T-matrix analysis of one-dimensional weakly coupled bound states

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The ground-state energy of the Hamiltonian $-(1/2)d^2/dx^2+\lambda V(x)$ is analyzed in terms of the zeros of a perturbative expansion for the inverse of the T matrix, and an expression for $(-2E)^{1/2}$ correct to order λ^4 is obtained. Modifications of the results for long-range potentials of the type $V(x)\to -a_{\pm}|x|^{-n}$, $n=1,\ldots,4$ at $x\to\pm\infty$ are discussed. The problem of three-body bound states is considered, leading to an expression for the ground-state energy of He-like atoms with nuclear charge $\alpha \gg 1$, in a strong magnetic field.

I. INTRODUCTION

It has been observed[1] that a short-range attractive potential always produces a bound state in one or two dimensions. This interesting property allows one to obtain some general results about the bound states in the weak coupling limit. In particular, for the one-dimensional Hamiltonian

$$H=-\frac{1}{2}\frac{d^2}{dx^2}+\lambda V(x), \tag{1}$$

Abarbanel, Callen, and Goldberger[2] have derived a formal series for the ground-state energy $E(\lambda)$ of the form

$$-(-2E)^{1/2}=\lambda\int dx\, V(x)+\lambda^2\int dx\, dy\, V(x)|x-y|V(y)+O(\lambda^3). \tag{2}$$

For range-long potentials, these results require modifications. For example, it has been shown by Blankenbecler, Goldberger, and Simon[3] that if $V(x)\to -ax^2$ as $x\to\pm\infty$,

$$-(-2E)^{1/2}=(\lambda+4a\lambda^2\ln\lambda)\int dx\, V(x)+O(\lambda^2). \tag{3}$$

Another example of long-range potentials is that of a hydrogen atom in a strong magnetic field for which

$$H=\tfrac{1}{2}p^2-\frac{\alpha}{r}+\frac{\gamma}{8}(x^2+y^2). \tag{4}$$

Under a scale transformation

$$p\to(\tfrac{1}{4}\gamma)^{1/4}p,\quad r\to(4/\gamma)^{1/4}r \tag{5}$$

the Hamiltonian becomes

$$H'=(\tfrac{1}{4}\gamma)^{1/2}\left(\frac{p^2}{2}-\frac{\alpha(4/\gamma)^{1/4}}{r}+\tfrac{1}{2}(x^2+y^2)\right). \tag{6}$$

For $\gamma\to\infty$, the essential problem reduces to weakly coupled motion in the z direction and one obtains[4] for the ground state,

$$E\underset{\gamma\to\infty}{\sim}\tfrac{1}{2}\gamma^{1/2}-2\alpha^2\left[\tfrac{1}{2}\ln(\tfrac{1}{4}\gamma)^{1/2}-\ln\ln(\tfrac{1}{4}\gamma)^{1/2}\right]^2. \tag{7}$$

This result is of direct practical importance and has been used[5] in dispersion relations to obtain accurate predictions for Zeeman energy shifts. Several other significant results[6] have been obtained by Simon and Klaus, in particular, about the uniqueness of the bound states.

In the derivation of most of the results pertaining to the bound states in one-dimensional weakly coupled potentials, the analysis has been in terms of the wave functions. Hausmann[7] has analyzed the bound states using the Lippmann-Schwinger equation but for the wave function. The discussion in terms of the wave functions, while being direct, is generally quite complicated requiring a careful incorporation of boundary conditions. We would like to suggest that the T matrix provides a more convenient tool for the analysis of bound states as poles of the T matrix. It has the advantage that one would then be working in the momentum representation and have access to integral equations of the Lippmann-Schwinger type for the T matrix. A particularly convenient form is the one provided by Noyes[8] which gives us a perturbative expansion for essentially the inverse of the T matrix thus allowing a perturbative description of the poles of the T matrix and hence the bound-state energies.

In the present note we analyze the bound-state energies for attractive one-dimensional potentials using the Noyes form of the T matrix. In Sec. II we discuss the general results for short-range potentials and show that

$$-(-2E)^{1/2}=\lambda\int dx\,V(x)+\lambda^2\int dx\,dy\,V(x)V(y)|x-y|$$
$$+\tfrac{1}{6}\lambda^3\int dx\,dy\,dz\,V(x)V(y)V(z)(|x-y|+|y-z|+|z-x|)^2$$
$$+\tfrac{1}{6}\lambda^4\int dx\,dy\,dz\,dt\,V(x)V(y)V(z)V(t)(|x-y|^3+6|x-y|^2|x-z|+3|x-y|^2|z-t|$$
$$+6|x-y||y-z||z-t|)+O(\lambda^5). \tag{8}$$

