# SINGULAR PERTURBATION EXPANSIONS IN QUANTUM PHYSICS 

## A TUTORIAL REVIEW

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## ABSTRACT

Several examples from both many- and one-body quantum physics of bound states in which the application of some scheme of "successive approximations" does not automatically lead to a regular (i.e., convergent power series) perturbation theory but rather to a singular one are illustrated.

## I. INTRODUCTION

In a great many problems in physics and engineering one is finally confronted with a differential equation, in one or many variables, which one is either unable to solve analytically or unable or unwilling (or both) to recur to numerical techniques to achieve a solution.

A conmon procedure has been to attempt a method of successive approximations by doing a perturbation expansion about the known solution

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* Work sponsored in part by CONACYT and ININ.
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of a certain part of the original problem. In quantum mechanics this solvable part of the Schrödinger equation may be, e.g., the hydrogenic atom, the harmonic oscillator, etc., or, in many-body physics, it may be the ideal (i.e., non-interacting) gas of particles, or even some Hartree-Fock independent particle model. The complete solution for, say, the ground state energy and wavefunction, is then expressed as a power series in a coupling parameter $\lambda$ (which multiplies the part of the hamiltonian called the 'perturbation'). For sufficiently small $\lambda$ the first few terms of this power series generally suffice for a satisfactory description of the full solution. This is known as regular perturbation theory, if the power series converges.

However, not all such problems of differential equations, in either quantum physics or engineering, allow in principle a perturbative solution as a power series in the coupling parameter $\lambda$ but rather give rise to expansions in $\lambda$ which are non-analytic ${ }^{(1)}$. That is, the expansion may contain fractional powers of $\lambda$, logarithm terms in $\lambda$ and even so-called essential singularity terms like $\mathrm{e}^{- \text {const } \lambda^{-1}}$. Singular perturbation theory is generally accepted as constituting these latter kind of problems or as power series perturbation expansions which do not converge (whether or not they are asymptotic). In fact some of the most interesting perturbation problems are of the singular type and it is our purpose here to give a brief survey of some examples of singular perturbation theory taken from both one-body and many-body quantum physics.

## II. SOME EXAMPLES FROM MANY-BODY PHYSICS

## a) The Electron Gas.

In the many-body perturbation treatment ${ }^{(2)}$ for the ground state energy of $N(\gg 1)$ point charges of mass $m$ and charge e submersed in a rigid uniform background of equal total but opposite charge (so as to ensure net neutrality) one finds divergent contributions to the perturbation series beginning in the second order of the coupling parameter $r_{S} \equiv r_{0} / a_{0}$, where $r_{0}$ is a measure of the interparticle separations and is defined in terms of the volume per particle $\mathrm{V} / \mathrm{N}=4 \pi \mathrm{r}_{\mathrm{O}}{ }^{3} / 3$ and $\mathrm{a}_{0} \equiv \hbar 2 / \mathrm{me}^{2}$ is the first Bohr radius. A rearrangement of the (diverging) series, or, alternatively, an infinite partial summation over the most divergent contri-
butions (Feynman diagrams) to the perturbation series, allows obtaining a finite but non-analytical correction to the unperturbed (plane-wave Hartree-Fock) energy value, namely a $\ln r_{s}$ term as first discovered by Macke ${ }^{(3)}$ in 1950. Gell-Mann and Brueckner ${ }^{(4)}$ recalculated this term and the subsequent one (which is a constant) by doing the "random phase approximation" (RPA). Dubois ${ }^{(5)}$ in 1959 and Carr and Maradudin ${ }^{(6)}$ in 1964 determined the coefficients of the next two terms (finding again a in $r_{S}$ term) by sumaing to infinite order and evaluating the next most divergent Feynman diagrams beyond the RPA. The resulting expansion for the ground state energy per particle is

$$
\begin{align*}
& \mathrm{E}_{\mathrm{O}} / \mathrm{N} \underset{\mathrm{r}_{\mathrm{c}} \ll 1}{\sim} \mathrm{r}_{\mathrm{s}}^{-2}\left[\mathrm{a}-\mathrm{br} \mathrm{r}_{\mathrm{s}}+\mathrm{c}_{1} \mathrm{r}_{\mathrm{s}}^{2} \ln \mathrm{r}_{\mathrm{s}}-\mathrm{c}_{2} \mathrm{r}_{\mathrm{s}}{ }^{2}+\right.  \tag{1}\\
& \left.+c_{3} r_{s}{ }^{3} \ln r_{s}+c_{4} r_{s}^{3}+O\left(r_{s}^{4} \ln r_{s}\right)\right]
\end{align*}
$$

and clearly gives a weak-coupling, singular perturbation expansion. The (positive) coefficients $a, b, c_{1}$ to $c_{4}$ are known and found in the literature cited above.

