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Non-relativistic bound-state problems in momentum space

T W Chiu

Physics Department, National Taiwan University, Taipei, Taiwan, Republic of China

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Abstract. The non-relativistic bound-state problem is studied in momentum space with emphasis on the potentials which are divergent at large distances. The Schrödinger integral equation is solved by the collocation method. In contrast to the bound-state problem in coordinate space, solving this type of eigenproblem in momentum space does not yield the correct eigenvalues unless the 'infrared' divergent potential is regularised. A regularisation method is introduced and illustrated with two examples, namely the simple harmonic oscillator and the linearly rising potential. Finally the quarkonium systems are studied with the regulated linear plus Coulomb potential.

1. Introduction

The bound-state problems in non-relativistic quantum mechanics are usually solved via the Schrödinger equation in coordinate space. Examples are the square well, simple harmonic oscillator and Coulomb potential. These have exact analytic solutions. Other potentials which do not have analytic solutions are often treated by the perturbation or semiclassical methods. Although the problems with a simple central potential can be handled most easily with a differential equation approach, many problems in many-body and high energy physics lead naturally to integral equations in momentum space which cannot be transformed into a simple equation in coordinate space. Examples are relativistic bound-state equations. To develop techniques for handling relativistic bound-state problems in momentum space, it is instructive to test them in the non-relativistic regime where most problems are well understood. This motivates our present study.

In this paper, we solve the non-relativistic bound-state problems in momentum space, with emphasis on the potentials which are divergent at large distances (e.g., a linearly rising potential). In momentum space, the Schrödinger equation is an integral equation which can be solved numerically by the collocation method [1]. If we pick an 'infrared' divergent potential (e.g., the simple harmonic oscillator) and try to solve this problem by the collocation method, we find that the eigenvalues do not agree with those obtained via the Schrödinger differential equation. The discrepancy is due to the fact that the kernel is not square integrable. The kernel must be regularised before we can obtain the correct eigenvalues. At this point, let us discuss some salient features distinguishing the differential equations from the integral equations. Loosely speaking, a differential equation is '*local*'. It cannot conceive any information which is far away from the point of observation. Thus it cannot 'see' the 'infrared' divergence occurring at large distances. Furthermore boundary conditions have to be specified before the solutions can be obtained. We usually choose the boundary conditions such that the

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wavefunctions are well behaved at the origin and at infinity. On the other hand, an integral equation is 'global'; it incorporates all information from all points (including infinity) through the kernel. Thus the 'infrared' divergence at infinity affects every point of observation, then invalidates the collocation method. To overcome this difficulty, we regularise the 'infrared' divergent potential energy by levelling it off beyond a certain point (see figures 2 and 3). Doing this renders the kernel to be square integrable and yields the correct eigenvalues and eigenfunctions.

In the next section, we formulate the bound-state problem in momentum space and review the basic ideas of the collocation method. Three examples are discussed, namely Coulomb, linear and harmonic oscillator. Although the Coulomb potential is not 'infrared' divergent, we include it here for the sake of completeness. In § 3, we employ the techniques developed in § 2 to study the quarkonium system which is a bound state of a quark and an antiquark. It is well known that the quarkonium mass spectra can be fitted by many non-relativistic potential models [2]. We use the Cornell potential (Coulomb+linear) and their parameters to fit charmonium ($c\bar{c}$) and bottomium ($b\bar{b}$). Our results are in good agreement with the Cornell results.

