Causality and universality in low-energy quantum scattering

H.-W. Hammer\textsuperscript{a} and Dean Lee\textsuperscript{b,a}

\textsuperscript{a}Helmholtz-Institut für Strahlen- und Kernphysik (Theorie) and
Bethe Center for Theoretical Physics,
Universität Bonn, D-53115 Bonn, Germany

\textsuperscript{b}Department of Physics, North Carolina State University, Raleigh, NC 27695, USA

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Abstract

We generalize Wigner’s causality bounds and Bethe’s integral formula for the effective range to arbitrary dimension and arbitrary angular momentum. Moreover, we discuss the impact of these constraints on the separation of low- and high-momentum scales and universality in low-energy quantum scattering.

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In quantum mechanics causality requires that no scattered wave propagates before the incident wave first reaches the scatterer. This constraint ensures a scattering amplitude which is analytic in the upper half plane as a function of energy $E$ \[1, 2\]. For the case of finite-range interactions the constraints of causality were first investigated by Wigner \[3\]. The time delay between the incoming wave and the scattered outgoing wave can be computed from the energy derivative of the elastic phase shift, \(\Delta t = 2\hbar d\delta/dE\). If $d\delta/dE$ is negative, this implies a time advance of the outgoing wave. However, the time advance cannot be arbitrarily large since the incoming wave must first enter the interaction region before the scattered wave can exit. Since the derivative of the phase shift with respect to the energy is involved, this argument places a bound on the effective range of the scattering amplitude.

Wigner bounds are particularly interesting in the context of low-energy scattering and universality. Universality at low energies arises when there is a large separation between the short-distance scale of the interaction and the long-distance scales given by the average particle spacing and thermal wavelength. One example of low-energy universality is the unitarity limit, which refers to an idealized system where the range of the interaction is zero and the $S$-wave scattering length is infinite. It has been studied most thoroughly for two-component fermions. In nuclear physics, cold dilute neutron matter is close to the unitarity limit. However, most recent interest in unitarity-limit physics is driven by experiments with cold $^6$Li and $^{40}$K atoms using magnetically-tuned Feshbach resonances. For reviews of recent cold atom experiments, see Refs. \[4, 5\]. Theoretical overviews of ultracold Fermi gases and their numerical simulations are given in \[6, 7\]. A general review of universality at large scattering length can be found in \[8\].

Several experiments have also investigated strongly-interacting $P$-wave Feshbach resonances in $^6$Li and $^{40}$K \[9–13\]. An important issue here is whether the physics of these strongly-interacting $P$-wave systems is universal, and if so, what are the relevant low-energy parameters. A resolution of these issues would provide a connection between, for example, the atomic physics of $P$-wave Feshbach resonances and the nuclear physics of $P$-wave alpha-neutron interactions in halo nuclei. Some progress towards addressing these questions has been made utilizing low-energy models of $P$-wave atomic interactions \[14 \[19\] and $P$-wave alpha-neutron interactions \[20 \[23\]. A renormalization group study showed that scattering should be weak in higher partial waves unless there is a fine tuning of multiple parameters \[24\].

In this letter, we answer the question of universality and the constraints of causality for arbitrary dimension $d$ and arbitrary angular momentum $L$. Our analysis is applicable to any finite-range interaction that is energy independent, non-singular, and spin independent. We present generalizations of Bethe’s integral formula for the effective range \[25\] and Wigner bounds for arbitrary $d$ and $L$. Our results can be viewed as a generalization of the analysis of Phillips and Cohen \[26\], who derived a Wigner bound for the $S$-wave effective range for short-range interactions in three dimensions. Here we show that for $2L + d \geq 4$, causal wave propagation produces a fundamental obstruction to reaching the scale-invariant limit for finite range interactions. Instead we find the emergence of the effective range as a second relevant low-energy parameter that cannot be tuned to zero without violating causality. For the case of shallow bound states, we show that this second low-energy parameter also parametrizes the size of the bound-state wavefunction. Complementary work was carried out by Ruiz Arriola and collaborators. A discussion of the Wigner bound in the context of chiral two-pion exchange can be found in \[27\] while correlations between the scattering
We consider two non-relativistic spinless particles in \( d \) dimensions with a rotationally-invariant two-body interaction. We let \( L \) label the absolute value of the top-level angular momentum quantum number \( \frac{\mu}{2} \). For \( d \geq 2 \), \( L \) can be any non-negative integer. For \( d = 1 \), the notion of rotational invariance reduces to parity invariance. Here we assume a parity-symmetric interaction and write \( L = 0 \) for even parity and \( L = 1 \) for odd parity. We analyze the two-body system in the center-of-mass frame using units with \( \hbar = 1 \) for convenience. With reduced mass \( \mu \) and energy \( p^2/(2\mu) \), we rescale the radial wavefunction \( R^{(p)}_{L,d}(r) \) as

\[
u^{(p)}_{L,d}(r) = (pr)^{(d-1)/2} R^{(p)}_{L,d}(r).
\]