In Sec. III, we consider the modifications required by bound states for long-range potentials. In addition to obtaining the results (3) and (7), we are able to derive expressions

$$-(-2E)^{1/2}=\lambda\int dx\,V(x)+\lambda^2\int dx\,dy\,V(x)V(y)|x-y|+2\lambda^3(a_++a_-)(\ln\lambda)\left(\int dx\,V(x)\right)^2+O(\lambda^3) \tag{9}$$

for $V(x)\to -a_\pm|x|^{-3}$ at $x\to\pm\infty$ and

$$-(-2E)^{1/2}=\lambda\int dx\,V(x)+\lambda^2\int dx\,dy\,V(x)V(y)|x-y|$$
$$+\tfrac{1}{2}\lambda^3\int dx\,dy\,dz\,V(x)V(y)V(z)(|x-y|+|y-z|+|z-x|)^2$$
$$+\tfrac{4}{3}\lambda^4(a_++a_-)(\ln\lambda)\left(\int dx\,V(x)\right)^3+O(\lambda^4) \tag{10}$$

for $V(x)\to -a_\pm x^{-4}$ at $x\to\pm\infty$. In Sec. IV, we consider the bound states for the Hamiltonian

$$H=-\frac{1}{2}\frac{d}{dx_1^2}-\frac{1}{2}\frac{d^2}{dx_2^2}$$
$$+\lambda_1 u(x_1)+\lambda_2 v(x_2)+\lambda_3 w(|x_1-x_2|). \tag{11}$$

In order to simplify the problem we introduce an approximation which may be reasonable in general. This allows us to obtain an expression for the binding energy which is valid when λ_3 is small compared to λ_1 and λ_2. We include the modifications due to long-range interactions and use our results to obtain an approximate expression for the binding energy of He-like atoms with nuclear charge $\alpha\gg 1$, in a strong magnetic field, analogous to expression (7) for the hydrogen atom. This expression is found to agree quite well with a simple variational expression for the energy.

II. SHORT-RANGE POTENTIALS

We begin the T matrix discussion of the bound states with the Lippmann-Schwinger equation for the T matrix:

$$\langle p|T|q\rangle=\langle p|\lambda V|q\rangle+\sum_k\frac{\langle p|\lambda V|k\rangle\langle k|T|q\rangle}{E-\frac{1}{2}k^2+i\eta}, \tag{12}$$

where the total energy $E=\frac{1}{2}q^2$. For the analysis of the bound states it is preferable to use the Noyes[8] form of the equation which is obtained by writing

$$\langle k|T|q\rangle=f(k,q)\langle q|T|q\rangle, \tag{13}$$

where $\langle q|T|q\rangle$ is the forward scattering amplitude and $f(q,q)=1$. This relation leads to

$$\langle q|T|q\rangle=\langle q|\lambda V|q\rangle\Big/\left(1-\sum_k\frac{\langle q|\lambda V|k\rangle f(k,q)}{E-\frac{1}{2}k^2+i\eta}\right) \tag{14}$$

with $f(k,q)$ satisfying the integral equation

$$f(k,q)=\frac{\langle k|\lambda V|q\rangle}{\lambda V_0}+\sum_{k'}\left(\langle k|\lambda V|k'\rangle-\frac{\langle k|\lambda V|q\rangle\langle q|\lambda V|k'\rangle}{\lambda V_0}\right)\times\frac{f(k',q)}{(E-\frac{1}{2}k'^2+i\eta)}, \tag{15}$$

where $V_0=\langle q|V|q\rangle$. The bound states correspond to the zeros of the function in the denominator of expression (14). Now, since Eq. (15) allows an iterative solution for $f(k,q)$, one can locate the zeros of the denominator and hence obtain the bound-state energy perturbatively. Before proceeding with the perturbative derivation of the

one-dimensional bound-state energy, we note that in n dimensions the denominator in (14) is

$$D(E)=1-\int \frac{d^nk}{(2\pi)^n}\frac{\langle q|\lambda V|k\rangle f(k,q)}{(E-\frac{1}{2}k^2+i\eta)}. \tag{16}$$

It is easily seen that the integral diverges in the limit $E\to 0$ for $n\leq 2$ so that $D(E)$ always has a zero in these cases for $\lambda\to 0$ if the potential is attractive. This explains the well-known fact that an attractive short-range potential always produces a bound state in one or two dimensions howsoever small be the coupling, but not in three dimensions.

