Resonant-state-expansion Born approximation with a correct eigen-mode normalisation

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Abstract
The Born approximation (Born 1926 Z. Phys. 38 802) is a fundamental result in physics, it allows the calculation of weak scattering via the Fourier transform of the scattering potential. As was done by previous authors (Ge et al 2014 New J. Phys. 16 113048) the Born approximation is extended by including in the formula the resonant-states (RSs) of the scatterer. However in this study unlike previous studies the included eigen-modes are correctly normalised with dramatic positive consequences for the accuracy of the method. The normalisation of RSs used in the previous RS expansion Born approximation or resonant-state expansion (RSE) Born approximation made in Ge et al (2014 New J. Phys. 16 113048) has been shown to be numerically unstable in Muljarov et al (2014 arXiv:1409.6877) and by analytics here. The RSs of the system can be calculated using my recently discovered RSE perturbation theory for dispersive electrodynamic scatterers (Muljarov et al 2010 Europhys. Lett. 92 50010; Doost et al 2012 Phys. Rev. A 85 023835; Doost et al 2013 Phys. Rev. A 87 043827; Armitage et al 2014 Phys. Rev. A 89; Doost et al 2014 Phys. Rev. A 90 013834) and normalised correctly to appear in spectral Green’s functions and hence the RSE Born approximation via the flux-volume normalisation which I recently rigorously derived in Armitage et al (2014 Phys. Rev. A 89), Doost et al (2014 Phys. Rev. A 90 013834), Doost (2016 Phys. Rev. A 93 023835). In the case of effectively one-dimensional systems I find a RSE Born approximation alternative to the scattering matrix method.

Keywords: resonant-state expansion, Born approximation, numerical validation, eigen-mode normalisation

(Some figures may appear in colour only in the online journal)

1. Introduction
Fundamental to scattering theory, the Born approximation consists of taking the incident field in place of the total field as the driving field at each point inside the scattering potential, it was first discovered by Max Born and presented in [1]. The Born approximation gave an expression for the differential scattering cross section in terms of the Fourier transform of the scattering potential. The Born approximation is only valid for weak scatterers as we will see in the numerical demonstrations.

In this paper I provide an extension to the Born approximation which allows an arbitrary number of resonant states (RSs) to be taken into account. I have named this extension to the Born approximation the resonant-state-expansion (RSE) correction to the Born approximation or the RSE Born approximation. An almost identical approach is already available in the literature [2] however its derivation differed by including an unstable normalisation formula for the RS eigen-modes of the system which was then subsequently used to expand Born’s approximation incorrectly. The normalisation derived in [13] and used in the previous RSE Born approximation made in [2] has been shown to be numerically unstable in [8] and shown to be unstable using analytics in appendix C. Furthermore the numerical study made in [2] only included a single RS in the expansion of the Born approximation, most likely to avoid divergence caused by their incorrect normalisation of the RSs.
Recently there has been developed [3] a rigorous perturbation theory called resonant-state expansion (RSE) which was then applied to one-dimensional (1D), two-dimensional (2D) and three-dimensional (3D) systems [4–7, 9, 10] which only calculates the modes and makes no use of them. The RSE accurately and efficiently calculates RSs of an arbitrary system in terms of an expansion of RSs of a simpler, unperturbed one. RSs are normalised correctly to appear in spectral Green’s functions (GFs) via the flux volume normalisation [7] and hence the RSE Born approximation. In the limit where an infinite number of these resonances are included in the RSE Born approximation we will observe convergence of the method towards the exact solutions. That the RSE can reproduce both the correctly normalised RS fields as well as frequencies was demonstrated in [4] with my convergence and extrapolation algorithm.

The concept of RSs was first conceived and used by Gamow in 1928 in order to describe mathematically the process of radioactive decay, specifically the escape from the nuclear potential of an alpha-particle by tunnelling. Mathematically this corresponded to solving Schrödinger’s equation for outgoing boundary conditions (BCs). These states have complex frequency $\omega$ with negative imaginary part meaning their time dependence $\exp(-i\omega t)$ decays exponentially, thus giving an explanation for the exponential decay law of nuclear physics. The consequence of this exponential decay with time is that the further from the decaying system at a given instant of time the greater the wave amplitude. An intuitive way of understanding this divergence of wave amplitude with distance is to notice that waves that are further away have left the system at an earlier time when less of the particle probability density had leaked out. There already exists numerical techniques for finding eigen-modes such as finite element method (FEM) and finite difference in time domain (FDTD) method to calculate resonances in open cavities. However determining the effect of perturbations which break the symmetry presents a significant challenge as these popular computational techniques need large computational resources to model high quality modes. Also these methods generate spurious solutions which would damage the accuracy of the RSE Born approximation if included in the basis.