2. Three examples

In momentum space, the Schrödinger equation is

$$\left(E-\frac{p^2}{2\mu}\right)\psi(\boldsymbol{p})=\int\frac{d^3\boldsymbol{q}}{(2\pi)^3}\,V(\boldsymbol{p}-\boldsymbol{q})\psi(\boldsymbol{q}) \tag{1}$$

where E is the energy eigenvalue and μ is the mass of the particle. The wavefunction in coordinate space can be obtained by the Fourier transformation

$$\psi(\boldsymbol{r})=\frac{1}{(2\pi)^3}\int d^3\boldsymbol{p}\,\exp(i\boldsymbol{p}\cdot\boldsymbol{r})\psi(\boldsymbol{p}). \tag{2}$$

We perform the partial wave decomposition as follows:

$$\psi(\boldsymbol{p})=\sum_{l,m}\frac{U_l(p)}{p}\,Y_{lm}(\hat{p}) \tag{3}$$

$$\begin{aligned}V(\boldsymbol{p}-\boldsymbol{q})\equiv V(p,q,x)&=\sum_l\frac{(2l+1)}{4\pi}\,P_l(x)\,V_l(p,q)\\&=\sum_{l,m}Y_{lm}(\hat{p})\,Y_{lm}(\hat{q})\,V_l(p,q)\end{aligned} \tag{4}$$

where x is the cosine of the angle between $\hat{p}$ and $\hat{q}$, P_l is the Legendre polynomial and Y_{lm} is the spherical harmonic.

Substituting (3) and (4) into (1) and integrating over the angular variables, we obtain

$$\left(E-\frac{p^2}{2\mu}\right)U_l(p)=\int_0^\infty\frac{dq}{(2\pi)^3}\,pqV_l(p,q)\,U_l(q) \tag{5}$$

where

$$V_l(p,q)=2\pi\int_{-1}^{1}dx\,P_l(x)\,V(p,q,x). \tag{6}$$

Equation (5) is a linear integral equation which can be solved numerically by the collocation method.

The essence of the collocation method is to discretise the momentum variables in (5). This turns equation (5) into a set of simultaneous algebraic equations:

$$EU_l(p_i) = \sum_{j=1}^{n} \left(\frac{p_j^2}{2\mu} \delta_{ij} + \frac{\Delta_j}{(2\pi)^3} p_i p_j V_l(p_i, p_j) \right) U_l(p_j) \qquad i = 1, \ldots, n \tag{7}$$

where $\{p_1 \ldots p_n\}$ is the set of discrete momentum mesh points, δ_{ij} is the Kronecker δ function and Δ_j is the weight corresponding to dq in (5). The eigenproblem of equation (7) can be solved numerically.

2.1. *Coulomb potential* ($V = -\alpha/r$)

In momentum space, the potential kernel is

$$V(p, q, x) = -\frac{4\pi\alpha}{p^2 + q^2 - 2pqx}. \tag{8}$$

If we substitute (8) into (6), the integration can be evaluated analytically to yield

$$V_l(p, q) = -\frac{8\pi^2\alpha}{pq} Q_l \frac{p^2 + q^2}{2pq} \tag{9}$$

where Q_l is the Legendre polynomial of the second kind. However, (9) is not suitable for the collocation method due to the singularity of Q_l at $p = q$. To avoid this singularity, we shall integrate equation (6) numerically by Gaussian integration. Notice that such a singularity would be absent in the case of a Yukawa potential ($V = -(\alpha/r)e^{-mr}$) where the argument of Q_l in (8) is replaced by $(p^2 + q^2 + m^2)/2pq$. For $\mu = 0.92$, $\alpha = 0.5236$ and 100 mesh points which are distributed according to

$$p_i = 0.92 \left(\frac{i}{101 - i} \right) \qquad i = 1, \ldots, 100$$

we obtain the energy eigenvalues listed in table 1 in comparison with the exact eigenvalues. Higher energy eigenvalues have been omitted. The eigenfunction of the ground state is plotted in figure 1, which is in good agreement with the exact Coulomb wavefunction in momentum space [3]. The more mesh points we use, the higher the accuracy of the eigenvalues and eigenfunctions we obtain.

2.2. *Linearly rising potential* ($V = ar$)

First, let us solve this problem in coordinate space because the solution is not readily available in most textbooks. The Schrödinger equation of the linearly rising potential is

$$\frac{d^2U_l}{dr^2} + 2\mu \left(E - ar - \frac{l(l+1)}{2\mu r^2} \right) U_l = 0 \qquad \hbar = 1 \tag{10}$$

where U_l is the radial wavefunction and l is the angular momentum quantum number.

