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# Nonperturbative corrections to bound states of the quasipotential equation by Padé approximants

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A nonperturbative approach to the relativistic bound-state problem is tested in a simplified version of quantum electrodynamics. The approach used is based on applying Padé approximants to a perturbation series of quasipotentials derived from an inhomogeneous quasipotential equation. The resultant nonperturbative form of the quasipotential is used in solving the homogeneous quasipotential equation (relativistic Schrödinger equation). The size of the nonperturbative results of the Lamb shift is compared with that of the perturbative results. As with real quantum electrodynamics for point particles, this simplified model we use to test our approach gives complex energies if the coupling constant is larger than some critical value. The change of this critical value of the coupling constant which results from using a nonperturbative form of the potential is computed.

## I. INTRODUCTION

Todorov has recently proposed a new local version of the quasipotential equation for the relativistic bound-state problem.[1] The quasipotential equation, unlike the Bethe-Salpeter equation, is a three-dimensional one-time formulation of the two-body problem. Although the equation is relativistically invariant, Todorov's particular one-time formulation of the problem leads to a bound-state equation similar to the Schrödinger equation. This feature, together with its locality, is a very desirable aspect since it permits simple numerical techniques for solutions of the eigenvalue problem. If the Born term in quantum electrodynamics is considered, then exact solutions are obtained which are accounted for in a much more complicated way in other approaches.[1] In addition, in the static limit, this approach yields equations that are the conventional one-body bound-state equations for spin-0 or spin-$\frac{1}{2}$ particles in a Coulomb field, namely the Klein-Gordon and Dirac equations. It yields predictions for the $\alpha^4$ fine-structure splittings for the two-body problem in a much simpler way than the more conventional approaches.[1] Krapchev, Rizov, and Todorov[2] have recently computed the $\alpha^5 \ln\alpha$ corrections due to radiative effects in the case of scalar electrodynamics with vector photons with this approach for arbitrary particle masses $m_1$ and $m_2$.

In this paper we examine the quasipotential approach to quantum electrodynamics for the case where the coupling constant is not small. Thus, in this approach, we wish to examine the size of the Lamb shift for large $Z$ or, equivalently, bound-state energies for strongly coupled QED. This necessitates a nonperturbative approach to the bound-state problem. Here we consider a simplified version of QED with scalar photons instead of vector photons. We also consider only the static limit in which one of the particles becomes infinitely massive.

In Sec. II a review is given of the quasipotential equation for scalar particles. We follow very closely the discussion given by Todorov in Ref. 1. The relativistic Balmer formula derived there, and also given in this paper, has two shortcomings when the coupling is not weak. First, it includes only the effects of the lowest-order diagram. Second, it leads to complex energies if the coupling strength $\alpha$ is large enough. This latter aspect is related to the problem of singular potentials. One might speculate that by incorporating higher-order corrections in a nonperturbative way, he might not only adjust the first shortcoming but might also modify to some extent the problem of the singular potential, which seems to be a common problem of many relativistic bound-state equations.

Any nonperturbative approach must agree in the limit of small coupling with the perturbative results. In Sec. III the higher-order corrections are considered perturbatively. In the process, it is found that the local feature of the quasipotential cannot be maintained. In order to avoid the infrared problem, the quasipotential is modified by accounting for the fact that the bound particle is off its mass shell. Within the context of this quasipotential approach, which is an on-energy-shell equation, this leads to a nonlocal contribution to the potential. As it turns out, this

nonlocal formulation leads to a comparatively simple determination of the ground-state energy.

In Sec. IV Padé approximants[3] are used to calculate the ground state of scalar hydrogen nonperturbatively. The quantity that is computed nonperturbatively is the quasipotential. As the Padé approximants are derived from a perturbation series, the nonperturbative form of the quasipotential necessarily reduces to the perturbative form in the limit of small coupling. By applying dispersion techniques to the approximation, one obtains a form of the quasipotential equation that has the same structure as the perturbative form of the equation. Although the perturbative results can be computed exactly, numerical techniques are needed to compute the nonperturbative results.

In a problem such as the one presented in this paper, the primary aim of numerical calculations is not to obtain agreement between theory and experiment. Strongly coupled real QED deals with spin-$\frac{1}{2}$ particles and massless vector gluons rather than scalar particles and massless scalar gluons. Also, a realistic calculation of large-$Z$ Lamb shifts should take into account finite nuclear size. Nevertheless, numerical calculations have a theoretical importance. There are two basic questions that must be and can only be answered by numerical calculations.

For $\alpha<1$, the size of the nonperturbative values of the Lamb shift must be compared with the perturbative values. Are the differences large or small, and for what value of $\alpha$ does the difference become significant? Second, only a numerical calculation will determine whether or not the value of $\alpha$ at which complex energies appear is altered when one sums up the perturbation series of potentials into a nonperturbative form. If it is, is it displaced upward or downward from $\alpha=1$ and by how much? The results of the calculation and the techniques used are discussed in Sec. V.

## II. QUASIPOTENTIAL EQUATION FOR SCALAR PARTICLES

### A. Off-shell kinematics and covariant form of the quasipotential equation

The quasipotential equation is a relativistic Lippmann-Schwinger type equation for the invariant scattering amplitude $T$

$$T+V+VGT=0\ . \tag{2.1}$$

In this paper $T$ will refer to the elastic scattering of two spinless particles of masses $m_1$ and $m_2$ with initial (final) momenta $p_1$ and $p_2$ ($q_1$ and $q_2$). Its relation to the $S$ matrix is given by

$$\begin{aligned}\langle q_1q_2|S|p_1p_2\rangle &= (2\pi)^6 4p_1^0p_2^0\delta(\vec{q}_1-\vec{p}_1)\delta(\vec{q}_2-\vec{p}_2)\\ &\quad+(2\pi)^4 i\delta(q_1+q_2-p_1-p_2)\\ &\quad\times T(q_1q_2;p_1p_2)\ .\end{aligned} \tag{2.2}$$

Rather than regard (2.1) as an off-energy-shell equation, as is usually done, we define it as an off-mass-shell (on-energy-shell) equation. One proceeds off the mass shell in such a way that the 4-momenta squared always satisfy the relation

$$q_1^2-q_2^2=p_1^2-p_2^2=-(m_1^2-m_2^2)\ . \tag{2.3}$$

The total 4-momentum is the timelike vector

$$P=q_1+q_2=p_1+p_2,\quad P^2=-w^2<0\ . \tag{2.4}$$

The center-of-mass energies $E_1$ and $E_2$ of particles 1 and 2 are defined in the invariant way

$$\begin{aligned}E_1&=-\frac{1}{w}P\cdot q_1=-\frac{1}{w}P\cdot p_1=\frac{w^2+m_1^2-m_2^2}{2w}\ ,\\ E_2&=-\frac{1}{w}P\cdot q_2=-\frac{1}{w}P\cdot p_2=\frac{w^2+m_2^2-m_1^2}{2w}\ ,\end{aligned} \tag{2.5}$$

with their sum given by the center-of-mass energy $w$. The relative 4-momenta $q$ and $p$ are two spacelike vectors defined by

$$q=\frac{E_2}{w}q_1-\frac{E_1}{w}q_2,\quad p=\frac{E_2}{w}p_1-\frac{E_1}{w}P_2\ , \tag{2.6}$$

and are orthogonal to $P$: $P\cdot q=P\cdot p=0$. In the nonrelativistic limit, when $w\to m_1+m_2$, we have

$$\frac{1}{w}E_i=\frac{m_i}{m_1+m_2}\ ,\quad i=1,2 \tag{2.7}$$

so that $q$ and $p$ go into the conventional nonrelativistic relative momenta.

The quasipotential equation, unlike the Bethe-Salpeter equation, is a three-dimensional one-time formulation of the two-body problem. Rather than ascribe an individual time variable to each particle, a single spacelike surface defined to be perpendicular to the total four-momentum $P$ acts as the time variable in the problem. Furthermore, it follows from the orthogonality of the relative momenta $p$ and $q$ to the total momentum $P$ that the relative time variable vanishes in the center-of-mass frame.[4] As a consequence, the troublesome concept of relative time plays no role in this approach.