The interaction is assumed to be energy independent and have a finite range \( R \) beyond which the particles are non-interacting. Writing the interaction as a real symmetric operator with kernel \( W(r, r') \), we have the radial Schrödinger equation

\[
p^2 u^{(p)}_{L,d}(r) = \left[ -\frac{d^2}{dr^2} + \frac{4L + 2d - 4}{4r^2} \right] u^{(p)}_{L,d}(r) + 2\mu \int_0^R dr' W(r, r') u^{(p)}_{L,d}(r').
\]

The normalization of \( u^{(p)}_{L,d}(r) \) is chosen so that for \( r \geq R \),

\[
u^{(p)}_{L,d}(r) = \sqrt{\frac{pr\pi}{2}} p^{L+d/2-3/2} \left[ \cot \delta_{L,d}(p) J_{L+d/2-1}(pr) - Y_{L+d/2-1}(pr) \right].
\]

Here \( J_{\alpha} \) and \( Y_{\alpha} \) are the Bessel functions of the first and second kind, and \( \delta_{L,d}(p) \) is the phase shift for partial wave \( L \). The phase shifts are directly related to the elastic scattering amplitude \( f_{L,d}(p) \), where

\[
f_{L,d}(p) \propto \frac{p^{2L}}{p^{2L+d-2} \cot \delta_{L,d}(p) - ip^{2L+d-2}}.
\]

In addition to having finite range, we assume also that the interaction is not too singular at short distances. Specifically, we require that the effective range expansion defined below in Eq. (5) converges for sufficiently small \( p \) and that \( \frac{d}{dr} u^{(p)}_{L,d} \) is finite and \( u^{(p)}_{L,d} \) vanishes as \( r \to 0 \). For example, these short-distance regularity conditions are satisfied for a local potential, \( W(r, r') = V(r)\delta(r-r') \), provided that \( V(r) = O(r^{-2+\epsilon}) \) as \( r \to 0 \) for positive \( \epsilon \). In our discussion, however, we make no assumption that the interactions arise from a local potential. The treatment of spin-dependent interactions with partial wave mixing is beyond the scope of this analysis. For coupled-channel dynamics without partial wave mixing the analysis can proceed by first integrating out higher-energy contributions to produce a single-channel effective interaction. In order to satisfy our condition of energy-independent interactions, this should proceed using a technique such as the method of unitary transformation described in Ref. [31–33].

The effective range expansion is

\[
p^{2L+d-2} \left[ \cot \delta_{L,d}(p) - \delta_{(d \mod 2),0} \frac{2}{\pi} \ln (p\rho_{L,d}) \right]
\]

\[
= -\frac{1}{a_{L,d}} + \frac{1}{2} r_{L,d} p^2 + \sum_{n=0}^{\infty} (-1)^{n+1} P^{(n)}_{L,d} p^{2n+4}.
\]

\[\text{(5)}\]
The term $\delta_{(d \mod 2),0}$ is 0 for odd $d$ and 1 for even $d$. $a_{L,d}$ is the scattering parameter, $r_{L,d}$ is the effective range parameter, and $P^{(n)}_{L,d}$ are the $n$th-order shape parameters. $\rho_{L,d}$ is an arbitrary length scale that can be scaled to any nonzero value. The rescaling results in a shift of the dimensionless coefficient of $p^{2L+d-2}$ on the right-hand of Eq. (5), and we define $\bar{\rho}_{L,d}$ as the special value for $\rho_{L,d}$ where this coefficient is zero.

