Perturbation Theory for Singular Potentials in Quantum Mechanics

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Abstract

We study perturbation theory in certain quantum mechanics problems in which the perturbing potential diverges at some points, even though the energy eigenvalues are smooth functions of the coefficient of the potential. We discuss some of the unusual techniques which are required to obtain perturbative expansions of the energies in such cases. These include a point-splitting prescription for expansions around the Dirichlet (fermionic) limit of the δ-function potential, and performing a similarity transformation to a non-Hermitian potential in the Calogero-Sutherland model. As an application of the first technique, we study the ground state of the δ-function Bose gas near the fermionic limit.

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1 Introduction

Perturbation theory is an old and often used method for studying problems in quantum mechanics which are close to some exactly solvable problems [1]. However, there are many models in which the traditional formulas of perturbation theory lead to divergent expressions for the energies even at fairly low orders, although the actual energy eigenvalues are known to be perfectly finite numbers. This situation typically (but not always) arises if the perturbing potential is singular, that is, if it blows up at certain points in the configuration space. We are therefore forced to develop new kinds of perturbative techniques if we wish to expand such problems around the exactly solvable points.

We will discuss two such techniques here. The first one is used in the presence of a δ-function potential in one dimension [2], of which the δ-function Bose gas is a more general case [3]. We will find that an expansion around the Neumann (bosonic) point, where the coefficient of the δ-function potential is zero, is rather straightforward. However, an expansion around the Dirichlet (fermionic) point, where the coefficient is infinity, diverges at second order in perturbation theory. We can obtain finite answers at that order by using a point-splitting prescription. After discussing all this in a one-particle model in Secs. 2 and 3, we generalise the discussion to the δ-function Bose gas in Sec. 4.

The other technique discussed is used in the case where the perturbing potential has a scale-invariant inverse-square form; this leads to the wave functions vanishing as a power of the two-particle separation whenever a pair of particles approach each other. An important example is the Calogero-Sutherland model in one dimension [4, 5], which has been studied extensively in recent years from many points of view (see [6] for a partial list of references). In Sec. 5, we show that this model can be studied perturbatively around the noninteracting bosonic limit by performing a similarity transformation of the Hamiltonian which takes into account the power-law form of the wave functions near coincident points. This leads to a perturbation which has a non-Hermitian form; one can then employ the usual Rayleigh-Schrödinger perturbation theory. As a byproduct, we prove that the energies get no contributions beyond the leading one or two orders in perturbation theory when the external (one-body) potential is either simple harmonic or zero; the wave functions however do get contributions to higher orders.

Historically, the method of using a non-Hermitian perturbation was perhaps first used to study models of anyons in two dimensions [7], in order to study the spectrum near the bosonic limit [8]. There is a vast literature on this subject, so we will not discuss it here. We should also briefly mention that there are other treatments of perturbation theory for singular potentials in two and higher dimensions, either in quantum mechanics [9] or in Chern-Simons field theories [10]. We will only consider one-dimensional models here which are technically simpler but have not been discussed as extensively.

In this work, we will not be exhaustive in our list of examples of singular potentials. Further, certain parts of our discussion are not new, and all the models we will study are

exactly solvable. We should therefore explain the motivations behind our presentation. Our main aim is to introduce the reader to a class of problems in which the usual form of perturbation theory fails, and to indicate some ways of dealing with such problems. A more complete study of this subject would certainly be worthwhile but we will not attempt that here. Secondly, the models considered here would not remain exactly solvable if we introduced additional non-singular interactions or external potentials; however, such additional terms would not change the nature of the new perturbative techniques which are designed to address the singular parts of the interactions. It is therefore better to study the nature of these new techniques in exactly solvable models so that we can easily check that these methods do give the right answers.

In our discussion, we will use the following expression from Rayleigh-Schrödinger perturbation theory to quadratic order in a perturbation V. If $H = H_0 + V$, and the exact normalised eigenstates $\psi_n(0)$ and eigenvalues $E_n(0)$ of H_0 are known, then the eigenstates of H to first order in V and the eigenvalues to second order in V are given by [1]

$$\begin{aligned} \psi_n &= \psi_n(0) + \sum_{l \neq n} \psi_l(0) \, \frac{\langle \psi_l(0)|V|\psi_n(0)\rangle}{E_n(0) - E_l(0)} \; , \\ E_n &= E_n(0) + \langle \psi_n(0)|V|\psi_n(0)\rangle + \sum_{l \neq n} \frac{\langle \psi_n(0)|V|\psi_l(0)\rangle \langle \psi_l(0)|V|\psi_n(0)\rangle}{E_n(0) - E_l(0)} \; . \end{aligned} \tag{1}$$

If there is a degeneracy at energy $E_n(0)$, then we have to modify the procedure at first order in V by first diagonalising the matrix $V_{ln} = \langle \psi_l(0)|V|\psi_n(0)\rangle$. However, we will not have to face this problem in any of the models discussed in this paper, because the matrix elements V_{ln} will always turn out to be zero for any two states for which $E_n(0) = E_l(0)$.

In Sec. 5, we will also need the general form of perturbation theory at second and higher orders. The only information we will actually use is that, at all orders in V higher than the first, the change in the energy E_n of the state ψ_n involves products of matrix elements like

$$\langle \psi_n(0)|V|\psi_{l_k}(0)\rangle \; \langle \psi_{l_k}(0)|V|\psi_{l_{k-1}}(0)\rangle \; ... \langle \psi_{l_2}(0)|V|\psi_{l_1}(0)\rangle \; \langle \psi_{l_1}(0)|V|\psi_n(0)\rangle \; , \tag{2}$$

where $k \geq 1$, and all the intermediate states $l_1, l_2, ..., l_k$ are different from n [1].