To illustrate the iterative procedure for the perturbative evaluation of bound-state energy in one dimension, we consider the first-order solution for $f(k,q)$,

$$f(k,q)=\langle k|\lambda V|q\rangle/\lambda V_0, \tag{17}$$

which leads to

$$D(E)=1-\frac{1}{2\pi}\int dk\frac{\langle q|\lambda V|k\rangle\langle k|\lambda V|q\rangle}{\lambda V_0(E-\frac{1}{2}k^2+i\eta)}. \tag{18}$$

One then uses the expression

$$\langle q|\lambda V|k\rangle=\int dx\,\lambda V(x)e^{i(k-q)x}, \tag{19}$$

and carries out the k integration to get

$$D(E)=1+\frac{i\lambda}{q}\int dx\,dy\,\frac{V(x)V(y)}{V_0}e^{iq(|x-y|+x-y)}. \tag{20}$$

Expanding the exponential function for $q\to 0$ and retaining only the first two terms to be consistent with the order of the iteration, we have

$$D(E)=1+\frac{i\lambda}{q}V_0-\frac{\lambda}{V_0}\int dx\,dy\,V(x)V(y)|x-y|\,dx\,dy. \tag{21}$$

From the condition that $D(E)$ should vanish at bound-state energies and the relation $q=\sqrt{2E}$, one finally obtains

$$-(-2E)^{1/2}=\lambda\int dx\,V(x)+\lambda^2\int dx\,dy\,V(x)V(y)|x-y|, \tag{22}$$

which agrees with the expression (2) of Abarbanel, Callen, and Goldberger.[2] We proceed along the same lines but include the next two terms in the iterative solution for $f(k,q)$:

$$f(k,q)=\frac{\langle k|\lambda V|q\rangle}{\lambda V_0}+\int\frac{dk'}{2\pi(E-\frac{1}{2}k'^2+i\eta)}\left(\langle k|\lambda V|k'\rangle-\frac{\langle k|\lambda V|q\rangle\langle q|\lambda V|k'\rangle}{\lambda V_0}\right)$$
$$\times\left[\frac{\langle k'|\lambda V|q\rangle}{\lambda V_0}+\int\frac{dk''}{2\pi(E-\frac{1}{2}k''^2+i\eta)}\right.$$
$$\left.\times\left(\langle k'|\lambda V|k''\rangle-\frac{\langle k'|\lambda V|q\rangle\langle q|\lambda V|k''\rangle}{\lambda V_0}\right)\frac{\langle k''|\lambda V|q\rangle}{\lambda V_0}\right]. \tag{23}$$

One again uses expression (19) for the potential matrix elements, integrates over the k, k', and k'' variables, carries out an expansion in powers of q, and finally obtains from the condition that $D(E)=0$ at bound-state energies,

$$-(-2E)^{1/2}=\lambda\int dx\,V(x)+\lambda^2\int dx\,dy\,V(x)V(y)|x-y|$$
$$+\tfrac{1}{6}\lambda^3\int dx\,dy\,dz\,V(x)V(y)V(z)(|x-y|+|y-z|+|z-x|)^2$$
$$+\tfrac{1}{6}\lambda^4\int dx\,dy\,dz\,dt\,V(x)V(y)V(z)V(t)$$
$$\times(|x-y|^3+6|x-y|^2|x-z|+3|x-y|^2|z-t|+6|x-y||y-z||z-t|). \tag{24}$$

We have evaluated these terms for a particle in a square well of depth v_0 and width a, to get

$$(-2E)^{1/2}=av_0-\tfrac{1}{3}a^3v_0^2+\tfrac{1}{5}a^5v_0^3-\tfrac{46}{315}a^7v_0^4 \tag{25}$$

which agrees with the iterative solution for the bound-state energy obtained by solving the equation

$$(-2E)^{1/2}=[2(v_0+E)]^{1/2}\tan\{[2(v_0+E)]^{1/2}\tfrac{1}{2}a\} \tag{26}$$

for the square well. Of course, expression (24) is meaningful only if the integrals occurring in it exist; i.e., the potentials are of short range.

III. LONG-RANGE INTERACTIONS

In this section we discuss the modifications required if the interactions are of long range. It may be noted that the case of $V(x) \to a_\pm |x|^{-1}$ for $x \to \pm\infty$ requires special consideration, since V_0 in Eq. (15) is not defined for this potential and therefore one cannot use the analysis in terms of the forward-scattering amplitude. We first discuss the potentials for which

$$V(x) \to -a_\pm |x|^{-n} \text{ for } x \to \pm\infty, \quad n = 2, 3, 4. \tag{27}$$