Let $u^{(p)}_{L,d}$ and $u^{(p')}_{L,d}$ be radial solutions of the Schrödinger equation for two different momenta. We construct the Wronskian of the two solutions,

$$u^{(p)}_{L,d} \frac{d}{dr} u^{(p')}_{L,d} - u^{(p')}_{L,d} \frac{d}{dr} u^{(p)}_{L,d},$$

and evaluate at some radius $r \geq R$. Taking the limits $p' \to 0$ and then $p \to 0$, we find that for any $r \geq R$,

$$r_{L,d} = b_{L,d}(r) - 2 \lim_{p \to 0} \int_0^r dr' \left[ u^{(p)}_{L,d}(r') \right]^2,$$

where $b_{L,d}(r)$ is defined as follows. For $d = 2$ and $d = 4$, $b_{L,d}(r)$ can contain logarithmic terms analog to Eq. (5). For the special case $2L + d = 2$, we have

$$b_{L,d}(r) = \frac{2r^2}{\pi} \left\{ \ln \left( \frac{r}{2a_{L,d}} \right) + \gamma - \frac{1}{2} \right\} \left[ \frac{\pi}{2a_{L,d}} \left( \frac{r}{2} \right)^2 + \frac{1}{4} \right],$$

where $\gamma$ is the Euler-Mascheroni constant and for $2L + d = 4$,

$$b_{L,d}(r) = \frac{4}{\pi} \left[ \ln \left( \frac{r}{2a_{L,d}} \right) + \gamma \right] - \frac{4}{a_{L,d}} \left( \frac{r}{2} \right)^2 + \frac{\pi}{a_{L,d}} \left( \frac{r}{2} \right)^4.$$

For the generic case of $2L + d$ any positive odd integer or any even integer $\geq 6$:

$$b_{L,d}(r) = -\frac{2\Gamma(L + \frac{d}{2} - 2)\Gamma(L + \frac{d}{2} - 1)}{\pi} \left( \frac{r}{2} \right)^{-2L-d+4} - \frac{4}{L + \frac{d}{2} - 1} \frac{1}{a_{L,d}} \left( \frac{r}{2} \right)^2 + \frac{2\pi}{\Gamma(L + \frac{d}{2})\Gamma(L + \frac{d}{2} + 1)} \frac{1}{a_{L,d}^2} \left( \frac{r}{2} \right)^{2L+d}. $$

The formula in Eq. (10) for $L = 0$ in three dimensions was first derived by Bethe [25] and extended by Madsen for general $L$ [34]. The results presented here give the generalization to arbitrary $d$ and arbitrary $L$.

Since the integrand in Eq. (7) is positive semi-definite, $r_{L,d}$ satisfies the upper bound

$$r_{L,d} \leq b_{L,d}(r)$$

for any $r \geq R$. For $d = 3$ our results are equivalent to the causality bound derived by Wigner [3]. As noted in the introduction, the time delay between the incoming wave and the scattered outgoing wave is proportional to the energy derivative of the elastic phase shift, $d\delta_{L,d}/dE$. Since the incoming wave must first enter the interaction region before the scattered wave can exit, causality places a bound on $d\delta_{L,d}/dE$. The precise quantum
mechanical statement of this causality requirement is that the reciprocal logarithmic derivative \( u_{L,d}^{(p)} / d r u_{L,d}^{(p)} \) has a non-negative energy derivative. This fact can be derived from the Wronskian in Eq. (6), and a detailed derivation of this connection will be given in Ref. [35]. For finite-range interactions \( p^{2L+d-2} \cot \delta_{L,d} \) has a convergent effective range expansion, and \( d\delta_{L,d}/dE \) at zero energy is proportional to the effective range \( r_{L,d} \). For \( d = 3 \), the Wigner causality bound in zero-energy limit is equivalent to the bound in Eq. (11) on the effective range. For \( S \)-wave interactions in three dimensions the upper bound on the effective range was discussed in Ref. [26]. It was observed that for fixed \( a_{L,d} \) the zero-range limit \( R \to 0 \) is possible only when \( r_{L,d} \) is negative. The constraint becomes more severe for larger \( 2L+d \). For \( 2L+d \geq 4 \), the limit \( R \to 0 \) at fixed \( a_{L,d} \) produces a divergence in the effective range, \( r_{L,d} \leq b_{L,d}(R) \to -\infty \).