The paper is organised as follows, section 2 outlines the derivation of the RSE Born approximation, section 3 discusses normalisations of RSs by other authors, section 4 outlines the application of the RSE Born approximation to planar slabs, section 5 gives the numerical validation of the new method along with a comparison of the alternative RSE approaches.

### 2. Derivation of the RSE Born approximation

I will in the following section re-derive the method for calculating the full GF of an open electromagnetic system in the same way as [2] however unlike previous authors I use the numerically stable normalisation of RSs which I derived in [7]. These methods are required to calculate transmission and scattering cross-section from the dispersive RSE perturbation theory with mathematical rigour and accuracy.

For an electrodynamic system with local frequency dependent dielectric permittivity tensor $\varepsilon_0(r)$ and permeability $\mu = 1$, where $r$ is the 3D spatial position, Maxwell’s wave equation for the electric $E(r)$-field with a current source $J(r)$ oscillating at frequency $\omega$, which can be real or complex, is

$$-\nabla \times \nabla \times E(r) + k^2 \varepsilon_0(r)E(r) = ik\frac{4\pi}{c}J(r). \quad (1)$$

The time-dependent part of the field is given by $\exp(-i\omega t)$ with the complex eigen-frequency $\omega = ck$, where $c$ is the speed of light in vacuum.

The GF of an open electromagnetic system is a tensor $G_0$, which satisfies Maxwell’s wave equation equation (1) with a delta function source term,

$$-\nabla \times \nabla \times G_0(r, r') + k^2 \varepsilon_0(r)G_0(r, r') = i\delta(r - r'). \quad (2)$$

where $\delta$ is the unit tensor. Physically, the GF describes the response of the system to a point current with frequency $\omega$, i.e. an oscillating dipole.

The importance of $G_0$ comes from the fact we can see from equation (2) that equation (1) can be solved for $E(r)$ by convolution of $G_0$ with the current source $J(r')$

$$E(r) = \int G_0(r, r')ik\frac{4\pi}{c}J(r')dr'. \quad (3)$$

Inside the system we can use the RSE to calculate the GF. In appendix A I derive for dispersive systems (for which I have recently developed a dispersive RSE perturbation theory [9, 10]) a convenient form of the spectral GF, valid inside the scatterer only,

$$\hat{G}_k(r, r') = \sum_n \frac{E_n(r) \otimes E_n(r')}{2k(k - k_n)}. \quad (4)$$

The $E_n$ are RSs of the open optical system and are defined as the eigen-solutions of Maxwell’s wave equation,

$$\nabla \times \nabla \times E_n(r) = k^2 \varepsilon_0(r)E_n(r), \quad (5)$$

satisfying the outgoing wave BCs. I have also taken the resonant to be embedded in free space ($\varepsilon = 1$) without loss of generality. Here, $k_n$ is the wave-vector eigen-value of the RS numbered by the index $n$, and $E_n(r)$ is its electric field eigen-function. The RSs which are solutions of equation (5) are either stationary or decaying in time. Modes appearing in equation (4) are normalised [7, 10] according to the flux-volume normalisation

$$\delta_{0,k_n} + 1 = \int_{V} E_n(r) \cdot \frac{\partial(k^2 \varepsilon_0(r))}{\partial(k^2)} |_{k = k_n} E_n(r)dr + \lim_{k \to k_n} \int_{S_k} E_n \cdot \nabla E - E \cdot \nabla E_n dS, \quad (6)$$

where the first integral is taken over an arbitrary simply connected volume $V$ enclosing the inhomogeneity of the system and the centre of the spherical coordinates used, and the second integral is taken over its surface $S_k$. This normalisation is required [7] for the validity of the spectral representation equation (4). Numerically equation (6) has been validated by
its use in RSE perturbation theory [4–7, 9, 10]. A discussion of the dispersive RSE for nano-particles is given in appendix B.

The generalisation of my equation (6) to \( k_0 = 0 \) modes is attributable solely to E A Muljarov in [7], however that part of the proof of the normalisation can only be further generalised to dispersive systems using the spectral GF equation (4) derived in appendix A. The required derivation is identical except that it makes use of the rigorously derived spectral GF equation (4) instead of the identical GF derived in a less mathematically rigorous way for non-dispersive systems. This last step is vital for the accuracy of the method. Further I note that just as I explained in [10] \( \hat{\varepsilon}_k \) must be a real symmetric matrix or a scalar in order to calculate the dispersion factor as shown.

