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THE SOLUTION OF THE DELTA FUNCTION MODEL FOR HELIUM-LIKE IONS*

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ABSTRACT

A one dimensional Fredholm integral equation is derived for the ground state solution of the delta-function model for two electron Helium-like ions. This equation is solved numerically; the perturbation series is developed through $E^{(20)}$ and compared with the solution of the integral equation. The series is further analyzed in terms of the singularity which determines its radius of convergence.

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Introduction

The δ-function model for He-like 2-electron systems is a one-dimensional analogue of the physical He problem in which the two particles are constrained to move along the real line and all coulombic terms are replaced by δ-functions. It is a natural generalization of the δ-function model for the hydrogen atom in which the single electron is constrained to the real line and the coulombic attraction term is replaced by a single δ-function. Such a model for 2-electron systems is not the only one which has been suggested. Benson, White, and Byers-Brown[1] have also considered the so called Hooke's law He atom in which the coulombic attraction terms are replaced with harmonic oscillator potentials and the repulsion term is left unchanged.

δ-functions have been used for some time as models to study the real coulomb problem. Quite recently several authors have used these potentials to study collections of a large number of interacting boson-fermion systems.[2] This study will concentrate on the simplest such system, the two electron ions.

The point of the study is really twofold. We will attempt to answer the question, how well does the model correspond to reality and where or how does it fail to do so? This can be done by solving the model exactly and we present a potentially exact solution. In the second part of the paper we obtain the perturbation energies through 20th order. We attempt to analyze the convergence of the series they constitute, in order to investigate for a specific problem where such

a perturbation series breaks down and what happens when it does.

Section I describes the Hamiltonian, the perturbation, the solution of the unperturbed problem; some general remarks about the solution of the perturbed problem are included as well. Section II contains the method of exact solution, a discussion of the integral equation and a presentation of numerical results. Section III presents some theoretical and numerical arguments about the nature of the computed results. Section IV contains a derivation of the equations for the perturbation series and a listing of the perturbation energies through 20th order. Section V attempts an analysis of these perturbation energies in terms of the singularity which determines the radius of convergence of the series they constitute.

I. Statement of Problem

The Hamiltonian for the model described in the introduction is in suitable units:

$$-\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - \delta(x) - \delta(y) + \lambda\,\delta(x-y) \qquad (1)$$

Here $\lambda = 1/Z$, where Z is the charge on the nucleus; thus λ measures the strength of the perturbation. $\lambda = 0$ defines the unperturbed problem and non - 0 λ represents a finite interaction between the two particles of strength λ. The unperturbed problem is separable. The solution consists of a single bound state of energy -1, a singly excited continuum beginning at $E = -\frac{1}{2}$, obtained by exciting one of the particles to the continuum and a doubly excited continuum beginning at $E = 0$, obtained by exciting both particles to the continuum

Using the Weyl comparison theorem[3] one may determine the number of bound states which equation (1) possesses.

For finite positive λ the potential is bounded below by the unperturbed potential; thus there exists at most one bound state. For negative λ the potential is bounded below by the potential of equation (2), with two interactions of strength λ.

$$\left\{-\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - \delta(x) - \delta(y) + \lambda\left[\delta(x-y) + \delta(x+y)\right]\right\}\psi = E\psi \tag{2}$$

This problem (which is exactly soluble) also has only one bound state[4]; thus the original problem has also <u>at most</u> one bound state. Furthermore for negative λ the potential of (1) is bounded above by the unperturbed potential; thus there must exist <u>at least</u> one bound state. These two statements together imply the existence of a single bound state for negative λ. The argument is equally valid for positive $\lambda < 1$, where the bound state of equation (2) disappears. Beyond this point all that can be said is that there may exist at most a single bound state. The continuum solutions of (1) begin at $E = -\frac{1}{2}$, just as in the unperturbed problem. These continuum solutions may in fact be constructed from the unperturbed problem by taking the simple anti-symmetric combination $\varphi_b^0(x)\varphi_e^0(y) - \varphi_b^0(y)\varphi_e^0(x)$ where $\varphi_b^0(x) = e^{-|x|}$, $\varphi_e^0(x) = \sin kx$ or $\cos k[|x|+\Delta]$, $\tan k\Delta = 1/k$. Whether the bound state crosses into continuum cannot be answered by arguments of this general nature.

II. Method of Exact Solution

We solve equation (1) exactly with a 2-dimensional Fourier

transform. Letting

$$G(k_1, k_2) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{ik_1x} e^{ik_2y} \psi(x,y)\,dx\,dy,$$

G satisfies equation (3):

$$\frac{1}{2}(k_1^2 + k_2^2 + p^2)G(k_1, k_2) - \int_{-\infty}^{\infty} e^{ik_2y}\psi(0,y)$$
$$-\int_{-\infty}^{\infty} e^{ik_1x}\psi(x,0)\,dx + \lambda\int_{-\infty}^{\infty} e^{i(k_1+k_2)x}\psi(x,x)\,dx = 0 \qquad (3)$$

with $E = -p^2/2$.

We are interested in the symmetric ground state solution, $\psi(x,y) = \psi(y,x)$; $\psi(-x,y) = \psi(x,y)$; $\psi(x,-y) = \psi(x,y)$. This implies $\psi(x,0) = \psi(0,x)$ and that $\psi(x,0)$ and $\psi(x,x)$ $(\psi(x,x) = \psi(-x,x) = \psi(-x,-x))$ are even functions of x. Writing

$$F(k) = \int_{-\infty}^{\infty} e^{ikx}\psi(x,0)\,dx$$
$$H(k) = \int_{-\infty}^{\infty} e^{ikx}\psi(x,x)\,dx$$

(3) becomes

$$G(k_1, k_2) = \frac{F(k_1) + F(k_2) - \lambda H(k_1+k_2)}{\frac{1}{2}(k_1^2 + k_2^2 + p^2)} \qquad (4)$$

That is, the unknown function G of the two variables k_1 and k_2 may be expressed in terms of two unknown functions, F and H, each of which depend only on a single variable, and a known denominator which depends on k_1 and k_2. These two functions F and H are obviously related in some way; they are obtained by Fourier transforming a single function $\psi(x,y)$ along with x axis and along the line y = x respectively. Below we deduce what that relation is. But the essential point is that via equation (4) the problem of determing the unknown function G of two variables simplifies to the problem of determing the two

(related) functions of one variable, F and H.