Table 1. Coulomb energy levels ($\mu = 0.92$, $\alpha = 0.5236$,100 mesh points).

n	1	2	3
E(collocation)	−0.126 367	−0.032 991	−0.016 017
$E = -\mu\alpha^2/2n^2$	−0.126 112	−0.031 528	−0.014 012

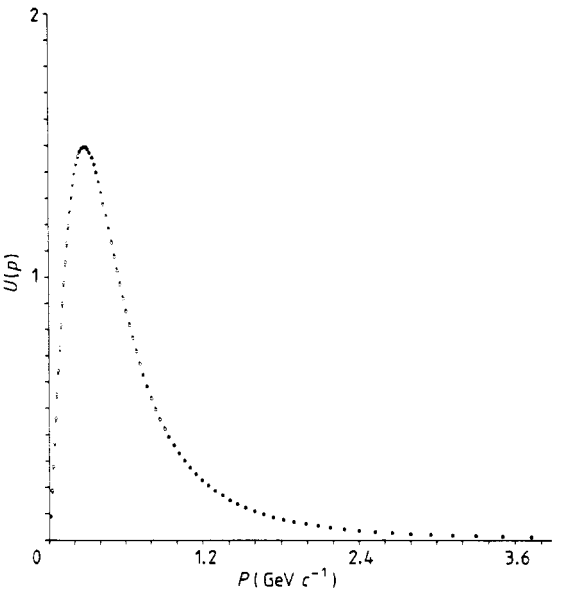

Figure 1. Normalised ground-state Coulomb wavefunction in momentum space (○: collocation solution, +: analytic solution).

For $l = 0$, we have

$$d^2U_0/dr^2 + 2\mu(E - ar)U_0 = 0. \tag{11}$$

Introducing a new variable

$$Z \equiv (2\mu a)^{1/2}(r - E/a)$$

equation (11) can then be transformed to

$$d^2U_0/dZ^2 - ZU_0 = 0. \tag{12}$$

Solutions are pairs of linearly independent Airy functions given on p 446 of Abramowitz and Stegun [4]. They are

$$\begin{aligned} &A_i(Z) \qquad B_i(Z) \\ &A_i(Z) \qquad A_i(Z\exp(2\pi i/3)) \\ &A_i(Z) \qquad A_i(Z\exp(-2\pi i/3)). \end{aligned} \tag{13}$$

Now we must impose the boundary condition $U_0(0) = 0$ in order to obtain the energy eigenvalues. The energy eigenvalues are determined from the zeros of $A_i(Z)$, i.e.

$$E = -[a/(2\mu a)^{1/3}]Z_0 \qquad A_i(Z_0) = 0. \tag{14}$$

The first few zeros of $A_i(Z)$ (see [4], table 10.13, p 478) are

−2.338 11	−9.022 65
−4.087 95	−10.040 17
−5.520 56	−11.008 52
−6.786 71	−11.936 01
−7.944 13	−12.828 78.

For $\mu = 0.92$ and $a = 0.182\,63$, the corresponding energy eigenvalues are

0.614 20	2.370 152
1.073 86	2.637 443
1.450 19	2.891 818
1.782 79	3.135 460
2.086 84	3.369 981 ....