The analysis for such potentials may be illustrated by considering an integral of the type

$$I = \int_{-\infty}^{\infty} dx\, V(x)\, e^{iq|x-y|}, \tag{28}$$

which for example occurs in Eq. (20). This integral can be written as

$$I = \int_{-1/q}^{1/q} dx\, V(x) e^{iq|x-y|} + \int_{1/q}^{\infty} dx\, V(x) e^{iq|x-y|} + \int_{-\infty}^{-1/q} dx\, V(x) e^{iq|x-y|} \tag{29}$$

$$\underset{q\to 0}{\sim} \int_{-1/q}^{1/q} dx\, V(x) \sum_{j=0}^{n-1} \frac{1}{j!} (iq|x-y|)^j + O(q^{n-1}). \tag{30}$$

To extract the leading terms, the prescription then is to retain terms up to order $|x-y|^{n-1}$ and integrate from $-1/q$ to $1/q$. Since $q \sim \lambda$, the integral can equivalently be carried out between the limits $(-1/\lambda, 1/\lambda)$. This immediately leads to the following results:

for $n = 2$,

$$-(-2E)^{1/2} = \lambda \int dx\, V(x) + 2\lambda^2 (\ln\lambda)(a_+ + a_-) \int dx\, V(x) + O(\lambda^2), \tag{31}$$

for $n = 3$,

$$-(-2E)^{1/2} = \lambda \int dx\, V(x) + \lambda^2 \int dx\, dy\, V(x)V(y)|x-y| + 2\lambda^3 (\ln\lambda)(a_+ + a_-)\left(\int V(x)\, dx\right)^2 + O(\lambda^3), \tag{32}$$

for $n = 4$,

$$\begin{aligned} -(-2E)^{1/2} = {} & \lambda \int dx\, V(x) + \lambda^2 \int dx\, dy\, V(x)V(y)|x-y| \\ & + \tfrac{1}{6}\lambda^3 \int dx\, dy\, dz\, V(x)V(y)V(z)(|x-y| + |y-z| + |z-x|)^2 \\ & + \tfrac{4}{3}\lambda^4 (\ln\lambda)(a_+ + a_-)\left(\int V(x) dx\right)^3 + O(\lambda^4). \end{aligned} \tag{33}$$

Relation (31) is a slight generalization of result (3) obtained by Blankenbecler, Goldberger, and Simon and reduces to their expression for $a_+ = a_- = a$, while the remaining two relations are new results.

For potentials of the type

$$V(x) \to -a_\pm |x|^{-1} \text{ for } x \to \pm\infty, \tag{34}$$

the forward scattering amplitude is not defined and hence one cannot use Eqs. (14) and (15). Alternatively, we may analyze the bound states in terms of the backward scattering amplitude. The corresponding equations are obtained by writing

$$\langle k|T|q\rangle = g(k,q)\langle -q|T|q\rangle, \tag{35}$$

where $\langle -q|T|q\rangle$ is the backward scattering amplitude and $g(-q,q) = 1$. On substituting this relation in Eq. (12), one obtains

$$\langle -q|T|q\rangle = \langle -q|\lambda V|q\rangle \Big/ \left(1 - \sum_k \frac{\langle -q|\lambda V|k\rangle\, g(k,q)}{E - \frac{1}{2}k^2 + i\eta}\right), \tag{36}$$

with $g(k,q)$ satisfying the integral equation

$$g(k,q)=\frac{\langle k|\lambda V|q\rangle}{\lambda V_1}+\sum_{k'}\left(\langle k|\lambda V|k'\rangle-\frac{\langle k|\lambda V|q\rangle\langle -q|\lambda V|k'\rangle}{\lambda V_1}\right)\times\frac{g(k',q)}{E-\frac{1}{2}k'^2+i\eta},\tag{37}$$

where $V_1=\langle -q|V|q\rangle$. The bound states once again correspond to the zeros the denominator of expression (36). Though this function is somewhat more complicated in the general case than the corresponding function in Eq. (14), it has the advantage that it is well defined for potentials (34) which have a Coulomb tail.

We retain the leading iterative solution for $g(k,q)$,

$$g(k,q)=\langle k|\lambda V|q\rangle/\lambda V_1,\tag{38}$$

which leads to an expression

$$D_1(E)=1-\int\frac{dk}{2\pi}\frac{\langle -q|\lambda V|k\rangle\langle k|\lambda V|q\rangle}{(E-\frac{1}{2}k^2+i\eta)(\lambda V_1)},\tag{39}$$

for the denominator in Eq. (36). For potential $V(x)$ in (34) one has the leading behavior

$$\langle k|V|q\rangle\underset{k,q\to 0}{\sim}(a_++a_-)\ln|k-q|.\tag{40}$$

We substitute this in (39) and carry out the k integration to obtain

$$D_1(E)=1+\tfrac{1}{2}\lambda(a_++a_-)(\ln|2E|)/|2E|^{1/2}.\tag{41}$$

This is zero for

$$-(-2E)^{1/2}=(a_++a_-)\lambda(\ln\lambda+\ln\ln\lambda)+O(\lambda)\tag{42}$$

which gives the energy of the bound state.

