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The absence of positive energy bound states for a class of nonlocal potentials

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Abstract
We generalize in this paper a theorem of Titchmarsh for the positivity of Fourier sine integrals. We then apply the theorem to derive simple conditions for the absence of positive energy bound states (bound states embedded in the continuum) for the radial Schrödinger equation with nonlocal potentials which are superpositions of a local potential and separable potentials.

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1. Introduction

Nonlocal separable two-body interactions have often been used in nuclear physics and many-body problems because of the fact that the two-body Schrödinger equation is easily solvable for them, and leads to closed expressions for a large class of such interactions. They have also been used very systematically with Faddeev equations for the three-body problem. Their main feature is that the partial-wave t-matrix has a very simple form, and can be continued off the energy-shell in a straightforward manner, a feature which is most important, as is well known, in nuclear physics, and in the Faddeev equations [1] (we shall quote often this book. See especially chapter 12). The only problem with such potentials is the existence of positive energy bound states, i.e. bound states embedded in the continuous spectrum [2][3], [3][4]. This is a general feature with nonlocal potentials, whether short-range or not, in contrast to the case of local potentials for which positive energy bound states exist only if the potential is long-range and oscillating at infinity [1, 4]. Such states are, of course,

[3] In these papers [2], the inverse problem for separable potentials, including the possibility of positive energy bound states, was solved for the first time, and the complete solution was given explicitly. The case where a local potential is also present was considered first by Chadan [3].
[4] We shall follow the notation of this book.

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undesirable, and should be avoided. Their main feature is that they are highly unstable, in the sense that a slight change in the potential makes them disappear, or shifts them far away, whereas, for the usual bound states with negative energy, i.e. below the continuous spectrum, we have the continuity theorem [1, 4].

Although nonlocal separable potentials have been used for decades now, as said earlier, the only paper we know in which the absence of positive energy bound states is shown for a particular class of nonlocal potentials is the paper of Zirilli [5], in which the author shows the absence of such states for general nonlocal potentials which are dilatation analytic in the sense of Combes. The purpose of the present paper is to give other simple conditions for the absence of these states for nonlocal potentials which are the sum of a local potential and a separable potential.

The three-dimensional Schrödinger equation for the scattering of a particle by a general nonlocal interaction reads

$$(\Delta + E)\Psi(\vec{k},\vec{r}) = \int U(\vec{r},\vec{r}\,')\Psi(\vec{k},\vec{r}\,')\,\mathrm{d}\vec{r}\,'. \tag{1}$$

Separable interactions are those for which

$$\begin{cases} U(\vec{r},\vec{r}\,') = \displaystyle\sum_{l=0}^{\infty}\sum_{n=1}^{N_l}\varepsilon_{nl}u_{nl}(r)u_{nl}(r')P_l(\cos\theta), \\ r = |\vec{r}|, \qquad r' = |\vec{r}\,'|, \qquad \cos\theta = \dfrac{\vec{r}\cdot\vec{r}\,'}{rr'}, \qquad \varepsilon_{nl} = \pm 1. \end{cases} \tag{2}$$

A more general class consists of separable interactions plus a local potential $V(r)$, which we assume to be spherically symmetric [3].

Remark. As is seen here, changing each u to $-u$ does not change the potential, and hence the equation. This is the reason why one had also to add the ε_{nl}. It can be seen that $\varepsilon = 1$ corresponds to a repulsive interaction, whereas $\varepsilon = -1$ leads to an attractive one [2, 3].

In the present paper, we shall consider the case where only one separable term is present in each angular momentum state:

$$U(\vec{r},\vec{r}\,') = \sum_l \varepsilon_l u_l(r)u_l(r')P_l(\cos\theta) + V(r)\delta(r - r'). \tag{3}$$

It is for this class of potentials that we are going to obtain simple conditions for the absence of positive energy bound states.

As usual, in order to secure the self-adjointness of the Hamiltonian, and the existence of a decent scattering theory, one must impose some conditions on $u_l(r)$ and $V(r)$. It turns out that sufficient conditions for being on the safe side are the following [3]:

$$\begin{cases} u_l(r) \text{ and } V(r) \text{ are both real, and locally } L^1 \text{ for } r \neq 0,\ V(r) \geqslant 0, \\ \displaystyle\int_0^{\infty} r^2|u_l(r)|\,\mathrm{d}r < \infty, \qquad \int_0^{\infty} rV(r)\,\mathrm{d}r < \infty. \end{cases} \tag{4}$$

Making use of the partial wave decomposition

$$\Psi(\vec{k},\vec{r}) = \sum_{l=0}^{\infty}(2l+1)\mathrm{i}^l\frac{\psi_l(k,r)}{kr}P_l(\cos\theta), \tag{5}$$

we obtain the radial Schrödinger equation

$$\begin{cases} \left[\dfrac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \dfrac{l(l+1)}{r^2}\right]\psi_l(k,r) = \varepsilon_l U_l(r)\displaystyle\int_0^{\infty} \\ U_l(r')\psi_l(k,r')\,\mathrm{d}r' + V(r)\psi_l(k,r), \\ U_l(r) = (4\pi)^{1/2} r u_l(r), \qquad \psi_l(k,0) = 0. \end{cases} \tag{6}$$

