].
$$
 (45)

The comparison is made in Table I. The λ -values differ at most by 3% , and generally by much less. There is no column in Table I for the Born approximation, since it can never yield a bound state.

⁷ This was derived by using the identity

 $\int_{0}^{\infty} r^{-1}\left\{e^{-\sigma r}-e^{-\tau r}\right\}\left\{\mathrm{Ei}\left(-\alpha r\right)-\mathrm{Ei}\left(-\beta r\right)\right\}dr$ $=Li_2(-\tau/\alpha)+Li_2(-\sigma/\beta)-Li_2(-\sigma/\alpha)-Li_2(-\tau/\beta)$ valid for α , β , τ , σ with positive real parts. Here Ei(-z) is the exponential integral

$$
\mathrm{Ei}(-z) = -\int_{z}^{\infty} r^{-1}e^{-r}dr; \quad \mathrm{Re}z > 0.
$$

⁸ L. Lewin, *Dilogarithms and Associated Functions* (Macdonald, London, 1958).

⁹ J. M. Blatt and J. D. Jackson, Phys. Rev. 76, 18 (1949).

A particularly interesting object for comparison is $\lambda(0)$, the coupling required to just barely bind a state with zero energy. The exact result is known¹⁰ to be

$$
\lambda^{\text{EX}}(0) = 1.683.
$$

We find from (44) [or directly from (37)] that

$$
\lambda^{QB}(0) = \frac{\ln 4/3}{\ln 32/27} = 1.693
$$

so the agreement here is to about 0.6%. [This may be

TABLE I. The coupling λ required to give a bound state with binding energy κ^2 . Here "EX" means the Blatt-Jackson "exact" result (45), and "QB" means the quasi-Born approximation (44).

κ	λ EX	λQB
	1.683	1.693
0.2	2.129	2.154
0.4	2.570	2.611
0.6	3.036	3.009

¹⁰ R. G. Sachs and M. Goeppert-Mayer, Phys. Rev. 53, 991 $(1938).$

TABLE II. The coupling λ required to give a scattering length a_s .
Here "EX" means the Blatt-Jackson result (50), "QB" means the
quasi-Born approximation (49), and "B" means the ordinary Born approximation (46).

a_{s}	λ EX	λ ^{QB}	$\lambda^{\mathbf{B}}$
3.0	2.793	2.988	$-.3.0$
5.0	2.220	2.342	-5.0
10.0	1.932	1.977	-10.0
∞	1.683	1.693	∞
-10.0	1.478	1.473	10.0
-5.0	1.300	1.298	5.0

contrasted with an N/D calculation¹¹ using the Born approximation to give the discontinuity in T across the left-hand cut. The lowest order solution of the coupled equations for N and D gives $\lambda(0)=1$, the second-order solution gives $\lambda(0) = \infty$, and the exact solution gives $\lambda(0)=2.80$. A computer solution¹¹ of the coupled N/D equations using second Born approximation for the lefthand cut gives $\lambda(0) = 1.70$.

IV. YUKAWA POTENTIAL: SCATTERING LENGTHS

The Born approximation (34) gives the scattering length here as $\sigma^B(E)=2\pi \int |f^B(E,\theta)|^2 \sin\theta d\theta=$

$$
a_s{}^B = -\lambda. \tag{46}
$$

The quasi-Born approximation (33) gives instead The quasi-Born approximation (52) gives

$$
a_s^{\text{QB}} = -\lambda \left[1 + \frac{J(0)}{4 \ln 4/3 (1 - J(0))} \right]. \tag{47}
$$

We have already noted that

$$
J(0) = \left(\frac{\ln 32/27}{\ln 4/3}\right) \lambda = 0.5906\lambda
$$
 (48)

so (47) becomes

$$
a_s^{\text{QB}} = -\lambda \left\{ \frac{1 - 0.0774\lambda}{1 - 0.5906\lambda} \right\}.
$$
 (49)