It is possible to obtain the bound-state energy for Hamiltonian (6), for $\gamma\to\infty$, by using the above result (42). We first note that Eq. (36) is valid for the three-dimensional Hamiltonian as well. Specifically for the Hamiltonian in (6), we take the unperturbed Hamiltonian to consist of the kinetic energy and the simple harmonic potential, so that the states $|k\rangle$ contain harmonic oscillator states for motion in the xy plane and free states for for motion in the z direction; the "weak" Coulomb potential $(-\alpha)(4/\gamma)^{1/4}(1/r)$ serves as the λV perturbation. Now, since the oscillator energies are separated by finite energies, for the limit $k\to 0$ one needs to include only the ground state in the summation of the oscillator states. This reduces the problem to a one-dimensional problem with the effective potential being given by an expectation value of $1/r$ between the oscillator states. Thus we have

$$\left\langle k\left|\frac{1}{r}\right|q\right\rangle=\frac{1}{\pi}\int dx\,dy\,dz\,e^{-(x^2+y^2)}e^{i(q-k)z}\left(\frac{1}{r}\right)\underset{k,q\to 0}{\sim}-2\ln|k-q|,\tag{43}$$

from which it follows that the bound-state energy for the Hamiltonian in (6) can be obtained from Eq. (42) with $\lambda=\alpha(4/\gamma)^{1/4}$. Including the oscillator energy and multiplying by $(\frac{1}{4}\gamma)^{1/2}$, one finally gets

$$E\underset{\gamma\to\infty}{\sim}\tfrac{1}{2}\gamma^{1/2}-2\alpha^2[\tfrac{1}{2}\ln(\tfrac{1}{4}\gamma)^{1/2}-\ln\ln(\tfrac{1}{4}\gamma)^{1/2}+O(1)]^2.\tag{44}$$

This expression agrees with the known results.[4]

IV. THE THREE-BODY PROBLEM

In this section we discuss the problem of a bound state for the Hamiltonian

$$H=-\frac{1}{2}\frac{d^2}{dx_1^2}-\frac{1}{2}\frac{d^2}{dx_2^2}+\lambda_1u(x_1)+\lambda_2v(x_2)+\lambda_3w(|x_1-x_2|),\tag{45}$$

in the weak coupling limit $\lambda_i\to 0$. The general problem is much too complicated so that one is forced to make some approximations. In particular, we obtain an expression for the bound-state energy which is valid if $\lambda_3\ll\lambda_1,\lambda_2$.

First consider the case of short-range interactions. If the particles are to be bound, at least one of the two potentials, $u(x_1)$ or $v(x_2)$, has to be attractive. Let us assume that $v(x_2)$ is attractive and that particle 2 is bound with the ground-state energy ϵ_0 given by expression (24),

$$\epsilon_0=-\tfrac{1}{2}\Big(\lambda_2\int dx\,v(x)+\lambda_2^2\int dx\,dy\,v(x)v(y)|x-y|+\frac{1}{6}\lambda_2^3\int dx\,dy\,dz\,v(x)v(y)v(z)(|x-y|+|y-z|+|z-x|)^2+\frac{1}{6}\lambda_2^4\int dx\,dy\,dz\,dt\,v(x)v(y)v(z)v(t)\times(|x-y|^3+6|x-y|^2|x-z|+3|x-y|^2|z-t|+6|x-y||y-z||z-t|)+O(\lambda_2^5)\Big)^2.\tag{46}$$

We now analyze the scattering of particle 1 in the forward direction by the potential

$$\lambda V = \lambda_1 u(x_1) + \lambda_3 w(|x_1 - x_2|)\,, \tag{47}$$

with particle 2 being in the ground state both in the initial and the final state. Let the states of particle 2 be designated by $|i\rangle$ and the corresponding energy by ϵ_i, $i=0$ being the ground state with the energy given by Eq. (46). Then the three-body bound-state energy is given by the position of the zero of the denominator function

$$D(E) = 1 - \int \frac{dk}{2\pi} \sum_i \frac{\langle q,0|\lambda V|k,i\rangle f(k,i;q,0)}{E - \epsilon_i - \frac{1}{2}k^2 + i\eta}\,, \tag{48}$$