For simplicity, we begin with the S-wave ($l = 0$). We shall see later how to generalize the results to higher waves. Consider now first the case where we have no local potential V present:

$$\begin{cases} \psi'' + k^2\psi = \varepsilon U(r)\displaystyle\int_0^\infty \psi(k, r')U(r')\,\mathrm{d}r', \\ \varepsilon = \pm 1, \qquad \displaystyle\int_0^\infty r|U(r)|\,\mathrm{d}r < \infty. \end{cases} \tag{7}$$

It can then be shown that the positive energy bound states with energies k_ν^2 ($k_\nu > 0$) are given by the simultaneous roots of the following two equations [2, 3]

$$\begin{cases} \widetilde{U}(k_\nu) = 0, \\ \varepsilon + \dfrac{2}{\pi} P \displaystyle\int_0^\infty \frac{\widetilde{U}^2(p)}{p^2 - k_\nu^2} p^2\,\mathrm{d}p = 0, \end{cases} \tag{8}$$

where

$$\widetilde{U}(p) = \int_0^\infty U(r) \frac{\sin pr}{p}\,\mathrm{d}r, \tag{9}$$

and P means the principal value of the integral. Under our conditions (7) on $U(r) = \sqrt{4\pi} r u(r)$, it is obvious that $p\widetilde{U}(p)$ is a bounded and differentiable function for all $p \geqslant 0$, and vanishes at $p = \infty$ by the Riemann–Lebesgue lemma [6]. Everything is then quite meaningful in the integral in (8): there is absolute convergence at $p = \infty$, and the principal value part is well-defined since $\widetilde{U}(p)$ is differentiable. One can then show that if $k_\nu \to \infty$, the principal value integral vanishes [2, 3]. It follows that positive energy bound states cannot go to infinity, and therefore, that they are finite in number. In fact, this integral can also be written as a nice Fourier cosine integral, as shown in appendix A, if one assumes also $U \in L^1(0, \infty)$:

$$\begin{cases} \varepsilon + \dfrac{2}{\pi} P \displaystyle\int_0^\infty \cdots = \varepsilon + \int_0^\infty \omega(r) \cos kr\,\mathrm{d}r, \\ \omega(r) \in L^1(0, \infty). \end{cases} \tag{10}$$

This formula shows that, under the integrability condition on $U(r)$, given in (7), the principal value integral is a bounded and continuous function of k, and vanishes at infinity, so that the whole expression goes to $\varepsilon (= \pm 1)$. Therefore, from (8), there cannot be positive energy bound states beyond some value of k^2.

In any case, as was shown by Gourdin and Martin [2], one may have any number of positive energy bound states by choosing $u(r)$ appropriately through the inverse problem techniques for separable potentials.

Let us look now to the case where a local positive potential is also present [3]:

$$\begin{cases} \psi'' + k^2\psi = V(r)\psi(k, r) + \varepsilon U(r)\displaystyle\int_0^\infty U(r')\psi(k, r')\,\mathrm{d}r'. \\ \varepsilon = \pm 1, \qquad \displaystyle\int_0^\infty rV(r)\,\mathrm{d}r < \infty, \qquad V(r) \geqslant 0. \end{cases} \tag{11}$$

Here, we assume that the Schrödinger equation with only the local potential:

$$\begin{cases} \varphi'' + k^2\varphi = V\varphi, \\ \varphi(k, 0) = 0, \qquad \varphi'(k, 0) = 1, \end{cases} \tag{12}$$

can be solved explicitly and we know $\varphi(k, r)$. When $V = 0$, we get, of course, $\varphi = \sin kr/k$. Since V is assumed positive, there are no negative energy bound states, and one can show that the set $\{\varphi(k,r);\, k \in [0,\infty)\}$ is complete in $L^2(0,\infty)$, [1, 3, 4] and can be used to define integral transforms quite similar to Fourier sine transform. Like $\sin kr/k$, $\varphi(k,r)$ is an even entire function of k of exponential type r. In fact, we have, for every fixed $r > 0$,

$$\varphi(k,r) \underset{|k|\to\infty}{=} \frac{\sin kr}{k}[1 + o(1)]. \tag{12a}$$

Also, it can be shown that, as for $\sin kr/k$, the zeros of φ, for every fixed r, are all real if $V(r) > 0$, and, therefore, because of (12a), are given asymptotically by $k_n = \pm n\pi/r$. One well-known example is, naturally, $V(r) = l(l+1)/r^2, l \geqslant 0$, which leads to a Hankel transform in which, instead of $\sin kr$, one has to deal with the appropriate Bessel function. The potential here is outside the class defined in (11), but one can still show the completeness, as is well-known ([7]: in this book, one finds many examples of eigenfunction expansions related to various differential equations of second order). We can now define

$$\widetilde{U}(k) = \int_0^\infty U(r)\varphi(k,r)\,\mathrm{d}r. \tag{13}$$

When $V = 0$, we go back, of course, to (9). Using now this integral transform with (11), one then obtains that now the positive energy bound states of (11) are given by the simultaneous roots of the following two equations:

$$\begin{cases} \widetilde{U}(k_\nu) = 0, \\ \varepsilon + \dfrac{2}{\pi} P \displaystyle\int_0^\infty \frac{\widetilde{U}^2(p)}{p^2 - k_\nu^2} \frac{p^2}{|F(p)|^2}\,\mathrm{d}p = 0, \end{cases} \tag{14}$$

where $F(k)$ is the Jost function of local potential V, i.e. of equation (12) [1, 3]. It is known that $F(k)$, which is a continuous function for $k \geqslant 0$, never vanishes for $k \in [0,\infty)$, and $F(\infty) = 1$. Again, it is easily shown, under conditions (7) and (4) on $U(r)$ and $V(r)$, that the principal value integral is well defined [3]. The similarity with (8) is to be noted here. So, one may hope that if a sufficient condition on $U(r)$ is found to forbid positive energy bound states in (7), a similar condition may be expected for (11), for a given $V(r)$.