Happily for this problem one also possesses a strong-coupling theory. This was developed by Carr ${ }^{(7)}$ and others in 1961, following an earlier suggestion by Wigner ${ }^{(8)}$ in 1934 that for $r_{S} \gg 1$ the electrons would go onto the sites of a perfect lattice, (giving us the so-called 'Wigner solid'). The strong-coupling theory perturbs about this perfect, classical lattice (all potential energy) in terms of perturbing kinetic energy contributions which introduce first harmonic zero-point energy, then anharmonic corrections, etc., to the leading Coulomb lattice energy $-a / r_{S}$. The result is

$$
\begin{equation*}
E_{0} / N \underset{r_{s} \gg 1}{\sim}-\frac{a}{r_{s}}+\frac{b}{r_{s}{ }^{3 / 2}}-\frac{c}{r_{s}{ }^{2}}-\frac{d}{r_{s}^{5 / 2}}+0\left(\frac{e^{- \text {const } r_{s}}{ }^{1 / 2}}{r_{s}}\right) \tag{2}
\end{equation*}
$$

where the positive coefficients a to $d$ are found in the literature $i_{1 / 2}$ Again one begins with a power series expansion not in $r_{s}$ but in $r_{s}^{-1 / r}$ (and hence non-regular); but eventually "exponential" terms related to
intersite overlapping electron clouds also appear.
b) Bosons with short-ranged forces.

For a many-boson system with central pair interactions (no matter how singular, as with hard cores) one can apply analogous many-body infinite summation techniques and express the ground state energy per particle, at low particle density $\rho \equiv N / V$, in terms of the "dimensionless smallness parameter ${ }^{\prime \prime} \sqrt{\rho \mathrm{a}^{3}}$, where $a$ is the well-known scattering length depending entirely on the free two-body problem. The result, to which very laboriously have contributed Lenz ${ }^{(9)}$ in 1929, Lee, Huang and Yang (10) since 1957, $\mathrm{Wu}^{(11)}$ as well as Pines and Hugenholtz ${ }^{(12)}$ and also Beliav ${ }^{(13)}$ in 1959, is just

$$
\begin{align*}
\mathrm{E}_{0} / \mathrm{N} \underset{\rho \mathrm{a}^{3} \ll 1}{\sim} \frac{2 \pi \hbar^{2}}{\mathrm{~m}} \rho \mathrm{a}[ & 1+\mathrm{c}_{1} \sqrt{\rho \mathrm{a}^{3}}+\mathrm{c}_{2} \rho \mathrm{a}^{3} \ln \rho \mathrm{a}^{3}+ \\
& \left.+O\left(\rho \mathrm{a}^{3}\right)+O\left[\left(\rho \mathrm{a}^{3}\right)^{3 / 2} \ln \rho \mathrm{a}^{3}\right]\right], \tag{3}
\end{align*}
$$

where we again see the singular nature of the resulting perturbation expansion in the new smallness parameter $\sqrt{\rho a^{3}}$. The coefficients, $c_{1}$ and $c_{2}$ have been determined and appear in the literature.

It is possible to think of several many-boson as well as manyfermion systems interacting via a simplified two-body interaction potential (Fig. 1, snset) consisting of a hard core of diameter c surrounded by an atractive square well of range $b$ and depth $-v_{0}$. In this case, standard effective range theory ${ }^{(14)}$ gives us the expression for the scattering length (in units of the hard core diameter) as

$$
\begin{equation*}
a / c=1+\frac{b-c}{c}\left[1-\frac{\tan \sqrt{\frac{m v_{0}}{\hbar^{2}}}(b-c)}{\sqrt{\frac{m v_{0}}{\hbar^{2}}}(b-c)}\right] \text {, } \tag{4}
\end{equation*}
$$