(15)

Now let us solve this problem in momentum space by the collocation method. The potential kernel is

$$V(p, q, x) = -8\pi a/(p^2+q^2-2pqx)^2. \tag{16}$$

With 100 mesh points distributed according to

$$p_i = 0.92\left(\frac{i}{101-i}\right) \qquad i = 1, \ldots, 100$$

the eigenvalues turn out to be totally nonsensical. They are

1.093 32
2.786 22
4.771 47
7.135 02
9.995 08
⋮

(17)

in complete disagreement with those listed in (15). The discrepancy is due to the fact that the kernel

$$K(p, q) \equiv 2\pi pq \int_{-1}^{1} \mathrm{d}x\, P_l(x)\, V(p, q, x)$$

of the linear potential is not square integrable:

$$\int_0^\infty \mathrm{d}p \int_0^\infty \mathrm{d}q\, |K(p, q)|^2 < \infty.$$

To overcome this difficulty, we regulate the linear potential as illustrated in figure 2. This amounts to levelling off the divergent potential after exceeding a certain distance. Many different regularisations had been tried but could not yield better results. This can be understood as follows. If we regulate the divergent potential by replacing it at large distances with a monotonic decreasing potential, a potential barrier is artificially created and the 'tunnelling' through the barrier would affect the energy eigenvalues and eigenfunctions at small distances. Such 'tunnelling' effects could be reduced to a minimum if the barrier is infinitely thick. The reglarisation in figure 2 satisfies this requirement and in fact yields the best results. The regularised potential kernel is

$$V(p, q, x) = (2\pi)^3 ab\delta^3(\boldsymbol{p}-\boldsymbol{q}) + \frac{4\pi a}{(p^2+q^2-2pqx)^2}[2\cos b(p^2+q^2-2pqx)^{1/2} - 2 + b(p^2+q^2-2pqx)^{1/2}\sin b(p^2+q^2-2pqx)^{1/2}]. \tag{18}$$

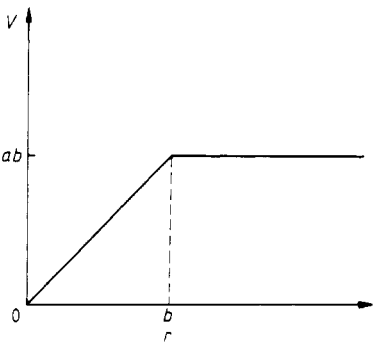

Figure 2. Regularised linear potential.

Using the regularised kernel, the energy eigenvalues come out to agree with those obtained via differential equations. They are summarised in table 2. We have dropped those eigenvalues bigger than ab because they no longer correspond to the bound states of the regularised potential. By adjusting the value of the parameter b, we can have as many eigenvalues as we wish. We also note that the low lying eigenvalues are insensitive to the parameter b.

Table 2. Energy eigenvalues of a regularised linear potential ($\mu = 0.92$, $a = 0.182\,63$, $l = 0$, $V_0 = 0$, 100 mesh points).

$b = 5$	$b = 10$	$b = 15$	$b = 20$	Solutions of equation (15)
0.612 840	0.613 820	0.613 590	0.613 361	0.614 20
	1.073 464	1.073 190	1.072 913	1.073 86
	1.449 486	1.449 486	1.449 175	1.450 19
	1.768 493	1.782 072	1.781 732	1.782 79
		2.086 100	2.085 743	2.086 84
		2.369 154	2.369 034	2.370 15
		2.630 881	2.636 308	2.637 44
			2.890 668	2.891 82
			3.134 264	3.135 46
			3.368 180	3.369 98
			3.586 697	

In this example we have seen clearly the difference between solving 'infrared divergent' potential problems in coordinate space and in momentum space. In coordinate space we must impose boundary conditions to ensure the eigenfunctions are well behaved at the origin and at infinity. These boundary conditions have indeed forced us to quantise the energy. On the other hand, in momentum space, we do not have the freedom of imposing the boundary conditions on the integral equation. We must regulate the 'infrared divergent' potential as we have done in figure 2. This is equivalent to shifting the potential energy origin and then setting $V = 0$ for $r > b$.

We also studied the higher angular momentum ($l \neq 0$) states. The results are summarised in table 3. The energy levels of $l > 0$ are in good agreement with those obtained by using the large l asymptotic expansion [11].

Table 3. Energy eigenvalues of a regularised linear potential ($\mu = 0.92$, $a = 0.182\,63$, $b = 10.0$, $V_0 = 0.0$, 100 mesh points).