To obtain equations for F and H, note that inverse Fourier transforming G gives back the function ψ (x,y) in terms of integrals over F and H. We use this expression and the definitions of $F(k) = \int e^{ikx}\psi(x,0)$ and $H(k) = \int e^{ikx}\psi(x,x)$ to get two coupled integral equations for the functions F and H. Thus

$$\psi(x,y) = \frac{1}{(2\pi)^2}\iint e^{-ik_1x}e^{-ik_2y}\,G(k_1,k_2)\,dk_1\,dk_2$$

$$= \frac{1}{(2\pi)^2}\iint e^{-ik_1x}e^{-ik_2y}\left[\frac{F(k_1)+F(k_2)-\lambda H(k_1+k_2)}{\frac{1}{2}(k_1^2+k_2^2+p^2)}\right]dk_1\,dk_2$$

and

$$F(k) = \int e^{ikx}\psi(x,0)\,dx = \frac{1}{(2\pi)^2}\iiint e^{i(k-k_1)x}\left[\frac{F(k_1)+F(k_2)-\lambda H(k_1+k_2)}{\frac{1}{2}(k_1^2+k_2^2+p^2)}\right]dk_1\,dk_2\,dx$$

$$H(k) = \int e^{ikx}\psi(x,x)\,dx = \left(\frac{1}{2\pi}\right)^2\iiint e^{i(k-k_1-k_2)x}\left[\frac{F(k_1)+F(k_2)-\lambda H(k_1+k_2)}{\frac{1}{2}(k_1^2+k_2^2+p^2)}\right]dk_1\,dk_2\,dx\,.$$

These simplify to

$$F(k) = \frac{1}{2\pi}\int\frac{[F(k)+F(k')]\,dk'}{\frac{1}{2}(k^2+k'^2+p^2)} - \frac{\lambda}{2\pi}\int\frac{H(k+k')}{\frac{1}{2}(k^2+k'^2+p^2)}\,dk'$$

and

$$H(k) = \frac{2}{2\pi}\int\frac{F(k-k')\,dk'}{\frac{1}{2}[(k-k')^2+k'^2+p^2]} - \frac{\lambda}{2\pi}H(k)\int\frac{dk'}{\frac{1}{2}[(k-k')^2+k'^2+p^2]}$$

which further simplify to

$$F(k) = \frac{1}{\pi}\int\frac{F(k')}{k^2+k'^2+p^2} + \frac{F(k)}{\sqrt{k^2+p^2}} - \frac{\lambda}{\pi}\int\frac{H(k')\,dk'}{(k^2+(k-k')^2+p^2)}$$

and

$$H(k) = \frac{2}{\pi}\int\frac{F(k')}{[(k'-k)^2+k'^2+p^2]} - \frac{\lambda\,H(k)}{\sqrt{k^2+2p^2}}$$

The second of these equations gives H in terms of an integral over F which may then be substituted into the first to give a single integral equation for the function F:

$$F(k) = \frac{1}{\pi}\int \frac{F(k')\,dk'}{k^2+k'^2+p^2} + \frac{F(k)}{\sqrt{k^2+p^2}} - \frac{2\lambda}{\pi^2}\int \frac{dk'}{[(k'-k)^2+k^2+p^2]}\int \frac{F(k'')\,dk''}{[(k''-k')^2+k''^2+p^2]}\,\frac{\sqrt{2p^2+k'^2}}{(\sqrt{2p^2+k'^2}+\lambda)} \tag{5}$$

The integral over k' in the last term of (5) may be worked out explicitly. Equation (5) is thus of the form

$$F(k)\,\phi(k) = \int_{-\infty}^{\infty} K(k,k')\,F(k')\,dk' \tag{6}$$

with

$$\phi(k) = 1 - \frac{1}{\sqrt{k^2+p^2}} \tag{7}$$

and

$$K(k,k') = \frac{1}{\pi}\,\frac{1}{k^2+k'^2+p^2} - \frac{2\lambda}{\pi^2}\int_{-\infty}^{\infty} \frac{dk''}{[k^2+(k-k'')^2+p^2]}\,\frac{1}{[k'^2+(k'-k'')^2+p^2]}\,\frac{\sqrt{2p^2+k''^2}}{(\sqrt{2p^2+k''^2}+\lambda)} \tag{8}$$

Thus the bound state solutions of equation (1) are the normalizable solutions of (6) with ϕ and K given by (7) and (8); the eigenvalues $E = -p^2/2$ are the values of p^2 which for each λ allow such normalizable solutions.

Equation (6) is (almost) of the standard Fredholm type. It may in fact be cast in this form provided the function $\phi(k)$ never vanishes. If this is the case (i.e. if $p^2 > 1$) we may write

$$\tilde{F}(k) = \mu \int_{-\infty}^{\infty} \tilde{K}(k,k')\tilde{F}(k')\,dk' \tag{9}$$

with $\tilde{F}(k) = F(k)\sqrt{\phi(k)}$, $\tilde{K}(k,k') = \dfrac{K(k,k')}{\sqrt{\phi(k)}\sqrt{\phi(k')}}$ and μ an eigenvalue. We then seek solutions of this standard Fredholm integral equation of the second kind[5] with eigenvalue $\mu = 1$. i.e. the dependence of p on λ is fixed by requiring that an eigenvalue μ of (9) be 1. Furthermore since K is symmetric in k and k' and square integrable for <u>all</u> values of $\lambda > 0$ and $p^2 > 0$ (see Appendix I), $\tilde{K}$ is also symmetric in k and k' and square integrable for all values of $\lambda > 0$, but now only for all values of $p^2 > 1$. This guarantees that (1) eigenvalues μ exist and (2) they are discrete and (3) the corresponding eigenfunctions F are normalizable.[5] Thus we determine p(λ) by solving (9) with fixed λ by adjusting p so that $\mu = 1$.

This was done numerically. Since $\psi(x,0)$ is even in x, so is F(k) ($= \int e^{ikx}\psi(x,0)\,dx$) even in k; thus we need only consider positive k by replacing K (k,k') with (K(k,k') + K(k,-k')) in (5) or (9). The integral may then be transformed easily to an integral over the interval (0,1) in a variety of ways, e.g. by letting x = k'/(k'+1). The integrand then is well behaved over the new interval (0,1) (because $K(k,k') \to 0$ like $1/k'^2$ for large k') and an approximate integration scheme may be expected to work very well. The numerical results of Table I and Figure I were obtained this way using a Gauss Legendre integration scheme of first 10, then 20 points. (Hardly any improvement was observed by increasing the number of points to 20, and the tables present the 10 point results.) The results were obtained using equation (5), not (9). Replacing the integral of (5) with a finite sum converts (5)

to a homogeneous finite set of simultaneous equations in the values of the unknown function F ($\frac{x}{1-x}$) at the quadrature points x_i . λ is fixed and p varied until this set has a solution, i.e. until the determinant of the set of simultaneous equations = 0.