which clearly becomes unity when the attraction vanishes. The interaction parameters $b, c$ and $v_{o}$ have been adjusted in the literature to the twoboson systems: $\mathrm{He}^{4}-\mathrm{He}^{4}(15)$ and two alpha particles ${ }^{(16)}$; to the two-
fermion systems: $\mathrm{He}^{3}-\mathrm{He}^{3}$ (same interaction as between $\mathrm{He}^{4}$ ) and nucleonnucleon systems ${ }^{(17)}$ like neutron-proton, proton-proton, etc. If we take $b$ as approximately $3 c$ we can display these widely different dynamical systems on a single graph of $a / c$ vs. $\sqrt{m_{0} / h^{2}}(b-c)$, the "attractive strength', Fig.1. We note first of all that of the two-body problems considered only the neutron-proton system, in the spin-triplet ( ${ }^{3} \mathrm{~S}_{1}$ ) state, and the alpha-alpha one, without Coulomb repulsions, are sufficiently attractive so as to bind the pair. (Recall that $\sqrt{\mathrm{mv}_{\mathrm{o}} / \mathrm{h}^{2}}(\mathrm{~b}-\mathrm{c})=\pi / 2$ is exactly the condition for a square well depth $v_{0}$ and range (b-c) to bind a particle of mass $\mathrm{m} / 2$ with zero energy). Secondly, we notice that although the remaining two-body systems considered here do not bind, the attraction is sufficiently great so that the corresponding scattering length is negative. For the many-boson system whose ground state at very low densities is described by Ec. (3) this means that, because of the non-regular term $\sqrt{\rho^{3}}$, the energy of the $N$-particle system not only can become negative but also complex. But this we know (although some think this to mean a breakdown of the theory) means the appearance of a nonstationary state with a finite lifetime which could very well be a metastable quantum state consisting of very brief formations of $n$-body clusters $(2<n<N)$ which undoubtedly occurs before the $N$-body cluster (e.g., liquid $\mathrm{He}^{4}$ ) is stably formed at higher densities.
c) Fermions with short-ranged interactions.

A similarly heroic effort has been carried out for the manyfermion problem, beginning with Lenz ${ }^{(9)}$ in 1929 and ending with Baker ${ }^{(17)}$ in 1971. The result, again a singular expansion in the "smallness parameter ${ }^{\prime \prime} \mathrm{k}_{\mathrm{F}}$, where the Fermi momentum $\mathrm{k}_{\mathrm{F}}$ is defined through the particle density $\rho \equiv N / V=\nu \mathrm{k}_{\mathrm{F}}{ }^{3} / \mathrm{b} \pi^{2}$ for a $v$-species fermion system, is (for $v=4$ : balanced nuclear matter):

$$
\begin{align*}
& E_{0} / N \underset{k_{F}{ }^{\lll 1}}{\sim} \\
& \frac{3}{5} \frac{\hbar^{2} k_{F}}{2 m}+c_{1}\left(k_{F} a\right)^{3}+c_{2}\left(k_{F} a\right)^{4}+c_{3}\left(k_{F} a\right)^{5}  \tag{5}\\
&+c_{4}\left(k_{F} a\right)^{6} \ln \left|k_{F} a\right|+c_{5}\left(k_{F} a\right)^{6}+\ldots
\end{align*}
$$

The coefficients $c_{1}$ through $c_{5}$ have been determined in the literature
and their dependence on purely two-body scattering parameters specified.


Fig. 1 Scattering length a (in units of c) for the hard-core-plus-attrac-tive-square-well potential shown in inset, vs. $\sqrt{m v_{0} / \hbar^{2}}(b-c)$ which is a measure of the attractiveness of the well, for $b=3 c$. The pole at $\pi / 2$ designates the well strength at which the first zero-energy bound state appears. The open dots refer to the empirical values reported in the literature for the different two-body systems. Note that upper scale is linear while the bottom is logarichmic.
d) BCS theory of superconductivity.

The Bardeen-Cooper-Schrieffer (BCS) theory ${ }^{(18)}$ of superconductivity is well-known to lead, as the relevant (electron-phonon) coupling parameter $\lambda \rightarrow 0$, to a lower energy per electron of the "superconduct ing" relative to that of the 'normal" state by an amount

$$
\begin{equation*}
\underset{\text { Super }}{\mathrm{E}} \longrightarrow \underset{\text { normal }}{\mathrm{E}}-\mathrm{Nce} \mathrm{e}^{-\mathrm{co} / \lambda}, \tag{6}
\end{equation*}
$$

where $c$ and $c_{0}$ are positive. constants. Thus, the two problems, "complete" (superconducting) and 'unperturbed" (normal), are not connected by a regular perturbation theory but rather by a singular one, in fact, by an extremely singular one called an "essential singularity". Namely, the function $f(\lambda)=e^{-c / \lambda}$ can easily be seen to have no Taylor series expansion in $\lambda$ since $\left[f^{(n)}(\lambda)\right]_{\lambda=0} \equiv 0$, for all $n$th order derivatives.