2 The δ-function potential in a box

We begin with a particle which is restricted to move in one dimension in the range $-1 \leq x \leq 1$. At the two end points $|x| = 1$, we demand that the wave functions should vanish. We impose a δ-function potential at the origin. The Hamiltonian is

$$H = - \frac{1}{2m} \frac{\partial^2}{\partial x^2} + \frac{c}{m} \, \delta(x) \; , \tag{3}$$

where c must be a real constant for H to be Hermitian. (We set Planck's constant $\hbar = 1$). We will only consider the subspace of wave functions which are even functions of x, since the odd functions vanish at the origin and are therefore unaffected by the δ-function potential. The δ-function is equivalent to imposing the boundary condition

$$\psi'(0+) \;=\; -\;\psi'(0-) \;=\; c\psi(0)\;, \tag{4}$$

where the primes denote derivatives with respect to x, and $0+$ and $0-$ denote the limits x approaching the origin from the right and left respectively. (Note that $c = 0$ gives us the Neumann boundary condition $\psi'(0) = 0$, while $c = \infty$ gives the Dirichlet boundary condition $\psi(0) = 0$). It is clear that this probem is exactly solvable; the (unnormalised) eigenstates and eigenvalues of H are given by

$$\begin{aligned} \psi_n &= \sin\,[\,\alpha_n(1-|x|)\,]\;, \\ E_n &= \frac{\alpha_n^2}{2m}\;, \\ \text{where}\quad \alpha_n\,\cot\alpha_n &= -\;c\;. \end{aligned} \tag{5}$$

The normalised eigenstates and energies for $c = 0$ are given by

$$\begin{aligned} \psi_n(x;0) &= \sin\,[\,(n\,+\,\frac{1}{2})\pi(1\,-\,|x|)\,]\;, \\ E_n(0) &= \frac{(n\,+\,\frac{1}{2})^2\pi^2}{2m}\;, \end{aligned} \tag{6}$$

where $n = 0, 1, 2, ...$ If we expand the energies in (5) around their values at $c = 0$, the leading order terms are

$$E_n(c) \;=\; \frac{1}{2m}\,[\,(n+\frac{1}{2})^2\pi^2 \;+\; 2c \;-\; \frac{c^2}{(n\,+\,\frac{1}{2})^2\pi^2} \;+\; ...\,]\;. \tag{7}$$

For $c = \infty$, the eigenstates and energies are

$$\begin{aligned} \psi_n(x;\infty) &= \sin\,[\,(n\,+\,1)\pi(1\,-\,|x|)\,]\;, \\ E_n(\infty) &= \frac{(n\,+\,1)^2\pi^2}{2m}\;, \end{aligned} \tag{8}$$

where $n = 0, 1, 2, ...$ The energies in (5) can be expanded around their values at $c = \infty$ in powers of $1/c$ as

$$E_n(c) \;=\; \frac{(n+1)^2\pi^2}{2m}\,[\,1 \;-\; \frac{2}{c} \;+\; \frac{3}{c^2} \;+\; ...\,]\;. \tag{9}$$

We will now study how the expansions in (7) and (9) can be obtained by using perturbation theory around $c = 0$ and ∞ respectively. Using the expressions in (1) with

$V = (c/m)\delta(x)$, we recover the results in (7); at second order, we have to use the easily derivable identity

$$\sum_{l \neq n} \frac{4}{(n \ + \ \frac{1}{2})^2 \ - \ (l \ + \ \frac{1}{2})^2} \ = \ - \ \frac{1}{(n \ + \ \frac{1}{2})^2} \ , \tag{10}$$

where the sum over l runs from 0 to ∞.

We now have to discover how to perform perturbation theory around $c = \infty$ in powers of $1/c$. We begin as follows. If $\psi_n(x;c)$ and $E_n(c)$ are the exact results for the problem at any value of c, then the Feynman-Hellmann theorem says that with the perturbation $V = (c/m)\delta(x)$,

$$\frac{dE_n}{dc} \ = \ \langle \psi_n | \ \frac{1}{m} \ \delta(x) \ | \psi_n \rangle \ = \ \frac{1}{m} \ |\psi_n(0;c)|^2 \ . \tag{11}$$

Using (4), this implies that

$$\frac{dE_n}{d(1/c)} \ = \ - \ \frac{1}{m} \ |\psi_n'(0+;c)|^2 \ . \tag{12}$$

Therefore, the change in energy to first order in $1/c$ can be obtained by taking the perturbation to be

$$\tilde{V} \ = \ - \ \frac{1}{2cm} \ \delta''(x) \ . \tag{13}$$

Here, it is understood that when we compute $\langle \psi_n | \tilde{V} | \psi_n \rangle$, i.e., when calculating $\psi'(0;c)$, we must take the limit $x \to 0$ either always from the right $(0+)$ or always from the left $(0-)$. This is because $\psi(x;c)$ has a cusp at the origin for all $c > 0$; hence the two limiting values of $\psi'(0;c)$ are equal in magnitude but have opposite signs.

Eq. (13) is one of the main results of this paper. It has not been discussed much in the literature before except for a brief mention in Ref. [11] (there is a minor error in the relevant equation in that paper). It is straightforward to check that using this potential as the perturbation does give the correct first order change in energy if we use the $c = \infty$ results in (8) as the uperturbed wave functions. However, if use (13) in the second order expression for the energy in (1), we obtain a divergent sum. We therefore have to *regularise* the sum in some way. We do this as follows. From the first order result for ψ_n in (1), we find that for $x > 0$,

$$\begin{aligned} \psi_n'(x;c) \ = \ & - \ \ (n+1)\pi \ \cos \ [\ (n+1)\pi(1-x) \ ] \\ & + \ \ \frac{2(n+1)\pi}{c} \ \sum_{l \neq n} \ \frac{(-1)^{l+n}(l+1)^2 \ \cos \ [\ (l+1)\pi(1-x) \ ]}{(n+1)^2 \ - \ (l+1)^2} \ . \end{aligned} \tag{14}$$

It is clear that if we naively set $x = 0$ in (14), the sum over l will diverge.