Blatt and Jackson⁹ have given an interpolation formula for λ as a function of a_s :

$$
\lambda = 1.683[1.000 + 1.348a_s^{-1} + 1.275a_s^{-2}+ 0.322a_s^{-3} - 3.028a_s^{-4} - 1.326a_s^{-5}],
$$
 (50)

which is expected to be a good approximation for λ near the critical value $\lambda(0)=1.683$, where a zero-energy resonance makes a_s infinite. The comparison between (46), (49), and (50) is made in Table II. We see that the quasi-Born approximation agrees very well with Blatt and Jackson, and that the Born approximation does very badly. For $|\lambda|$ < 1.3 the exact and quasi-Born results will, of course, both approach the Born approximation. For $|a_s| < 3$ the Blatt-Jackson formula can no longer be relied upon.

V. YUKAWA POTENTIAL: CROSS SECTIONS

The Born approximation (31) to the scattering amplitude is

$$
f^{\mathbf{B}}(E,\theta) = \lambda/(1+4k^2\sin^2\theta/2). \tag{51}
$$

The quasi-Born approximation adds a correction term
 $f^{\text{QB}}(E,\theta) = f^{\text{B}}(E,\theta) + g(E)$, (52)

$$
F^{\mathbf{Q}\mathbf{B}}(E,\theta) = f^{\mathbf{B}}(E,\theta) + g(E), \qquad (52)
$$

where $g(E)$ is given by (32) as

$$
g(E) = \frac{-\lambda}{4k^2} \frac{J(E+i\epsilon)}{1 - J(E+i\epsilon)}
$$

$$
\times \frac{\ln^2((1-ik)/(1-2ik))}{\ln([2-2ik]^2/[1-2ik][3-2ik])}
$$
(53)

and $k = (E)^{1/2} > 0$. The quasi-Born result for $J(E+i\epsilon)$ was presented in Sec. III.

It would be tedious to compare (52) with exact results for a large assortment of energies, angles, and couplings. We will instead make the comparison only for the total cross section. The Born approximation gives this as

$$
\sigma^{\mathbf{B}}(E) = 2\pi \int_0^{\pi} |f^{\mathbf{B}}(E,\theta)|^2 \sin\theta d\theta = \frac{4\pi\lambda^2}{1+4k^2}.
$$
 (54)

(47)
$$
\sigma^{QB}(E) = 2\pi \int_0^{\pi} |f^B(E,\theta) + g(E)|^2 \sin\theta d\theta
$$

$$
= \sigma^B(E) + \frac{2\pi\lambda}{k^2} \ln(1+4k^2)
$$

(48)
$$
\times \text{Reg}(E) + 4\pi |g(E)|^2. \quad (55)
$$

The comparison of (55) with exact results will test not only the validity of the quasi-Born approximation for the ^s wave (as was the case in Secs. III and IV) but will also check that the other partial waves are given by the Born approximation alone, as implied by Eq. (52).

The calculation of $\sigma^{QB}(E)$ from (55) is quite messy, but it was not necessary to use a computer. Unfortunately, we have not been able to find exact results in the literature to compare with $\sigma^{QB}(E)$, so we were forced to sum up partial-wave cross sections calculated from s-, p -, and d -wave phase shifts.¹² The comparison of these "exact" cross sections with the quasi-Born approximation (55) and the Born approximation (54) is made in Figs. 1–4, for $\lambda = 0.1, 1, 1.\overline{5}, 2$.

The agreement between exact and quasi-Born cross sections is generally excellent, and always very much better than for the ordinary Born approximation. The exact zero-energy cross sections become infinite at $\lambda = 1.683$, so the comparison is not very meaningful for

n Y.T. Fung (private communication).

¹² These were very kindly provided by C. Schwartz and Y. T. Fung.

FIG. 1. Scattering cross section versus $k = (E)^{1/2}$ for the Yukawa potential V(r) = $\nu r^{-1}e^{-r}$ at a coupling value $\lambda = 0.1$. The curves respectively, exact, lowest order quasi-
"EX", "QB" and "B" are, respectively, exact, lowest order quasi-Born approximation, and lowest order ordinary Born approximation.