2. Absence of positive energy bound states

We consider first the simple case where $V = 0$, and so we have (8) and (9). Now, a very simple condition to forbid simultaneous roots of the two equations in (8) is to see whether one can choose $U(r)$ in such a way as to have $\widetilde{U}(p) > 0$ for all $p \geqslant 0$. In this case, there cannot be any real common roots. Here, one can use the following theorems for Fourier sine and cosine transforms[5]:

Theorem 1 (Titchmarsh). *Let $f(x)$ be non increasing over $(0,\infty)$, integrable over $(0,1)$, and let $f(x) \to 0$ as $x \to \infty$. Then $F_s(k) \geqslant 0$, where F_s is the Fourier sine transform of f. In fact, $F_s(k) > 0$ for $k > 0$ if $f(x)$ is strictly decreasing.*

Theorem 2 (Titchmarsh). *Let $f(x)$ be a bounded function, which decreases steadily to zero as $x \to \infty$ and is convex. Then $F_c(k)$, the Fourier cosine transform of $f(x)$, is positive and belongs to $L^1(0,\infty)$.*

[5] Reference [6], p 169, theorem 123, p 170, theorem 124.

The first theorem applies directly to (8) and (9), and leads to the somewhat trivial:

Theorem A. *If $U(r)$ is a strictly decreasing function of r, is $L^1(0,1)$, and $rU(r) \in L^1(1,\infty)$, the Schrödinger equation (7) has no positive energy bound states. Note here that if U is L^1 at the origin, rU also is L^1, so that the integrability condition on rU, shown in (7), reduces to $rU \in L^1$ at infinity. And since U is decreasing, one has, of course, $U(\infty) = 0$.*

Remark 1. In fact, any function $U(r) = ru(r)$ of positive type satisfying the integrability conditions given in (4) would lead, of course, to the same result. Theorem 1 is just a simple criterion. The purpose of theorem A is to prepare for what follows.

We have now to look at (11)–(14), where $V(r) > 0$. In order to find a simple condition as above, we must first generalize theorem 1 of Titchmarsh to the integral transform (13). A simple generalization is:

Theorem 3. *In order for $\widetilde{U}(k)$ defined by (13) to be positive, it is sufficient that $U(r)$ be of the form*

$$U(r) = \varphi_0(r) \int_r^\infty \varphi_0(t) g(t)\, \mathrm{d}t \int_r^t \frac{\mathrm{d}u}{\varphi_0^2(u)}, \tag{15}$$

where $\varphi_0(r) = \varphi(k = 0, r)$, and $g(r)$ is any positive function, which is such that $r^2 g(r) \in L^1(0,1)$, and $rg(r) \in L^1(1,\infty)$. Moreover, from the assumptions on $g(r)$, one gets also that $U(r) \in L^1(0,1)$, $rU(r) \in L^1(1,\infty)$, and $U(r)$ is a decreasing function, so that $U(\infty) = 0$.

The proof of this theorem will be given in appendix B.

In order to make (15) more precise, we must of course show that the last integral on the right-hand side is meaningful, i.e. $\varphi_0(r) \neq 0$ for all $r > 0$, and that the whole integral is convergent at $t = \infty$. These follow from the differential equation for $\varphi_0(r)$, which is (12) at $k = 0$:

$$\begin{cases} \varphi_0''(r) = V(r)\varphi_0(r), & V(r) > 0, \\ \varphi_0(0) = 0, & \varphi_0'(0) = 1, \end{cases} \tag{16}$$

and where one assumes that $rV(r) \in L^1(0,\infty)$. On the basis of this assumption, one can show that [1, 3]

$$\varphi_0(r) > 0, \qquad \forall r > 0, \tag{17a}$$

and

$$\begin{cases} \varphi_0(r) = r[1 + o(1)], & \text{as } r \to 0, \\ \varphi_0(r) = Ar + B + o(1), & \text{as } r \to \infty, \end{cases} \tag{17b}$$

where $A > 1$, and $B < 0$. In short, $\varphi_0(r)$ is an increasing convex function of r since, from (17a), $\varphi_0''(r) > 0$, and it grows linearly as $r \to \infty$. Using the above properties of $\varphi_0(r)$, it is now quite easy to show that the right-hand side of (15) is quite meaningful under the conditions given on $g(r)$ (appendix B).