State	Energy eigenvalue
1S	0.613 820
1P	0.882 564
2S	1.073 464
1D	1.115 554
2P	1.282 658
3S	1.449 486
2D	1.478 212
3P	1.628 090
4S	1.768 493
3D	1.791 106

2.3. Spherical harmonic oscillator ($V = \frac{1}{2}kr^2$)

The Schrödinger equation of the radial wavefunction of a spherical harmonic oscillator is

$$\frac{d^2U_l}{dr^2} + \frac{2\mu}{\hbar^2}\left(E - \tfrac{1}{2}kr^2 - \frac{l(l+1)\hbar^2}{2\mu r^2}\right)U_l = 0.$$

For $l = 0$, the energy levels [5] are

$$E = (2n + \tfrac{3}{2})\hbar\omega \qquad \omega = (k/\mu)^{1/2} \qquad n = 0, 1, 2, \ldots . \tag{19}$$

In momentum space, the regularised potential (figure 3) kernel is

$$V(p, q, x) = 4\pi^3 kb^2\delta^3(\boldsymbol{p} - \boldsymbol{q}) + 4\pi k|\boldsymbol{p} - \boldsymbol{q}|^{-5}\{(b^2|\boldsymbol{p} - \boldsymbol{q}|^2 - 3)\sin|\boldsymbol{p} - \boldsymbol{q}|b + 3b|\boldsymbol{p} - \boldsymbol{q}|\cos|\boldsymbol{p} - \boldsymbol{q}|b\}$$

where

$$|\boldsymbol{p} - \boldsymbol{q}| = (p^2 + q^2 - 2pqx)^{1/2}. \tag{20}$$

For $\mu = 0.92$, $k = 0.92$ and $b = 5.0$, we obtain the energy eigenvalues listed in table 4. They are in excellent agreement with the analytical formula (16) except the last one. Here we only get 11.3 . . . while the exact value is 11.50. This is because this eigenvalue

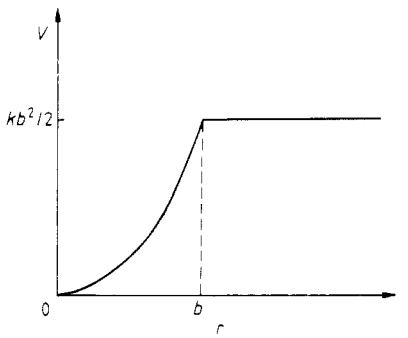

Figure 3. Potential energy of a regularised spherical harmonic oscillator.

Table 4. Energy eigenvalues of a spherical harmonic oscillator ($\mu = 0.92$, $k = 0.92$, $b = 5.0$, $\hbar = 1$, $V_0 = 0.0$).

100 mesh points	1.4946	3.4915	5.4890	7.4865	9.4756	11.3194
150 mesh points	1.4976	3.4962	5.4951	7.4937	9.4836	11.3257

is right at the top of the regulated potential well ($\frac{1}{2}kb^2 = 11.50$), and the transmission of the wavefunction decreases the energy eigenvalue. In fact the situation was set up deliberately to see how well we can determine the eigenvalues when they are close to the top of the potential well. In table 2, for the case of the linearly rising potential, we also see that the energy eigenvalues close to the top of the regularised potential well are decreased due to the 'leakage' of the wavefunction. We also notice that the accuracy of the eigenvalues can be improved by increasing the number of mesh points (table 4).

3. Quarkonium

It is well known that the mass spectra of the quark-antiquark bound states can be fitted by many non-relativistic potential models [6]. In this section, we investigate this bound-state problem in momentum space by the techniques developed in the last section.