Our results are exact only for the case where the interaction vanishes for \( r \geq R \). For exponentially-bounded interactions of \( O(e^{-r/R}) \) at large distances, the results should still be accurate with only exponentially small corrections. For an exponentially-bounded but otherwise unknown interaction, the non-negativity condition for \( b_{L,d}(r) - r_{L,d} \) can be used to determine the minimum value for \( R \) consistent with causality. As an example, we plot \( b_{L,3}(r) - r_{L,3} \) for alpha-neutron scattering in Fig. 1. In the plot, we show results for the \( S_{1/2} \), \( P_{1/2} \), and \( P_{3/2} \) channels. We note that a qualitatively similar plot was introduced for nucleon-nucleon scattering in the \( S \)-wave spin-singlet channel [36]. The non-negativity condition gives \( R \geq 1.1 \) fm for \( S_{1/2} \), \( R \geq 2.6 \) fm for \( P_{1/2} \), and \( R \geq 2.1 \) fm for \( P_{3/2} \). For comparison, the alpha root-mean-square radius and pion Compton wavelength are both about 1.5 fm. Since the minimum values for \( R \) are not small when compared with these, our analysis suggests some caution when choosing the cutoff scale for an effective theory of alpha-neutron interactions.

At this point we comment on our requirement that the interactions are energy independent. For energy-dependent interactions it possible to generate any energy dependence for the elastic phase shifts even when the interaction \( W(r, r'; E) \) vanishes beyond some finite
radius $R$ for all $E$. Under these more general conditions there are no longer any Wigner bounds and the constraints of causality seem to disappear. However, it is misleading to regard interactions of this more general type as having finite range. As noted in the introduction, the scattering time delay is given by the energy derivative of the phase shift. The energy dependence of the interaction can by itself generate large negative time delays and thereby reproduce the scattering of long-range interactions. In this sense the range of the interaction as observed in scattering is set by the dependence of $W(r, r'; E)$ on the radial coordinates $r, r'$ as well as the energy $E$. In this case the bound in Eq. (11) can be viewed as an estimate for the minimum value of this interaction range.

We now consider the scattering amplitude in the low-energy limit $p \to 0$ while keeping the interaction range $R$ fixed. In the low-energy limit the scattering amplitude depends on just one dimensionful parameter when $2L + d \leq 3$. For $2L + d = 1$ and $2L + d = 3$ the relevant parameter is $a_{L,d}$, and for $2L + d = 2$ it is $\bar{\rho}_{L,d}$. When $2L + d \geq 4$ a second dimensionful parameter appears in the non-perturbative low-energy limit. In the limit $|a_{L,d}| \to \infty$, the upper bounds on the effective range reduce to the form $\bar{\rho}_{L,d} \leq \frac{e\gamma}{2}$ for $2L + d = 4$, and

$$r_{L,d} \leq -\frac{2\Gamma(L + \frac{d}{2} - 2)\Gamma(L + \frac{d}{2} - 1)}{\pi} \left(\frac{r}{2}\right)^{2L-d+4}$$

(12)

for $2L + d \geq 5$. There is no way to suppress the $p^2 \ln(p\bar{\rho}_{L,d})$ term in the effective range expansion for $2L + d = 4$ by fine-tuning parameters because the bound forbids tuning the argument of the logarithm to 1 as $p \to 0$. Similarly, for $2L + d \geq 5$ the upper bound in Eq. (12) and the negative coefficient on the right-hand side prevent setting $r_{L,d}$ to zero to eliminate the term $\frac{1}{2}r_{L,d}p^2$. Hence in both cases we are left with two relevant parameters in the non-perturbative low-energy limit. This corresponds to two relevant directions near a fixed point of the renormalization group, and the universal behavior is characterized by two low-energy parameters. For the case of $P$-wave neutron-alpha scattering in three dimensions, this issue was already discussed in [20]. Proper renormalization of an effective field theory for $P$-wave scattering requires the inclusion of field operators for the scattering volume and the effective range at leading order. In the renormalization group study of [24], the emergence of multiple relevant directions around a fixed point was observed for the repulsive inverse square potential.

For $2L + d \geq 4$ this second dimensionful parameter has a simple physical interpretation for shallow bound states. Consider a bound state at $p = ip_I$ in the zero binding-energy limit $p_I \to 0^+$. Let $P_>(r)$ be the probability of finding the constituent particles with separation larger than $r$:

$$P_>(r) = \int_r^\infty dr' \left| \tilde{u}_{L,d}^{(ip_I)}(r') \right|^2,$$

(13)

where $\tilde{u}_{L,d}^{(ip_I)}$ is the normalized wave function. For $2L + d \leq 3$, the probability $P_>(r)$ equals 1 in the limit $p_I \to 0^+$ for any $r$. At sufficiently low energies the physics at short distances is irrelevant, and the bound state wavefunction is spread over large distances. For $2L + d \geq 4$, however, the situation is different. For $2L + d = 4$ the probability is logarithmically dependent on $\bar{\rho}_{L,d}$ and can be tuned to any value between 0 and 1 [33]. Similarly for $2L + d \geq 5$,

$$P_>(r) \to \frac{2\Gamma(L + \frac{d}{2} - 2)\Gamma(L + \frac{d}{2} - 1)}{(-r_{L,d})\pi} \left(\frac{r}{2}\right)^{2L-d+4}$$