We introduce now the second independent solution of (16)

$$\begin{cases} \chi_0(r) = \varphi_0(r) \displaystyle\int_r^\infty \frac{\mathrm{d}u}{\varphi_0^2(u)}, & \chi_0(0) = 1, \\ W(\varphi_0, \chi_0) = \varphi_0'\chi_0 - \varphi_0\chi_0' = 1. \end{cases} \tag{18}$$

From its definition, $\chi_0(r) > 0$ for all $r \geqslant 0$. Also, since $\chi_0'' = V\chi_0$, $\chi_0(r)$ is, like φ_0, a convex function of r. From the second part of (17b), it is now easily seen that

$$\chi_0(\infty) = \frac{1}{A} < 1. \tag{19}$$

Since $\chi_0(0) = 1$, it follows that $\chi_0(r)$ is a decreasing convex function of r. At any rate, using the definition of χ_0 given in (18) in formula (15), we find

$$U(r) = \int_r^\infty [\chi_0(r)\varphi_0(t) - \varphi_0(r)\chi_0(t)]\, g(t)\, \mathrm{d}t. \tag{20}$$

From this formula, it is immediately found that, under the assumptions of theorem 3 on $g(r)$, one has (appendix B)

$$U \in L^1(1, 0), \qquad \text{and} \qquad U(\infty) = 0. \tag{21}$$

Now, from (15), we have $U(r) > 0$, and differentiating (20) twice, we find (remember that $g(r)$ is positive)

$$U''(r) - V(r)U(r) = g(r), \tag{22}$$

which shows that $U(r)$ is also a convex function of r, and since $U(0) > 0$, and $U(\infty) = 0$, U is a decreasing convex function of r.

Remark 2. As we see from the above analysis, $U(r)$ given by (15) is less general than $U(r)$ of theorem 1 of Titchmarsh where $U(r)$ had to be only L^1 at $r = 0$, whereas here $U(0)$ is finite. Also, $U(r)$ of Titchmarsh was only a decreasing function, whereas here we have our $U(r)$ is even convex. The reason for all these shortcomings is that theorem 3 is a restricted form of the more general theorem whose proof will be given in a separate paper. In any case, theorem 3 now applies directly to (13), and leads to:

Theorem B. *Given $V(r)$, in order for (11) to have no positive energy bound states, it is sufficient for $U(r)$ to be of the form (15), where $g(r)$ is any positive function such that $r^2 g(r) \in L^1(0, 1)$ and $rg(r) \in L^1(1, \infty)$.*

Remark 3. Condition (11) on $V(r)$ is sufficient, but is not necessary in general. Examples for (13) are many. We just mention the Hankel transform (see footnote 5), using Bessel functions $\sqrt{r}J_{\ell+\frac{1}{2}}(r)$ instead of sine, which correspond to

$$V(r) = \frac{\ell(\ell+1)}{r^2}, \qquad \ell \geqslant 0. \tag{23}$$

We have

$$\widetilde{F}_\nu(k) = \int_0^\infty f(r)\sqrt{kr}\, J_\nu(kr)\, \mathrm{d}r, \tag{24}$$

where $\nu = \ell + \frac{1}{2}$. Then, for $a > 0$, we have [7]:

$$f(r) = r^{-1/2}, \qquad \widetilde{F}_\nu(k) = k^{-1/2};$$
$$f(r) = r^{-1/2}(r^2 + a^2)^{-1/2}, \qquad \widetilde{F}_\nu(k) = \sqrt{k} I_{\frac{\nu}{2}}\left(\tfrac{1}{2}ak\right) K_{\frac{\nu}{2}}\left(\tfrac{1}{2}ka\right);$$
$$f(r) = r^{-1/2}\,\mathrm{e}^{-ax}, \qquad \widetilde{F}(k) = \frac{k^{\frac{1}{2}-\nu}}{(a^2+y^2)^{1/2}}[(a^2+y^2)^{1/2} - a]^\nu;$$

and

$$f(r) = r^{-1/2}\,\mathrm{e}^{-ax^2}, \qquad \widetilde{F}(k) = \frac{\sqrt{\pi}}{2}\sqrt{\frac{k}{a}}\exp\left(-\frac{k^2}{8a}\right) I_{\frac{\nu}{2}}\left(\frac{k^2}{8a}\right);$$

etc. It is known that I_ν and K_ν do not vanish on the positive real axis for $\nu > 0$ [9].

3. Generalizations

1. Using the results obtained in the papers of Mills and Reading [3], it is possible to generalize (15) to the case of a local potential plus a finite sum of separable potentials. However, the conditions one obtains are cumbersome, and we shall not reproduce them here.
2. So far, we have restricted ourselves to $\ell = 0$ (S-wave) in (6). One can consider the case $\ell \neq 0$ along similar lines, and one gets results similar to theorems A and B. Details will be given in a separate paper.
3. In this paper, we have considered the case where $g(t)$ is a function. However, $g(t)$ may be a generalized function. This will be dealt with in detail in the separate paper mentioned above. To conclude, consider just the simplest case where $g(t) = \lambda\delta(t - r_0)$, λ and r_0 both positive. One finds then:

$$U(r) = \lambda\varphi_0(r_0)\varphi_0(r)\int_r^{r_0} \frac{\mathrm{d}u}{\varphi_0^2(u)}\theta(r_0 - r) = \lambda\varphi_0(r_0)[\chi_0(r) - \chi_0(r_0)]\theta(r_0 - r), \tag{25}$$

   which has a finite range, and is finite at the origin since $\chi_0(1) = 1$. For $g(t)$ given by a finite sum of delta functions, one gets a finite sum of such $U(r)$.
4. We have been considering only the case where the local potential is positive. However, it is easy to extend the results to the case where $V(r)$ is negative and small enough. Indeed, it is seen from bound (B.3), where one has to replace $V(r)$ by $|V(r)|$ everywhere, that if V is small enough, the second term on the right-hand side of (B.2) can be made smaller than the first term. It follows that now $K(r, t)$ is negative. Similar observation can be made on (B.11), ..., (B.16). And since, as seen in (7), U and $-U$ are equivalent, we can consider now a U which is negative, increasing, and $U(\infty) = 0$. The analysis of appendix B goes through without modification, and we get again theorems 3, B and 5 for $-U(r)$, provided $V(r)$ is small enough. This suggests that all our formulae and theorems may be true as long as $V(r)$ has no bound states, i.e. $\varphi_0(r)$ does not vanish on $(0, \infty]$. The proof needs different techniques which we shall exhibit in a separate paper.