## III. SOME ACADEMIC ONE-BODY EXAMPLES

a) Shallow attractive well in 1-, 2- and 3-dimensions. It is well-known that in three dimensions a square well potential $v(r) \equiv v_{0} \theta(a-r)$ supports a bound state for a particle of mass $m$ if and only if

$$
\begin{equation*}
v_{o} a^{2} \geq \hbar^{2} \pi^{2} / 8 m \tag{7}
\end{equation*}
$$

(cf. e.g., Fig.1, put $b-c=a$ and replace $m$ by $2 m$ ). Also of common knowledge is the fact that in one dimension a square well potential $v(x) \equiv-v_{0} \theta(a-\mid x!)$ always has a bound state, no matter how shallow the depth $v_{O}$, and that the bound state energy $E$ tends to $0^{-}$as $\mathrm{v}_{\mathrm{O}} \rightarrow 0^{+}$like

$$
\begin{equation*}
\underset{\mathrm{v}_{0} \rightarrow 0^{+}}{\longrightarrow}-\frac{\mathrm{m}}{2 \hbar^{2}} \mathrm{v}_{0}^{2} \mathrm{a}^{2}+\text { higher order terms, } \tag{8}
\end{equation*}
$$

i.e., analytically in $v_{0}$. Less well-known is the two-dimensional square well case $v(r, \phi)=-v_{0} \theta(a-r)$ where, as the binding energy approaches $0^{-}$ but as ${ }^{\text {(19) }}$

$$
\begin{equation*}
E \underset{v_{o} \rightarrow 0^{+}}{\longrightarrow}-\frac{\hbar^{2}}{\mathrm{ma}^{2}} e^{-\frac{2 \hbar^{2}}{\mathrm{ma}^{2} \mathrm{v}_{0}}} \tag{9}
\end{equation*}
$$

i.e., non-analytically. Thus a regular perturbation theory for this problem does not exist.
b) The single- and double-delta attractive well. A very simple model for $\mathrm{H}_{2}{ }^{+}$, (or even for the inversion spectrum of $\mathrm{NH}_{3}$ where the nitrogen atom oscillates between two potential minima) is the double oscillator well ${ }^{(20)}$ or the infinite square well with a finite repulsive square harrier placed in its center ${ }^{(21)}$, both in one dimension. A even simpler such model is the double attractive delta well problem ${ }^{(22)}$. Consider first a particle of mass $m$ in the single well

$$
\begin{equation*}
v(x)=-\frac{\hbar^{2}}{2 m} \frac{\lambda}{a} \delta(x) ; \quad \lambda, a>0 \tag{10}
\end{equation*}
$$

The negative energy level is given by

$$
\begin{align*}
& E_{1}<0, \quad K_{1}^{2} \equiv \frac{2 m}{\hbar^{2}}\left|E_{1}\right|, \quad u^{\prime \prime}(x)-K_{1}^{2} u(x)=-\frac{\lambda}{a} \delta(x) u(x), \\
& u( \pm \infty)=0 \Rightarrow u(x)=e^{-K_{1}|x|},|x|>0 \tag{11}
\end{align*}
$$

At $x=0$ the first derivative of the wave function $u(x)$ is discontinuous, namely

$$
\begin{equation*}
\left.u^{\prime}(x)\right|_{x=0^{+}}-\left.u^{\prime}(x)\right|_{x=0^{-}}=-\frac{\lambda}{a} u(0), \tag{12}
\end{equation*}
$$

which immediately gives the eigenvalue equation

$$
\begin{equation*}
K_{1}=\frac{\lambda}{2 \mathrm{a}} \tag{13}
\end{equation*}
$$

The double-well problem

$$
\begin{equation*}
v(x)=-\frac{\hbar^{2}}{2 m} \frac{\lambda}{a}[\delta(x-a)+\delta(x+a)], \tag{14}
\end{equation*}
$$

on the other hand, is easily seen to give the bound state energy $\mathrm{E}_{2}<0$ solution, with $K_{2}{ }^{2} \equiv \frac{2 m}{\hbar^{2}}\left|E_{2}\right|$,

$$
\begin{align*}
u(x) & =e^{-x_{2} x} & & \text { for } x>a \\
& =A \cosh K_{2} x & & \text { for }-a<x<a  \tag{15}\\
& =e^{K_{2} x} & & \text { for } x<-a .
\end{align*}
$$