Todorov postulates the equation

$$T_P(q,p)+V_P(q,p)+\int\frac{d^4k}{(2\pi)^3}V_P(q,k)G_P(k)T_P(k,p)\delta(P\cdot k)=0\ . \tag{2.8}$$

In the center-of-mass frame, where

$$P=(w,\vec{0}),\quad q=(0,\vec{q}),\quad p=(0,\vec{p}),\tag{2.9}$$

the time components of all relative four-momenta (including the intermediate variable $k$) vanish. In this frame, the covariant quasipotential equation takes on the three-dimensional form

$$T_w(\vec{q},\vec{p})+V_w(\vec{q},\vec{p})+\int\frac{d^3k}{(2\pi)^3}V_w(\vec{q},\vec{k})G_w(\vec{k})T_w(\vec{k},\vec{p})=0\ ,\tag{2.10}$$

where $G_w(\vec{k})=G_P(k)/w$.

### B. Definition of the quasipotential and Green's function: The homogeneous quasipotential equation

The quasipotential equation is identical in form to the Lippmann-Schwinger equation of nonrelativistic quantum mechanics. In nonrelativistic quantum mechanics, this equation (on energy shell) allows one to construct the scattering amplitude $T$ from the potential $V$. In quantum field theory, it is not the potential that is given but rather the perturbative expansion of $T$. The link between $T$ and the quasipotential $V$ is made by imposing the following assumption.

(i) Equation (2.10) is satisfied order by order by the Feynman perturbative expansion of $T$.

In particular, with $G$ assumed to be independent of the coupling constants and $T=T_1+T_2+\cdots$, the quasipotential $V$ has the perturbative expansion $V=V_1+V_2+\cdots$, with

$$V_1=-T_1,\quad V_2=-T_2+T_1GT_1\ .\tag{2.11}$$

The second and third assumptions fix the Green's function $G$ uniquely.

(ii) For a Hermitian potential Eq. (2.10) should imply the on-shell elastic unitarity condition.

(iii) For spinless particles, $(G_w(\vec{k}))^{-1}$ is a linear function of $k^2$. These lead to[1]

$$G_w(\vec{k})=\frac{1}{2w}(k^2-b^2-i\epsilon)^{-1}\ ,\tag{2.12}$$

where

$$b^2(w)=\frac{1}{4w^2}[w^4-2(m_1^2+m_2^2)w^2+(m_1^2-m_2^2)^2]\tag{2.13}$$

is the on-shell value of the center-of-mass momentum squared of each of the two particles.

The Green's function $G$ has the same form as that which occurs in the nonrelativistic Lipmann-Schwinger equation. By making appropriate assumptions regarding the factorization of the residue of the pole of $T$ at the bound states, Todorov shows how one can obtain a relativistic form of the Schrödinger equation from (2.10):

$$2w(q^2-b^2(w))\psi_w(\vec{q})+\int\frac{d^3k}{(2\pi)^3}V_w(\vec{q},\vec{k})\psi_w(\vec{k})=0\ .\tag{2.14}$$

If the quasipotential $V_w$ is local $[V_w=V_w(\vec{q}-\vec{k})]$, then (2.14) is equivalent to a local Schrödinger equation (homogeneous quasipotential equation) in coordinate space:

$$\left(-\frac{\nabla^2}{2m_w}+v_w(\vec{r})\right)\psi_w(\vec{r})=\frac{b^2}{2m_w}\psi_w(\vec{r})\ ,\tag{2.15}$$

where $m_w$ is the relativistic reduced mass

$$m_w=\frac{m_1m_2}{w}$$

and (2.16)

$$v_w(\vec{r})=\frac{1}{(2\pi)^3}\int d^3k\,\frac{e^{i\vec{k}\cdot\vec{r}}V_w(\vec{k})}{4m_1m_2}\ .$$

Notice that for weak binding $m_w\to m_1m_2/(m_1+m_2)$, the nonrelativistic reduced mass.

## III. SCALAR ELECTRODYNAMICS WITH SCALAR PHOTONS

### A. The relativistic Balmer formula

The model we wish to examine is a simplified version of quantum electrodynamics consisting of two charged (complex) scalar fields $\psi_1$ and $\psi_2$ of masses $m_1$ and $m_2$ interacting by way of a neutral scalar photon field $A$. The Lagrange function describing the interaction is patterned after real electrodynamics and has the normal-ordered form

$$\mathcal{L}_I(x)=[g_1:\psi_1^*(x)\psi_1(x):+g_2:\psi_2^*(x)\psi_2(x):]A(x)\ .\tag{3.1}$$

As $V_1=-T_1$, the lowest-order approximation for the potential is

$$V=V_1=-g_1g_2/(\vec{q}-\vec{p})^2\ .\tag{3.2}$$

The coupling constants $g_1$ and $g_2$ have the dimensions of mass. In order to emphasize the similarity between this model and quantum electrodynamics, we introduce a dimensionless quantity $\alpha$ by setting

$$g_1g_2=16\pi m_1m_2Z_1Z_2\alpha\equiv16\pi m_1m_2\alpha_Z\ .\tag{3.3}$$

This leads to a relativistic Schrödinger equation of the form

$$\left(\frac{-\nabla^2}{2m_w}-\frac{\alpha_Z}{r}\right)\psi_w(\vec{r})=\frac{b^2}{2m_w}\psi_w(\vec{r})\ .\tag{3.4}$$

In the rest of this paper we take $Z_1=Z_2=1$ and $\alpha_Z$

$\equiv \alpha$.[5] As has been pointed out by Todorov,[1] the energy dependence of $m_w$ along with the $w$ dependence of $b^2$, (2.13), take proper care of relativistic recoil effects, which in other approaches are accounted for in a much more complicated way. In particular, (3.4) can be solved exactly giving the O(4)-symmetric result

$$w^2 = m_1^2 + m_2^2 + 2m_1 m_2 (1 - \alpha^2/n^2)^{1/2} . \tag{3.5}$$

In the limit of small coupling, the binding energy is

$$\begin{aligned}(m_1 + m_2) - w &= m_1 + m_2 \left[1 - \left(1 - 2\,\frac{m_1 m_2}{(m_1 + m_2)^2}\,(1 - (1 - \alpha^2/n^2)^{1/2})\right)^{1/2}\right] \\ &= \frac{m_1 m_2}{m_1 + m_2}\,\frac{\alpha^2}{2n^2} \\ &= \frac{m_R \alpha^2}{2n^2} .\end{aligned} \tag{3.6}$$

This, of course, is the usual nonrelativistic Balmer formula.

Let us consider the ground state $n = 1$. If the coupling is strong enough so that $\alpha > 1$, then the energy becomes complex. Such occurrences of complex energies for large enough couplings arise in the solution of other relativistic bound-state equations, the Dirac equation being a prime example. Case[6] has demonstrated that this is an indication that the Coulomb potential for the Dirac equation is a singular potential[7] for large enough coupling. In the Dirac equation, the radial wave function has an essential singularity at the origin if $\alpha$ is large enough. By more careful handling of this singularity in $\alpha$, Case demonstrates that one may in fact obtain a real spectrum for larger $\alpha$, but the resulting spectrum depends on an undetermined constant. He interprets this constant as a cutoff parameter to be determined by using a more realistic potential that does not display such singular behavior.

The present example is similar to the Dirac case in that complex energies appear if $\alpha$ is large enough. In order to see how it is different, we simplify matters by considering the case $m_1 \to \infty$ and $n = 1$. In this case, the binding energy is

$$m - \mathcal{E} = m(1 - (1 - \alpha^2)^{1/2}), \quad m = m_2 \tag{3.7}$$

where $\mathcal{E}$ is the total energy of the bound particle. The corresponding Schrödinger equation is

$$\left(\frac{-\nabla^2}{2m} - \frac{\alpha}{r}\right)\psi(\vec{r}) = \frac{b^2}{2m}\,\psi(\vec{r}), \quad b^2 = \mathcal{E}^2 - m^2 . \tag{3.8}$$

The ground-state wave function and solution are

$$\psi(\vec{r}) = \frac{e^{-r/a}}{(\pi a^3)^{1/2}}, \quad a = \frac{1}{m\alpha}, \quad \frac{b^2}{2m} = -\frac{m\alpha^2}{2} \tag{3.9}$$

and does not display an essential singularity for large coupling as does the Dirac case. In other words, viewed as an eigenvalue equation with the eigenvalue $b^2/2m$, real eigenvalues are obtained for all $\alpha$. However, real energies are found only for a restricted range of $\alpha$ if $\mathcal{E}^2 = m^2 + b^2$ is to remain positive.