 $k \leq 0.5$; the scattering lengths in Table II provide a more illuminating comparison at these low energies.

VI. YUKAWA POTENTIAL: SECOND APPROXIMATION

In order to test the speed of convergence of the series expansion (15) in powers of the reduced kernel, we have performed a second order calculation of the critical coupling $\lambda(0)$ required to just barely give a bound state with zero energy. This is, of course, a quantity that cannot be calculated by any ordinary Born approximation. We will calculate it as the root of

$$
J(0)=1
$$
, (56) in the sense of Eq. (21), i.e.,

where $J(W)$ is given in the second quasi-Born approximation by (19).

The integrals required to calculate $J_{(2)}(0)$ are difficult to do in closed form, though presumably straightforward for a computer. To lighten our labor we will not use the vertex function (40) employed until now, but will instead take¹³

$$
\Gamma(r,k) = e^{ikr}r
$$

or since we are at zero energy

$$
\Gamma(r,0) = r. \tag{57}
$$

This behaves correctly at $r=0$, but not at $r=\infty$. Since (57) is far from ideal, the work of this section will serve to test a statement made in Ref. 2, that even a poor vertex function can give very good results if calculations are carried to sufhcient order in the reduced kernel.

The first quasi-Born approximation (37) now gives

$$
J_{(1)}(0) = \lambda/2 \tag{58}
$$

so that the critical coupling in this order is $\lambda(0)=2$, about 19% too high.

The function $J_{(2)}(0)$ appearing in (19) is

$$
J_{(2)}(0) = \frac{\int d^3r d^3r' d^3r'' \frac{\Gamma^*(r,0) V(r) V(r'') V(r') \Gamma(r',0)}{r |r-r'| |r'-r'|r'}}{(4\pi)^3 \int_0^\infty V(r) |\Gamma(r,0)|^2 dr}
$$

A straightforward calculation using (57) gives here

$$
J_{(2)}(0) = \lambda^2 \ln\frac{4}{3} = 0.2877\lambda^2. \tag{59}
$$

Therefore, $J(0)$ is given by the second-order formula (19) as $J(0) = \frac{1}{2}\lambda + 0.0377\lambda^2$. (60)

$$
J(0) = \frac{1}{2}\lambda + 0.0377\lambda^2. \tag{60}
$$

The convergence is obviously quite rapid in the neighborhood of $\lambda = 2$. The critical value $\lambda(0)$ defined by (56) ls now

$$
\lambda(0) = 1.765\tag{61}
$$

as compared with the exact value¹⁰ λ (0)= 1.683 and the first-order value 2.000. The error is reduced from 19% to 5% in going to second order.

VII. OTHER POTENTIALS

The s-wave vertex function we have been using

$$
\Gamma(r,k) = e^{ikr}(1 - e^{-r})\tag{40}
$$

happens to be the ideal choice for the Hulthen potential

$$
V(r) = -\lambda \left[e^r - 1 \right]^{-1} \tag{62}
$$

$$
\begin{aligned} \left[(-d^2/dr^2) + V(r)/\eta_1(W) - W\right] \Gamma(r,k) &= 0\\ \eta_1(W) &= \lambda/(1-2ik) \, ; \quad k = (W)^{1/2}. \end{aligned} \tag{63}
$$

The reduced kernel $K_1(W)$ will have an eigenvalue zero in place of $\eta_1(W)$, so we can expect the series (15) to converge quite rapidly. In particular, the function $J(W)$ is given in the lowest order $[Eq. (18)]$ by

$$
J(W) = \eta_1(W) = \lambda / (1 - 2ik)
$$
 (64)

FIG. 2. Same as Fig. 1, with $\lambda = 1.0$.