III. Theoretical Discussion of Results

Figure 1 shows a smooth curve which starts at E = -1 with slope ½ and increases up to E = -½ at about λ = 2.65 where it stops; the slope of the curve at this point is 0. One might ask why doesn't the curve cross into the continuum; or why does it stop at all; or why does it stop where it does; or why is the slope 0 at this point?

Physically one might expect the bound state to disappear by making the repulsive interaction between the two particles large enough. This apparently happens in the real 3-dimensional He problem[6] at λ = 1.1184 , but not at the onset of the continuum but within the continuum and not with 0 slope. Thus physical arguments and analogy with the real He problem do not alone provide the answers to these questions.

Some of them may be answered by examining equation (5) in the vicinity of the point $p^2 = 1$ (E = -½). For $p^2 \leq 1$, equation (5) completely changes character; when the factor ϕ has a zero it is no longer possible to construct equation (9) from (5). (This required division of K (k,k') by $\sqrt{\phi(k)}\sqrt{\phi(k')}$). Even so, it is possible to rule out some of the possibilities suggested in the first paragraph through use of the square integrability of K (k,k') for all $p^2 > 0$, $\lambda > 0$. A square integrable kernel defines perhaps the simplest

completely continuous (compact) transformation.[7] Equation (5) may be put in the form

$$NF - KF = \mu F, \tag{10}$$

where N is a bounded normal transformation; K is a completely continuous transformation and μ is an eigenvalue. The solutions of eq. (5) are solutions of eq. (10) with eigenvalues $\mu = 0$. A theorem due to Neumann and Weyl[8] states that the continuous spectrum of a normal transformation is invariant under the addition of a completely continuous transformation. The continuous spectrum (all of the spectrum) of the normal transformation in question is the range of the function ϕ. As long as $p^2 > 1$ the range of ϕ is bounded away from 0. This implies the continuous eigenvalues of (10) are also bounded away from 0 also. This means that the only solutions of (10) with eigenvalue 0 are bound, a fact we knew anyway.

As for the questions outlined above, suppose first of all, $E(\lambda)$ exists only for $\lambda \leq \lambda_0$ and $E(\lambda_0) \leq \bar{E} < -\frac{1}{2}$. Then one could easily compute a variational $\tilde{E}$ for $(\lambda_0 + \delta) > \lambda > \lambda_0$, with δ small enough, which would provide an upper bound for such λ sufficiently close to λ_0 below $E = -\frac{1}{2}$. $\tilde{E} = E(\lambda_0) + (\lambda - \lambda_0)\left[\frac{\int \psi(x,x)^2 dx}{\int \psi(x,y)^2 dx dy}\right]$ $= E(\lambda_0) + E'(\lambda_0)(\lambda - \lambda_0)$. ($E'(\lambda)$ is a decreasing function of λ and is finite ($=\frac{1}{2}$) at $\lambda = 0$). By hypothesis this could not be a bound state. But a continuum state cannot have energy $< -\frac{1}{2}$. This provides the required contradiction. Similarly neither can $E(\lambda)$ exist for $\lambda < \lambda_0$ (i.e. in an open interval) with $E(\lambda) \leq \bar{E} < -\frac{1}{2}$, and not exist for $\lambda \geq \lambda_0$. If this were so we could define the completely continuous operator of equation (9) at the point $(\lambda_0, \lim_{\lambda \to \lambda_0} p(\lambda) = p_0)$. Let F_i be a sequence of solutions of (9) corresponding to $(\lambda_i, p(\lambda_i))$

with $\lambda_i \to \lambda_0, E_0 = -\frac{p_0^2}{2}$. From the sequence of functions $\tilde{K}(\lambda_0, p_0; k, k')$ F_i one can then extract a convergent subsequence.[7] Using this subsequence and arguing as below, one can define a solution at the point λ_0, p_0. This provides the required contradiction.

Having dealt with these two simpler cases, suppose now that $E(\lambda) \to -\frac{1}{2}$ as $\lambda \to \lambda_0$ for some λ_0 (including the case $\lambda_0 = \infty$). Then we have a sequence of normalizable eigenfunctions F_i, and a sequence of points $(\lambda_i, p(\lambda_i))$ such that $p(\lambda_i) \to 1$; $\lambda_i \to \lambda_0$ and

$$F_i(k)\phi_i(k) = \int K_i(k,k')\, F_i(k')\, dk'$$

$$K_i(k,k') \equiv K(\lambda_i, p(\lambda_i); k, k') \qquad \phi_i = \left(1 - \frac{1}{\sqrt{k^2 + p(\lambda_i)^2}}\right)$$

$$K_i \to K_0(k,k') \equiv K(\lambda_0, 1; k, k') \qquad \phi_i \to \phi_0 = \left(1 - \frac{1}{\sqrt{k^2+1}}\right)$$

Again, since K is square integrable for all non-0 λ and p, K_i and K_0 are completely continuous transformations. Furthermore $K_i \to K_0$ strongly, i.e. in the sense of the norm $\|K_i - K_0\| \to 0$. Since K_0 is completely continuous we can extract a convergent subsequence from the bounded sequence of functions $K_0 F_i$ such that $K_0 F_i \to \psi$ in the mean. Since $K_0 F_i = (K_0 - K_i + K_i) F_i$ and $K_i \to K_0$ strongly we also have $K_i F_i \to \psi$ Thus $\phi_i F_i \to \psi$, which means the sequence $\phi_0 F_i$ as well as F_i itself converge also, $F_i \to \frac{\psi}{\phi_0} \equiv F$. Thus F_i converges to a function $F = \frac{\psi}{\phi_0}$ which may or may not be normalizable. ($\phi_0(0) = 0$) If F is normalizable then $\|F\| = \lim_i \|F_i\| = 1$. This implies that ψ is not identically 0 (otherwise F would have 0 norm), and that $\psi(0) = 0$, so that F has finite norm). If F is not normalizable, then again ψ cannot be identically 0, and $\psi(0)$ must still be 0.

This is so because $\psi(k)$ is finite: $|\psi(k)| \leq \lim_i |\int K_0(k,k') F_i(k') dk'| \leq \lim_i |\int K_0^2(k,k') dk'| < \infty$ (the F_i's are assumed normalized). Assuming without proof, as we do below, that the limit and the integral may be interchanged, we have $\psi(k) = \lim_i \int K_0(k,k') F_i(k') dk' = \int K_0(k,k') F(k') dk' = \int K_0(k,k') \frac{\psi(k')}{\phi_0(k')} dk'$. Since $\phi_0(k') = o(k'^2)$, the term on the right is infinite unless $K_0(k,k')\psi(k') = o(k'^{(1+\alpha)}), \alpha > 0$ for small k'. $K_0(k,0) \neq 0$, so in order that $\psi(k)$ be finite, we must have $\psi(k') = o(k'^{(1+\alpha)})$ for small k'. Note this does <u>not</u> imply that $F = \frac{\psi}{\phi_0}$ is necessarily normalizable.