with $f(k,i;q,0)$ satisfying the integral equation

$$f(k,i;q,0) = \frac{\langle k,i|\lambda V|q,0\rangle}{\lambda V_0} + \int \frac{dk'}{2\pi} \sum_j \left(\langle k,i|\lambda V|k',j\rangle - \frac{\langle k,i|\lambda V|q,0\rangle\langle q,0|\lambda V|k',j\rangle}{\lambda V_0}\right) \frac{f(k',j;q,0)}{(E - \epsilon_j - \frac{1}{2}k'^2 + i\eta)}\,, \tag{49}$$

where $E - \epsilon_0 = \frac{1}{2}q^2$ and $\lambda V_0 = \langle q,0|\lambda V|q,0\rangle$, analogous to Eq. (15). The matrix elements of λV are given by

$$\langle k,i|\lambda V|k',j\rangle = \lambda_1 \int dx\, u(x) e^{i(k'-k)x}\delta_{ij} + \lambda_3 \int dx\, w(x) e^{i(k'-k)x}\langle i|e^{i(k'-k)x_2}|j\rangle\,. \tag{50}$$

We now introduce our major approximation by replacing ϵ_i and ϵ_j by ϵ_0 in the summation over the states. Since u connects only the diagonal elements in the space of i, j states, this introduces errors only in terms of second or higher order in λ_3. It may be observed that the errors tend to zero in the region of large k or k' integrations. The approximation may therefore be worthwhile even in cases where λ_3 is not small. Of course, the results are rigorous up to terms which are first order in λ_3. With this approximation, the summation over i and j can be carried out, leading to

$$D(E) = 1 - \int \frac{dk}{2\pi} \frac{\langle q,0|\lambda V|k\rangle f(k;q,0)}{E - \epsilon_0 - \frac{1}{2}k^2 + i\eta}\,, \tag{51}$$

and

$$f(k;q,0) = \frac{\langle k|\lambda V|q,0\rangle}{\lambda V_0} + \int \frac{dk'}{2\pi} \left(\langle k|\lambda V|k'\rangle - \frac{\langle k|\lambda V|q,0\rangle\langle q,0|\lambda V|k'\rangle}{\lambda V_0}\right) \frac{f(k';q,0)}{(E - \epsilon_0 - \frac{1}{2}k'^2 + i\eta)}\,. \tag{52}$$

These equations can be analyzed to give the bound-state energy in the weak-coupling limit and to first order in λ_3.

It should be noted that while there is no pole in the integrand of Eq. (52), the w-matrix elements are not smooth near $k'=0$ because of factors of the type $\langle 0|\exp[i(k'-k)x_2]|0\rangle$ observed in Eq. (50). The origin of this nonsmooth behavior is essentially the fact that $w(|x_1 - x_2|)$ may not be small for $x_1 \to \infty$, if $x_2 \to \infty$. However, one can then argue that every successive iteration brings in terms which are of higher order either in λ_1 or in $(\lambda_3/\lambda_1, \lambda_3/\lambda_2)$. Hence the leading terms in the first order of λ_3 are obtained from the first two terms in the iterative solution for $f(k,i;q,0)$. Finally, for carrying out the k and k' integrations, we use the integral representation (19) for the potentials and use

$$\psi(x_2) = |2\epsilon_0|^{1/4} \exp(-|2\epsilon_0|^{1/2}|x_2|) \tag{53}$$

for the bound-state wave functions[1] in evaluating the integrals in the x_2 space. For example, the first iterative solution for $f(k,i;q,0)$ leads to

$$D(E) = 1 + \frac{i\lambda_1}{q} \int dx\, dy\, \frac{u(x)u(y)}{u_0} e^{iq(|x-y|+x-y)} + \frac{\lambda_3 w_0 |\epsilon_0|^{1/2}}{(2|E-\epsilon_0|)^{1/2}(|\epsilon_0|^{1/2} + |E-\epsilon_0|^{1/2})}\,, \tag{54}$$

where

$$u_0 = \int u(x)dx\,, \tag{55}$$

$$w_0 = \int w(x)dx\,. \tag{56}$$

Using higher-order iterative solutions for $f(k,i;q,0)$, analogous to Eq. (23) but retaining only the leading

terms in the first order of λ_3, we finally obtain

$$E=-\tfrac{1}{2}\Big(\lambda_1\int dx\,u(x)+\lambda_1^2\int dx\,dy u(x)u(y)|x-y|$$
$$+\tfrac{1}{6}\lambda_1^3\int dx\,dy\,dz\,u(x)u(y)u(z)(|x-y|+|y-z|+|z-x|)^2$$
$$+\tfrac{1}{6}\lambda_1^4\int dx\,dy\,dz\,dt\,u(x)u(y)u(z)u(t)(|x-y|^3+6|x-y|^2|x-z|$$
$$+3|x-y|^2|z-t|+6|x-y||y-z||z-t|)\Big)^2$$
$$+\epsilon_0-\lambda_1\lambda_2\lambda_3\frac{w_0u_0|v_0|}{|\lambda_1u_0|+|\lambda_2v_0|}+O(\lambda^6)+O(\lambda_3\lambda^2)+O(\lambda_3^2)\,, \tag{57}$$

where ϵ_0 is defined in (46), λ stands for λ_1 or λ_2, and

$$v_0=\int v(x)dx\,. \tag{58}$$

To the order specified, this is a rigorous result for short-range potentials.