4. Conclusion

As was said in the introduction, nonlocal separable potentials are widely used in few-body problems in nuclear physics [1]. In the kernels of Faddeev equations, or in more general equations for higher number of particles, one needs the T-matrices of the subsystems in unphysical regions off the energy-shell, and it is known that analytic continuation from the physical region of energy is a difficult problem, and is very sensitive to small errors. This is the reason for the wide use of nonlocal separable potentials, for which the Schrödinger equation can be solved exactly, and often analytically, something which allows the analytic continuation of T-matrices off the energy-shell in a straightforward manner.

The only problem for nonlocal potentials in general is the occurrence of positive energy bound states, which are highly unstable and unphysical. This is clearly seen in equations (8) or (14), which show that the energies of such states are given by the simultaneous roots of two generally transcendental functions. Changing $u(r)$ slightly in those two equations makes the coincidence disappear, and there will remain in general no more positive energy bound states. This is why it seems appropriate to avoid from the beginning the accidental occurrence of such unphysical states, and this is the justification for the present work. The condition we derive for the absence of positive energy bound states, although simple, is not very restrictive since $g(t)$ in (15) or (20), except for being positive, and to satisfy the usual integrability conditions at the origin and at infinity, conditions satisfied by all decent potentials, is arbitrary, and can have any shape and be as large as one wishes. We end up by noting that one can, of course, avoid positive energy bound states by having $u(r)$ small enough in order to avoid the second equation in (8), or equivalently (10) and (A.19), to have zeros, but this is not very interesting since $u(r)$ has to be small.

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Appendix A

We have, from our assumptions, that $U(r)$ belongs to the following class:

$$U(r) \in L^1(0,\infty), \qquad rU(r) \in L^1(0,\infty). \tag{A.1}$$

Let us assume first that $U(r) > 0$, and define

$$\widetilde{u}(p) \equiv p\widetilde{U}(p) = \int_0^\infty U(r)\sin pr\,\mathrm{d}r, \tag{A.2}$$

The function $\widetilde{u}(p)$ is a bounded continuous function, and $\widetilde{u}(0) = \widetilde{u}(\infty) = 0$. But we have more. Indeed, differentiating (A.2) with respect to p under the integral sign, we get

$$\dot{\widetilde{u}}(p) = \int_0^\infty [rU(r)]\cos pr\,\mathrm{d}r, \tag{A.3}$$

which is again a bounded continuous function, and $\dot{\widetilde{u}}(\infty) = 0$. Therefore, $\widetilde{u}(p)$ is, in fact, $C^1[0,\infty)$. If we now introduce

$$W(r) = \int_r^\infty U(t)\,\mathrm{d}t, \tag{A.4}$$

because of the second part of (A.1), it is immediately seen that W is a bounded and continuous function for $r > 0$ and

$$W(r) \in L^1(0,\infty), \qquad \lim_{r\to 0,\infty} rW(r) = 0. \tag{A.5}$$

Introducing $U = -W'$ in (A.2), and integrating by parts, we find that $\widetilde{u}(p)$ can also be written as

$$\widetilde{u}(p) = p\int_0^\infty W(r)\cos pr\,\mathrm{d}r. \tag{A.6}$$

Now, if we assume, to begin with, that $U(r)$ is also a decreasing function, it follows that $W(r)$ is bounded and convex, and $W(\infty) = 0$. Therefore, from theorem 2, we have

$$\frac{\widetilde{u}(p)}{p} \in L^1(0,\infty), \tag{A.7}$$

which shows that the integral in (8) is absolutely convergent at $p = \infty$. Moreover, since $\widetilde{u}(p)$ is C^1, there is also no problem for the existence and even Hölder continuity of the principal value integral [6].

Let us now write the integral in (8) as follows:

$$G(k) = P\int_0^\infty \frac{\widetilde{u}^2(p)}{p^2-k^2}\,\mathrm{d}p = P\int_0^\infty \frac{\widetilde{u}^2(p)}{2p}\left[\frac{1}{p-k} + \frac{1}{p+k}\right]\mathrm{d}p. \tag{A.8}$$

Changing p to $-p$ in the second integral, it is easily found that

$$G(k) = \frac{1}{2} P \int_{-\infty}^{\infty} \frac{\widetilde{u}(p)}{p} \frac{\widetilde{u}(p)}{p-k} \, \mathrm{d}p. \tag{A.9}$$

If we now use (A.2) for one $\widetilde{u}(p)$, and (A.6) for the second one, we find

$$G(k) = \frac{1}{2} \int_0^{\infty} U(r) \, \mathrm{d}r \int_0^{\infty} W(r') \, \mathrm{d}r' P \int_{-\infty}^{\infty} \frac{\sin pr \cos pr'}{p-k} \, \mathrm{d}p. \tag{A.10}$$