The vanishing of $\psi(0)$ implies that the limiting function $F = \frac{\psi}{\phi_0}$ is also a solution of equation (5') below, provided that $K_0(0,0) \neq 0$.

$$F(k)\,\phi_0(k) = \int K_0(k,k') F(k')\, dk' - \int \frac{K_0(0,k') K_0(0,k)}{K_0(0,0)} F(k')\, dk' \qquad (5'),$$

since the last term on the right is identically 0. That is , the original square integrable symmetric kernel $K_0(k,k')$ may be replaced by the new square integrable symmetric kernel:

$$K_0(k,k') - \frac{K_0(0,k') K_0(0,k)}{K_0(0,0)} \equiv K_1(k,k')$$

of (5') provided $K_0(0,0) \neq 0$. The reason for constructing this new kernel is that we may now proceed in exactly the same manner which led us to equation (9). That is, since $K_1(0,k') = o(k')$; $K_1(k,0) = o(k)$, we may divide K_1 by $\sqrt{\phi_0(k)}\sqrt{\phi_0(k')}$. Letting $\tilde{F}(k) = \sqrt{\phi_0(k)}\, F(k)$, $\tilde{K}_1(k,k') = K_1(k,k')/(\sqrt{\phi_0(k)}\sqrt{\phi_0(k')})$, $\tilde{F}$ satisfies the standard Fredholm integral equation of the second kind:

$$\tilde{F}(k) = \mu \int \tilde{K}_1(k,k') \tilde{F}(k') dk',$$

μ an eigenvalue. Direct calculation shows that eigensolutions with $\mu = 1$ do not exist. This calculation is performed by fixing μ at 1, p at 1 and replacing the integral with a finite quadrature sum.As λ varies the

determinant of the corresponding set of simultaneous equations remains bounded away from 0. The variation in this determinant with λ is indicated in Table II. The single point $\lambda_0 = 2.66736$ where $K_0(0,0) = 0$ (at this point one may not construct $K_1(k,k')$) emerges as the only point where E (λ) may cross over into the continuum. At all other points λ, $p = 1$, solutions of (5') do not exist. One of the consequences of this results is, for example, that E <u>cannot</u> tend asymptotically to $-\frac{1}{2}$ as $\lambda \to \infty$, a fact which was not at all obvious either from physical arguments or from the general shape of the computed curve.

The numerical evidence that the analysis is correct is very convincing. It is a simple matter to calculate the value of λ for which $K_0(0,0) = 0$. Alternatively (this was actually done first) one may solve equation (5) by quadrature and let λ increase to determine p as a function of λ. The curve levels off and $\longrightarrow$ 1 as $\lambda \to \lambda_0$. The two calculations fix λ_0 at 2.66736 in entirely independent ways.

What can be said about the slope of the function $E(\lambda)$ at $\lambda = \lambda_0$. Numerically the slope seems to be going to 0. The Hellman-Feynman theorem applied to equation (1) gives $\frac{dE}{d\lambda} = \frac{\int \psi(x,x)^2 dx}{\int \psi(x,y)^2 dx\, dy}$ i.e. the slope is every where positive. Since the 2nd order energy is always negative,[6] i.e. since $\frac{d^2E}{d\lambda^2} < 0$, the slope is a decreasing function of λ. At any point λ_0 where $\frac{dE}{d\lambda} = 0$, either $\int \psi(x,x)^2 dx$ must be 0, i.e. $\psi(x,x)$ must be 0 almost everywhere, or $\int \psi(x,x)^2 dx$ must remain finite and $\int \psi(x,y)^2 dx\, dy$ must become infinite. $\psi(x,x)$ cannot vanish for the nodeless

ground state; thus if ever $\frac{dE}{d\lambda} = 0$, $\psi_\lambda(x,y)$ must be non-normalizable at that point. i.e. the solution must be a continuum solution. The Weyl-Neumann theorem insures that at $E = -\frac{1}{2}$ ($p = 1$), a continuum solution must exist. (A bound solution may be degenerate with it however). At the point ($\lambda_0 = 2.66736$, $p = 1$) A unique (numerical) solution of (5) was found. The uniqueness insures that it must be an approximation to the continuum solution guaranteed by the Weyl Neumann theorem, and explains why the slope of the curve is 0 at this point, $\int \psi(x,y)^2 dx dy = \infty$. It was thought at first that this continuum solution was a simple delta function. If $K_0(0,k)$ were identically 0 a delta function, $\delta(k)$ would satisfy eq. (5) exactly. $K_0(0,k)$ is however not identically 0 (though it remains small) and the exact continuum solution is more complicated than a simple δ -function.

To summarize, using the complete continuity of the operator we have been able to show that (1) $E(\lambda)$ must either cross or touch the line $E = -\frac{1}{2}$ which bands the continuum; (2) it cannot touch or cross the line $E = -\frac{1}{2}$ except at the single point $\lambda = \lambda_0$ where $K_0(0,0) = 0$; and (3) it does in fact touch there with 0 slope. The solution at this point goes over from bound to continuum. (It is conceivable but highly unlikely that the bound state could reappear beyond this point in the continuum.)

IV. The Perturbation Solution of Equation I

It is of interest to determine how well these results can be reproduced with high order perturbation theory. Though equation (1) has the exact solution described in the previous two sections,

the real 3-dimensional problem does not permit an exact solution. Perturbation theory is in fact often the only way of solving difficult problems and in this example we have an excellent opportunity to see how well it does in describing the true result.

W. Byers Brown has worked out the first three of these perturbation energies and Stillinger and White[4] have repeated the calculation in a very interesting article that examines many electron problems with an H_o that involves the hyper-spherical average of the true H. For the two electron δ -function model this circular average gives rise to a 2 dimensional H atom Hamiltonian with an attraction term $(2\sqrt{2}-\lambda)/(\sqrt{2}\pi r)$. Thus for $\lambda > 2\sqrt{2}$ this term changes sign; the attraction becomes repulsion; one might expect that the series of perturbation energies would break down for values of $\lambda > 2\sqrt{2}$ since for such values the H_o problem does not have a bound state solution. Indeed the λ_o of the previous section is fairly close to 2.828.