Various schemes exist to evaluate the surface integral limit in equation (6) such as analytic methods in [3, 7, 8] or numerically extending the surface into a non-reflecting, absorbing, perfectly matched layer where it vanishes.

The derivation of the RSE Born approximation by Kristensen et al [2] has been made using the normalisation introduced by Leung et al [13] the limit of infinite volume \( V \) is taken:

\[
1 = \lim_{V \to \infty} \int_V \frac{\partial(k^2 \hat{\varepsilon}_k(r))}{\partial(k^2)} \left|_{k=k_0} \right. E_0^e(r) dr + \frac{i}{2k_0} \oint_{\partial S} E_2^e(r) dS.
\]

(7)

It was numerically found [11] that the surface term was leading to a stable value of the integral for the relatively small volumes available in 2D FDTD calculations and high-Q modes. However, it was discovered at the time that this was not the case for low-Q modes. It was wrongly shown by Muljarov et al [8] that equation (7) is actually diverging in the limit \( V \to \infty \), and therefore the expansion of the Born approximation in [2] and the normalisation equation (7) are incorrect. In appendix C I provided a mathematically rigorous disproof of some of E A Muljarov’s points and make some correct points about the unsuitability of equation (7) for the RSE perturbation theory myself. Hence although being a cornerstone of the scattering theory of open systems the correct expansion of the Born approximation in terms of RSEs to the exact solution was not previously available.

Analogously to [2] the derivation of the RSE Born approximation of Ge et al [2] is made but in this case using my correct normalising formula for modes.

That the \( E_n^e(r) \) and \( k_0 \) can be calculated accurately by the RSE perturbation theory and normalised correctly by equation (6) makes possible the RSE Born approximation.

The free space GF \( \hat{G}_k^{\beta} \) is now introduced

\[
-\nabla \times \nabla \times \hat{G}_k^{\beta}(r, r') + k^2 \hat{G}_k^{\beta}(r, r') = \hat{\delta}(r - r'),
\]

(8)

which has the solution,

\[
\hat{G}_k^{\beta}(r, r') = -\frac{e^{ik|\mathbf{r} - \mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|} \hat{\mathbf{i}}.
\]

(9)

The systems associated with \( \hat{\varepsilon}_k \) and \( \hat{G}_k^{\beta} \) are related by the Dyson equations perturbing back and forth with

\[
\Delta \hat{\varepsilon}_k(r) = \hat{\varepsilon}_k(r) - \hat{I} \]

(2),

\[
\hat{G}_k^i(r, r') = \hat{G}_k^{\beta}(r, r') - k^2 \int \hat{G}_k^{\beta}(r, r'') \Delta \hat{\varepsilon}_k(r'') \hat{G}_k^{\beta}(r'', r') dr''
\]

(10)

\[
\hat{G}_k(r', r'') = \hat{G}_k^{\beta}(r', r'') - k^2 \int \hat{G}_k^{\beta}(r', r') \Delta \hat{\varepsilon}_k(r') \hat{G}_k^{\beta}(r', r'') dr'
\]

(11)

Combining equations (10) and (11) it is obtained as in [2]

\[
\hat{G}_k(r, r') = \hat{G}_k^{\beta}(r, r') - k^2 \int \hat{G}_k^{\beta}(r, r') \Delta \hat{\varepsilon}_k(r') \hat{G}_k^{\beta}(r', r'') dr''
\]

(12)

or using equation (A1) instead

\[
\hat{G}_k(r, r') = \hat{G}_k^{\beta}(r, r') - k^2 \int e^{ik(r-r')} \hat{\delta}(r') dr' - k^2 \int e^{ik(r-r')} \hat{\delta}(r') dr' - k^2 \int e^{ik(r-r')} \hat{\delta}(r') dr'.
\]

(13)

Therefore substituting equation (4) and equation (9) in to equation (12) and using equation (13) because both \( r, r'' \) are far from the scatterer we arrive at the RSE Born approximation

\[
\hat{G}_k(r, r') = -\frac{e^{i|\mathbf{r} - \mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|} \hat{\mathbf{i}}
\]

(14)