Although quantum chromodynamics (QCD) is the candidate theory for the strong interaction, so far nobody has succeeded in deriving the interaction potential energy between quark-antiquark from the underlying theory. Here we choose the Cornell potential energy [7], which is a linear plus Coulomb potential

$$V_c(r) = -\tfrac{4}{3}\alpha/r + ar + V_0 \qquad V_0 \text{ is a constant.} \tag{21}$$

Because of the infrared divergence, we must regulate the linearly rising potential as

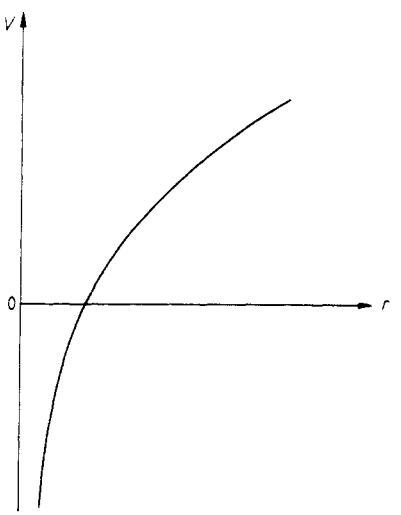

Figure 4. Cornell potential energy of quarkonium.

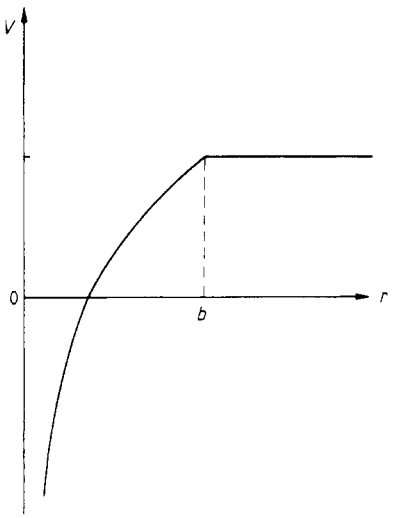

Figure 5. Regularised potential energy of quarkonium.

we have done in the last section. The regulated potential kernel is

$$V(p, q, x) = -\frac{16\pi}{3}\frac{\alpha}{(p^2+q^2-2pqx)} + (2\pi)^3(ab+V_0)\delta^3(\boldsymbol{p}-\boldsymbol{q}) + \frac{4\pi a}{(p^2+q^2-2pqx)^2}[2\cos b(p^2+q^2-2pqx)^{1/2} - 2 + b(p^2+q^2-2pqx)^{1/2}\sin b(p^2+q^2-2pqx)^{1/2}]. \quad (22)$$

First, we study the charmonium ($c\bar{c}$) system. Using the parameters $m_c = m_{\bar{c}} = 1.84$ GeV ($\mu = 0.92$ GeV), $\alpha = 0.39$, $a = 0.182\,63$, $b = 10.0$ and $V_0 = -0.842$ GeV, we obtain the $c\bar{c}$ spectrum shown in table 5. The mass of the bound state was computed according to

$$M = m_c + m_{\bar{c}} + \text{energy eigenvalue}.$$

Table 5. $c\bar{c}$ bound states ina regularised linear plus Coulomb potential. Parameters used are $m_c = 1.84$ GeV, $v_0 = -0.842$ GeV, $a = 0.182\,63$, $\alpha = 0.39$ and $b = 10.0$.

State	Mass (MeV)	Mass (MeV) in reference [8]
1S	3095	3095
1P	3524	3522
2S	3686	3684
1D	3809	3810
2P	3967	
3S	4110	4110
2D	4194	4190
3P	4337	
4S	4464	4460
3D	4527	
4P	4627	
5S	4642	4790

Next we study the bottomium ($b\bar{b}$) system. Using parameters $m_b = m_{\bar{b}} = 5.17$ GeV ($\mu = 2.585$ GeV), $\alpha = 0.39$, $a = 0.182\,63$, $b = 10.0$ and $V_0 = -0.710$ GeV, we obtain the $b\bar{b}$ mass spectrum shown in table 6.