One way of getting the perturbation series is to expand everything in equation (5) in powers of λ and equate the coefficient of each term to 0. The algebra soon becomes very involved and it is slightly easier, but entirely equivalent, to expand the Fourier transform of equation (1) directly. When that is done one has the infinite set of equations:

$$\frac{1}{2}(k_1^2+k_2^2-2E^{(0)})G^{(n)}(k_1,k_2) - F^{(n)}(k_1) - F^{(n)}(k_2)$$
$$= \sum_{i=1}^{n} E^{(i)}G^{(n-i)}(k_1,k_2) - H^{(n-1)}(k_1+k_2) \qquad (11)$$

$n = 0, 1, 2, \cdots$

where

$$G(k_1, k_2) = \sum \lambda^n G^{(n)}(k_1, k_2)$$

$$E = \sum \lambda^n E^{(n)} \quad , \quad -\frac{p_0^2}{2} = E^{(0)}$$

$$F(k) = \sum \lambda^n F^{(n)}(k)$$

$$H(k) = \sum \lambda^n H^{(n)}(k)$$

Thus

$$G^{(n)}(k_1, k_2) = \frac{F^{(n)}(k_1) + F^{(n)}(k_2) - H^{(n-1)}(k_1+k_2) + \sum_{i=1}^{n} E^{(i)} G^{(n-i)}}{\frac{1}{2}(k_1^2 + k_2^2 + p_0^2)}$$

It is easy to see inductively that

$$G^{(n)}(k_1, k_2) = \sum_{i=0}^{n} \frac{A_n^i(k_1) + A_n^i(k_2)}{[\frac{1}{2}(k_1^2 + k_2^2 + p_0^2)]^{i+1}} + \sum_{i=1}^{n} \frac{B_n^i(k_1+k_2)}{[\frac{1}{2}(k_1^2 + k_2^2 + p_0^2)]^{i}}$$

The A_n^i's and B_n^i's obey the following recurrence scheme:

$$A_{n+1}^0 = F^{(n+1)}$$

$$A_{n+1}^1 = E^{(n+1)} A_0^0 + E^{(n)} A_1^0 + \cdots E^{(1)} A_n^0$$

$$\vdots$$

$$A_{n+1}^m = E^{(n+2-m)} A_{m-1}^{m-1} + \cdots E^{(1)} A_n^{m-1}$$

$$\vdots$$

$$A_{n+1}^{n+1} = E^{(1)} A_n^n$$

and

$$B_{n+1}^1 = -H^{(n)}$$

$$B_{n+1}^2 = E^{(n)} B_1^1 + \cdots E^{(1)} B_n^1$$

$$\vdots$$

$$B_{n+1}^m = E^{(n+2-m)} B_{m-1}^{m-1} + \cdots E^{(1)} B_n^{m-1}$$

$$\vdots$$

$$B_{n+1}^{n+1} = E^{(1)} B_n^n$$

As in section II, we inverse Fourier transform $G^{(n)}(k_1, k_2)$ to get $\psi^{(n)}(x,y)$ and then use the definitions of F and H to obtain the two nth order equations for $F^{(n)}$ and $H^{(n)}$,

$$F^{(n)}(k)\left(1-\frac{1}{\sqrt{k^2+p_0^2}}\right) = \frac{1}{2\pi}\int \frac{F^{(n)}(k')\,dk'}{\frac{1}{2}(k^2+k'^2+p_0^2)} + \frac{1}{2\pi}\int \sum_{i=1}^{n} \frac{\left[A_n^i(k)+A_n^i(k')\right]dk'}{\left[\frac{1}{2}(k^2+k'^2+p_0^2)\right]^{i+1}} + \frac{1}{2\pi}\int \sum_{i=1}^{n} \frac{B_n^i(k')\,dk'}{\left[\frac{1}{2}(k^2+(k-k')^2+p_0^2\right]^{i}} \tag{12}$$

and

$$H^{(n)}(k) = \frac{1}{\pi}\int \sum_{i=0}^{n} \frac{A_n^i(k')\,dk'}{\left[\frac{1}{2}(k'^2+(k-k')^2+p_0^2)\right]^{i+1}} + \frac{1}{2\pi}\sum_{i=1}^{n} B_n^i(k)\int \frac{dk'}{\left[\frac{1}{2}\left[(k-k')^2+k'^2+p_0^2\right]\right]^{i}} \tag{13}$$

here $p_0^2 = 2$. Equation (12) is an inhomogeneous integral equation for $F^{(n)}$; the inhomogeneity involves the unknown n^{th} order energy $E^{(n)}$ which is determined by requiring that the equation have a solution.

i.e. that

$$\frac{1}{2\pi}\int \sum_{i=2}^{n} \frac{\left[A_n^i(k)+A_n^i(k')\right]dk'}{\left[\frac{1}{2}(k^2+k'^2+p_0^2)\right]^{i+1}} + \frac{1}{2\pi}\int \frac{E^{(n)}\left(A_0^0(k)+A_0^0(k')\right)}{\left[\frac{1}{2}(k^2+k'^2+p_0^2)\right]^2}$$

$$+ \frac{1}{2\pi}\int \sum_{i=1}^{n-1} \frac{E^{(i)}\left(A_{n-i}^0(k)+A_{n-i}^0(k')\right)}{\left(\frac{1}{2}(k^2+k'^2+p_0^2)\right)^2} + \frac{1}{2\pi}\int \sum_{i=1}^{n} \frac{B_n^i(k')dk'}{\left(\frac{1}{2}(k^2+(k-k')^2+p_0^2)\right)^i}$$

be orthogonal to the homogeneous solution, $F^{(0)}(k) = \frac{1}{k^2+1}$. This uniquely fixes $E^{(n)}$. (All of the terms but the second in the inhomogeneous term involve energies and functions of order $\leq$ n -1 which are assumed known.) With this choice of $E^{(n)}$, (12) has a solution which is uniquely determined by requiring that $F^{(n)}$ be orthogonal to $F^{(0)}$ (intermediate normalization convention). Once we have $F^{(n)}$ we calculate $H^{(n)}$ directly using equation (13). All of the terms on the right are now known. Again this entire procedure was carried out numerically by replacing the integrals with finite quadrature sums, after transforming the semi-infinite interval $(0,\infty)$ to (0,1) with $x = \frac{k}{k+1}$. Furthermore, as equations (12) and (13) are written, it is clear that at no time does one need the functions B_n^i and A_n^i at points other than the original set of quadrature points. That is, no interpolation scheme is necessary. In this way the perturbation energies through 20th order were calculated using 20, 32, and 50 quadrature points. The results are listed in table III along with the first three analytic results.[4] The functions $F^{(n)}$ and $H^{(n)}$ were also retained in the calculation and are available, but not listed here. Convergence does seem to have been reached with the 32 quadrature points.