 13 This choice was made in Sec. X of Ref. 2, and the calculation was carried there as far as the first approximation (58). [This $\Gamma(r,k)$ happens to be ideal for the Coulomb potential.]

and all higher order terms vanish. Therefore, the binding energy is given by (17) as

$$
B = -k^2 = \left[(\lambda - 1)/2 \right]^2 \quad (\lambda > 1). \tag{65}
$$

This is the exact answer for B .

It is more useful here to compare solutions of the scattering problem. The scattering length in the Born approximation (34) is

$$
a_s^{\ \mathrm{B}} = -2\lambda \sum_{\nu=1}^{\infty} \frac{1}{\nu^3} = -2\lambda \zeta(3) \,, \tag{66}
$$

where ζ is the Riemann zeta function, $\zeta(3)$ = 1.202. The quasi-Born approximation (33) is ⁰

$$
a_s^{\text{QB}} = -2\lambda \{\zeta(3) + (\lambda/1 - \lambda)\}.
$$
 (67)

$$
a_s^{EX} = -2\lambda \sum_{\nu=1}^{\infty} (\nu^3 - \nu \lambda)^{-1}
$$

=
$$
a_s^{QB} - 2\lambda^2 \left\{ \frac{1}{8(4-\lambda)} + \frac{1}{27(9-\lambda)} + \cdots \right\}.
$$
 (68)

For instance, at the critical value $\lambda=1$ the Born approximation gives $a_s^B = -2.4$, while a_s^{QB} and a_s^{BX} go to infinity, their difference being 3.5% of a_n ^B. The approximation (67) becomes poor when λ approaches 4, where a second bound state appears.

For the record, we will give some results for the exponential potential

$$
V(r) = -\lambda e^{-r}.
$$
 (69)

Using the vertex function (40), we find now that the lowest quasi-Born approximation (37) gives

$$
J(0) = \frac{11}{16}\lambda, \qquad (70)
$$

FIG. 3. Same as Fig. 1, with $\lambda = 1.5$. Observe that σ^{QB} and σ^{BX} become very large at low energies, in response to a virtual state which becomes bound at $\lambda = 1.68$. This virtual state is not detected by σ^{B} .

¹⁴ R. Jost and A. Pais, Phys. Rev. 82, 840 (1951). The scattering length can be derived with a little work from their Eq. (36), p. 845, or from, Eqs. (98) and (118) of Ref. 2.

FIG. 4. Same as Fig. 1, with $\lambda = 2.0$. Here σ^{QB} and σ^{EX} are very These results may be contrasted with the exact value¹⁴ large at low energy in response to a shallow bound state at $E \cong -0.04$. Again, σ^B is not affected.

so that the critical λ for a bound state at zero energy is $\lambda(0) = 16/11 = 1.455$, which is 0.6% higher than the exact value¹⁵ λ (0)=1.446. The scattering lengths (34) and (33) turn out to be

$$
a_s{}^{\mathbf{B}} = -2\lambda\,,\tag{71}
$$

$$
a_s^{\text{QB}} = -2\lambda \{ (1 - 0.11\lambda) / (1 - 0.69\lambda) \}.
$$
 (72)

VIII. DISCUSSION

We must confess to some surprise that our lowest order approximation works so well. To understand the reason, it is necessary to consider the bound-state and scattering problems separately. The former is exactly solved by the lowest quasi-Born approximation if the vertex $| \Gamma \rangle$ happens to be an eigenfunction of the kerne $K(W)$, as it was for the Hulthen potential in Sec. VII. Hence, our success in calculating binding energies and the critical coupling $\lambda(0)$ for the Yukawa and exponential potentials might perhaps mean only that the vertex function $e^{ikr}[1-e^{-r}]$, which is an exact eigenfunction of the Hulthén kernel, is also close to ideal for any potential of unit range.

But this does not explain why the scattering calculation also turns out so well. Suppose we are able to find an ideal vertex function, as was the case in Sec. VIII. The reduced kernel $K_1(W)$ is then not zero, but still has all its original eigenvalues, except the largest. The magnitude of the second largest eigenvalue $\eta_2(W)$ will therefore govern the rate of convergence of the expansion (15) in powers of $K_1(W)$. The correction to the lowest quasi-Born approximation (20) will be much less than indicated by $|\eta_2(W)|$, because the Born term accounts to some extent for all the $\eta_{\nu}(W)$. [However, the only case for which the lowest quasi-Born approximation gives the scattering amplitude exactly is for a separable potential, in which case $K(W)$ has only one nonzero eigenvalue.)