Matching $u(x)$ and $u^{\prime}(x)$ at, say $x=a$, gives, respectively,

$$
e^{-K_{2} a}=A \cosh K_{2} a,
$$

$$
\begin{equation*}
-K_{2} e^{-\mathrm{K}_{2} a}-K_{2} A \sinh K_{2} a=-\frac{\lambda}{a} e^{-K_{2} a}, \tag{16}
\end{equation*}
$$

which allows elimination of the constant $A$ and gives the new eigenvalue equation

$$
\begin{equation*}
\frac{\lambda}{\mathrm{K}_{2} \mathrm{a}}-1=\tanh \mathrm{K}_{2} \mathrm{a} \leq 1 \Leftrightarrow \mathrm{~K}_{2} \geq \frac{\lambda}{2 \mathrm{a}} \equiv \mathrm{~K}_{1}, \tag{17}
\end{equation*}
$$

so that $\mathrm{E}_{2}<\mathrm{E}_{1}$. Hence $\mathrm{H}_{2}{ }^{+}$is more stable than H and $\mathrm{H}^{+}$unbound. More importantly, the $\mathrm{H}_{2}^{+}$state cannot be gotten by regular perturbation theory since, on taking very large separation $a \rightarrow \infty$, we have

$$
\begin{equation*}
\tanh K_{2} a \xrightarrow[a \rightarrow \infty]{\longrightarrow} 1-2 e^{-2 K_{2} a} \simeq \frac{\lambda}{K_{2} a}-1, \tag{18}
\end{equation*}
$$

or

$$
E_{2} \underset{a \rightarrow \infty}{\longrightarrow} E_{1}\left(1-2 e^{\left.-\frac{2 K_{2}}{a^{-1}}\right)} .\right.
$$

That is, the total (double-well) energy tends to the unperturbed (singlewell) energy non-analytically in the smallness parameter $\mathrm{a}^{-1} \rightarrow 0$.
c) The quartic anharmonic oscillator ${ }^{(23)}$. We have here the hamiltonian

$$
\begin{align*}
H & =-\frac{d^{2}}{d x^{2}}+x^{2}+\lambda x^{4}  \tag{19}\\
& \equiv H_{O}+\lambda H_{1}, \quad H_{1} \equiv x^{4} .
\end{align*}
$$

TABIE I

| N | $\sum_{n=0}^{n} a_{n}(0.2)^{n}$ |
| :---: | :---: |
| 1 | 1.150000 |
| 3 | 1.153750 |
| 5 | 1.176999 |
| $\vdots$ | ! |
| 10 | $-2.442698$ |
| $\vdots$ | $\vdots$ |
| 13 | 168.895730 |
| $\vdots$ | : |
| 15 | 3,0005.179546 |
| 50 | $\sim \pm 10^{4}$ |
| 1,000 | $\sim \pm 10^{2,000}$ |

Table I. Rayleigh-Schrödinger series, partially summed to order $N$, for the ground statc energy of the anharmonic oscillator Ec. (19) for $\lambda=0.2$. (See Ref.26).



Fiy. 2 Potential well (dashed curve) of the quartic anharmonic oscillator hamiltonian for both positive and negative quartic perturbation $\mathrm{x}^{4}$.

The standard Rayleigh-Schrodinger, i.e., regular, perturbation series for the ground state energy $E_{0}(\lambda)$ in $\lambda$

$$
\begin{equation*}
E_{o}(\lambda)=\sum_{n=0}^{\infty} a_{n} \lambda^{n} \tag{20}
\end{equation*}
$$

where standard perscriptions apply in the determination of the $a_{n}$ 's, diverges for all $\lambda$. This was apparently first noted by Kramers (24) who discovered that $a_{n}$ goes like $(n!)^{2}$ for $n \rightarrow \infty$, which by the Cauchy ratio test indicates divergence of the series. The divergence, moreover, is not at all obvious from the first few orders (so that it would go entirely unnoticed in a standard quantum mechanical exercise.) as Table I shows.