V. He-LIKE ATOMS IN A STRONG MAGNETIC FIELD

The Hamiltonian for a two-electron atom in a strong magnetic field is given by

$$H=\tfrac{1}{2}p_1^2+\tfrac{1}{2}p_2^2-\frac{\alpha}{r_1}-\frac{\alpha}{r_2}+\frac{1}{r_{12}}+\frac{\gamma}{8}(x_1^2+y_1^2+x_2^2+y_2^2)\,, \tag{59}$$

where α is the charge of the nucleus. Under the scale transformation

$$p_i\to(\tfrac{1}{4}\gamma)^{1/4}p_i\,,\quad r_i\to(4/\gamma)^{1/4}r_i\,, \tag{60}$$

the Hamiltonian becomes

$$H'=\Big(\frac{\gamma}{4}\Big)^{1/2}\Big(\tfrac{1}{2}p_1^2+\tfrac{1}{2}p_2^2-\frac{\alpha(4/\gamma)^{1/4}}{r_1}-\frac{\alpha(4/\gamma)^{1/4}}{r_2}+\frac{(4/\gamma)^{1/4}}{r_{12}}+\tfrac{1}{2}(x_1^2+y_1^2+x_2^2+y_2^2)\Big)\,. \tag{61}$$

For $\gamma\to\infty$, the problem reduces essentially to one-dimensional motion in the z direction, but with the potential having a Coulomb tail. As was mentioned before, for a potential with a Coulomb tail, the forward scattering amplitude is not defined. However, one can analyze the bound-state energy in terms of poles of the backward scattering amplitude.

The denominator function for the backward scattering is

$$D_1(E)=1-\int\frac{dk}{2\pi}\sum_i\frac{\langle -q,0|\lambda V|k,i\rangle g(k,i;q,0)}{E-\epsilon_i-\frac{1}{2}k^2+i\eta}\,, \tag{62}$$

with

$$g(k,i;q,0)=\frac{\langle k,i|\lambda V|q,0\rangle}{\lambda V_1}+\int\frac{dk'}{2\pi}\sum_j\Big(\langle k,i|\lambda V|k',j\rangle-\frac{\langle k,i|\lambda V|q,0\rangle\langle -q,0|\lambda V|k',j\rangle}{\lambda V_1}\Big)\frac{g(k',j;q,0)}{(E-\epsilon_j-\frac{1}{2}k'^2+i\eta)}\,, \tag{63}$$

where $\lambda V_1=\langle -q,0|\lambda V|q,0\rangle$, analogous to Eq. (37). As before we replace ϵ_i and ϵ_j by ϵ_0 and carry out the summation over i and j to obtain

$$D_1(E)=1-\int\frac{dk}{2\pi}\frac{\langle -q,0|\lambda V|k\rangle g(k;q,0)}{E-\epsilon_0-\frac{1}{2}k^2+i\eta}\,, \tag{64}$$

and

$$g(k;q,0)=\frac{\langle k|\lambda V|q,0\rangle}{\lambda V_1}+\int\frac{dk'}{2\pi}\Big(\langle k|\lambda V|k'\rangle-\frac{\langle k|\lambda V|q,0\rangle\langle -q,0|\lambda V|k'\rangle}{\lambda V_1}\Big)\frac{g(k';q,0)}{(E-\epsilon_0-\frac{1}{2}k'^2+i\eta)}\,. \tag{65}$$

These equations can be used to analyze the ground-state energy of Hamiltonian (61). For this we take the unperturbed Hamiltonian to consist of the kinetic energy, the simple harmonic potential, and the term

$-\alpha(4/\gamma)^{1/4}(1/r_2)$ so that the states consist of oscillator wave functions in the x and y variables, free-particle wave functions in the z_1 variables, and weakly coupled bound states in the z_2 variable with the ground-state energy

$$\epsilon_0 = -\frac{4\alpha^2}{\gamma^{1/2}}\left[\tfrac{1}{2}\ln\left(\frac{\gamma}{4}\right)^{1/2} - \ln\ln\left(\frac{\gamma}{4}\right)^{1/2}\right]^2, \tag{66}$$

as given in Eq. (44). The scattering potential is

$$\lambda V = -\alpha\left(\frac{4}{\gamma}\right)^{1/4}\left(\frac{1}{r_1}\right)+\left(\frac{4}{\gamma}\right)^{1/4}\left(\frac{1}{r_{12}}\right). \tag{67}$$