The change of the order of integrations is justified because both $U(r)$ and $W(r)$ are $L^1(0, \infty)$ [6]. Now, since

$$\sin pr \cos pr' = \tfrac{1}{2}[\sin p(r+r') + \sin p(r-r')], \tag{A.11}$$

and [6]

$$P \int_{-\infty}^{\infty} \frac{\sin xy}{y - y_0} \, \mathrm{d}y = \pi \cos xy_0, \tag{A.12}$$

we finally have

$$G(k) = \frac{\pi}{2} \int_0^{\infty} U(r) \cos kr \, \mathrm{d}r \int_0^{\infty} W(r') \cos kr' \, \mathrm{d}r' = \frac{\pi}{2} \widetilde{U}_c(k) \widetilde{W}_c(k). \tag{A.13}$$

The first integral being a bounded and continuous function, and the second one $L^1(0, \infty)$ by the second theorem of Titchmarsh, as we saw before, it follows that $G(k)$ is also $L^1(0, \infty)$. We can now write $G(k)$ as a Fourier cosine transform [6, 10]

$$G(k) = \int_0^{\infty} \omega(r) \cos kr \, \mathrm{d}r, \tag{A.14}$$

where $\omega(r)$ is given by the convolution

$$\omega(r) = \frac{\pi}{2} \int_0^{\infty} U(t)[W(|r-t|) + W(r+t)] \, \mathrm{d}t. \tag{A.15}$$

And since both U and W are $L^1(0, \infty)$, it follows, from the convolution theorem of two L^1 functions, that $\omega(r)$ is also $L^1(0, \infty)$ [6].

So far, we have been assuming that $U'(r) < 0$. However, in (A.15), no reference is made to the derivative of U. If $U(r)$ satisfies only (A.1), again all factors inside the integral in (A.15) are $L^1(0, \infty)$, and so is $\omega(r)$. One may expect therefore that (A.14) and (A.15) are true under (A.1) only. The direct proof of this assertion needs more elaborate reasoning by using the methods of [6, chapter 2]. We shall not reproduce it here.

We come now to the sign of $U(r)$ itself. So far, we have been assuming $U(r)$ to be positive. However, in the main text, the assumption we made is only the one shown in (7), with no reference to the sign of $U(r)$. We have therefore to extend our result to the case where $U(r)$ is oscillating. But this is all easy. Indeed, we can separate the positive and negative parts of $U(r)$, and write

$$U(r) = U_+(r) - U_-(r) \tag{A.16}$$

where both U_+ and U_- are positive, and, of course, satisfy separately (7). We have now

$$\widetilde{U}^2(p) = \widetilde{U}_+^2(p) + \widetilde{U}_-^2(p) - 2\widetilde{U}_+(p)\widetilde{U}_-(p). \tag{A.17}$$

It is now trivial to apply our previous reasoning separately to each of the three terms here. To summarize, introducing $W_\pm$ as in (A.4), and reducing our assumptions (A.1) to their essential parts, we have

Theorem 4. *Under the assumptions*

$$U(r) \in L^1(0,1), \qquad rU(r) \in L^1(1,\infty), \tag{A.18}$$

the second formula in (8) can be written as

$$\varepsilon + \frac{2}{\pi} P \int \cdots = \varepsilon + \frac{\pi}{2}\int_0^\infty \omega(r)\cos kt \, \mathrm{d}t, \tag{A.19}$$

where

$$\begin{aligned}\omega(r) = \frac{\pi}{2}\int_0^\infty & U_+(t)[W_+(|r-t|) + W_+(r+t)]\,\mathrm{d}t \\ & + \frac{\pi}{2}\int_0^\infty U_-(t)[W_-(|r-t|) + W_-(r+t)]\,\mathrm{d}t \\ & - \pi\int_0^\infty U_-(t)[W_+(|r-t|) + W_+(r+t))\,\mathrm{d}t,\end{aligned} \tag{A.20}$$

and $\omega(r) \in L^1(0,\infty)$*. In the third integral, one can, of course, exchange U and W, and have* $U_+(t)[W_- \cdots]$.

Appendix B

Proof of theorem 3. We wish to show that given $V(r) > 0$, which defines the integral transform (13), and under suitable conditions on $U(r) > 0$, $\widetilde{U}(k)$ is positive. For this purpose, we use the following integral representation for $\varphi(k,r)$, which comes from the Gel'fand–Levitan theory of inverse problems [1, 3]:

$$\varphi(k,r) = \frac{\sin kr}{k} + \int_0^r K(r,x)\frac{\sin kx}{k}\,\mathrm{d}x. \tag{B.1}$$

The kernel $K(r,x)$, defined only for $0 \leqslant x \leqslant r$, satisfies the Volterra integral equation[6]:

$$K(r,x) = \frac{1}{2}\int_{\frac{r-x}{2}}^{\frac{r+x}{2}} V(s)\,\mathrm{d}s + \int_{\frac{r-x}{2}}^{\frac{r+x}{2}}\mathrm{d}s\int_0^{\frac{r-x}{2}} V(s+u)K(s+u,s-u)\,\mathrm{d}u. \tag{B.2}$$