In spite of these differences, it is probable that if the $\alpha$ singularity can be eliminated (or shifted to larger values of $\alpha$) in this simplified problem, then a similar solution can be found in the more realistic theories that involve spin and vector photons.

### B. Higher-order corrections: The case of scalar hydrogen

The bound-state energy formula given in Eq. (3.5) gives complex energies for $\alpha > 1$ if $n = 1$. Even for $\alpha$ smaller than 1, however, (3.5) is not correct, as the radiative corrections have not been accounted for. One might speculate that by incorporating these higher-order corrections in a nonperturbative way into the quasipotential (thereby using a more realistic potential) we can obtain a formula for the Lamb shift for $\alpha \leq 1$ and extend the range of $\alpha$ for which real bound-state energies are obtained.

The nonperturbative technique to be employed is the Padé approximant.[3] The Padé approximant uses the perturbative expansion, however, and therefore a series expansion of $V$ must first be found. The expansion we shall use for $V$ is

$$V = V_1 + V_2 = -T_1 - T_2 + T_1 G T_1 . \tag{3.10}$$

The Born term is $T_1$. The sum of vacuum-polarization, vertex with self-energy corrections, box,

and cross-box diagrams comprises $T_2$, and $T_1GT_1$ is the iterated Born diagram. In this paper we examine scalar hydrogen, that is, the one-body problem. In Appendix A it is shown that in the static limit $m_1 \to \infty$ the iterated Born diagram cancels the sum of the box and cross box contributions.[8] The diagrams are given in Figs. 1–5. The only diagrams that contribute are written in subtracted dispersion form in the momentum transfer $t$. The various subtractions are used to account for charge, mass, and wave-function renormalization:

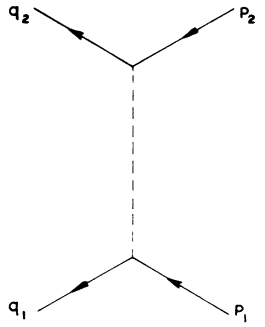

FIG. 1. Born diagram.

$$V = \frac{16\pi m^2\alpha}{t - i\epsilon} - 16m^4\alpha^2 \int_{4m^2}^{\infty} dt' \left(\frac{t' - 4m^2}{t'}\right)^{1/2} \frac{1}{t'^2} \frac{1}{t' - t - i\epsilon}$$

$$+ 32m^4\alpha^2 \int_{4m^2}^{\infty} dt' \frac{1}{t'(t'^2 - 4m_\Delta{}^2 t')^{1/2}} \ln\left[\frac{(t' - 4m_\Delta{}^2)^{1/2} + (t' - 4m^2)^{1/2}}{(t' - 4m_\Delta{}^2)^{1/2} - (t' - 4m^2)^{1/2}}\right] \frac{1}{t' - t - i\epsilon} \quad . \tag{3.11}$$

The first term of the quasipotential is the Born diagram. The next term refers to the subtracted vacuum polarization diagram and the third term is the subtracted vertex diagram. This quasipotential has been modified to apply to the bound-state problem. In particular, the infrared divergence has been avoided in the last integral (the vertex) by accounting for the fact that the bound particle is off its mass shell:

$$-p^2 = (p^0)^2 - \vec{p}^2 = \mathcal{E}^2 - \vec{p}^2 = m_\Delta{}^2 < m^2 \ . \tag{3.12}$$

This same method of dealing with infrared divergences is used in Ref. 2. This technique for avoiding the infrared divergence is similar to the one used by Erickson and Yennie,[9] but, as we shall see, is simpler to implement.

### C. Nonlocal potentials and the infrared problem for bound states

In many cases the quasipotential is local. However, this local feature cannot be maintained, as it depends on the potential's being a function of $(\vec{p} - \vec{q})^2$. In particular, in order to avoid infrared divergences one accounts for the binding of the particle by taking it off its mass shell (on energy shell). In the case of the vertex, this leads to a $\vec{p}^2$ and $\vec{q}^2$ dependence in the last term of the quasipotential (3.11). The self-energy term is, of course, local and is written as a weighted sum of Yukawa potentials. The vertex form appears in the quasipotential as the integral

$$\int \frac{d^3q}{(2\pi)^3} \frac{V(\vec{p} - \vec{q}, m_\Delta{}^2)}{4m^2} \bar{\psi}(\vec{q}) \ . \tag{3.13}$$

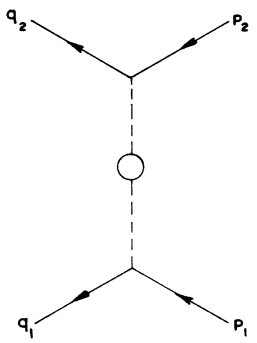

FIG. 2. Vacuum polarization.

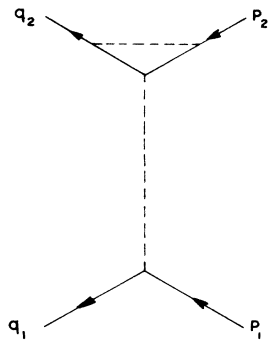

FIG. 3. Vertex (off mass shell, on energy shell).

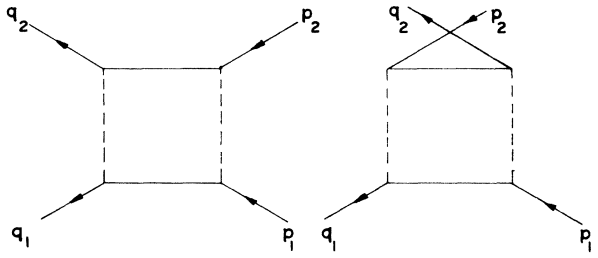


FIG. 4. Box and cross-box diagrams.

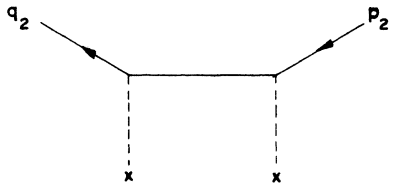


FIG. 5. Iterated Born diagram. This cancels the contribution to $V^{(2)}$ of the diagrams in Fig. 4 in the static limit ($m_1 \to \infty$).

If this is transformed to $\vec{r}$ space, then one obtains the form

$$\int d^3r' \mathcal{U}(\vec{r}, \vec{r}')\psi(\vec{r}') , \tag{3.14}$$

where $\mathcal{U}$ is the double Fourier transform of $V$ in the variables $\vec{p}$ and $\vec{q}$. A particularly simple form can be found for $\mathcal{U}(\vec{r}, \vec{r}')$ by writing the spectral function in the vertex integral as a spectral integral over the variable $m_\Delta^2$. That is,

$$\int_{4m^2}^{\infty} \frac{dt'}{t'} \ln\left[\frac{(t'-4m_\Delta^2)^{1/2}+(t'-4m^2)^{1/2}}{(t'-4m_\Delta^2)^{1/2}-(t'-4m^2)^{1/2}}\right] \frac{1}{(t'^2-4m_\Delta^2 t')^{1/2}} \frac{1}{t'-t-i\epsilon}$$
$$= \int_{4m^2}^{\infty} \frac{dt'}{t'} \frac{1}{t'-t-i\epsilon} \int_{4m^2}^{\infty} \frac{dv'}{v'-4m_\Delta^2-i\eta} \rho(t', v') , \tag{3.15}$$

where $\rho(t', v')$ is the double-spectral function in the momentum transfer and the particle mass:

$$\rho(t', v') = \frac{\theta(t'-v')}{t'^{1/2}(t'-v')^{1/2}} . \tag{3.16}$$

Using this and

$$v' - 4m_\Delta^2 = v' - 4m^2 + 4\vec{p}^2 + 4\mathfrak{b}^2 \quad (\mathfrak{b}^2 = -b^2) , \tag{3.17}$$

one obtains the following integro-differential quasipotential equation:

$$\left[\frac{-\nabla^2}{2m} - \frac{\alpha}{r} + \mathcal{U}(r)\right]\psi(\vec{r}) + \int d^3r' \mathcal{U}_v(\vec{r}, \vec{r}')\psi(\vec{r}') = \frac{b^2}{2m}\psi(\vec{r}) , \tag{3.18}$$

where

$$\mathcal{U}(r) = -\frac{2m^2\alpha^2}{\pi} \int_{4m^2}^{\infty} dt' \left(\frac{t'-4m^2}{t'}\right)^{1/2} \frac{1}{t'^2} \frac{e^{-r\sqrt{t'}}}{r} \tag{3.19}$$

and $\mathcal{U}_v$ has the symmetric form

$$\mathcal{U}_v(\vec{r}, \vec{r}') = \frac{\alpha^2}{16\pi^2} \int_{4m^2}^{\infty} \frac{dt'}{t'} \int_{4m^2}^{\infty} dv' \frac{\theta(t'-v')}{[t'(t'-v')]^{1/2}} \left(\frac{e^{-r\sqrt{t'}}}{r} + \frac{e^{-r'\sqrt{t'}}}{r'}\right) \frac{\exp\{\frac{1}{2}[-(v'-4m^2+4\mathfrak{b}^2)^{1/2}]|\vec{r}-\vec{r}'|\}}{|\vec{r}-\vec{r}'|} . \tag{3.20}$$