A very simple heuristic proof of the divergence of the RS series exists. Fig. 2 shows a graph (dashed curve) of the potential well for both $\lambda>0$ and $\lambda<0$. Clearly, stationary states (of real energy) are possible only for the former case, while for $\lambda<0$ even the lowest energy state will be a non-stationary (resonance) state with a finite lifetime since the particle can tumnel away through the "shoulders" of the well. However, if a convergent expansion (20) existed at all, it would converge regardless of the sigh of $\lambda$. But for $\lambda<0$ this expansion would yield a real (perhaps negative) energy in contradiction with Fig. 2; therefore, it cannot converge.

Inspite of this divergence of the series, a sequence of Pade approximants ${ }^{(25)}$ constructed on the basis of the coefficients $a_{n}$, with $\mathrm{n}=0,1, \ldots, 2 \mathrm{~N}$, for the $\left[\mathrm{N}, \mathrm{N}\right.$ lapproximant is seen ${ }^{(26)}[$ Table II] to converge very well and quickly to the exact answer $\mathrm{E}_{\mathrm{O}}^{\text {exact }}(0.2)=1.118292$ obtainable by numerical integration of the Schrodinger equation.
d) Spiked oscillators ${ }^{(27)}$. This is the name given to the class of problems defined by the hamiltonian

$$
\begin{align*}
H & =-\frac{d^{2}}{d x^{2}}+x^{2}+\frac{\lambda}{|x|^{\alpha}} ; \quad \alpha>0  \tag{21}\\
& \equiv H_{0}+\lambda H_{1} ; \quad H_{1} \equiv|x|^{-\alpha} .
\end{align*}
$$

For $\alpha>2$, two notable surprises occur ${ }^{(28)}$ : a) as $\lambda \rightarrow 0$ the $n^{\text {th }}(n=0,1,2 \ldots$ )

TABLE II

| $N$ | $E_{0}[N, N]$ for $\lambda=0.2$ |
| :---: | :---: |
| 1 | 1.111111 |
| 2 | 1.117541 |
| 3 | 1.118183 |
| 4 | 1.118272 |
| 5 | 1.118288 |
| 6 | 1.118292 |
| 7 | 1.118292 |

$E_{o}^{\text {exact }}(0.2)=1.118292$
Table II Value of succesive [ $N, N$ ] Padé approximants constructed on the first $2 N+1$ coefficients $a_{n}$ of the RS series (20). See Ref. 26 .
state $E_{n}(\lambda)$ dos not become $E_{n}(0) \equiv(2 n+1) \quad$ (the ground and excited states of $\mathrm{H}_{\mathrm{O}}$ ) but rather the corresponding $\mathrm{n}^{\text {th }}$ state of $\mathrm{H}_{\mathrm{O}}$ supplemented by Dirichlet boundary conditions, i.e., $H_{0, D B C}$ (namely that at $x=0$ the solution vanish). Thus, instead of the nth state approaching the states on the left-hand column of Fig. 3, it goes into those of the right-hand column, as $\lambda \rightarrow 0$. Specifically, the ground state wave function of $H_{0, D B C}$ is $x e^{-x^{2} / 2}$ whereas that of $H_{0}$ is just $e^{-x^{2} / 2}$ (energy eigenvalue of 1 ) and the former, moreover, is degenerate with $|x| e^{-x^{2} / 2}$ both having energy eigenvalue of 3 . A so-called "vestigial effect" (of the interaction) remains. Also, b) an asymptotic series in fractional powers of $\lambda$ for the eigenvalues of $H$ results. Table Ill summarizes the results obtained by enploying WKB techniques to solve the Schrodinger equation for small $\lambda$. We see that not only fractional powers of $\lambda$ appear, and also $\lambda \ln \lambda$ terms, but even $\lambda^{2} \ln ^{2} \lambda$ terms. Note the similarity of these expansions with those of many-body theory mentioned in Chapter II above.

- $\frac{\frac{E_{0}(0)}{\text { state\# }}}{0}$


2


3


Fig. 3 First few wave functions of the one dimensional oscillator hamiltonian (left column) together with the associated energy eigenvalue $(2 n+1), n=0,1,2, \ldots$ Same, but for oscillator hamiltonian subjected to Dirichlet boundary conditions (DBC), i.e., that the wave function vanish at $x=0$. Note that the lowest energy is 3 , instead of 1 as before, and that each energy level is doubly-degenerated.