V. Analysis of Perturbation Energies:

The sign changes every third term (beyond $E^{(2)}$) in the sequence of perturbation energies was something of a surprise. In the real He problem all of the available variation perturbation energies (beyond $E^{(3)}$) are negative. Stillinger was able to fit this sequence of numbers to a singularity of the type $A(\rho-\lambda)^{\theta}+B(\lambda)$ where $B(\lambda)$ is assumed to have no singularity as close as or closer than ρ to the origin. This was possible because the expansion of $(\rho-\lambda)^{\theta}$ also gives rise to a series with constant signs and indeed the fit was quite good.[6] Furthermore we have already argued in Sections II and III that the bound state disappears at $\lambda = \lambda_0 =$ 2.66736; and a term of the type $(2.66736-\lambda)^{\theta}$, $\theta > 1$, in the analytic expression for $E(\lambda)$ would account for this behavior as well as for the observed 0 slope at $\lambda = 2.66756$ and the general shape of the curve in Figure I.

The nonconstancy in sign of the perturbation energies precludes the existence (or at least the importance) of such a term however. Nevertheless, can one say anything about the analytic behavior of $E(\lambda)$ by looking at the terms in the series? It is well known that the radius of convergence of a series representation of a function is determined entirely by the location in the complex plane of the singularity of the function which lies nearest to the origin.[9] It is also known that the convergence of a series is determined entirely by the behavior of its high index coefficients. Thus the behavior of these high index coefficients must reveal the nature and position of the

nearest singularity. It is just this idea that enabled Stillinger to evaluate ρ and θ with the first 20 terms in the perturbation series for He.

Quite recently W. Byers Brown and B. McLeod have succeeded in identifying the singularities of certain 1-dimension Strum-Liouville eigenvalue problems which depend on a perturbation parameter λ as branch points in the complex plane where two or more eigenvalues coalesce.[9,10] Byers Brown has been able to locate these controlling branch points for all of the low lying states of the linear rotor in a perturbing Stark Field.[11]

We attempt here to use Byers Brown's method of analysis on our perturbation energies, although the original problem itself actually does not belong to the category of problems for which the approach is strictly applicable. Nevertheless if one assumes $E(\lambda) = A(\lambda^2 - 2\lambda R\cos\phi + R^2)^{\theta} + B(\lambda)$, where B has no singularity as close or closer to the origin than R then the high index coefficient $E^{(n)}$ will behave like the high index coefficient in the expansion of the first term. Writing

$$A(\lambda^2 - 2\lambda R\cos\phi + R^2)^{\theta} = A'\left(1 + \frac{2\lambda x}{R} + \frac{\lambda^2}{R^2}\right)^{\theta}$$

with $x = -\cos\phi$, and expanding $\left(1 + \frac{2\lambda x}{R} + \frac{\lambda^2}{R^2}\right)^{\theta}$ out, the expansion coefficients $\sum \frac{\lambda^n}{R^n} F_n^{\theta}(2x)$ are ultraspherical polynominals and obey a 3 term recurrence relation[12]

$$F_{n+1}^{\theta}(2x) = \frac{2x(\theta - n)}{(n+1)} F_n^{\theta}(2x) + \frac{(2\theta + 1 - n)}{(n+1)} F_{n-1}^{\theta}(2x)$$

If our assumption is correct, then the high index $E^{(n)} R^n$ should obey this same three term recurrence relation for some choice of R, θ, and x. One may test the hypothesis by using three consecutive

such equations (involving $E^{(n)}$, $E^{(n+1)}$, $E^{(n+2)}$, $E^{(n+3)}$, $E^{(n+4)}$) to determine the three unknowns R, θ, and x. As n increases, that is, the next set of three equations is used, the computed values of R, θ, and x change. If they change only slightly and begin to tend toward definite limits then our hypothesis is probably correct. For every n the three equations may be reduced to a single cubic equation in R^2; a quadratic equation in θ (with coefficients that depend on R), and a linear equation in x (with coefficients that depend on θ and R). We look for real positive R, real θ, and real x such that $|x| \leq 1$, which change only slightly as we change n. Each equation in the set of three which determine R, θ, and x is of the form:

$$r_{m+1} r_m R^2 = 2x \frac{(\theta - m)}{m+1} R r_m + \frac{(2\theta + 1 - m)}{m+1}, \quad m = n, n+1, n+2,$$

where $r_m = \frac{E_m}{E_{m-1}}$ $\qquad n \geq 1$

The results of this calculation for various values of n are presented in Table IV. Although there are some bad discrepancies, particularly at n = 12 and 15, the numbers do suggest the presence of a singularity of the branch point type in the analytic expression for E as a function of λ. The point lies in the complex plane at a radius R with $2.7 < R < 3.0$. One might be tempted to make other guesses about the singularity. Some of these were tried but nothing gave results as good as the single branch point described above.

How does this result relate to our previous assertion that at the point $\lambda_0 = 2.66736$ the bound state disappeared and that at this point $\frac{dE}{d\lambda} = 0$? If $R < \lambda_0$ then the series would tell us

nothing about the behavior of E(λ) at λ_0 since it is not valid there. If however R $> \lambda_0$, as it seems to be, what is the series describing in the interval $[\lambda_0, R)$, where it still converges? First of all, it is possible for $\frac{dE}{d\lambda}$ to be 0 at λ_0 : only the <u>high</u> index coefficients are determined by the branch point singularity; there certainly must exist another term in the expression for $E(\lambda)$ = $A(\lambda^2+2x\lambda R+R^2)^{\sigma}+B(\lambda)$. (This is so because we know asymptotically E $\rightarrow -\frac{\lambda^2}{4}$). This second term makes it possible for $\frac{dE}{d\lambda}$ to vanish at λ_0 even though the first term does not. (In the Stillinger analysis of the variation perturbation energies for the true He problem it was the presence of just such a term which made $\frac{dE}{d\lambda} \neq 0$ at λ = 1.1184). If in fact R is $> \lambda_0$ we may examine the curve in the vicinity of λ_0 by using the series itself, both for the function and its derivative, since for $|\lambda| < R$ the series converges uniformly and absolutely. When this is done it is indeed found that $E^*(\lambda) = \sum_0^{20} \lambda^n E^{(n)}$ has a maximum near λ_0, at λ_0^* = 2.65171 and beyond that point decreases; i.e. for $\lambda > \lambda_0^*, E'(\lambda) < 0$. The true eigenvalue E(λ) is however everywhere increasing. This means that for $R > \lambda > \lambda_0^*$, the series, though it is convergent, is converging to a non-physical result. It further implies that the behavior of E(λ) is the region of λ_0 is as described in Section II. $E(\lambda)$ cannot cross into the continuum; for if it did the series would describe such a crossing and it does not do so; it instead converges to a non-physical decreasing function for $\lambda > \lambda_0^*$.