Notice that the term involving $|\vec{r}-\vec{r}'|$ has a rather long-range contribution for $v' \sim 4m^2$, unlike the other Yukawa parts. In spite of this nonlocal form, one can compute the perturbation analytically for small $\alpha$. By avoiding the infrared divergence in this way (off mass shell, on energy shell) one obtains a simple alternative to the more conventional techniques. Furthermore, when numerical solutions are needed, the semilocal form (3.18) is easier to handle than the momentum-space form.

### D. Perturbative calculation of the ground state of scalar hydrogen

In order to examine nonperturbative techniques for computing the Lamb shift for the relativistic one-body problem (scalar hydrogen) we must obtain a perturbative answer as a check on the small coupling limits of the nonperturbative result. The wave function is an $S$ state, and one may write the resultant

radial equation as

$$\left[-\frac{1}{2m}\frac{d^2}{dr^2}-\frac{\alpha}{r}-\frac{m^2\alpha^2}{\pi}\int_{4m^2}^{\infty}\frac{dt'}{t'^2}\left(\frac{t'-4m^2}{t'}\right)^{1/2}\frac{e^{-r\sqrt{t'}}}{r}\right]u(r)$$
$$+\frac{\alpha^2}{2\pi^2}\int_0^{\infty}dr'\int_{4m^2}^{\infty}dv'\int_{4m^2}^{\infty}\frac{dt'}{t'}\frac{\theta(t'-v')}{[t'(t'-v)]^{1/2}}\left(\frac{e^{-r\sqrt{t'}}}{r}+\frac{e^{-r'\sqrt{t'}}}{r'}\right)$$
$$\times\left[\frac{\sinh(r'\lambda(v'))e^{-r\lambda(v')}\theta(r'-r)}{\lambda(v')}+(r\rightleftharpoons r')\right]u(r')=\frac{b^2u(r)}{2m}\ , \tag{3.21}$$

where

$$\lambda(v')=\tfrac{1}{2}(v'-4m^2+4b^2)\equiv\lambda\ . \tag{3.22}$$

The ground-state wave function is

$$u(r)=2re^{-r/2a}/a^{3/2},\quad a=1/m\alpha\ . \tag{3.23}$$

Taking expectation values gives (after appropriate changes of variables)

$$\frac{b^2}{2m}=m\alpha^2\left[-\frac{1}{2}-\frac{\alpha^3}{4\pi}\int_0^1\frac{dy\,y(1-y)^{1/2}}{(\alpha y^{1/2}+1)^2}\right.$$
$$\left.+\frac{2\alpha^3}{\pi}\int_0^1dx\int_0^1\frac{dz\,z}{(1-z)^{1/2}}\frac{1}{(\alpha(xz)^{1/2}+2)^2-\lambda^2y^2z^2}\left(\frac{1}{(\alpha+\lambda)^2}-\frac{z}{4(\alpha(zx)^{1/2}+1)^2}\right)\right]. \tag{3.24}$$

If the integrands are expanded in powers of $\alpha$, the integrals that appear in the coefficients of $\alpha^5$ can be evaluated exactly, giving

$$\frac{b^2}{2m}=-\frac{m\alpha^2}{2}-\frac{m\alpha^5}{15\pi}+\frac{2m\alpha^5}{3\pi}\left(\ln\frac{1}{\alpha^2}-2-2\ln2\right), \tag{3.25}$$

or

$$\mathcal{E}=m\left[1-\frac{\alpha^2}{2}-\frac{\alpha^4}{2}-\frac{\alpha^5}{15\pi}+\frac{2\alpha^5}{3\pi}\left(\ln\frac{1}{\alpha^2}-2-2\ln2\right)\right] \tag{3.26}$$

as the energy of the ground state. Our result differs from the result given by Fronsdal and Huff.[8] In place of the term $-2-2\ln2$ they have approximately $-\frac{15}{4}-2\ln2$. A detailed comparison of this method of handling the vertex with the more conventional Bethe sum approach and the Erickson and Yennie approach will be presented in a future paper on the nonperturbative treatment of real hydrogen (vector photons and spin-$\frac{1}{2}$ particles).[10] Any nonperturbative approach should yield the above energy for small $\alpha$.

## IV. PADÉ APPROXIMANTS AND A NONPERTURBATIVE CALCULATION OF THE GROUND STATE OF SCALAR HYDROGEN

### A. The Lamb shift for general $\alpha$ and related problems

In studying the Lamb shift for general $\alpha$ there are two related aims to keep in mind. From the point of view of atomic physics, one could obtain nonperturbative Lamb-shift calculations for large $Z$ values and perhaps for superheavy elements ($Z>137$).[11] For superheavy elements, one would run into the problem of complex energies unless a way of introducing some type of cutoff is found. Pieper and Greiner are able to shift this singular behavior away by using the Coulomb potential of a charge distribution rather than a point.[12] Erickson extrapolates the spectrum for the Lamb shift from small $Z$ to general $Z$ by using convenient functional forms for the spectrum that are correct for small $Z$, are finite for all $Z$, and vanish for infinite $Z$.[13] In the context of the quasipotential approach, what we wish to do is obtain an improved Lamb shift for larger coupling ($Z$ or $\alpha$) by extrapolating the potential by use of Padé approximants of the perturbation series of the potential. Conceivably, the $\alpha$ singularity will be deflected by including higher-order terms nonperturbatively without imposing a charge distribution.[14]

From the point of view of particle physics, a study of the Lamb shift for general $\alpha$ is of interest in light of what it might say about the problem of strong binding and quark models. For example, Schwinger has speculated that the quarks may in fact be magnetic monopoles with a magnetic charge $\alpha^*\sim137$ (as opposed to $\alpha\sim\frac{1}{137}$).[15] The Lamb shift may play a major role in determining the spectrum that such a quark (dyon) model would imply. Barut has examined a dyon model by relating it to representations of groups such as O(4), O(4, 1),

and O(4, 2).[16] However, he is not faced with problems of complex energies at large coupling constants.[17] There are two problems that must be met by the quasipotential approach in this context. Is it possible to obtain real energies for large $\alpha$ and, if so, is the binding deep?[18] As this second problem is a two-body problem, it will not be treated in this paper.[19]

### B. Padé approximants

Any nonperturbative scheme for computing the energy spectrum must agree with the perturbative answer for small coupling constants. The Padé approximant[3] has this feature. The reason is that the Padé approximant (PA) is derived from a perturbation series (or Taylor series) in the coupling constant (or expansion variable). Given a formal series expansion of the form

$$f(x) = \sum_{m=0}^{\infty} f_m x^m , \tag{4.1}$$

the $[N/M]$ PA is uniquely defined as the ratio of polynomials

$$f^{[N/M]}(x) = \frac{\sum_{n=0}^{N} p_n x^n}{\sum_{m=0}^{M} q_m x^m}$$

$$= f(x) + O(x^{N+M+1}) . \tag{4.2}$$

Padé approximants give one a way to extrapolate the partial sum of a series. In many instances it provides a way of accelerating the convergence of a slowly convergent series or of resumming a formally divergent series into a convergent sequence of approximants.[20]

Unlike a power series, PA's allow one to approximate functions near their poles. The stability of the position of these zeros of the denominator is an important aspect. This feature was used by Basdevant, Bessis, Zinn-Justin, and others to compute the masses of meson-meson resonances by finding the pole positions of the PA's to the scattering amplitude.[21] Padé approximants appear to be the most successful method of obtaining physical features of strongly interacting systems from a formal Lagrangian field theory.