We now use the result

$$\sum_{l=-\infty}^{\infty} \ \exp \ (ilx) \ = \ 2\pi \ \sum_{p=-\infty}^{\infty} \ \delta \ (x - 2\pi p) \ , \tag{15}$$

which follows from the completeness of the functions $\exp(ilx)$ in any interval in x of length 2π. The right hand side of (15) is zero in the neighbourhood of $x = 0$ except exactly at the point $x = 0$. We therefore set the left hand side of the equation equal to zero *in the limit* $x \to 0$, although it diverges precisely at $x = 0$. This implies that

$$\lim_{x\to 0} \sum_{l\neq n} \cos\ (l+1)x \ = \ -\ \frac{3}{2}\ , \tag{16}$$

since l runs from 0 to ∞. We now subtract (16) from the summation in (14), and then take the limit $x \to 0+$, to obtain a finite result

$$\begin{aligned} \psi_n'(0+;c) \ &= \ (-1)^n\ (n+1)\pi\ \Big[\ 1\ -\ \frac{2}{c}\ \Big(\ \frac{3}{2}\ +\ (n+1)^2\ \sum_{l\neq n} \frac{1}{(n+1)^2\ -\ (l+1)^2}\ \Big)\ \Big]\ , \\ &= \ (-1)^n\ (n+1)\pi\ [\ 1\ -\ \frac{3}{2c}\ ]\ . \end{aligned} \tag{17}$$

Substituting this in (12), we obtain the correct second order result in (9).

Basically, we see that our regularisation of the energies at second order consists of using the first order wave functions *not* at the point $x = 0$, but rather at the point $x = 0+$ (or $0-$). In the language of quantum field theory, this is called a point-splitting prescription. Note also that the second order change in the ground state energy ($n = 0$) in (9) is *positive*, although the formula in (1) would suggest that it should be negative (since $E_n(0) < E_l(0)$ for all $l \neq n$); this peculiarity is a consequence of the regularisation.

We will not pursue perturbation theory beyond second order near $c = \infty$. It seems likely that a similar point-splitting prescription will also work at higher orders, but this requires a much more detailed analysis.

3 Combination of δ-function and simple harmonic potentialss

We now consider another exactly solvable example of the regularised perturbation theory described in the previous section. The motivation for studying a second example is to confirm that the point-splitting prescription is sound, and that it also works if the particle feels a potential in addition to the δ-function. We take the additional potential to be simple harmonic [2]. Thus

$$H \ = \ -\ \frac{1}{2m}\ \frac{\partial^2}{\partial x^2}\ +\ \frac{c}{m}\ \delta(x)\ +\ \frac{1}{2}\ m\omega^2 x^2\ . \tag{18}$$

Once again, we restrict our attention to the subspace of even wave functions. The exact eigenstates and energies are given in Ref. [2]. In particular, the energies are given by the

transcendental equation

$$\frac{\Gamma\left(\,\frac{3}{4}\,-\,\frac{E}{2\omega}\,\right)}{\Gamma\left(\,\frac{1}{4}\,-\,\frac{E}{2\omega}\,\right)}\;=\;-\;\frac{c}{2}\;. \tag{19}$$

From (19), we can compute the first three terms in an expansion for E_n around $c = 0$ and $c = \infty$. Near $c = 0$,

$$\frac{E_n}{\omega}\;=\;n+\frac{1}{2}+\frac{c}{\sqrt{\pi m\omega}}\frac{(n-1)!!}{n!!}-\frac{c^2}{2\pi m\omega}\left(\,\frac{(n-1)!!}{n!!}\,\right)^2\,[\,\psi(\frac{n}{2}+1)-\psi(\frac{n}{2}+\frac{1}{2})\,]\;, \tag{20}$$

where $n = 0, 2, 4, ...$, we define

$$\begin{aligned} p\;!!\;&\equiv\;p(p-2)(p-4)...2\quad\text{if}\quad p\quad\text{is even and}\quad\geq 2\;,\\ &\equiv\;p(p-2)(p-4)...1\quad\text{if}\quad p\quad\text{is odd and}\quad\geq 1\;,\\ &\equiv\;1\quad\text{if}\quad p=0\quad\text{or}\quad -1\;, \end{aligned} \tag{21}$$

and $\psi(z) = d\log\Gamma(z)/dz$ is the digamma function [12] (not to be confused with the wave function ψ_n). Near $c = \infty$,

$$\frac{E_n}{\omega}\;=\;n+\frac{1}{2}-\frac{2}{c}\sqrt{\frac{m\omega}{\pi}}\,\frac{n!!}{(n-1)!!}+\frac{2m\omega}{c^2\pi}\left(\,\frac{n!!}{(n-1)!!}\,\right)^2\,[\,\psi(\frac{n}{2}+1)-\psi(\frac{n}{2}+\frac{1}{2})\,]\;, \tag{22}$$

where $n = 1, 3, 5, ...$ The difference of digamma functions in (20) and (22) is given by

$$\begin{aligned} \psi(\frac{n}{2}+1)-\psi(\frac{n}{2}+\frac{1}{2})\;&=\;2\,\log 2\quad\text{if}\quad n=0\;,\\ &=\;2\,[\,\log 2\,+\,\sum_{k=1}^{n}\,\frac{(-1)^k}{k}\,]\quad\text{if}\quad n\quad\text{is even and}\quad\geq 2\;,\\ &=\;2\,[\,-\,\log 2\,-\,\sum_{k=1}^{n}\,\frac{(-1)^k}{k}\,]\quad\text{if}\quad n\quad\text{is odd and}\quad\geq 1\;. \end{aligned} \tag{23}$$

We will now derive the expressions (20) and (22) using perturbation theory.

For $c = 0$, the exact eigenstates and energies are

$$\begin{aligned} \psi_n\;&=\;(m\omega)^{1/4}\,H_n(y)\,\exp\,(-y^2/2)\;,\\ E_n\;&=\;(\,n\,+\,\frac{1}{2}\,)\,\omega\;, \end{aligned} \tag{24}$$

where $n = 0, 2, 4, ...$, and H_n is the Hermite polynomial of degree n in the dimensionless variable $y = x\sqrt{m\omega}$. To be explicit [12],

$$H_n(y)\;=\;\left(\,\frac{n!}{2^n\sqrt{\pi}}\,\right)^{1/2}\,\sum_{m=0}^{n/2}\,\frac{(-1)^m\,(2y)^{2m}}{(\frac{n}{2}-m)!\,(2m)!}\;. \tag{25}$$

We now use the second-order formula in (1) and discover that the results match (20) provided the following identities are true

$$\sum_{l\neq n} \frac{(l-1)!!}{l!!} \frac{1}{l-n} \;=\; \frac{1}{2} \frac{(n-1)!!}{n!!} \left[\psi(\frac{n}{2} \;+\; 1) \;-\; \psi(\frac{n}{2} \;+\; \frac{1}{2}) \right] , \tag{26}$$

where the sum over l runs over $0, 2, 4, ...$ For $n = 0$, this identity is given in Ref. [13], but for $n \geq 2$, we have not yet found it in the literature. However we have checked it numerically by computing the summation on the left hand side from $l = 0$ to $L = 2 \times 10^7$ and setting the remainder (from $l = L+2$ to $l = \infty$) equal to $\sqrt{2/(\pi L)}$ by using Stirling's formula. We find that the two sides of (26) match upto 10^{-9} for $n = 0$ to 100.