The vector \( \mathbf{A}_n^e \) is defined as a Fourier transform of the RSEs,

\[
\mathbf{A}_n^e = \int e^{ik\cdot \mathbf{r}} \hat{\delta}(r') \mathbf{E}^e_n(r') \, dr'.
\]

(16)

I note that the fast Fourier transform method is available. Furthermore I note that for the inverse scattering problem at resonance the inverse Fourier transform is also available. The first two terms in equation (15) correspond to the standard Born approximation, the final summation term corresponds to the RSE correction to the Born approximation.
A simple corollary of this theory is as follows, we can see from the arguments just stated that from equation (10) if r'' is inside the resonator and r ≫ r'' then

\[
\hat{G}_i(r, r'') = -\frac{e^{ik |r-r'|}}{4\pi |r - r''|} \hat{I} + k \frac{e^{ikr''}}{4\pi} \sum_n \frac{A_n(k_n) \otimes E_n(r'')}{2(k - k_n)},
\]

(17)

or using equation (A1) instead

\[
\hat{G}_k(r, r'') = -\frac{e^{ik |r-r'|}}{4\pi |r - r''|} \hat{I} + k^2 \frac{e^{ikr''}}{4\pi} \sum_n \frac{E_n(r) \otimes A_n(-k_n'')}{2(k - k_n)},
\]

(19)

similarly from equation (11) if r is inside the resonator and r'' ≫ r then

\[
\hat{G}_k(r, r'') = -\frac{e^{ik |r-r'|}}{4\pi |r - r''|} \hat{I} + k^2 \frac{e^{ikr''}}{4\pi} \sum_n \frac{E_n(r) \otimes A_n(-k_n'')}{2(k - k_n)},
\]

(20)

other permutations are possible.

3. Other normalisations

3.1. Normalisation by Sauvan and co-workers

The rigorously derived normalisation of Sauvan and co-workers that they gave in [16] as

\[
2 = \int_V E_n(r) \cdot \frac{\partial (k^2 \hat{E}_n(\mathbf{r}))}{\partial (k^2)} \mid_{k=k_n} E_n(r) dr
- \int_V H_n(r) \cdot \frac{\partial (k^2 \hat{H}_n(\mathbf{r}))}{\partial (k^2)} \mid_{k=k_n} H_n(r) dr.
\]

(21)

requires that the integral V be continued into a perfectly matched layer where it is attenuated to zero, thus eliminating the need for surface terms in the normalisation. As such it is most suitable for FEM and FDTD calculations. Further I note that just as I explained in [10] \( \hat{E}_n(\mathbf{r}) \) must be a real symmetric matrix or a scalar in order to calculate the dispersion factor as shown.

I generate this normalisation by combining the RSE normalisation for \( \mathbf{H}_n \) and \( \mathbf{E}_n \). I note that this alternative approach to deriving Sauvan’s normalisation was discussed with E A Muljarov at some point but without discussing \( k_n = 0 \) modes. I also note that \( k_n = 0 \) modes have only \( \mathbf{H} \) field or \( \mathbf{E} \) field component by Maxwell’s equations because they are curl free modes. \( k_n = 0 \) are by definition modes which satisfy the condition of being curl free. These two points explain why the addition of \( k_n = 0 \) modes to Sauvan and co-worker’s normalisation takes the form it does. Actually the RSE normalisation for \( \mathbf{H}_n \) modes was first shown to me in an email attachment, by E A Muljarov several years ago but without any derivation and without \( k_n = 0 \) modes or differential dispersion factor included.

The rigorous derivation of the relationship between normalised \( \mathbf{E}_n \) and \( \mathbf{H}_n \) modes appearing in the spectral GF of Maxwell’s wave equations for \( \mathbf{E} \)-field and \( \mathbf{H} \)-field can be found in appendix D of my PhD thesis [18].

Clearly as the perturbation is increased there is a critical perturbation strength at which the RSE becomes less efficient than FDTD and FEM and beyond this point one should use the RSE Born approximation with the normalisation of \[16\] and FDTD or FEM.

3.2. Radiation mode normalisation

I have recently written a paper on the RSE Born approximation for waveguides with dispersion [10]. I found that such modes for cylindrical/effectively-2D waveguides can be normalised by reducing Maxwell’s equation to effectively 2D and replacing the operation \( \nabla \times \nabla \times \) with a suitable linear operator \( L \) invariant along the length of the waveguide. A similar approach is found in [17] and further comparison of the two methods is required.