Quantum electrodynamics is a success of the perturbative approach to field theory. As $\alpha \sim \frac{1}{137}$, the PA's do not differ significantly from the perturbation series. However, if $Z$ is large or one wishes to consider strong-coupling QED, then the perturbative approach is inadequate. Crater,[22] Gammel and Menzel,[23] Garibotti, Pellicoro, and Villiani,[24] and Graffi and Grecchi[25] have examined the convergence of PA's in the case of QED. Crater showed that the $[1/1]$ Padé approximant of the Born, ladder, and cross-ladder diagram has poles that display the correct O(4) symmetry but do not have the right positions. However, this situation changes if more terms are included. In particular, Gammel and Menzel[23] and Crater[22] demonstrated that one could find the bound states very accurately by locating the poles of the diagonal Padé approximants to the series of ladder and cross-ladder diagrams generated by the eikonal approximation. So, given a series of Feynman diagrams in QED, one is led to expect that the PA's would have poles whose position would converge to the correct bound-state energies. However, from a practical point of view, there is no reason to use PA's on the series. The reason is that one could, of course, obtain the position of the poles directly from the eikonal form without the use of Padé approximants.[26] Using the PA's in this way is not very efficient. We intend to use them in a more efficient way.

The eikonal approximation can be derived very easily from the quasipotential approach, as has been shown by Todorov.[1] This is essentially because of the similarity of the quasipotential equation and the nonrelativistic Lippmann-Schwinger equation. For bound states, the most efficient way to find the spectrum is to solve the homogeneous equation (relativistic Schrödinger equation) rather than look for poles in the scattering amplitude $T$. This suggests a more efficient use of the PA summation scheme. Instead of computing bound states by looking at poles of Padé approximants of Feynman diagrams, we solve the homogeneous quasipotential equation in which the potential $V$ is a Padé resummation of a perturbation series of $V$'s.

Solving for the eigenvalue of the homogeneous equation with the Coulomb potential is equivalent to finding the poles in the eikonal approximation to the sum of ladder and cross-ladder diagrams.[27] What set of diagrams corresponds to solving the homogeneous equation with the effective potential defined by the Padé sum of a perturbation series of $V$'s? This question can be answered only in a speculative, heuristic way. But, let us suppose that $V = \alpha V_{\text{Born}} + \alpha^2 V_{\text{vac}}$. Then $V_{\text{eff}} = \alpha V_{\text{Born}}/(1 - \alpha V_{\text{vac}}/V_{\text{Born}})$. This effective potential is essentially an iterated sum of self-energy corrections. Since solving the homogeneous quasipotential equation is equivalent (in terms of finding the eigenvalue) to iterating the inhomogeneous equation to all orders, we conjecture that the equivalent set of diagrams would be the "eikonal" approximation of all ladder and cross-ladder type diagrams with the exchange lines containing zero, one, two, ... vacuum-polarization corrections.

### C. Nonperturbative dispersion form of the quasipotential

The quasipotential given in Eq. (3.11) is of the form

$$V=\alpha V_1+\alpha^2 V_2 . \tag{4.3}$$

From this partial sum of the perturbation series for $V$, we can construct the [1/1] PA

$$V^{[1/1]}=\frac{\alpha V_1}{1-\alpha V_2/V_1} . \tag{4.4}$$

This form, however, is not convenient to work with. The reason is that it does not allow one to perform Fourier transforms easily, as the variables $t$ and $v=4m_{\Delta}^2$ in $V_2$ do not appear in a simple way. That is, $V^{[1/1]}$ is not given as a dispersion integral over the variables $t$ and $v$. This can be corrected, however, by using subtraction techniques to rewrite (4.4) in terms of dispersion integrals.

In order to illustrate this technique, we consider first just the Born graph and the self-energy graph. According to (3.11), $V$ is given by

$$V=16\pi m^2\alpha\left(\frac{1}{t}+\alpha\Pi(t+i\epsilon)\right), \tag{4.5}$$

where

$$\Pi(t+i\epsilon)=\frac{1}{\pi}\int_{4m^2}^{\infty}\frac{dt'\rho(t')}{t'(t'-t-i\epsilon)} \tag{4.6}$$

and

$$\rho(t')=-m^2\left(\frac{t'-4m^2}{t'}\right)^{1/2}\frac{1}{t'} . \tag{4.7}$$

From Eq. (4.4) we find

$$V^{[1/1]}(t+i\epsilon)=16\pi m^2\alpha\,\frac{1}{t}\,\frac{1}{[1-\alpha t\Pi(t+i\epsilon)]} . \tag{4.8}$$

As has been mentioned, this is not a convenient form for performing Fourier transforms. However, one can rewrite this as a dispersion integral if proper account of the $\alpha=0$ behavior is made by a subtraction at $t=0$. In that case

$$V^{[1/1]}(t+i\epsilon)=\frac{16\pi m^2\alpha}{t}+\frac{16\pi m^2\alpha^2\Pi(t+i\epsilon)}{1-\alpha t\Pi(t+i\epsilon)} , \tag{4.9}$$

and one then computes the discontinuity across the cut starting at $t=4m^2$ of the second term in this equation.[28] This gives

$$V^{[1/1]}(t+i\epsilon)=16m^2\pi\alpha\left[\frac{1}{t}+\frac{\alpha}{\pi}\int_{4m^2}^{\infty}\frac{dt'\rho(t')}{t'|1-\alpha t'\Pi(t'+i\epsilon)|^2}\,\frac{1}{t'-t-i\epsilon}\right] . \tag{4.10}$$

In the range $4m^2\leq t'<\infty$, $\Pi(t'+i\epsilon)$ has both a real and an imaginary part.

The $r$-space form of this potential is

$$V^{[1/1]}(r)=-\frac{\alpha}{r}+\frac{1}{\pi}\int_{4m^2}^{\infty}dt'\,\frac{\rho(t')}{t'|1-\alpha t'\Pi(t'+i\epsilon)|^2}\,\frac{e^{-r\sqrt{t'}}}{r} . \tag{4.11}$$

The second term in the potential is like the vacuum-polarization term in (3.19). The difference is due to the appearance of the denominator $1/|1-\alpha t'\Pi(t'+i\epsilon)|^2$.

Next, include the nonlocal vertex part in $V_2$. Then in place of (4.8) we have

$$V^{[1/1]}(t+i\epsilon,\,v+i\eta)=16\pi m^2\alpha\,\frac{1}{t}\,\frac{1}{1-\alpha t\Pi(t+i\epsilon,\,v+i\eta)}$$

$$=\frac{16\pi m^2\alpha}{t}\left[1+\frac{\alpha t\Pi(t+i\epsilon,\,v+i\eta)}{1-\alpha t\Pi(t+i\epsilon,\,v+i\eta)}\right] , \tag{4.12}$$

where now $\Pi$ is defined as

$$\Pi(t+i\epsilon,\,v+i\eta)=\frac{1}{\pi}\int_{4m^2}^{\infty}\frac{\rho_1(t')}{t'(t'-t'-i\epsilon)}+\frac{1}{\pi^2}\int_{4m^2}^{\infty}dt'\int_{4m^2}^{\infty}dv'\,\frac{\rho_2(t',v')}{t'(t'-t-i\epsilon)(v'-v-i\eta)} , \tag{4.13}$$

with

$$\rho_1(t')=-m^2\left(\frac{t'-4m^2}{t'}\right)^{1/2}\frac{1}{t'} \tag{4.14}$$

and

$$\rho_2(t',v')=\frac{2\pi m^2\Theta(t'-v')}{[t'(t'-v')]^{1/2}} . \tag{4.15}$$

We wish to find an expression for the potential analogous to the perturbative form (3.11). Recall that it

consists of a Coulomb piece, a local vacuum contribution, and a nonlocal part. In (4.12), the Coulomb term has been split off. We note that

$$\Pi(t+i\epsilon, -\infty) = \frac{1}{\pi} \int_{4m^2}^{\infty} dt' \frac{\rho_1(t')}{t'(t'-t-i\epsilon)} \ . \tag{4.16}$$