It can be shown that this Volterra integral equation can always be solved by iteration, and leads to an absolutely convergent series, provided that $rV(r) \in L^1(0,\infty)$ [1, 3]. Moreover, one gets the upper bound (remember that here $V(r)$ is positive):

$$K(r,x) \leqslant \frac{1}{2}\int_{\frac{r-x}{2}}^{\frac{r+x}{2}} V(s)\exp\left[\int_0^{\frac{r+x}{2}} uV(u)\,\mathrm{d}u\right]\mathrm{d}s \leqslant \frac{1}{2}\mathrm{e}^{\int_0^\infty uV(u)\,\mathrm{d}u}\int_{\frac{r-x}{2}}^{\frac{r+x}{2}} V(s)\,\mathrm{d}s. \tag{B.3}$$

We can now use (B.1) on the right-hand side of (13), and we get, with a slight change of notation

$$\begin{cases}\widetilde{U}(k) = \displaystyle\int_0^\infty f(x)\frac{\sin kx}{k}\,\mathrm{d}x, \\ f(x) = U(x) + \displaystyle\int_x^\infty K(r,x)U(r)\,\mathrm{d}r.\end{cases} \tag{B.4}$$

The exchange of the order of integrations in going from (13) to (B.4) is legitimate because of bound (B.3), which shows that $K(\infty,x) = 0$ for all $x > 0$, and by the assumption that $U(\infty) = 0$, so that the integrals are all absolutely convergent at the upper limit.

[6] Reference [3], pp 43–5.

Now, in (B.4), $\widetilde{U}(k)$ is a Fourier sine transform, and we wish therefore to apply theorem 1 of Titchmarsh. We have therefore to show that $f(x)$ satisfies all the requirements of that theorem, namely:

$$\begin{cases} f(x) > 0, \\ f(x) \in L^1(0, 1), \\ f(x) \text{is steadily decreasing, and} \\ f(\infty) = 0. \end{cases} \tag{B.5}$$

Now, since $K(r, x)$ is positive in (B.4), in order to secure that $f(x)$ is also positive, it is sufficient to assume that

$$U(r) > 0. \tag{B.6}$$

Let us now check the second statement in (B.5). In (B.4), both U and K being positive, it is obvious that to secure that $f(x) \in L^1(0, 1)$, we must assume

$$U(r) \in L^1(0, 1). \tag{B.7}$$

That the integral $\int_x^\infty KU \,\mathrm{d}r$ in (B.4) is also $L^1(0, 1)$ follows now from the positivity of K and U, (B.7) and

$$K(r, 0) = 0 \qquad \text{uniformly in } r, \tag{B.8}$$

which is an obvious consequence of (B.2) and (B.3).

Concerning the last statement in (B.5), $f(\infty) = 0$, it is obvious in (B.4) and the fact that both U and K are positive, that we must assume

$$U(\infty) = 0, \tag{B.9}$$

and this is sufficient.

It remains to show that $f(x)$ is a decreasing function. From (B.4), we have

$$f'(x) = U'(x) - K(x, x)U(x) + \int_x^\infty \frac{\partial K(r, x)}{\partial x} U(r) \,\mathrm{d}r. \tag{B.10}$$

Now, differentiating (B.2) with respect to r and x, we also find

$$\begin{cases} \dfrac{\partial K(r, x)}{\partial r} + \dfrac{\partial K(r, x)}{\partial x} = F(r, x), \\ F(r, x) = \dfrac{1}{2} V\left(\dfrac{r + x}{2}\right) + \displaystyle\int_0^{\frac{r-x}{2}} V\left(\dfrac{r + x}{2} + u\right) K\left(\dfrac{r + x}{2} + u, \dfrac{r + x}{2} - u\right) \mathrm{d}u > 0. \end{cases} \tag{B.11}$$

Extracting $\partial K/\partial x$, using it in (B.10) and integrating by parts with respect to r, we finally find that we must have

$$f'(x) = U'(x) + \int_x^\infty K(r, x)U'(r) \,\mathrm{d}r + \int_x^\infty F(r, x)U(r) \,\mathrm{d}t < 0. \tag{B.12}$$

This condition is, obviously, very complicated, and nothing simple on U can be easily obtained from it. Let us therefore assume that U'' also exists. Differentiating (B.12), and using (B.11) at $r = x$:

$$\left[\frac{\partial K(r, x)}{\partial r} + \frac{\partial K(r, x)}{\partial x}\right]_{x=r} = F(r, r) = \frac{1}{2} V(r), \tag{B.13}$$

we find

$$f''(x) = U''(x) - \frac{1}{2} V(x)U(x) - K(x, x)U'(x) - \frac{\partial K}{\partial x}(x, x)U(x) + \int_x^\infty \frac{\partial^2 K(r, x)}{\partial x^2} U(r) \,\mathrm{d}r. \tag{B.14}$$

It is now well known that $K(r, x)$ satisfies the differential equation [1, 3]

$$\frac{\partial^2 K(r,x)}{\partial r^2} - \frac{\partial^2 K(r,x)}{\partial x^2} = V(r)K(r,x), \tag{B.15}$$

which can also be obtained from (B.2). If we replace now $\partial^2 K/\partial x^2$ obtained from (B.15) in (B.14), integrate by parts twice the integral containing $\partial^2 K/\partial r^2$, and use the fact that, because of (B.2), (B.3) and (B.9), all the integrated terms vanish at $r = \infty$, we finally find

$$f''(x) = [U''(x) - V(x)U(x)] + \int_x^\infty K(r,x)[U''(r) - UV]\,\mathrm{d}r. \tag{B.16}$$