For $k, k' \to 0$, one needs to include only the ground state of the oscillator states which essentially reduces the problem to a one dimensional problem with the effective potential being given by an expectation value between the oscillator ground states:

$$\left\langle k\left|\frac{1}{r_1}\right|k'\right\rangle = \frac{1}{\pi}\int dx_1 dy_1 dz_1 e^{-(x_1^2+y_1^2)} e^{i(k'-k)z_1}\left(\frac{1}{r_1}\right)$$
$$\underset{k,k'\to 0}{\sim} -2\ln|k-k'|, \tag{68}$$

and

$$\left\langle k\left|\frac{1}{r_{12}}\right|k'\right\rangle = \frac{1}{\pi^2}\int dx_1 dy_1 dz_1 dx_2 dy_2 \exp[-(x_1^2+y_1^2+x_2^2+y_2^2)]\, e^{i(k'-k)z_1}\left(\frac{1}{r_{12}}\right)$$
$$\underset{k,k'\to 0}{\sim} -2(\ln|k-k'|)e^{i(k'-k)z_2}. \tag{69}$$

For calculating the expectation value of this last expression between the bound-state wave functions of particle 2, we take the wave function to be the same as Eq. (53) but with ϵ_0 given by (66).

In order that $D_1(E)$ includes the leading terms in the first order of the interaction between the two electrons, we use the twice iterated solution for $g(k;q,0)$, i.e., the expression in Eq. (63) with the $g(k';q,0)$ on the right-hand side replaced by $\langle k|\lambda V|q,0\rangle/\lambda V_1$. We finally get

$$D_1(E) = 1 + 2\left(\frac{4}{\gamma}\right)^{1/4} \times\left(\frac{\ln|E-\epsilon_0|^{1/2}}{(2|E-\epsilon_0|)^{1/2}}\right)\left(\alpha - \frac{|\epsilon_0|^{1/2}}{|\epsilon_0|^{1/2}+|E-\epsilon_0|^{1/2}}\right), \tag{70}$$

which, to leading order in α, reduces to

$$D_1(E) = 1 + \left(\frac{4}{\gamma}\right)^{1/4}(2\alpha-1)\frac{\ln|E-\epsilon_0|^{1/2}}{(2|E-\epsilon_0|)^{1/2}}. \tag{71}$$

This expression is equated to zero to give the bound-state energy. Finally, including the oscillator energy and multiplying by $(\gamma/4)^{1/2}$, one gets the bound-state energy of the two-electron atom in a strong magnetic field:

$$E' \underset{\gamma\to\infty}{\sim} \gamma^{1/2} - 2\alpha(2\alpha-1)[\tfrac{1}{2}\ln(\tfrac{1}{4})^{1/2} - \ln\ln(\tfrac{1}{4}\gamma)^{1/2}]^2. \tag{72}$$

The above result is valid for $\alpha \gg 1$. It is interesting to compare this expression with a simple variational calculation for the ground-state energy of the scale transformed Hamiltonian (61). If we use oscillator ground-state wave functions for the x and y variables, and wave functions (53) for the z variable, one obtains for $\gamma \to \infty$,

$$E \approx (\tfrac{1}{4}\gamma)^{1/2}[2 + |2\epsilon_0| - (4\alpha-1)(4/\gamma)^{1/4}|2\epsilon_0|^{1/2}\ln|2\epsilon_0|^{1/2}], \tag{73}$$

where we have used the fact that ϵ_0 is expected to be small. Taking ϵ_0 as a variational parameter, one finds for the variational energy

$$E_{\text{var}} \approx \gamma^{1/2} - (2\alpha - \tfrac{1}{2})^2[\tfrac{1}{2}\ln(\tfrac{1}{4}\gamma)^{1/2} - \ln\ln(\tfrac{1}{4}\gamma)^{1/2}]^2. \tag{74}$$

This expression is equivalent to an independent-particle approximation with a screened nuclear charge of $z-\frac{1}{4}$ which may be compared with the corresponding charge of $z-\frac{5}{16}$ for the case of $\gamma = 0$. The variational expression agrees very well with expression (72). Even for He, the coefficients of the second term agree to within about 2%. Therefore though we derived expression (72) under an assumption that $\alpha \gg 1$, it may be a good approximation for He as well, i.e., for $\alpha = 2$.

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