Hence, we can extract a local piece from the second term of (4.12) by a subtraction at $v=-\infty$. This local piece can be written as a dispersion integral and is in fact just the second term of (4.10). The remaining part can be written as a double dispersion integral:

$$\frac{\alpha\Pi(t+i\epsilon, v+i\eta)}{1-\alpha t\Pi(t+i\epsilon, v+i\eta)} - \frac{\alpha\Pi(t+i\epsilon, -\infty)}{1-\alpha t\Pi(t+i\epsilon, -\infty)} = \frac{1}{\pi^2} \int_{4m^2}^{\infty} dt' \int_{4m^2}^{\infty} dv' \frac{P(t', v')}{t'(t'-t-i\epsilon)(v'-v-i\eta)} \ , \tag{4.17}$$

where

$$P(t, v) = -\frac{t}{4}\{\Pi_{2R} - 2\alpha t(\Pi_{1R}\Pi_{2R} + \Pi_{1I}\Pi_{2I}) + \alpha^2 t^2[\Pi_{2R}(\Pi_{1R}^2 - \Pi_{2R}^2 - \Pi_{1I}^2 - \Pi_{2I}^2) + 2\Pi_{1I}\Pi_{2I}\Pi_{1R}]\}$$

$$\times\{[(1-\alpha t(\Pi_{1R}+\Pi_{2R}))^2 + \alpha^2 t^2(\Pi_{1I}+\Pi_{2I})^2][(1-\alpha t(\Pi_{1R}-\Pi_{2R}))^2 + \alpha^2 t^2(\Pi_{1I}-\Pi_{2I})^2]\}^{-1} \tag{4.18}$$

and

$$\Pi(t+i\epsilon, v+i\eta) = \Pi_{1R} + \Pi_{2R} + i\Pi_{1I} + i\Pi_{2I} \ . \tag{4.19}$$

The $\Pi$'s are defined by (P.V. means principal value)

$$\begin{aligned}
\Pi_{1R} &= \frac{1}{\pi}\,\text{P.V.}\int_{4m^2}^{\infty} \frac{dt'}{t'}\frac{\rho_1(t')}{t'-t} + \frac{1}{\pi}\,\text{P.V.}\int_{4m^2}^{\infty}\frac{dt'}{t'(t'-t)}\,\text{P.V.}\int_{4m^2}^{\infty}\frac{dv'}{v'-v}\rho_2(t', v') \ , \\
\Pi_{2R} &= -\frac{\rho_2(t, v)}{t} \ , \\
\Pi_{1I} &= \frac{1}{\pi}\,\text{P.V.}\int_{4m^2}^{\infty}\frac{dt'}{t'}\frac{\rho_2(t', v)}{t'-t} \ , \\
\Pi_{2I} &= \frac{1}{\pi}\,\text{P.V.}\int_{4m^2}^{\infty}\frac{dv'}{v'-v}\rho_2(t, v') + \frac{\rho_1(t)}{t} \ .
\end{aligned} \tag{4.20}$$

This permits us to write an integro-differential quasipotential equation analogous to (3.18):

$$\left(-\frac{\nabla^2}{2m} - \frac{\alpha}{r} + \frac{\alpha^2}{\pi}\int_{4m^2}^{\infty}\frac{dt'}{t'}\frac{\rho_1(t')}{|1-\alpha t'\Pi(t'+i\epsilon, -\infty)|^2}\frac{e^{-r\sqrt{t'}}}{r}\right)\psi(\vec{r})$$

$$+\frac{\alpha^2}{32\pi^3}\int d^3r'\int_{4m^2}^{\infty}dt'\int_{4m^2}^{\infty}dv'\frac{P(t', v')}{t'}\left(\frac{e^{-r\sqrt{t'}}}{r'} + \frac{e^{-r\sqrt{t'}}}{r}\right)\frac{\exp(-\frac{1}{2}(v'-4m^2+b^2)^{1/2}|\vec{r}-\vec{r}'|)}{|\vec{r}-\vec{r}'|}\psi(\vec{r}') = \frac{b^2}{2m}\psi(\vec{r}) \ . \tag{4.21}$$

An alternative form of this equation which involves a single dispersion integral is obtained if one replaces the dispersion integral over $m_\Delta^2$ by a Fourier transform. The following equation together with (4.21) provide a way of checking on the rather complex numerical calculations

$$\left[-\frac{\nabla^2}{2m} - \frac{\alpha}{r} + \frac{\alpha^2}{\pi r}\int_{4m^2}^{\infty}dt'\frac{\rho_1(t')e^{-r\sqrt{t'}}}{t'|1-\alpha t'\Pi(t'+i\epsilon, \infty)|^2}\right]\psi(\vec{r}) + \frac{\alpha^2}{2\pi}\int d^3r' K(\vec{r}, \vec{r}')\psi(\vec{r}') = \frac{b^2}{2m}\psi(\vec{r}) \ , \tag{4.22}$$

where

$$K(\vec{r}, \vec{r}') = \int_{4m^2}^{\infty}dt'\int\frac{d^3p}{(2\pi)^3}e^{i\vec{p}\cdot(\vec{r}-\vec{r}')}[\eta(t', p^2) - \eta(t', \infty)]\left(\frac{e^{-r\sqrt{t'}}}{r} + \frac{e^{-r'\sqrt{t'}}}{r'}\right) , \tag{4.23}$$

with

$$\eta(t', \vec{p}^2) = \frac{\rho(t', \vec{p}^2)}{t'|1-\alpha t'\Pi(t'+i\epsilon, \vec{p}^2)|^2} \ , \quad \eta(t', \infty) = \frac{\rho_1(t')}{t'|1-\alpha t'\Pi(t'+i\epsilon, \infty)|^2} \tag{4.24}$$

and

$$\rho(t', \vec{p}^2) = 2m^2\left[\frac{1}{(t'^2-4m_\Delta^2 t')^{1/2}}\ln\left(\frac{(t'-4m_\Delta^2)^{1/2}+(t'-4m^2)^{1/2}}{(t'-4m_\Delta^2)^{1/2}-(t'-4m^2)^{1/2}}\right) - \frac{1}{2t'}\left(\frac{t'-4m^2}{t'}\right)^{1/2}\right] . \tag{4.25}$$

The term $\Pi(t'+i\epsilon,\infty)$ is the same integral as given in (4.16). In the general case

$$\Pi(t'+i\epsilon,\vec{p}^{\,2})=\frac{1}{\pi}\int_{4m^2}^{\infty}dt''\,\frac{\rho(t'',\vec{p}^{\,2})}{t''(t''-t'-i\epsilon)}\ . \tag{4.26}$$

The radial form of (4.21) is similar to that given in Eq. (3.21) except that the single- and double-spectral functions in (4.21) are nonperturbative forms. The radial form of (4.22) for the $S$ state is

$$\left(-\frac{1}{2m}\frac{d^2}{dr^2}-\frac{\alpha}{r}+\frac{\alpha^2}{\pi r}\int_{4m^2}^{\infty}dt'\eta(t',\infty)e^{-r\sqrt{t'}}\right)u(r)+\frac{\alpha^2}{\pi^2}\int_0^{\infty}dr'\,k(r,r')u(r')=\frac{b^2}{2m}\,u(r) \tag{4.27}$$

and is different in that the kernel $k(r,r')$ involves integrals of oscillating functions

$$k(r,r')=\int_0^{\infty}dp\sin pr\sin pr'\int_{4m^2}^{\infty}dt'[\eta(t',p^2)-\eta(t',\infty)]\left(\frac{e^{-r\sqrt{t'}}}{r}+\frac{e^{-r'\sqrt{t'}}}{r'}\right)\ . \tag{4.28}$$

However, the spectral functions themselves appear simpler.

### D. Solution of the nonperturbative form of the homogeneous quasipotential equation: General comments

Before giving details of the solution of the above equation for various values of $\alpha$, let us summarize our assumptions. The relativistic Lippmann-Schwinger equation (2.1) has a dual role in the quasipotential approach to quantum field theory. This is especially evident in our nonperturbative approach to the bound-state problem. The initial use of (2.1) is to find the perturbation series of potential-energy terms from a series of Feynman diagrams. One then uses the Padé approximant resummation scheme to obtain a nonperturbative form for $V$. This nonperturbative form of $V$ is then used in the homogeneous form of the quasipotential equation. As has been mentioned before, solving this equation is equivalent to finding the poles of the exact solution $T$ of (2.1) for a given potential $V$. In our case, the given $V$ is a nonperturbative form. Notice that formally iterating the quasipotential to all orders in the potential $V$ is equivalent to solving the [1/1] operator PA.[29] To see this, notice that the first two terms in the iteration are

$$T=-V+VGV\ . \tag{4.29}$$

Viewed as an operator expansion in powers of $V$, the [1/1] operator PA formed from this is

$$T^{[1/1]}=-(1+VG)^{-1}V\ , \tag{4.30}$$

which of course is the formal solution to (2.1) for a given $V$.