The accuracy of the eigenfunctions can be tested by studying the leptonic decay width of these vector quarkonium states. To lowest order the leptonic width of the s-wave quarkonium states is given by the Van Royen-Weisskopf formula [8]

$$\Gamma_{e^+e^-} = \frac{16\pi\alpha^2}{M^2} |\bar{\Psi}(0)|^2 e_q^2 C \tag{23}$$

where $e_q = \frac{2}{3}$ for $c\bar{c}$ and $-\frac{1}{3}$ for $b\bar{b}$, M is the mass of the vector meson, α is the fine structure constant, C is the QCD correction factor and $\bar{\Psi}(0)$ is the wavefunction at the origin in coordinate space. The $\bar{\Psi}(0)$ can be calculated from the wavefunction in momentum space:

$$\bar{\Psi}(0) \sim \int_0^\infty \mathrm{d}p\, pu(p).$$

However, the QCD correction factor C is difficult to calculate. However these QCD corrections cancel in the ratio $\Gamma_{e^+e^-}(ns)/\Gamma_{e^+e^-}(1s)$. These ratios are calculated and the results are listed in tables 7 and 8. Again we see almost no difference between our results and the Cornell results.

Table 6. $b\bar{b}$ bound states in a regularised linear plus Coulomb potential. Parameters used are $m_b = 5.17$ GeV, $V_0 = -0.71$ GeV, $a = 0.182\,63$, $\alpha = 0.39$ and $b = 10.0$.

State	Mass(MeV)	Mass (MeV) in reference [8]
1s	9 460	9 460
1P	9 956	9 960
2S	10 051	10 050
1D	10 208	10 200
2P	10 311	10 310
3S	10 396	10 400
2D	10 500	10 500
3P	10 594	10 600
4S	10 674	10 670
3D	10 753	10 750
5S	10 916	10 920
6S	11 135	11 140

Table 7. Leptonic decay widths of $c\bar{c}$. Parameters used are $m_c = 1.84$ GeV, $V_0 = -0.842$ GeV, $a = 0.182\,63$, $\alpha = 0.39$ and $b = 10.0$.

	Integral equation	Differential equation [8]
$\Gamma(2s)/\Gamma(1s)$	0.45	0.44
$\Gamma(3s)/\Gamma(1s)$	0.31	0.31
$\Gamma(4s)/\Gamma(1s)$	0.23	0.23
$\Gamma(5s)/\Gamma(1s)$	0.06	

Table 8. Leptonic decay widths of $b\bar{b}$. Parameters used are $m_b = 5.17$ GeV, $V_0 = -0.71$ GeV, $a = 0.182\,63$, $\alpha = 0.39$ and $b = 10.0$.

	Integral equation	Differential equation [8]
$\Gamma(2s)/\Gamma(1s)$	0.32	0.36
$\Gamma(3s)/\Gamma(1s)$	0.24	0.25
$\Gamma(4s)/\Gamma(1s)$	0.20	0.20
$\Gamma(5s)/\Gamma(1s)$	0.18	0.18
$\Gamma(6s)/\Gamma(1s)$	0.17	0.16

4. Conclusion

In this paper we have shown that the non-relativistic bound-state problem in momentum space can be solved numerically by the collocation method. In the case of a Coulomb potential, the 'moving' singularities of the kernel can be avoided by integrating the potential kernel numerically via Gaussian integration (equation (6)). There are a lot of other methods [9] for handling this type of 'moving' singularity. In the case of infrared divergent potentials (e.g. linearly rising potential), we must regularise the kernel to make it square integrable. A simple regularisation is introduced in this paper which amounts to levelling off the divergent potential after a certain distance is exceeded (see figure 2). Physically this means that the force disappears after exceeding a certain distance. Using this regularisation, we obtain the eigenvalues and eigenfunctions, in excellent agreement with those obtained by solving the Schrödinger differential equation. The cases studied are the linearly rising potential, the simple harmonic oscillator and the Coulomb plus linearly rising potential. An extension of the present technique to the relativistic bound-state problems will be reported in a forthcoming paper [10].

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