TABLA 111


| $\alpha$ | $v=\frac{1}{a-2}>0$ | $E_{0}(\lambda)-E_{0}(0)\left\{\begin{array}{l}\text { energy } \\ \text { shift }\end{array}\right.$ |
| :---: | :---: | :---: |
| $\alpha<5 / 2$ | - | $c_{1} \lambda+c_{2} \lambda^{2}+\ldots$ |
| $\alpha=5 / 2$ | - | $c_{1} \lambda+c_{2} \lambda^{2} \ln \lambda+c_{3} \lambda^{2}+\ldots$ |
| $5 / 2<\alpha<3$ | $1<v<2$ | $c_{1} \lambda+c_{2} \lambda^{\nu}+O\left(\lambda^{2}\right)$ |
| $\alpha=3$ | $v=1$ | $c_{1} \lambda l n \lambda+c_{2} \lambda+O\left(\lambda^{2} \ell^{2} \lambda\right)$ |
| $3<\alpha<4$ | $1 / 2<v<1$ | $c_{1} \lambda^{\nu}+c_{2} \lambda+O\left(\lambda^{2 v}\right)$ |
| $\alpha \geq 4$ | $v \leq 1 / 2$ | $c_{1} \lambda^{\nu}+O\left(\lambda^{2 v}\right)$ |
| $\alpha$ |  |  |

- E.M. Harrell, II, Ann. Phys. (N.Y.) 105 (1977) 379.

Table III Singular perturbation energy shifts for several values of the exponent $\alpha$ in the ground state of (21), with respect to the unperturbed value $E_{0}(0)=1$ for $\alpha \leq 2$, but $=3$ for $\alpha>2$. See Ref. 27.
e) Super-singular perturbations (29). An example of these is

$$
\begin{align*}
H & =\frac{d^{2}}{d x^{2}}+x^{2}+\lambda e^{x^{4}} \\
& \equiv H_{0}+\lambda H_{1} ; \quad H_{1} \equiv e^{x^{4}}, \tag{22}
\end{align*}
$$

where the matrix elements of $\mathrm{H}_{1}$ clearly diverge in the $\mathrm{H}_{\mathrm{O}}$ oscillator basis. The leading term in the energy shift of the ground state, as $\lambda \rightarrow 0$, is found to be the highly singular expression

$$
\begin{equation*}
E_{0}(\lambda)-E_{0}(0) \underset{\lambda \rightarrow 0^{+}}{\sim} K(-\ln \lambda)^{1 / 4} e^{-(-\ln \lambda)^{1 / 2}}, \tag{23}
\end{equation*}
$$

with K a positive constant.
f) Treatment of bound and resonant states. A beautifully simple example has appeared in the literature ${ }^{(30)}$ whereby both bound (stationary) and resonant (non-stationary) states can be analyzed within a singular perturbation scheme. This is the hamiltonian

$$
\begin{aligned}
H & =-\frac{d^{2}}{d x^{2}}-\alpha \delta(x)+\lambda x^{2}, \quad \alpha>0 \\
& \equiv H_{0}+\lambda H_{1}, \quad H_{1} \equiv x^{2}
\end{aligned}
$$

where the potential well is graphed in Fig. 4 for both $\lambda>0$ (top) and $\lambda<0$. Clearly, the latter gives rise, if at all, only to resonant states.

Consider first the case $\lambda \geq 0$. Expanding the eigenstates of Ec. (24) in terms of the complete set of eigenstates not of $H_{0}$, as is the usual practice, but of $-d^{2} / d x^{2}+\lambda x^{2}$, one can easily arrive at the eigenvalues $\varepsilon$ equation

$$
\begin{equation*}
\alpha \sum_{n=0}^{\infty} \frac{\phi_{2 n}^{2}(0)}{E_{2 n}-\varepsilon}=1 \quad \text { (for even states) } \tag{25}
\end{equation*}
$$

where the oscillator energies $E_{2 n}$ are

$$
\begin{equation*}
E_{m}=2 \sqrt{\lambda}(m+1 / 2) ; \quad m=0,1,2, \ldots \tag{26}
\end{equation*}
$$

and $\phi_{2 n}(x)$ the associated eigenstates. For odd states the levels are unshifted because $\phi_{2 n+1}(0) \equiv 0$ for $n=0,1,2, \ldots$, and thus


Fig. 4 Potential well for the hamiltonian Ec. (24) for both positive and negative $\lambda$.

$$
\begin{align*}
& \varepsilon=E_{2 n+1}=2 \sqrt{\lambda}(2 n+3 / 2) \quad \text { (for odd states), } \\
& n=0,1,2, \ldots \tag{27}
\end{align*}
$$