4. Application to planar systems

In this section we discuss the application of the RSE Born approximation to exactly solvable 1D scattering problems in electrodynamics. This is in order to prove the convergence of the new method to the exact solutions available for 1D problems in section 5. The dielectric profile is described by a scalar frequency independent dielectric profile, i.e. \( \varepsilon_1(z) = \varepsilon_2(z) = \varepsilon \). As unperturbed system we use a homogeneous planar slab of half width \( a \), so that

\[
\varepsilon(z) = \begin{cases} 
\varepsilon, & \text{for } |z| < a, \\
1, & \text{elsewhere}.
\end{cases}
\]

(22)

4.1. Wave equation and normalisation formula in 1D

In this sub-section I consider how Maxwell’s wave equation transforms to 1D. I also consider how the normalisation formula transforms to 1D.

Maxwell’s wave equations for a planar dielectric structure with permeability \( \mu = 1 \) surrounded by vacuum is reduced for 1D to the following equation:

\[
\partial_z^2 \mathbb{E}_n(z, t) = \varepsilon(z) \partial_t^2 \mathbb{E}_n(z, t).
\]

(23)

We take the transverse eigen-modes with index \( n \) to have zero in-plane wave number. The eigen-modes can be factorised as

\[
\mathbb{E}_n(z, t) = E_n(z) \exp(-ik_n t) \vec{y}
\]

(24)
with time independent part satisfying the wave equation:

\[ \left\{ \partial_z^2 + \varepsilon(z) k_n^2 \right\} E_n(z) = 0. \]  

(25)

The electric field and its first derivative are continuous everywhere. Eigen-modes of Maxwell’s wave equation for open systems have outgoing BCs.

In 1D non-dispersive systems the RSs \( E_n(z) \) with frequency \( k_n \) are orthogonal and normalised correctly in 1D according to [3]

\[
\int_{-a}^{a} \varepsilon(z) E_n(z) E_m(z) \, dz = \frac{\delta_{nm}}{i(k_n + k_m)},
\]

(26)

where \( z = \pm a \) are the positions of the boundaries of the unperturbed system.

4.2. RSs of the unperturbed slab

In this sub-section I give the RSs used to calculate the RSE Born approximation in section 5.

Solving the wave equation (25) for dielectric constant \( \varepsilon(z) \) given by equation (22), the electric field of RS \( n \), normalised according to equation (26), takes the form [3]

\[
E_n(z) = \begin{cases} 
(-1)^n A_n e^{-ik_n z}, & z < -a, \\
B_n \left[ e^{i\sqrt{\varepsilon_n} k_n z} + (-1)^n e^{-i\sqrt{\varepsilon_n} k_n z} \right], & |z| \leq a, \\
A_n e^{i\sqrt{\varepsilon_n} z}, & z > a,
\end{cases}
\]

(27)

where

\[
A_n = \frac{e^{-ik_n a}}{\sqrt{\alpha(\varepsilon_1 - 1)}}; \quad B_n = \frac{(-i)^n}{2\sqrt{\alpha \varepsilon_1}}
\]

(28)

with

\[
k_n = \frac{1}{2a \sqrt{\varepsilon_1}} (\pi n - i \ln \gamma), \quad n = 0, \pm 1, \pm 2, \ldots
\]

(29)

and

\[
\gamma = \frac{\sqrt{\varepsilon_1} + 1}{\sqrt{\varepsilon_1} - 1}
\]

(30)

the imaginary part of the wave vectors \( k_n \) are all the same.

4.3. The form of the RSE Born approximation in the 1D case

It is demonstrated in this section that the 1D RSE Born approximation can be used in conjunction with the RSE perturbation theory (to generate the normalised eigen-modes of planar systems with arbitrary dielectric profile and dispersion) [3, 4, 6, 10] to offer a possible alternative to the scattering matrix method of [15]. The same method for planar waveguides can be developed in an analogous way except the eigen-modes should be calculated as in [6, 10].