For $c = \infty$, we have the exact results

$$\begin{aligned} \psi_n &= (m\omega)^{1/4} \; H_n(|y|) \; \exp \; (-y^2/2) \; , \\ E_n &= \left(\; n \; + \; \frac{1}{2} \; \right) \omega \; , \end{aligned} \tag{27}$$

where $n = 1, 3, 5, ...,$ and H_n is given by

$$H_n(y) \;=\; \Big(\frac{n!}{2^n \sqrt{\pi}} \Big)^{1/2} \sum_{m=0}^{(n-1)/2} \frac{(-1)^m \; (2|y|)^{2m+1}}{(\frac{n-1}{2} - m)! \; (2m+1)!} \; . \tag{28}$$

On using perturbation theory with (13), we recover the first order $(1/c)$ result in (22), but we again obtain a divergence at second order. We therefore use the point-splitting prescription and Eqs. (1) and (12) to obtain the second order energy

$$\frac{E_n^{(2)}}{\omega} \;=\; \lim_{y\to 0+} \frac{16 m\omega}{c^2} \frac{n!}{((\frac{n-1}{2})!)^2 \pi^{3/4} 2^n} \sum_{l\neq n} \frac{\sqrt{l!} \; H_l'(y)}{(\frac{l-1}{2})! \; 2^{l/2} \; (n-l)} \; . \tag{29}$$

where we sum over $l = 1, 3, 5, ...$ As before, we can extract a finite value for the limit $x \to 0+$ by using the completeness relation for Hermite polynomials

$$\sum_{p=0}^{\infty} \; H_p^\star(z) \; H_p(y) \; \exp \; \left[\; -\frac{1}{2} \; (\; y^2 \; + \; z^2 \;) \; \right] \;=\; \delta \; (y - z) \; . \tag{30}$$

Setting $z = 0$, we get

$$\lim_{y\to 0+} \sum_{p=0,2,4,...} \frac{\sqrt{p!}}{(\frac{p}{2})! \; \pi^{1/4} 2^{p/2}} \; H_p(y) \;=\; 0 \; . \tag{31}$$

We use the differential relation $H_l'(y) = \sqrt{2l} H_{l-1}(y)$ [12], and subtract (31) from (29). We then discover that (29) agrees with (22) provided again that the identities in (26) hold.

The results in this section indicate the general method of regularising second order perturbation theory near $c = \infty$. Namely, we have to use the completeness relations which hold for the solutions at $c = \infty$, as exemplified by the relations (15) and (30), in order to obtain a series whose sum is actually finite in the limit $x \to 0+$, although it diverges if we naively set $x = 0$. We then have to subtract this sum from the second order perturbation result in order to get a finite result in the limit $x \to 0+$.

4 The δ-function Bose gas

Having convinced ourselves that perturbation theory does work in the one-particle problem with a δ-function potential, let us consider a many-body generalisation. We will study the δ-function Bose gas which has been studied extensively since it was first solved in Ref. [3] using the Bethe ansatz. Although the exact results are available, it is instructive to see how they can be recovered by using perturbation theory near $c = 0$ and ∞. We will consider N particles on a circle of circumference L. We will sometimes be interested in the thermodynamic limit $N, L \to \infty$, keeping the density $\rho = N/L$ fixed. The Hamiltonian is

$$H \;=\; -\;\frac{1}{2m}\;\sum_{1\le i\le N}\;\frac{\partial^2}{\partial x_i^2}\;+\;\frac{2c}{m}\;\sum_{1\le i<j\le N}\;\delta\;(\;x_i\;-\;x_j\;)\;. \tag{32}$$

Since the particles are identical bosons, the wave functions must be completely symmetric. There are $N!$ possible orderings of the particle coordinates, given by $0 \le x_{P_1} \le x_{P_2} \le ... \le x_{P_N} \le L$, where $(P_1, P_2, ..., P_N)$ is some permutation of the numbers $(1, 2, ..., N)$. If the wave functions are known for any one ordering, say $0 \le x_1 \le x_2 \le ...x_N \le L$, they are known for all other orderings by symmetry.

Now it is clear that the model describes noninteracting bosons for $c = 0$. For $c = \infty$, the wave functions vanish whenever any two particle coordinates coincide. We can then carry out the unitary transformation $\psi_P \to (-1)^P \psi_P$, where ψ_P denotes the wave function for the ordering P, and $(-1)^P$ denotes the sign of the permutation P. Under this transformation, the wave function becomes completely antisymmetric, i.e., fermionic. Thus $c = \infty$ denotes a system of noninteracting fermions. Note that this unitary transformation is only allowed if $c = \infty$. At any other value of c, the symmetric wave functions do not vanish for $x_i = x_j$, and the transformation would produce antisymmetric wave functions which are discontinuous at those coincident points.