Note that Ec. (25) could in principle be solved graphically for each $(\alpha, \lambda)$ pair since we know $\phi_{2 n}(0)$ and $E_{2 n}$. In fact, Ec. (20) becomes explicitly

$$
\begin{equation*}
1=\frac{\alpha}{\sqrt{\pi}} \lambda^{1 / 4} \sum_{n=0}^{\infty}(-)^{n}\binom{-1 / 2}{n} \frac{1}{2 \sqrt{\lambda}(2 n+1 / 2)-\varepsilon} \equiv \alpha F(\lambda, \varepsilon) . \tag{28}
\end{equation*}
$$

Using the binomial expansion $\left(1-S^{2}\right)^{-3 / 2}=\sum_{m=0}^{\infty}\binom{-1 / 2}{n} S^{2 m}$, as well as an obvious integral representation, we can write $F(\lambda, \varepsilon)$ as

$$
\begin{align*}
F(\lambda, \alpha) & =\frac{1}{2 \sqrt{\pi} \lambda^{1 / 4}} \int_{0}^{1} d S \frac{S^{-\frac{\varepsilon}{2 \sqrt{\lambda}}}}{\sqrt{S\left(1-S^{2}\right)}}  \tag{29}\\
& =\frac{1}{4 \lambda^{1 / 4}} \frac{\Gamma(1 / 4-\varepsilon / 4 \sqrt{\lambda})}{\Gamma(3 / 4-\varepsilon / 4 \sqrt{\lambda})}
\end{align*}
$$

the last step following from the integral representation of the beta func-
tion ${ }^{(31)}$

$$
\begin{equation*}
B(m+1, n+1) \equiv \frac{\Gamma(m+1) \Gamma(n+1)}{\Gamma(m+n+2)}=\int_{0}^{1} d t t^{m}(1-t)^{n} \tag{30}
\end{equation*}
$$

Changing variable $S \equiv e^{-\eta}$, and restricting ourselves to the lowest eigenvalue $\varepsilon \equiv-\tilde{\varepsilon}<0$, the rhs of Ec. (29) becomes

$$
\begin{equation*}
\frac{1}{2 \sqrt{2 \pi} \lambda^{1 / 4}} \int_{0}^{\infty} d n \frac{e^{-\frac{\tilde{\varepsilon}}{2 \sqrt{\lambda}}}}{\sqrt{\sinh \eta}} \xrightarrow[\lambda \rightarrow 0^{+}]{ } \frac{1}{\sqrt{2 \tilde{\varepsilon}}}, \tag{31}
\end{equation*}
$$

thus showing clearly the singular character of the problem. Because of the asymptotic series nature of the $\Gamma$ functions in Ec. (29), we conclude that a perturbation expansion for $\tilde{\varepsilon}(\lambda)$ in powers of $\lambda$ diverges for all $\lambda$, but is nevertheless asymptotic.

Finally, for $\lambda \equiv-\tilde{\lambda}<0$, one can define

$$
\begin{equation*}
F(\tilde{\lambda}, \tilde{\varepsilon}) \equiv F^{\prime}+i F^{\prime \prime}, \quad\left(F^{\prime}, F^{\prime} r e a l\right), \tag{32}
\end{equation*}
$$

and readily see that

$$
\begin{equation*}
F^{\prime \prime}=\left[e^{-\frac{\tilde{\varepsilon} \pi}{2 \sqrt{\lambda}}}\right] \underset{\substack{F^{\prime} \ll 0^{+}}}{\substack{ \\\lambda}} \tag{33}
\end{equation*}
$$

so that our scheme can be employed to study, systematically, the positions of the resonances.

## IV. CONCLUSIONS

We have illustrated several examples from quantum mechanics where a scheme of successive approximations will not yield a regular (i.e, convergent power series in some smallness parameter) perturbation theory but rather a singular one. The latter is either a diverging power series or a non-power series which may contain fractional powers, logarithmic terms or even essential singularities in the smallness parameter .

A11 the examples discussed, both physical and academic, are connected with the study of "condensed", i.e., self-bound, many- or one-
body quantum systems.

## ACKNOWLEDGEMENT

We thank the Venezuelan authorities and the Universidad Central de Venezvela, Caracas, where this paper was presented at the "IV Latin American Workshop on Condensed Matter Theories" in July, 1980. Our special thaks go to Prof. Lutz Dohnhert, who organized the Workshop, for his kind hospitality.

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