Simpler examples of this sort of behavior for a function and its perturbation series exist. Consider a hydrogen atom perturbed by an additional coulombic term of strength $-\frac{\lambda}{r}$; the ground state energy is $-\frac{(\lambda+1)^2}{2}$, for $\lambda > -1$. For $\lambda \leq -1$ the bound state disappears. However the perturbation series $-\frac{\lambda^2}{2} - \lambda - \frac{1}{2}$ converges for all values of λ , positive and negative as well. In the region $\lambda \leq -1$, the series converges to a non-physical increasing function.

VI. Conclusions

We have examined the solution of the delta-function model for He-like ions with interactions = $\lambda\delta(x-y)$, $\lambda = \frac{1}{Z}$. The exact solution was obtained by solving numerically a 1-dimensional Fredholm integral equation of the second kind. The bound state disappears at λ = 2.66736 and does not cross into the continuum. This is to be contrasted with the real He problem where the bound state disappears at a much smaller value of λ = 1.1184 and does appear to cross over into the continuum. The perturbation series for the ground state was developed through 20th order and the coefficients fit to a branch point in the complex plane at approximately R=2.9, cos ϕ =.5 and exponent 1.1. The perturbation converges to a non-physical result in the range R $>$ 2.66736.

It also seems likely that the general method of solution could be extended to many one dimensional particles interacting through δ -function potentials.

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Appendix I

The arguments of Section III depend upon the square integrability of the kernel of equation (5). The first term is obviously square integrable. The second term is as well:

$$\text{Let } K_2(k,k'') = \lambda \int \frac{dk'}{k^2+(k-k')^2+p^2} \cdot \frac{1}{(k'-k'')^2+k''^2+p^2} \frac{\sqrt{2p^2+k'^2}}{\left(\sqrt{2p^2+k'^2}+\lambda\right)}$$

then

$$K_2(k,k'') = \int K_1(k,k')\, K_1(k'',k')\, \phi(k')\, dk'$$

$$\text{with } K_1(k,k') = \frac{1}{k^2+(k-k')^2+p^2} \quad \text{and} \quad \phi(k') = \frac{\lambda\sqrt{2p^2+k'^2}}{\sqrt{2p^2+k'^2}+\lambda} > 0.$$

Thus using the Schwartz inequality,

$$|K_2(k,k'')| \le \left[\int K_1(k,k')^2 \phi(k')\, dk'\right]^{1/2} \left[\int K_1(k'',k')^2 \phi(k')\, dk'\right]^{1/2}$$

$$\le C \left[\int K_1(k,k')^2 \sqrt{2p^2+k'^2}\, dk'\right]^{1/2} \left[\int K_1(k'',k')^2 \sqrt{2p^2+k'^2}\, dk'\right]^{1/2}$$

with C some constant ≤ 1.

The first term is a function of k'', the second of k. We now maximize the norm of K_2.

$$\int K_2(k,k'')^2\, dk\, dk'' \le C^2 \int K_1(k,k')^2 \sqrt{2p^2+k'^2}\, dk'\, dk \cdot \int K_1(k'',k')^2 \sqrt{2p^2+k'^2}\, dk'\, dk''$$

$$\text{But } \int K_1(k,k')^2 \sqrt{2p^2+k'^2}\, dk'\, dk = \int \frac{1}{(k^2+k'^2+p^2)} \sqrt{2p^2+(k-k')^2}\, dk\, dk'$$

$$= \int_0^\infty \int_0^{2\pi} \frac{d\theta\, \rho\, d\rho\, \left[2p^2+\rho^2[\cos\theta-\sin\theta]^2\right]^{1/2}}{(\rho^2+p^2)^2} < \int_0^\infty \frac{\rho\, d\rho\, \sqrt{2}}{(\rho^2+p^2)^{3/2}} < \infty.$$

And thus $\|K_2\| < \infty$, all $\lambda > 0$, $p > 0$.

Table I. E (λ) Computed from Equation (5) and First 20 Terms of Perturbation Series

λ	$-2E^{+}$	$-2(\sum_{i=0}^{20} \lambda^{i} E^{(i)})$
0.00000	2.00000	2.00000
0.10000	1.90323	1.90323
0.20000	1.81281	1.81279
0.30000	1.72854	1.72852
0.40000	1.65025	1.65022
0.50000	1.57773	1.57769
0.60000	1.51078	1.51075
0.70000	1.44920	1.44916
0.80000	1.39276	1.39273
0.90000	1.34126	1.34122
1.00000	1.29445	1.29442
1.10000	1.25212	1.25209
1.20000	1.21403	1.21401
1.30000	1.17995	1.17993
1.40000	1.14964	1.14962
1.50000	1.12287	1.12286
1.60000	1.09942	1.09941
1.70000	1.07905	1.07904
1.80000	1.06154	1.06154
1.90000	1.04668	1.04668

Table I. (continued)

2.00000	1.03425	1.03426
2.10000	1.02408	1.02408
2.20000	1.01595	1.01596
2.30000	1.00968	1.00971
2.40000	1.00508	1.00518
2.50000	1.00207	1.00222
2.60000	1.00046	1.00075
2.65171		1.00056*
2.66736	1.00000**	1.00058
2.70000		1.00073
2.80000		1.00223
2.90000		1.00552
3.00000		1.01121

+ calculated from equation (5) with 10 quadrature points

* maximum of series in vicinity of λ_o

** λ_o

Table II. Determinant of Numerical Approximation of Equation (9) with $\tilde{K} \equiv \tilde{K}_1$ of Section III as a Function of λ

λ	Determinant
0.0	12.299
.2	10.475
.4	8.9458
.6	7.6426
.8	6.5170
1.0	5.5344
1.2	4.6694
1.4	3.9036
1.6	3.2237
1.8	2.6222
2.0	2.0988
2.2	1.6722
2.4	1.4408
2.6	2.7531
2.7	-4.6611
2.8	-1.2062
3.0	-.87210
3.5	-1.4361
4.0	-2.0874
4.5	-2.6782
5.0	-3.2034
7.5	-5.1088
10.0	-6.3038