It follows that, if we assume

$$U''(x) - V(x)U(x) > 0, \tag{B.17}$$

then

$$f''(x) > 0, \tag{B.18}$$

that is, $f(x)$ is a convex function. Now, as we saw before, $f(x)$ is positive and $f(\infty) = 0$. The convexity of $f(x)$ secures then that [11]

$$f'(x) < 0. \tag{B.19}$$

We have therefore completed all the sufficient conditions to secure (B.5), namely (B.6), (B.7), (B.9) and (B.17). We can therefore apply theorem 1 of Titchmarsh to $f(x)$, and obtain:

Theorem 5. *Under conditions (B.6), (B.7), (B.9) and (B.17), we have*

$$\widetilde{U}(k) = \int_0^\infty f(r)\frac{\sin kr}{k}\,\mathrm{d}r > 0. \tag{B.20}$$

In order to prove theorem 3 of the main text, we must now study (B.17) further, which we write as

$$U''(x) - V(x)U(x) = g(x), \qquad g(x) > 0. \tag{B.21}$$

For the time being, $g(x)$ is, of course, arbitrary. However, it must be such that the solution of (B.21) satisfies (B.6), (B.7) and (B.9). Equation (B.21) being a simple inhomogeneous linear differential equation of second order, it is well known, and can be checked in a straightforward manner, that a solution satisfying (B.9), i.e. $U(\infty) = 0$, is given by

$$U(r) = \int_r^\infty [\chi_0(r)\varphi_0(t) - \varphi_0(r)\chi_0(t)]g(t)\,\mathrm{d}t = \varphi_0(r)\int_r^\infty \varphi_0(t)g(t)\,\mathrm{d}t \int_r^t \frac{\mathrm{d}u}{\varphi_0^2(u)}, \tag{B.22}$$

where φ_0 and χ_0 were defined in the main text. From the properties of φ_0 and χ_0 we established there, one finds easily, from the last expression in (B.22), that

$$U(r) \underset{r\to\infty}{\simeq} Ar\int_r^\infty \frac{1}{A}g(t)\frac{1}{A^2}\left(\frac{1}{r} - \frac{1}{t}\right)\mathrm{d}t. \tag{B.23}$$

Since $g(t) > 0$, it follows that, in order to have the convergence of the integral at infinity, we must have $g(t) \in L^1(\infty)$. And this secures, of course, that $U(\infty) = 0$. Similarly, if we wish to have $U(r) \in L^1$ at infinity, we must have $tg(t) \in L^1$ at infinity. Indeed, taking B large enough, we have $\int_B^\infty U(r)\,\mathrm{d}r \cong \int_B^\infty [(\text{B.23})]\,\mathrm{d}r$. Everything being positive in (B.23), we can now exchange the orders of integration in r and t. Then it is immediately seen that if $tg(t)$ is L^1, so is $U(r)$. For having $rU(r) \in L^1$ at infinity, (7), and needed also in appendix A, one must have $t^2 g(t) \in L^1$ at infinity, etc.

Let us now look at what happens at $r = 0$, for we have to secure (B.7). We can again use now the behaviour of φ_0 and χ_0, given in the main text, in the middle expression in (B.22). One finds easily that

$$U(r) \underset{r\to 0}{\simeq} \left(\int_{r\to 0}^{\infty} \varphi_0(t)g(t)\,\mathrm{d}t\right) - \left(r\int_{r\to 0}^{\infty} \chi_0(t)g(t)\,\mathrm{d}t\right). \tag{B.24}$$

The first integral here is finite if $tg(t)$ is $L^1(0)$, and the second one also because we can put r inside the integral and make it larger. To have only $U \in L^1$, at the origin, it is obvious first that it is sufficient to replace in (B.24) the two integrals by $\int_{r\to 0}^{1} \cdots \mathrm{d}t$. Then we have

$$\int_0^1 U(r)\,\mathrm{d}r = \int_0^1 \mathrm{d}r \left[\int_r^1 [\varphi_0(t)g(t) - r\chi_0(t)g(t)\right]\mathrm{d}t. \tag{B.25}$$

Again, all the functions here being positive, we can exchange the orders of integration in each double integral. One finds then immediately that $t^2 g(t) \in L^1(0,1) \Rightarrow U \in L^1(0,1)$. In short, we have

$$\begin{cases} t^{\alpha} g(t) \in L^1(1,\infty) \Rightarrow r^{\alpha-1}U(r) \in L^1(1,\infty), & \alpha = 1, 2, \\ t^2 g(t) \in L^1(0,1) \Rightarrow U(r) \in L^1(0,1). \end{cases} \tag{B.26}$$

This completes the proof of the properties of $g(t)$ in theorem 3, in theorem B and elsewhere, and provides sufficient conditions on the properties of $U(r)$ needed in the main text and in appendix A.

Remark. In all rigour, $K(x,x)$ in (B.5) is infinite if $V(r)$ is not integrable at $r = 0$, as is seen in (B.2) and (B.3). This may happen since we assume only $rV(r)$ to be integrable at $r = 0$. However, one may first regularize the potential at $r = 0$, and proceed as we did. Then, it can be seen that the final form (B.7) is quite general, and independent of whether $V(x)$ is integrable or not at the origin. One can therefore remove the regularization in (B.7), and so condition (15) is quite general.

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