(14)

for $r \geq R$. For this case the characteristic size of the bound state wavefunction is $(-r_{L,d})^{1/(2L-d+4)}$.
For \( P \)-wave Feshbach resonances in alkali atoms our analysis must be modified to take into account long-range van der Waals interactions of the type 
\[ W(r, r') = -C_6 r^{-6} \delta(r - r') \]
for \( r, r' \geq R \). This raises various new issues such as the applicability of our approach to power law potentials and the appearance of non-analytic terms in the effective range expansion. These issues will be addressed in detail in [35]. Here we will briefly discuss the modifications for potentials with a van der Waals tail in three dimensions only. It is convenient to reexpress \( C_6 \) in terms of the length scale \( \beta_6 = (2\mu C_6)^{1/4} \). In the following, we set \( d = 3 \) and drop the \( d \) subscript. Instead of free Bessel functions, scattering states should be compared with exact solutions of the attractive \( r^{-6} \) potential [37, 38]. The effect of the interactions for \( r < R \) are described by a finite-range \( K \)-matrix \( K_L(p^2) \) which is analytic in \( p^2 \) [39],
\[ K_L(p^2) = \sum_{n=0,1,\ldots} K_L^{(2n)} p^{2n} \]
When phase shifts are measured relative to free spherical Bessel functions, the effective range expansion is no longer analytic in \( p^2 \). For \( L = 0 \), the leading non-analytic term is proportional to \( p^3 \). For \( L = 1 \) the non-analytic term is proportional to \( p^1 \), thereby voiding the usual definition of the effective range parameter.

For a pure van der Waals tail, however, one can still obtain useful information from our approach. The zero-energy resonance limit is reached by tuning the lowest-order \( K \)-matrix coefficient \( K_L^{(0)} \) to zero. It turns out that for \( L = 1 \) in this limit the \( p^1 \) coefficient in the effective range expansion also vanishes, and we can therefore define an effective range parameter for both \( S \)- and \( P \)-waves [38, 40],
\[ r_0 = [\Gamma (1/4)]^2 \left( \beta_6 + 3K_0^{(2)} \beta_6^{-1} \right) / (3\pi), \]
\[ r_1 = -36 [\Gamma (3/4)]^2 \left( \beta_6^{-1} - 5K_1^{(2)} \beta_6^{-3} \right) / (5\pi). \] (15)

For the case of single-channel scattering for alkali atoms, the coefficients \( K_L^{(2)} \) are negligible compared with \( \beta_6^2 \). This is also true for some multi-channel Feshbach resonance systems [41]. In these cases we observe that the upper bounds for \( r_L \) in Eq. (12) are satisfied for \( L = 0 \) and \( L = 1 \) when we naively take \( R \sim \beta_6 \). In general, there may be multi-channel systems where the coefficients \( K_L^{(2)} \) cannot be neglected. Nevertheless, the coefficients \( K_L^{(2)} \) should satisfy Wigner bounds similar to those derived here for the effective range. This may be a useful starting point for further investigations of multi-channel Feshbach resonances in alkali atoms.

In this letter, we have addressed the question of universality and the constraints of causality for arbitrary dimension \( d \) and arbitrary angular momentum \( L \). For finite-range interactions we have shown that causal wave propagation can have significant consequences for low-energy universality and scale invariance. We find that in certain cases two relevant low-energy parameters are required in the non-perturbative low-energy limit. In the language of the renormalization group, this corresponds to two relevant directions in the vicinity of a fixed point. In particular, we confirm earlier findings in the case three dimensions for \( P \)-wave scattering [20] based on renormalization arguments and for higher partial waves in general [24] in the framework of the renormalization group. The analysis presented here concerns only the question of universality in two-body scattering. Universality for higher few-body systems requires a detailed analysis for each system under consideration. Effective field theory and renormalization group methods may again provide a useful starting point here [42, 43]. Our results may help to clarify some of the conceptual and calculational issues relevant to few-body systems for general dimension and angular momentum and their simulation using short-range interactions.
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