In 1D the GF \( G_k(z, z') \) is the solution of the equation

\[
\left\{ \partial_z^2 + \varepsilon(z) k^2 \right\} G_k(z, z') = \delta(z - z'),
\]

(31)

which from equation (4) we can see is given by

\[
G_k(z, z') = \sum_n \frac{E_n(z) E_n(z')}{2k(k - k_n)}
\]

(32)

The free space GF is a solution of

\[
\left\{ \partial_z^2 + k^2 \right\} G_k(z, z') = \delta(z - z'),
\]

(33)

and is given by

\[
G_k(z, z') = -\frac{e^{ik(z'-z)}}{2ik}
\]

(34)

Hence in 1D the RSE Born approximation is greatly simplified to

\[
G_k(z, z') = \frac{e^{ik(z'-z)}}{2ik} + \frac{e^{ik(z'-z)}}{4} \int_{-a}^{a} \Delta \varepsilon_k(z') dz'
\]

(35)

where \( \Delta \varepsilon_k(z) = \sum_n A_n(k_1) A_n(k_1') \frac{e^{i(k_1+z)\sqrt{\varepsilon_n} k_n}}{2(k - k_n)} \]

(36)

In this section we calculate the 1D GF outside of the homogeneous slab by equation (22) where \( \varepsilon_1 = 2.25 \). We do this using the RSE Born approximation, analytically using BCs, and also using the spectral GF for comparison. We find that the RSE Born approximation requires less basis states to reach a required accuracy than the spectral GF and unlike the spectral GF is convergent outside the system.

I calculate three types of GF in this section, an analytic GF, the GF of equation (32) and the GF of equation (35). From these it is possible to use the formula derived in [4, 6] for normal incident and waveguide systems for the transmission \( T(k, z') \),

\[
T(k, z') = \left| 2kG(z', -a; k) \right|^2
\]

(38)
The analytic GF is found by solving Maxwell’s wave equation in 1D with a source of plane waves while making use of Maxwell’s BCs.

The procedure used to select the basis of RSs for the RSE Born approximation calculation is analogous to that described in [7] for the RSE perturbation theory. Namely, I choose the basis of RSs such that all RSs with $|k_x| < k_{\text{max}}(N)$ using a maximum wave vector $k_{\text{max}}$ chosen to select $N$ RSs.

From figure 1 we can see that unlike the standard Born approximation the RSE Born approximation is valid over an arbitrarily wide range of $k$ depending only on the basis size $N$ used. Furthermore we see that as the basis size increases the RSE Born approximation converges to the exact solution. The absolute error in the RSE Born approximation is approximately reduced by an order of magnitude each time the basis size is doubled. Absolute errors of $10^{-7}$–$10^{-4}$ are seen in the $k$ range shown for basis size $N = 401$.

From figure 2 we can see that unlike the GF calculated with the spectral equation (32) the RSE Born approximation is stable over an arbitrarily wide range of $z'$, where $z'$ is the coordinate of the point of transmission to, depending only on the basis size $N$ used. The transmission calculated via the spectral GF is diverging with distance of the point of transmission from the slab, this suggests that outside the system the RSE spectral GF is not converging or is divergent. Furthermore we see that the RSE Born approximation requires fewer RSs than the spectral GF method in order to produce a required absolute error, at all values of $z'$. Although these points were first noted by Ge et al [2] they were using the unstable normalisation leading to an incorrect GF and so the results upon which they based their conclusions cannot be relied upon.

6. Summary

In this work we have seen the Born approximation mathematically rigorously extended to include terms which take into account the resonances of the scattering potential using the exact same method as [2] except with correctly normalised modes. Further I have made comparisons in 1D between scattering calculated with the spectral GF and the scattering calculated using the RSE Born approximation. I have demonstrated that once the correct normalisation is used in the RSE Born approximation convergence towards the exact solution is obtained. I have found that the RSE Born approximation for finding the full GF outside of the system is superior to the other spectral GF method considered in terms of convergence and accuracy when the correct normalisation of the RSs is used.

It is demonstrated in this paper that the 1D RSE Born approximation can be used in conjunction with the RSE perturbation theory (to generate the normalised eigen-modes of planar systems with arbitrary dielectric profile) [3, 4, 6, 10] to offer a possible alternative to the scattering matrix method of [15]. In fact, given the superior efficiency of the RSE perturbation theory in comparison with FDTD and FEM for weak perturbations demonstrated in [7] it is likely that the RSE coupled with the RSE Born approximation will be an incredibly powerful scattering theory for weak scatterers.