For simplicity, we will limit our discussion only to the ground state wave function and the corresponding energy per particle. At $c = 0$, these are given by

$$\begin{aligned} \psi_0 &= \frac{1}{\sqrt{L^N}}\;, \\ \frac{E_0}{N} &= 0\;. \end{aligned} \tag{33}$$

We now consider the perturbative expansion around $c = 0$. At first order, the change in energy is found to be

$$\frac{E_0^{(1)}}{N} \;=\; \frac{c\;(N-1)}{L} \tag{34}$$

which is equal to $c\rho$ in the thermodynamic limit. This agrees with the result in Ref. [3]. At second order, there are non-zero matrix elements between ψ_0 and

$$\psi_{k,-k} \;\equiv\; \frac{1}{\sqrt{L^N N(N-1)}} \sum_{i\neq j} \exp\;[\; ik(x_i \;-\; x_j)\;]\;, \tag{35}$$

where $k = 2\pi n/L$ and $n = 1, 2, 3, ...$ The second order formula in (1) then gives

$$\frac{E_0^{(2)}}{N} \;=\; -\;\frac{c^2(N-1)}{6}\;. \tag{36}$$

This is indeed the correct answer (i.e., it agrees with the Bethe ansatz results) if we take the limit $c \to 0$ holding N and L *fixed*. However, it is *not* the correct result if we hold c fixed and take the thermodynamic limit, as can be seen from the fact that the right hand side of (36) diverges in that limit. The reason for this divergence is that the matrix element

$$\langle\psi_{k,-k}|V|\psi_0\rangle \;=\; \frac{2c\sqrt{N(N-1)}}{L} \tag{37}$$

can become comparable to or even larger than the energy denominator $E_0 - E_{k,-k}$ if we let $L \to \infty$. Second order perturbation theory breaks down in that case. In the thermodynamic limit, a different perturbation theory exists due to Bogoliubov [3], and it gives the result

$$\frac{E_0^{(2)}}{N} \;=\; -\;\frac{4}{3\pi}\;c^{3/2}\;\rho^{1/2}\;. \tag{38}$$

The presence of a fractional power of c clearly shows that this perturbation theory is rather different from the one we have been discussing so far. We emphasize that the divergence in our second order perturbation theory in the thermodynamic limit is not to be confused with the divergence which we have discussed in the Secs. 2 and 3; the two divergences are due to entirely different reasons.

We will now consider perturbation theory around the free fermion point $c = \infty$. Here we will again discover a divergence at second order perturbation theory which is similar to the ones discussed in the previous two sections, and the regularisation required to cure it is also very similar. However, unlike the expansion around $c = 0$, there is no additional divergence in the thermodynamic limit, and E_0/N does have an expansion in integer powers of the dimensionless parameter ρ/c.

At $c = \infty$, the ground state wave function ψ_0 in a particular ordering of the particle coordinates is given by $1/\sqrt{L^N N!}$ times the determinant of the matrix

$$M_{ij} \;=\; \exp\;[\; ik_i x_j\;]\;, \tag{39}$$

where the momenta k_i run over the N distinct values $(\pi/L)\ (1-N, 3-N, 5-N, ..., N-1)$. (Note that for $c = \infty$, the allowed values of the momenta are given by $n2\pi/L$ if N is odd, and $(n + \frac{1}{2})2\pi/L$ if N is even [3]). The ground state energy is given by

$$\frac{E_0}{N} \ = \ \frac{1}{2mN} \ \sum_i \ k_i^2 \ = \ \frac{\pi^2}{6mL^2} \ (\ N^2 \ - \ 1 \ ) \ . \tag{40}$$

Following the arguments leading upto (13), we can show that the perturbation around $c = \infty$ is described by the two-particle interaction

$$\tilde{V} \ = \ - \ \frac{1}{cm} \ \sum_{i<j} \ \delta''(\ x_i \ - \ x_j \ ) \ . \tag{41}$$

(The simplest way to derive this is to consider just two particles, and transform to the centre of mass and relative coordinates $X = (x_1 + x_2)/2$ and $x = x_1 - x_2$ respectively. The contact interaction then involves only the coordinate x which is a one-body problem as in the previous sections). Using this potential in first order perturbation theory yields the change in energy

$$\frac{E_0^{(1)}}{N} \ = \ - \ \frac{\pi^2}{3mcL^3} \ N \ (\ N^2 \ - \ 1 \ ) \ . \tag{42}$$

We now proceed to second order perturbation theory. To simplify the calculation, we will consider the thermodynamic limit; thus we will replace $\sum_{k_i}$ by $(L/2\pi) \ \int dk$ whenever convenient. It is useful to introduce the Fermi momentum

$$k_F \ = \ \pi\rho \ , \tag{43}$$

so that all the momenta k_i in the ground state lie within the range $[-k_F, k_F]$. We begin our analysis by observing that $\tilde{V}$ has non-zero matrix elements between the ground state ψ_0 and the excited states $\psi_{k_i', k_j'}$, where $\psi_{k_i', k_j'}$ differs from ψ_0 in having exactly two momenta k_i' and k_j' different from two momenta k_i and k_j; the other $N-2$ momenta are identical in the two states. The translation invariance of the interaction (41) implies that we must have

$$k_i \ + \ k_j \ = \ k_i' \ + \ k_j' \ , \tag{44}$$

where k_i' and k_j' must lie *outside* the range $[-k_F, k_F]$.

We then find that the second order energy is given by

$$\frac{E_0^{(2)}}{N} \ = \ \frac{2}{mc^2NL^2} \ \sum_{k_i<k_j} \ (\ k_i \ - \ k_j \ )^2 \ \sum_{k_i'<k_j'} \ \frac{(\ k_i' \ - \ k_j' \ )^2}{k_i^2 \ + \ k_j^2 \ - \ k_i'^2 \ - \ k_j'^2} \ , \tag{45}$$

which is again divergent since the sum over k_i' or k_j' runs over all values outside the range $[-k_F, k_F]$. Note that there are only three independent sums on the right hand side of

(45) since there is a constraint from momentum conservation (44); thus we can replace the sums by multiple integrals over k_i, k_j and k'_j of the form

$$\int_{-k_F}^{k_F} dk_i \int_{k_i}^{k_F} dk_j \int_{k_0}^{\infty} dk'_j \ , \tag{46}$$

where the lower limit of the k'_j integral is given by

$$\begin{aligned} k_0 &= k_F \quad \text{if} \quad k_i + k_j < 0 \ , \\ &= k_F + k_i + k_j \quad \text{if} \quad k_i + k_j > 0 \ . \end{aligned} \tag{47}$$