The eigenvalues we shall determine are the ground-state eigenvalues for various values of $\alpha$. Variational methods are quite adequate for this problem. The peculiar difficulties involved come mainly from the nonlocal potential-energy term which arises from the Padé summation of the Born, vacuum-polarization, and vertex diagrams with self-energy corrections. This term is dependent on the eigenvalue itself so that the eigenvalue appears nonlinearly. Although the mathematical theory of nonlinear eigenvalue problems is not well known or extensively studied, that is of no concern in this paper. In practice, we solve the problem iteratively by initially guessing a value of the energy and using this guess in the eigenvalue-dependent potential-energy term. This, in effect, linearizes the eigenvalue problem. The linearized equation is solved using a variational method. The eigenvalue obtained by solving this linearized problem is used to generate a second estimate for the eigenvalue to be used in the potential-energy term. This procedure, known technically as a contraction mapping, is repeated until the generated estimate of the eigenvalue is sufficiently close to the variationally computed eigenvalue.

The numerical calculations are lengthy but straightforward. The main difficulties stem from the fact that the nonperturbative form of the quasipotential involves a double integration of an integrand which itself is a function of a rather complex integral, Eq. (4.26). One also has the additional problem of applying a satisfactory variational method to the problem. We shall not discuss the details here. In Appendix B we discuss the type of variational method used. As described in detail there, there are three primary technical problems in the numerical calculations. Our approach to these relies heavily on Padé approximants. No physical hypothesis is involved here with these technical points. These points are the generation of eigenvalue estimates, the integrations, and extrapolations of variationally generated eigenvalues arising from a sequence of discretizations of the quasipotential equations.

### E. Solution of the nonperturbative form of the homogeneous quasipotential equation: Numerical results

In Table I the exact Coulomb results are given. In Table II we present the perturbative results from numerical integrations of (3.24) for $\alpha = 0.2$, 0.4, 0.6, 0.8, and 1.0. [Equation (3.25) is valid only for $\alpha \ll 1$.] We also give in Table II the relative change in the binding energy over the pure Coulomb results of Table I. In Table III the results of treating the radiative corrections nonperturbatively are given. The relative changes in the binding energy over the perturbative results of Table II are also given. Both the perturbative and nonperturbative effects of the vacuum polarization are small. To the accuracy employed in the numerical calculations, there was no difference between the two. The major effects are found when the vertex graphs with self-energy corrections are included. In order to facilitate comparisons with the perturbative results we define $\mathfrak{b} = (-b^2)^{1/2}$ in terms of which $\mathcal{E} = (m^2 - \mathfrak{b}^2)^{1/2} = m(1 - \mathfrak{b}^2/m^2)^{1/2}$. For the Coulomb potential alone we have $\mathfrak{b}/m = \alpha$ and $\mathcal{E} = m(1 - \alpha^2)^{1/2}$.

Our final calculations are of that value of $\alpha$ for which the energy $\mathcal{E}$ becomes complex. Recall that for the ground-state Coulomb problem in this model this point is reached when $\alpha = 1$. Numerical studies show that when the potential is modified to include radiative corrections nonperturbatively the point is shifted upward by 1.2% to $\alpha = 1.012$.

## V. CONCLUSION

The corrections to the energy levels obtained with a pure Coulomb potential $(-\alpha/r)$ range up to 15% and represent a repulsive contribution. The results displayed in Table III show that the use of a nonperturbative calculation results in a change up to 2% from corresponding perturbative calculations for $\alpha \leq 1.0$. The major repulsive contributions arise from the proper vertex correction with both the perturbative and nonperturbative potentials. The net effect of these higher-order corrections is not sufficient to produce a large shift in the critical value of $\alpha$ where $\mathcal{E}$ becomes complex.

It is not possible to provide an *a priori* estimate of the accuracy of the nonperturbative approach employed here. The convergence of the technique might be estimated by examining the results of higher-order Padé approximants (for example, the [1/2] and [2/1] PA's) to the potential.

As we pointed out in Sec. III, the origin of complex energies for large $\alpha$ is of a somewhat different nature in this scalar model than that which leads to complex $\mathcal{E}$ for vector photons.[30] Nevertheless, the fact that the qualitative features of radiative corrections are the same for both scalar and vector approaches suggests that a similar small shift will occur for vector photons. Studies on this question are now in progress.

The scalar interaction (2.1) employed here cannot produce real bound-state energies at large coupling $\alpha$, at least to the order of approximation of the potential considered here. Should this situation persist with more accurate potentials, it might have significant implications. Other scalar interactions such as the pseudoscalar nucleon-nucleon coupling differ from the interaction considered here mainly in their long-range behavior. This long-range behavior does not produce the problem of complex $\mathcal{E}$. It is possible that such difficulties can be avoided by using a more general (i.e., non-

TABLE I. Binding energies for the Coulomb potential. The variable $\mathfrak{b}/m$ is equal to $\alpha$ for the Coulomb potential and, like the dimensionless variable $(m - \mathcal{E})/m$, gives a measure of the binding energy.

| $\mathfrak{b}/m$ | $(m - \mathcal{E})/m$ | $\alpha$ |
|---|---|---|
| 0.200 00 | 0.020 20 | 0.200 00 |
| 0.400 00 | 0.083 48 | 0.400 00 |
| 0.600 00 | 0.200 00 | 0.600 00 |
| 0.800 00 | 0.400 00 | 0.800 00 |
| 1.000 00 | 1.000 00 | 1.000 00 |

TABLE II. Binding energies for the perturbative form of the Coulomb potential plus radiative corrections.

| $\mathfrak{b}/m$ | $(m - \mathcal{E})/m$ | $\alpha$ | Relative change over Coulomb results I |
|---|---|---|---|
| 0.199 70 | 0.020 14 | 0.200 00 | 0.0030 |
| 0.398 19 | 0.082 70 | 0.400 00 | 0.0094 |
| 0.595 65 | 0.196 76 | 0.600 00 | 0.0163 |
| 0.792 84 | 0.390 57 | 0.800 00 | 0.0239 |
| 0.990 46 | 0.862 20 | 1.000 00 | 0.1480 |

TABLE III. Binding energies for the nonperturbative form of the Coulomb potential plus radiative corrections.

| $\mathfrak{b}/m$ | $(m - \mathcal{E})/m$ | $\alpha$ | Relative change over perturbative results II |
|---|---|---|---|
| 0.199 70 | 0.020 14 | 0.200 00 | 0.0000 |
| 0.398 18 | 0.082 69 | 0.400 00 | 0.0001 |
| 0.594 56 | 0.195 95 | 0.600 00 | 0.0041 |
| 0.791 13 | 0.388 35 | 0.800 00 | 0.0057 |
| 0.987 58 | 0.842 88 | 1.000 00 | 0.0227 |

polynomial) interaction Lagrangian or by modifying the quasipotential equation so that the potential appears in conjunction with the mass terms.[4] The fact that some shift of the critical $\alpha$ was obtained here clearly illustrates its dependence on the structure of the interaction.