I have now derived an analogous theory for general wave equations [10].
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Appendix A. Derivation of alternative Green’s function and completeness

In order to simplify the RSE Born approximation and develop equation (6) we require an appropriate spectral form of the GF which is different from the one already proven in the literature. To obtain this correct form I start with the GF valid inside the scatterer only, which I derived in [5, 10],

\[
\hat{G}_\xi(r, r') = \sum_n \frac{E_n(r) \otimes E_n(r')}{2k_n(k - k_n)}. \tag{A1}
\]

Substituting equation (A1) in

\[
-\nabla \times \nabla \times \hat{G}_\xi(r, r') + k^2 \hat{\varepsilon}_\xi(r) \hat{G}_\xi(r, r') = \hat{I} \delta(r - r'),
\]

(A2)

gives for \( k \to \infty \),

\[
\hat{\varepsilon}(r) \sum_n \frac{(k + k_n)E_n(r) \otimes E_n(r')}{2k_n} = \hat{I} \delta(r - r'). \tag{A3}
\]

since throughout the derivation in this appendix we are considering the limit where \( k \to \infty \) at which \( \hat{\varepsilon}_\xi(r) = \hat{\varepsilon}(r) \), i.e. the system is non-dispersive at high frequencies.

Convolting equation (A3) with arbitrary finite functions and assuming the series are convergent we see that since \( k \to \infty \) we have the sum rule,

\[
\sum_n \frac{E_n(r) \otimes E_n(r')}{2k_n} = 0. \tag{A4}
\]

Combining equations (A1) and (A4) yields

\[
\hat{G}_\xi(r, r') = \sum_n \frac{E_n(r) \otimes E_n(r')}{2k(k - k_n)}. \tag{A5}
\]

Combining equation (A3) and equation (A4) leads to the closure relation

\[
\frac{\hat{\varepsilon}(r)}{2} \sum_n E_n(r) \otimes E_n(r') = \hat{I} \delta(r - r'), \tag{A6}
\]

which expresses the completeness of the RSs, so that any function can be written as a superposition of RSs. If in the perturbed system some of the series are not convergent or are instead conditionally convergent then we will not arrive at the sum rule and completeness, in which case I expect that the RSE Born approximation will still give convergence to the exact solution but only if a valid spectral Green’s function is used, such as equation (A1).

Appendix B. RSE for dispersive systems

Due to the problems with non-convergence of schur factorisation for the generalised eigen-value problem of perturbing nano-spheres dispersively, the RSE in [9] might tends to fail for non-symmetric perturbation when more than typically 500 basis states are used. This is an estimate based on the unreported RSE failures for half and quarter sphere perturbations using the generalised eigen-value problem form of the RSE, tests which I carried out for [7]. Therefore it is necessary to add linear dispersion through a second stage perturbation, a perturbation to the possibly complex conductivity [9].

To make this perturbation consider the problem of a perturbation to the conductivity \(-i\Delta \sigma(r)/k\mu\)

\[
-\nabla \times \nabla \times E_\mu(r) = k_\mu^2 \left[ \hat{\varepsilon}_\kappa(r) + i\Delta \sigma(r)/k_\mu \right] E_\mu(r). \tag{B1}
\]

\( \hat{\varepsilon}_\kappa \) could have in principle any dispersion for which the eigen-modes can be normalised, and which becomes non-dispersive in the limit of high frequency in order to make the sum rule for the GF.

In this appendixes Greek index letters denote perturbed modes and British (English) lower case index letters denote unperturbed modes.

Since

\[
E_\mu(r) = ik_\mu \int \hat{G}_{\hat{\varepsilon}_\kappa}(r, r') \Delta \sigma(r') E_\mu(r') dr', \tag{B2}
\]

where \( \hat{G}_{\hat{\varepsilon}_\kappa}(r, r') \) is given by equation (A5) and by equation (A6)

\[
E_\mu(r) = \sum_n b_n E_n(r), \tag{B3}
\]

where in equation (B3) \( E_n \) and \( k_n \) correspond to the unperturbed modes of equation (5), then following the derivation method of [3]

\[
2b_n k_\mu = \sum_a \left[ (iS_{ma} + 2k_\mu k_n) b_{n a} \right], \tag{B4}
\]

where

\[
S_{ma} = \int E_n(r) \cdot \Delta \sigma(r) E_m(r) dr \tag{B5}
\]

which can be solved for the eigen-modes \( E_n \) and eigen-value \( k_n \) of the perturbed problem.

For examples of fitting dispersion linear in wavelength to the dispersion of real materials for the purposes of RSE perturbation theory please see my [9] where a linear dispersive RSE is presented in terms of a generalised eigen-value problem.