We regularize the divergence in (45) using the method described in Sec. 2. We will briefly indicate the procedure here without going through all the details. In the matrix element $\langle \psi_0 | \tilde{V} | \psi_{k'_i,k'_j} \rangle$, let us consider one of the terms in $\tilde{V}$, say, $\delta''(x_1 - x_2)$. After performing the integrals over $x_3, x_4, ..., x_N$, we are left with integrals over $X = (x_1 + x_2)/2$ and $x = x_1 - x_2$ of the form $\int_0^L dX/L$ times

$$\int dx \, \delta(x) \, \cos \, [\frac{1}{2}(k'_i - k'_j)x] \, \cos \, [\frac{1}{2}(k_i - k_j)x] \, = \, \frac{1}{2} \int dx \, \delta(x) \, [\cos \, (k'_j - k_i)x + \cos \, (k'_j - k_j)x] \tag{48}$$

appearing in the numerator of the last term on the right hand side of (45). If we naively perform the integral in (48) by setting $x = 0$, we obtain the constant 1; this leads to the divergence in (45) when we integrate a constant over k'_j with the ranges shown in (46) and (47). To regularise that divergence, we first perform the integral over k'_j for $x \neq 0$, and then take the limit $x \to 0+$. We use the result

$$\frac{1}{2} \int_{k_0}^{\infty} dk'_j \, [\, \cos \, (k'_j - k_i)x \, + \, \cos \, (k'_j - k_j)x \,] \, = \, - \, k_F \, - \, \frac{1}{2} \, | \, k_i \, + \, k_j \, | \tag{49}$$

in the limit $x \neq 0$. This follows from the fact that

$$\int_{-\infty}^{\infty} dk \, \exp \, [ikx] \, = \, 2 \int_0^{\infty} dk \, \cos \, (kx) \, = \, 0 \tag{50}$$

if $x \neq 0$, and therefore

$$\int_K^{\infty} dk \, \cos \, (kx) \, = \, - \, \frac{\sin \, (Kx)}{x} \tag{51}$$

which equals $-K$ in the limit $x \to 0+$.

After subtracting the integral in (49) from the right hand side of (45), we are left with the convergent expression

$$\begin{aligned} \frac{E_0^{(2)}}{N} &= \frac{1}{4\pi^3 mc^2 \rho} \int_{-k_F}^{k_F} dk_i \int_{k_i}^{k_F} dk_j \, (\, k_i - k_j \,)^2 \, I(k_1, k_2) \ , \\ \text{where} \quad I(k_1, k_2) &= 2k_F + | \, k_i + k_j \, | - \frac{1}{2} \, (k_i - k_j)^2 \int_{k_0}^{\infty} dk'_j \, \frac{1}{(k'_j - k_i)(k'_j - k_j)} \ . \end{aligned} \tag{52}$$

On doing the integrals in (52) and using (43), we get

$$\frac{E_0^{(2)}}{N} \;=\; \frac{\pi^2\rho^4}{2mc^2}\;. \tag{53}$$

Collecting all the results near $c = \infty$, we find the first three terms in the energy per particle in the thermodynamic limit to be

$$\frac{E_0}{N} \;=\; \frac{\pi^2\rho^2}{6m}\,[\;1\;-\;2\,\frac{\rho}{c}\;+\;3\,\frac{\rho^2}{c^2}\;+\;...\;]\;. \tag{54}$$

This agrees with the results in [3].

5 The Calogero-Sutherland model

We now turn to another technique for dealing with singular potentials. Consider the Calogero-Sutherland model in which particles move on a line (or circle), and interact pairwise through an inverse-square potential. This potential is so singular that the wave functions vanish whenever two particles i and j approach each other. This property can create difficulties for the usual kind of perturbation theory if we perturb around a model in which the inverse-square potential is absent and the wave functions do not vanish at coincident points. We will discuss two different versions of the inverse-square model, one with particles placed in a simple harmonic potential on a line, and the other with particles on a circle with no external potential. The modification of perturbation theory required in the two cases is similar, but it is convenient to discuss them separately.

5.1 The Calogero model

Consider the Hamiltonian for N identical particles on a line [4]

$$H \;=\; -\;\frac{1}{2m}\;\sum_i \frac{\partial^2}{\partial x_i^2}\;+\;\frac{\lambda(\lambda-1)}{m}\;\sum_{i<j}\;\frac{1}{(x_i\;-\;x_j)^2}\;+\;\frac{m\omega^2}{2}\;\sum_i\;x_i^2\;, \tag{55}$$

where $\lambda \geq 0$. To make the problem completely well-defined, we have to specify that all wave functions vanish as $|x_i - x_j|^\lambda$ whenever particles i and j approach each other. Since the singular two-particle interactions prevent particles from crossing each other, there is no way of comparing the phase of the wave function for one configuration with the phase for another configuration in which two particles have been exchanged. In other words, we have the freedom to work with any phase convention relating the different possible orderings of the particle coordinates. We will choose to work with completely symmetric wave functions. Note that the inverse-square interaction in (55) vanishes for both $\lambda = 0$

and $\lambda = 1$. However, the condition on the wave functions implies that $\lambda = 0$ corresponds to noninteracting bosons, while $\lambda = 1$ corresponds to noninteracting fermions. The latter is true even though we are working with symmetric wave functions; the situation is very similar to the model in Sec. 4 with $c = \infty$.

It is particularly simple to solve the model at the two noninteracting values $\lambda = 0$ and 1, and we can consider doing perturbation theory about either point. It turns out that perturbation theory around $\lambda = 1$ is completely straightforward since all matrix elements of the perturbation (taken to be the inverse-square term in (55)) are finite. However, perturbation theory around $\lambda = 0$ is not so simple because even the first order result in (1) diverges. This can be seen from a simple counting of powers; if we define a relative coordinate $x = x_1 - x_2$, the wave functions for $\lambda = 0$ go to a non-zero constant as $x \to 0$. Then first order perturbation theory involves an integral like $\int dx/x^2$ which diverges at $x = 0$. (The same power counting shows that perturbation theory around any value of $\lambda \leq 1/2$ is divergent; the divergence is weakest (logarithmic) at $\lambda = 1/2$ [14]).