Table III. Perturbation Energies through $E^{(20)}$ from Equations (12) and (13)

n	$E^{(n)*}$		$E^{(n)**}$		$E^{(n)***}$		$E^{(n)+}$	
0	-1.0000000000	10^{0}	-1.0000000000	10^{0}	-1.0000000000	10^{0}	-1.0000000000	10^{0}
1	.4999999326	10^{0}	.4999999986	10^{0}	.5000000000	10^{0}	.5000000000	10^{0}
2	-.1627932533	10^{0}	-.1627934067	10^{0}	-.1627934091	10^{0}	-.1627934092	10^{0}
3	.1398905240	10^{-1}	.1398914636	10^{-1}	.1398914766	10^{-1}	.1398914769	10^{-1}
4	.1642785438	10^{-2}	.1642768751	10^{-2}	.1642768530	10^{-2}		
5	.1701195144	10^{-4}	.1700914062	10^{-4}	.1700913369	10^{-4}		
6	-.5274847304	10^{-4}	-.5274758660	10^{-4}	-.5274758623	10^{-4}		
7	-.1329127203	10^{-4}	-.1329105145	10^{-4}	-.1329105066	10^{-4}		
8	-.5184462535	10^{-6}	-.5185341371	10^{-6}	-.5185337783	10^{-6}		
9	.6698272423	10^{-6}	.6697904232	10^{-6}	.6697904388	10^{-6}		
10	.2166476123	10^{-6}	.2167350240	10^{-6}	.2167349914	10^{-6}		
11	.1292205044	10^{-7}	.1296951883	10^{-7}	.1296950809	10^{-7}		
12	-.1242513775	10^{-7}	-.1250616493	10^{-7}	-.1250616476	10^{-7}		
13	-.4532663805	10^{-8}	-.4609443248	10^{-8}	-.4609442100	10^{-8}		
14	-.3613440165	10^{-9}	-.3301789956	10^{-9}	-.3301786254	10^{-9}		

Table III. (continuted)

15	.2184271892	10^{-9}	.2872509315	10^{-9}	.2872509602	10^{-9}
16	.9849371486	10^{-10}	.1132885837	10^{-9}	.1132884976	10^{-9}
17	.3889517412	10^{-10}	.8610384952	10^{-11}	.8610269419	10^{-11}
18	.1551822806	10^{-10}	-.7538615228	10^{-11}	-.7538614284	10^{-11}
19	-.4327301642	10^{-11}	-.3053112289	10^{-11}	-.3052989534	10^{-11}
20			-.2269633262	10^{-12}	-.2268955848	10^{-12}

* 20, ** 32, *** 50 quadrature points, + reference (3)

Table IV. Calculated Location of Singularity From Perturbation Series

n*	R	x	Θ
0	2.48709	-.304675	1.00506
1	2.32952	-.531994	1.09351
2	3.05225	-.455821	1.04563
3	3.26928	-.533929	0.896274
4	3.02570	-.508510	1.05530
5	2.91419	-.503415	1.18401
6	3.01022	-.514613	1.02348
7	2.92230	-.507873	1.16779
8	2.92744	-.508036	1.15695
9	2.71314	-.490979	1.71100
10	2.87769	-.502320	1.29332
11	2.92077	-.503401	1.16053
12	2.43990 3.58377	-.468808 -.516634	2.79992** -1.56745
13	2.85221	-.497089	1.42019
14	2.91163	-.498344	1.17797
15	2.27117 3.44697	-.454410 -.506628	3.88184** -1.58211
16	2.83658	-.492697	1.53892

* index of first equation used to get R, x, Θ.

** neither of the two solutions listed seems to fit the pattern of the other results. This may be due to increasing inaccuracy in the perturbation energies.

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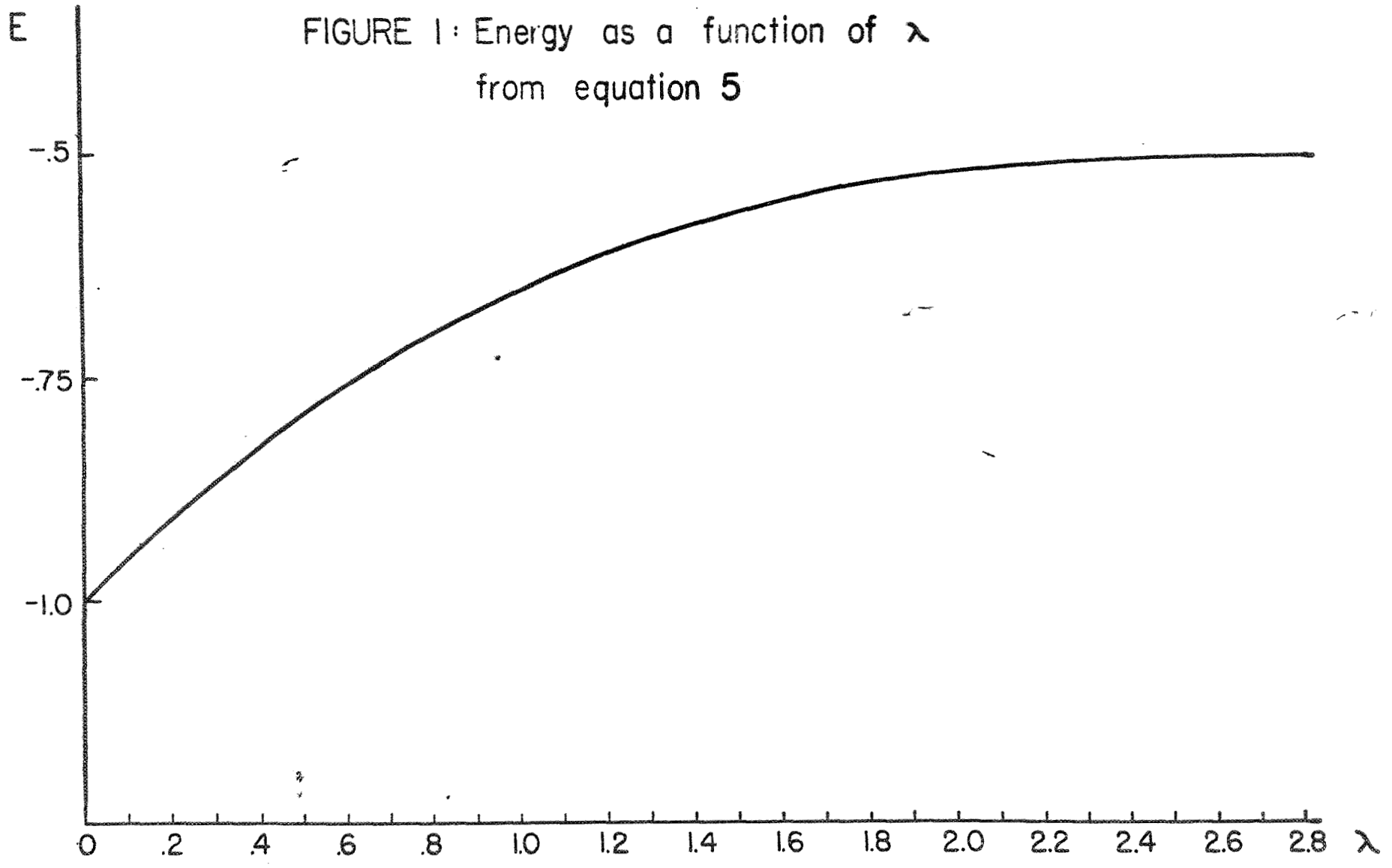

FIGURE 1: Energy as a function of λ from equation 5