The perturbation to \( \hat{\varepsilon}_\kappa \) can also be non-dispersive without resorting to generalised eigen-value problems, as treated in my [7]. To elaborate further on this point consider the problem of the non-dispersive perturbation \( \Delta \varepsilon(r) \)

\[
-\nabla \times \nabla \times E_\mu(r) = k_\mu^2 \left[ \hat{\varepsilon}_\kappa(r) + \Delta \varepsilon(r) \right] E_\mu(r). \tag{B6}
\]
Again $\tilde{\varepsilon}_k$ is dispersive as in equation (B1) for the same reasons. Equation (B6) is solved by [7]

$$\sum_{\alpha} \left( \delta_{\alpha\alpha} + \frac{\mathbf{V}_{\alpha\alpha}}{2\sqrt{k_n k_\alpha}} \right) c_{\alpha\mu} = \frac{1}{k_\mu} c_{\alpha\mu}, \quad (B7)$$

where

$$\mathbf{V}_{\alpha\alpha} = \int E_\alpha(r) \cdot \Delta\tilde{\varepsilon}(r) E_\alpha(r)dr \quad (B8)$$

and $b_{\alpha\mu} = c_{\alpha\mu}$. Please note that it is very important to be consistent with the signs of $\sqrt{k_\alpha}$ in the matrix elements of equation (B7).

Using the linear eigen-value approach outlined here it might be possible to treat an unperturbed Drude–Lorentz gold sphere with a non-dispersive shell, and perturb away the non-dispersive shell leaving in its place biological particles to be sensed as a perturbation. All perturbations must be within the boundaries of the unperturbed system due to convergence of the GF, see figure 2.

For a discussion of the eigen-functions of Maxwell’s equations in spherical coordinates please see [19].

**Appendix C. Proof of Kristensen normalisation**

In order for the normalisation of Kristensen et al to be correct it must be consistent with my equation (6), specifically the surface term $S_{\text{RSE}}$ in equation (6) must be mathematically equivalent to Kristensen’s surface term $S_{\text{KS}}$. Hence it should be that $S_{\text{RSE}} = S_{\text{KS}}$, where from [3] we have,

$$S_{\text{RSE}} = \frac{1}{2k_n} \oint_{S_k} \left[ E_n \cdot \frac{\partial E_n}{\partial r} - r \left( \frac{\partial E_n}{\partial r} \right)^2 \right] dr. \quad (C1)$$

and from equation (7) we have

$$S_{\text{KS}} = \lim_{V \to \infty} \frac{1}{2k_n} \oint_{S_k} E_n^2(r) dr. \quad (C2)$$

However considering the RSE Born approximation in 3D, specifically to ensure outgoing BCs equation (17) in particular driven by (convoluted with) a current vanishing proportional to $(k - k_n)$ as $k \to k_n$ so $E(r) \to E_n(r)$, we know that

$$\lim_{r \to \infty} E_n(r) = f(\theta, \phi) \frac{\hat{\mathbf{e}}_k \cdot \hat{\mathbf{r}}}{r}, \quad (C3)$$

where $r = (r, \theta, \phi)$ in spherical polar coordinates and $f(\theta, \phi) \propto A_{\text{R}}(\hat{\mathbf{r}}_{k_n})$, then substituting equation (C3) into equations (C1) and (C2) and equating $S_{\text{RSE}}$ and $S_{\text{KS}}$ gives,

$$\lim_{r \to \infty} S_{\text{RSE}} = \lim_{r \to \infty} S_{\text{KS}} = \frac{\oint_{S_k} \hat{\mathbf{e}}_k \cdot \hat{\mathbf{r}}}{2k_n r^2} \oint_{S_k} f^2(\theta, \phi) dS, \quad (C4)$$

a logically valid statement, therefore, $S_{\text{RSE}} = S_{\text{KS}}$ when $r \to \infty$ and so the normalisation of Kristensen et al is not wrong as it is stated. However in the RSE perturbation theory letting $r \to \infty$ in the normalisation of perturbed modes introduces huge errors because of the blow up of the RS mode fields far from the system causing blow up of error. By equation (C4), as $r$ grows one is essentially taking the difference of an exponentially growing surface term and an exponentially growing volume term to get the constant $1 + \delta_{k,0}$ for normalisation, this leads to large numerical errors for low-Q (leaky) modes [11]. Hence the Kristensen normalisation is numerically unstable.

In 1D Kristensen et al normalisation is actually correct for any finite $r$ that includes the system inhomogeneity [3].

The remaining problems with the Kristensen et al normalisation is that it is missing $k = 0$ modes, therefore it is incomplete. Also it does not have the conditions on $\tilde{\varepsilon}_k$ which should be the same as for my normalisation. That the RSs can be written in the form of (C3) aids the solution of the inverse scattering problem [10].

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