We therefore proceed as follows for perturbation theory around $\lambda = 0$. Let us denote the singular part of the wave functions at any value of λ by

$$\Delta(\lambda) \;=\; \prod_{i<j} \mid x_i \;-\; x_j \mid^{\lambda} . \tag{56}$$

Instead of solving $H\psi = E\psi$, we will solve $\tilde{H}\tilde{\psi} = E\tilde{\psi}$, where $\tilde{\psi} = \Delta^{-1}\psi$ does *not* vanish at coincident points, and

$$\begin{aligned} \tilde{H} \quad &= \quad \Delta^{-1}\, H\, \Delta \;=\; H_0 \;+\; \tilde{V} \;, \\ \text{where} \quad H_0 \quad &= \quad -\; \frac{1}{2m} \sum_i \frac{\partial^2}{\partial x_i^2} \;+\; \frac{m\omega^2}{2} \sum_i \; x_i^2 \;, \\ \text{and} \quad \tilde{V} \quad &= \quad -\; \frac{\lambda}{m} \sum_{i<j} \frac{1}{x_i - x_j} \left(\frac{\partial}{\partial x_i} \;-\; \frac{\partial}{\partial x_j} \right) . \end{aligned} \tag{57}$$

We now have to derive the formulas for perturbation theory with the *non-Hermitian* interaction $\tilde{V}$ given in (57). We can show that the required formulas are identical to those appearing in the usual Rayleigh-Schrödinger perturbation theory, such as Eqs. (1) and (2) [1]. We only have to remember to use the expressions exactly as given in (1) and schematically as given in (2). For instance, we cannot replace the matrix element $\langle\psi_n(0)|\tilde{V}|\psi_l(0)\rangle$ by the complex conjugate of $\langle\psi_l(0)|\tilde{V}|\psi_n(0)\rangle$ since $\tilde{V}$ is not Hermitian. This will become clearer after the discussion below.

The exact eigenstates and eigenvalues of the Hamiltonian H_0 have the general form

$$\begin{aligned} \Psi_n(x_i \;;\; \lambda = 0) \quad &= \quad P_n(x_i)\; G \;, \\ G \quad &= \quad \exp \left[\; -\; \frac{m\omega}{2} \sum_i \; x_i^2 \; \right] , \\ E_n^{(0)} \quad &= \quad \left(\; n \;+\; \frac{N}{2} \; \right) \omega \;, \end{aligned} \tag{58}$$

and P_n is a symmetric polynomial in the x_i of degree n. In order to discuss perturbation theory, it is convenient to use the following result [15]. Any symmetric polynomial $Q_n(x_i)$ of degree n can be written as a linear combination

$$Q_n(x_i) \;=\; \sum_l \; P_l(x_i) \;, \tag{59}$$

where the symmetric polynomials P_l all have degree $l \leq n$ and the wave functions $P_l G$ are eigenstates of H_0.

Let us now consider first order perturbation theory. We note that

$$\tilde{V} \;(\; P_n \; G \;) \;=\; \frac{\lambda N(N-1)}{2} \; P_n \; G \;+\; Q_l \; G \;, \tag{60}$$

where Q_l is a polynomial of degree $\leq n-2$. Using (59), $Q_l G$ is seen to be a superposition of eigenstates of H_0 with energy less than that of $P_n G$. Therefore $P_n G$ is orthogonal to $Q_l G$. Hence the first order change in energy is just

$$E_n^{(1)} \;=\; \frac{\lambda N(N-1)}{2} \;. \tag{61}$$

One might worry about degeneracies at this stage. To see that this is not a problem, consider two polynomials $P_n^{(1)}$ and $P_n^{(2)}$ of the same degree n such that $\psi^{(1)} = P_n^{(1)} G$ and $\psi^{(2)} = P_n^{(2)} G$ are degenerate and orthogonal eigenstates of H_0. The orthogonality together with the form in (60) shows that both the matrix elements $\langle \psi^{(1)} | \tilde{V} | \psi^{(2)} \rangle$ and $\langle \psi^{(2)} | \tilde{V} | \psi^{(1)} \rangle$ are zero. It is therefore unnecessary to worry about degenerate perturbation theory at first order. We also have the general result that $\langle \psi_l | \tilde{V} | \psi_n \rangle$ can be non-zero only if either $\psi_l = \psi_n$ or if the degrees of the respective polynomials satisfy $l \leq n-2$. This result will be used below.

We now consider higher order perturbation theory. From the general form given in (2), it is easy to see that there are *no* contributions to the energies at any order higher than the first. This is because the individual matrix elements in (2) can only be non-zero if the degrees of the polynomials satisfy $n \leq l_k - 2$, $l_k \leq l_{k-1}$, ..., $l_2 \leq l_1$ and $l_1 \leq n-2$. (These inequalities follow from the observation that the states ψ_{l_i} may be identical to each other, but they all have to be different from ψ_n). It is clear that all these inequalities cannot hold simultaneously; hence the product in (2) must necessarily be zero.

Our perturbation theory has therefore yielded the well-known result that the energies only get a contribution at first order in λ, and that this contribution is the same for all states as seen in (61). However the eigenstates can get contributions at any order in λ.

Before ending this subsection, we would like to emphasise that although the perturbation $\tilde{V}$ is not Hermitian, its derivation from the Hamiltonian in (55) guarantees that the perturbative changes in energies must be real. Note also that the eigenstates of $\tilde{H}$ are orthogonal with the integration measure $\Delta^2 \prod_i dx_i$, not with the measure $\prod_i dx_i$.