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## APPENDIX A: CANCELLATION OF BOX, CROSS-BOX, AND ITERATED BORN DIAGRAMS IN THE STATIC LIMIT

The second-order quasipotential has the form

$$V^{(2)} = -T^{(2)} + T^{(1)} G T^{(1)} \ . \tag{A1}$$

The contribution to $T^{(2)}$ for the two-particle scalar scattering amplitude consists of the vacuum diagram, the vertex with self-energy corrections, the box, and the cross-box diagrams. We wish to show here in outline form that in the static limit ($m_1 \to \infty$) the box and cross-box diagrams cancel the iterated Born term $T^{(1)} G T^{(1)}$. It is easiest to demonstrate this by use of the double dispersion relation form. For bound-state energies the box diagram has the form

$$\alpha^2 \int_{(m_1+m_2)^2}^{\infty} ds' \int_0^{\infty} dt' \, \frac{1}{s'-s} \, \frac{1}{t'-t} \, \frac{1}{(s't')^{1/2}} \, \frac{\theta(\eta(s',t'))}{[\eta(s',t')]^{1/2}} \ , \tag{A2}$$

where

$$\eta(s',t') = [(s'-(m_1+m_2)^2)(s'-(m_1-m_2)^2)t' - s'(\Delta m_1^{\,2} + \Delta m_2^{\,2})^2]/s' \ , \tag{A3}$$

with

$$\Delta m_i^{\,2} = m_i^{\,2} - m_{i\Delta}^{\,2}, \quad i = 1, 2 \ . \tag{A4}$$

The dispersion-relation form for the cross-box diagram is obtained by letting $s \to u$ in Eq. (A2). The iterated Born term has the double dispersion form

$$-2 \, \frac{\alpha^2}{s^{1/2}} \int_{(m_1+m_2)^2}^{\infty} ds' \int_0^{\infty} dt' \, \frac{1}{s'-s-i\epsilon} \, \frac{1}{t'-t-i\epsilon} \, \frac{1}{t'^{1/2}} \, \frac{\theta(\eta(s',t'))}{[\eta(s',t')]^{1/2}} \ . \tag{A5}$$

Consider now the static limit ($m_1 \to \infty$) of (A2). In taking the static limit the following definitions are useful. For $m_1 \gg m_2$ we define

$$\begin{aligned} s &= (m_1 + \mathcal{E})^2 = m_1^{\,2} + 2m_1 \mathcal{E} \ , \\ s' &= (m_1 + \mathcal{E}')^2 = m_1^{\,2} + 2m_1 \mathcal{E}' \ . \end{aligned} \tag{A6}$$

Making these substitutions and then taking the limit $m_1 \to \infty$ lead us to the following static form for the box:

$$\alpha^2 \int_m^{\infty} d\mathcal{E}' \, \frac{1}{\mathcal{E}'-\mathcal{E}} \times \int_0^{\infty} \frac{dt'}{t'-t} \, \frac{1}{t'^{1/2}} \, \frac{\theta((\mathcal{E}'^2-m^2)t' - \Delta m^4)}{[(\mathcal{E}'^2-m^2)t' - \Delta m^4]^{1/2}} \ , \tag{A7}$$

with $m = m_2$.

Likewise, one can show that in this limit, the cross box goes into

$$\alpha^2 \int_m^{\infty} d\mathcal{E}' \, \frac{1}{\mathcal{E}'+\mathcal{E}} \times \int_0^{\infty} \frac{dt'}{t'-t} \, \frac{1}{t'^{1/2}} \, \frac{\theta((\mathcal{E}'^2-m^2)t' - \Delta m^4)}{[(\mathcal{E}'^2-m^2)t' - \Delta m^4]^{1/2}} \ . \tag{A8}$$

Performing the same type of limits for the iterated Born contribution to $V^{(2)}$ gives us

$$-2\alpha^2 \int_m^{\infty} \frac{d\mathcal{E}' \, \mathcal{E}'}{\mathcal{E}'^2 - \mathcal{E}^2} \times \int_0^{\infty} \frac{dt'}{t'-t} \, \frac{1}{t'^{1/2}} \, \frac{\theta((\mathcal{E}'^2-m^2)t' - \Delta m^4)}{[(\mathcal{E}'^2-m^2)t' - \Delta m^4]^{1/2}} \ , \tag{A9}$$

which cancels the sum of (A7) and (A8).

## APPENDIX B: USE OF PADÉ APPROXIMANTS IN THE SOLUTION OF THE NONLINEAR EIGENVALUE PROBLEM

We shall outline in this appendix the numerical technique we used in finding the ground-state eigenvalue of the integro-differential quasipotential equation. The general form of the equation as exemplified in (3.21) and (4.27) is

$$-\frac{d^2}{dz^2} \, u(z) + q(z,\lambda) u(z) + \int_0^{\infty} dz' \, k(z,z',\lambda) u(z') = \lambda u(z) \ . \tag{B1}$$

As mentioned in the main part of this paper, there are three main numerical problems involved.

First of all, the nonlinear eigenvalue equation is linearized by letting $\lambda$ be fixed on the left-hand side of the equation. Call this value $\lambda_0$. The next step involves computing the function $q(z, \lambda_0)$ and the kernel $k(z, z', \lambda_0)$. This involves a double integral of a function which is itself a function of a rather complex integral. The method of integration used here was rather crucial in limiting the amount of time spent on the computer. We shall briefly outline it here and refer the reader to the article of Chisholm, Genz, and Rowlands[31] for a complete description and evaluation of the method.

The integration technique used is based on accelerating the convergence of a sequence of quadrature approximations (e.g., Simpson's rule at 3, 5, 9, 17, ... points). The acceleration techniques used are based on the type-I and type-II Padé approximants. Suppose one has a sequence of quadrature approximations $S_0, S_1, S_2, \ldots$ to an integral $S$. Then the type I accelerations are performed as follows. One forms the series

$$S_0 + (S_1 - S_2)x + (S_2 - S_1)x^2 + (S_3 - S_2)x^3 + \cdots . \quad \text{(B2)}$$

From this series, one forms diagonal $S^{[N/N]}(x)$ PA's or off-diagonal $S^{[(N+1)/N]}(x)$ PA's, depending on whether one has computed an odd or even number of quadrature approximations. One then evaluates these PA's at $x=1$. This technique is especially powerful in problems that have end- or interior-point singularities, as found in dispersion and principal-value integrals involved in computing $q(z, \lambda)$ and $k(z, z', \lambda)$. We used the type II or fixed point Padé approximants when the quadratures $S_i$ converge rather fast to $S$ or if the end-point singularities are rather mild or nonexistent. In the type II technique, one fits the computed $S_i$ to a function of the mesh size that has the form of a ratio of polynomials

$$S(h) = \frac{A + Bh^2 + Ch^4 + \cdots}{1 + Dh^2 + \cdots} . \quad \text{(B3)}$$

At $h=0$, $S(0)=A$ becomes the accelerated result of combining the various quadratures.

Once the integrals are evaluated, a variational technique is employed in computing the eigenvalue $\lambda$. A very efficient and rapidly convergent method for determining $\lambda$ is to discretize the problem and obtain a sequence of eigenvalues $\lambda(h_1), \lambda(h_2), \lambda(h_3) \cdots$. From this sequence of variationally computed eigenvalues one uses type II PA's to accelerate their convergence to the desired accuracy.

Let us call this result $\lambda_1$. One then uses this $\lambda$ in the left-hand side and goes through the entire procedure again obtaining a value $\lambda_2$. The aim now becomes one of consistency. That is, one would like the estimated eigenvalue and the computed one to be as close as desired. The variational technique leads to an equation of the form

$$f(\lambda_{i-1}) = \lambda_i , \quad i = 1, 2 . \quad \text{(B4)}$$

Beyond $i=2$ we desire an accelerated decrease of the difference between the estimated and computed eigenvalue. Suppose we defined

$$g(\lambda) = f(\lambda) - \lambda . \quad \text{(B5)}$$

Then the problem becomes one of finding the appropriate zero of $g(\lambda)$. From the first two guesses we have the equations

$$\begin{aligned} g(\lambda_0) &= f(\lambda_0) - \lambda_1 , \\ g(\lambda_1) &= f(\lambda_1) - \lambda_2 . \end{aligned} \quad \text{(B6)}$$

In the next estimate one does not use $\lambda_2$ but rather one assumes $g(\lambda)$ has the form

$$g(\lambda) = A + B\lambda . \quad \text{(B7)}$$

From (B6) one obtains the coefficients $A$ and $B$ and the third estimate is $-B/A = \lambda_2'$. This leads to a third equation of the form

$$g(\lambda_2') = f(\lambda_2') - \lambda_3 . \quad \text{(B8)}$$

Rather than use a linear interpolation again, we use the simple $[1/1]$ diagonal Padé approximant to generate a fourth estimate, as this gives a much more rapid convergence to the solution of $g(\lambda)=0$. That is, from (B1) and (B8) one finds the coefficients $A$ and $B$ in the rational form

$$g(\lambda) = \frac{A + B\lambda}{1 + C\lambda} . \quad \text{(B9)}$$

The fifth- and higher-order estimates are obtained in the same way.

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[4]This property along with the other properties of the classical limit of the quasipotential equation will be examined in a future publication by H. Crater and J. Naft.

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