¹⁵ T-Y. Wu and T. Ohmura, *Quantum Theory of Scatterin* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962), p. 80.

So we can therefore account for the success of the lowest quasi-Born approximation in scattering problems, provided that the second largest eigenvalue $\eta_2(E+i\epsilon)$ of the scattering kernel $K(W)$ is appreciably less than unity in absolute value. And conversely, the approximation must obviously be poor if $|\eta_2(E+i\epsilon)|$ approaches 1, since this is the condition for a second bound or nearly bound state. In this paper we have been interested in scattering for which the largest eigenvalue $\eta_1(E+i\epsilon)$ never gets very far outside the unit circle; hence we can understand our success if the eigenvalues $\eta_1(W)$ and $\eta_2(W)$ are not too close in magnitude.

How tightly packed are the $\eta_{\nu}(W)$? For the Hulthen potential the question can be answered exactly; in this case the ν th eigenvalue has the magnitude¹⁶

$$
|\eta_{\nu}(E+i\epsilon)| = \frac{|\lambda|}{\nu \lceil \nu^2 + 4E \rceil^{1/2}}.
$$
 (73)

Hence, $|\,\eta_2| / |\,\eta_1|$ is $\frac{1}{4}$ in the interesting case $E\!\!\ll\!\!1$ where the eigenvalues are largest, and $|\eta_2|/|\eta_1| \leq \frac{1}{2}$ at all energies. The rôle of $\eta_2(W)$ and higher eigenvalues can be seen very clearly from Eq. (68), which gives the exact scattering length for the Hulthen potential. For $\lambda \approx 1$ the percentage error in the quasi-Born approximation (67) drops to zero, since the scattering length is dominated by the shallow bound or virtual state, which is accounted for exactly by the ideal vertex (40). The difference between a_s^{EX} and a_s^{QB} remains roughly constant, being given in (68) by a sum of terms arising respectively from η_2 , η_3 , ... (When $\lambda \approx 4$ a second bound state appears and this difference becomes large.) The Born approximation (66) accounts approximately for the

contributions from all eigenvalues η_{ν} , so the success of the quasi-Born approximation should not have surprised us.

For the Yukawa potential it is known" that a second s-wave bound state appears at $\lambda \approx 5$. (The first p-wave state does not appear until $\lambda \approx 9$.) Hence at zero energy $|\eta_2/\eta_1| \approx 1.7/5 \approx 1/3$. As above, the Born term will partially account for η_2 , η_3 , etc., so when $|\eta_1| \approx 1$ (i.e., $\lambda \approx 2$) we should expect the error in the lowest quasi-Born approximation to be quite small.

In general, it is reasonable to guess that the $\eta_{\nu}(W)$ will decrease rapidly with ν for any short-range potential, because they satisfy a sum rule.¹⁸ tential, because they satisfy a sum rule.

$$
\sum_{\nu} \eta_{\nu}(W) = -k^{-1} \int_0^{\infty} V(r) e^{ikr} \sin kr dr , \qquad (74)
$$

the sum running over s-wave eigenvalues only. A purely attractive or repulsive potential will have all $\eta_{\nu}(0)$ of the same sign, so the convergence of the sum implies that they must vanish rather rapidly for $\nu \rightarrow \infty$.

In summary, we can say that the quasi-Born approximation works very well in scattering problems because ordinary potentials are effectively about 70% separable at low energies, and because the Born term accounts very well for the small higher $n_v(W)$, and, of course, dominates at high energy.

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¹⁶ Reference 2, Eq. (118).

¹⁷ Y. T. Fung (private communication). ¹⁸ Reference 2, Eq. (96).