5.2 The Sutherland model

We now consider the inverse-square model on a circle of circumference L with periodic boundary conditions [5]. The Hamiltonian for N particles is

$$H \;=\; -\;\frac{1}{2m}\;\sum_i\;\frac{\partial^2}{\partial x_i^2}\;+\;\frac{\lambda(\lambda-1)}{m}\;\sum_{i<j}\;\frac{\pi^2}{L^2\sin^2\;[\;\frac{\pi}{L}\;(\;x_i\;-\;x_j\;)\;]}\;. \tag{62}$$

We impose the same conditions on the wave functions at coincident points as in the previous subsection. To develop perturbation theory, we again perform a similarity transformation but now with a periodic function

$$\Delta(\lambda)\;=\;\prod_{i<j}\;|\sin\;[\;\frac{\pi}{L}\;(x_i\;-\;x_j)\;]\;|^\lambda\;. \tag{63}$$

This transforms the Hamiltonian into

$$\begin{aligned}
\tilde{H} \;&=\; \Delta^{-1}\;H\;\Delta\;=\;H_0\;+\;\tilde{V}\;,\\
\text{where}\quad H_0\;&=\;-\;\frac{1}{2m}\;\sum_i\frac{\partial^2}{\partial x_i^2}\;+\;\frac{\lambda^2\pi^2N(N^2-1)}{6mL^2}\;,\\
\text{and}\quad \tilde{V}\;&=\;-\;\frac{\lambda}{m}\;\frac{\pi}{L}\;\sum_{i<j}\;\cot\;[\;\frac{\pi}{L}(x_i-x_j)\;]\;(\;\frac{\partial}{\partial x_i}\;-\;\frac{\partial}{\partial x_j}\;)\;.
\end{aligned} \tag{64}$$

Note that H_0 has a λ dependent constant which will therefore appear in the energies of all the states. We now discuss perturbation theory with the interaction $\tilde{V}$.

The (unnormalised) eigenstates and eigenvalues of the noninteracting Hamiltonian H_0 are easy to derive. Consider a set of N integers $\{n_i\}=(n_1,n_2,...,n_N)$, each of which may be positive, negative or zero, and some of them may be equal to each other. Then we have

$$\begin{aligned}
\psi_{\{n_i\}}\;&=\;\exp\;[\;i\frac{2\pi}{L}\;(n_1x_1+n_2x_2+...+n_Nx_N\;)\;]\;+\quad\text{symmetrisation}\;,\\
E_{\{n_i\}}\;&=\;\frac{2\pi^2}{mL^2}\;\sum_i\;n_i^2\;.
\end{aligned} \tag{65}$$

The momentum of such a state is given by $(2\pi/L)\sum_i n_i$.

In order to discuss perturbation theory, it is convenient to introduce the concept of *squeezing* [5]. We say that a set of integers $\{n_i'\}$ can be obtained from another set $\{n_i\}$ by squeezing if (a) two integers in the first set, say, n_i' and n_j', are different from two integers in the second set, say, n_i and n_j, but all the other $N-2$ integers in the two sets are pairwise equal, and (b) $n_i'+n_j'=n_i+n_j$ but $|n_i'-n_j'|<|n_i-n_j|$. Thus the momentum of the states corresponding to the two sets are equal, but $E_{\{n_i'\}}<E_{\{n_i\}}$ according to (65).

We then find that the action of $\tilde{V}$ on the states is given by

$$\tilde{V}\ \psi_{\{n_i\}}\ =\ \Big(\ \frac{2\lambda}{m}\frac{\pi^2}{L^2}\ \sum_{i<j}\ |\ n_i\ -\ n_j\ |\ \Big)\ \psi_{\{n_i\}}\ +\ \sum_{\{n_i'\}}\ \psi_{\{n_i'\}}\ , \tag{66}$$

where the summation over states runs over the various possible sets $\{n_i'\}$ which can be obtained from the set $\{n_i\}$ by squeezing; all these states have lower energy than $\psi_{\{n_i\}}$ by the comment in the previous paragraph. We thus see that a matrix element $\langle\psi_{\{n_i'\}}|\tilde{V}|\psi_{\{n_i\}}\rangle$ can only be non-zero if $\{n_i'\}$ is either identical to $\{n_i\}$ or can be obtained from it by squeezing. Clearly, matrix elements between distinct but degenerate states are zero, so that we do not need to do any degenerate perturbation theory.

The first order change in energy is therefore given by

$$E^{(1)}_{\{n_i\}}\ =\ \frac{2\lambda}{m}\frac{\pi^2}{L^2}\ \sum_{i<j}\ |\ n_i\ -\ n_j\ |\ . \tag{67}$$

Once again, there is no contribution to the energies from any higher orders in perturbation theory due to the product form in (2); at least one of the matrix elements in that product must be zero following an argument very similar to the one used in the previous section (with the concept of "degree of polynomial" replaced by "squeezing").

We have thus recovered the result that there are only two λ dependent terms in the energy of any state. The term of order λ is given in (67) and it depends on the state, whereas the term of order λ^2 given in (64) is the same for all states.

6 Outlook

There are several issues which could be addressed in the future. For the δ-function problem near $c = \infty$ in Secs. 2-4, we could study perturbation theory at cubic and higher orders to see if a similar point-splitting regularisation can be devised to obtain finite answers at all orders in $1/c$.

We can also study a generalisation of the δ-function problem to higher dimensions. Given a bounded region M with boundary ∂M, it is known [16] that the Hamiltonian $H = -\vec{\nabla}^2$ is self-adjoint (and therefore has real eigenvalues and orthonormal eigenvectors) if we impose the boundary condition on all wave functions,

$$\hat{n}\cdot\vec{\nabla}\psi\ =\ c\psi \tag{68}$$

where $\hat{n}$ is the unit vector pointing inward and normal to the boundary ∂M, and c can be any real number. Once again, we can study perturbation theory near $c = 0$ (Neumann condition) or $c = \infty$ (Dirichlet condition). To do this, we first define a generalised δ-function and its derivatives which are non-zero only in an infinitesimal neighbourhood of

∂M. We can then use expressions like (1) or (13) where the perturbation V or $\tilde{V}$ involves that δ-function or its second derivative. Once again, we obtain a divergence in second order perturbation theory near $c = \infty$, and a regularisation is required to obtain finite answers. It would be interesting to study the precise form of the regularisation for an arbitrary region M.

The method of non-Hermitian perturbation has already been used in two-dimensional models such as anyons [8] and systems with other types of two-body correlations [17]. We can consider applications of this method to any model in which conventional perturbation theory diverges due to the singular nature of the wave functions in the vicinity of certain points in configuration space. We simply remove the singular part of the wave functions by a similarity transformation; we then obtain a new potential (generally non-Hermitian) whose matrix elements between non-singular wave functions need to be computed. The procedure will work if all such matrix elements can be shown to be finite.

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