Scattering states of a particle, with position-dependent mass, in a \( \mathcal{PT} \)-symmetric heterojunction

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Abstract

The study of a particle with position-dependent effective mass (pdem), within a double heterojunction is extended into the complex domain—when the region within the heterojunctions is described by a non-Hermitian \( \mathcal{PT} \)-symmetric potential. After obtaining the exact analytical solutions, the reflection and transmission coefficients are calculated and plotted as a function of the energy. It is observed that at least two of the characteristic features of non-Hermitian \( \mathcal{PT} \)-symmetric systems—namely left/right asymmetry and anomalous behaviour at spectral singularity, are preserved even in the presence of pdem. The possibility of charge conservation is also discussed.

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

1. Introduction

Ever since the pioneering work of Bender et al more than a decade ago, the fact that a class of non-Hermitian Hamiltonians admits real and discrete spectrum under certain conditions is well established [1, 2]. Non-Hermitian Hamiltonians having \( \mathcal{PT} \) symmetry (\( P \rightarrow \text{parity}, \; T \rightarrow \text{time reversal} \)) form a special class in this category, as they admit real and discrete spectrum for exact \( \mathcal{PT} \) symmetry and complex conjugate pairs of energy when this spacetime symmetry is spontaneously broken, the transition occurring at the so-called exceptional point [3, 4]. Naturally, numerous attempts have been made by various scientists to extend the framework of quantum mechanics into the complex domain [5–7]. Theoretical predictions for \( \mathcal{PT} \)-symmetric systems exist in quantum field theory, mathematical, atomic and solid-state physics, classical optics, etc [8]. A pair of coupled active LCR circuits—one with amplification the other with equivalent attenuation—exhibit \( \mathcal{PT} \) symmetry [9]. Of late, experimental confirmation of such non-Hermitian \( \mathcal{PT} \)-symmetric concepts have been observed in optics, in \( \mathcal{PT} \)-symmetric crystals with a complex refractive index distribution \( n(x) = n_0 + n_R(x) + i n_I(x) \), where \( n_0 \) represents a constant background index, \( n_R(x) \) is the real index profile (even) of the...
structure and $n_I(x)$ stands for the gain or loss component (odd) [10–17]. Unlike ordinary crystals, complex crystals show unique properties—e.g. violation of Fresnel’s law of Bragg scattering, double refraction, power oscillations, non-reciprocal diffraction, handedness or left–right asymmetry, anomalous transport, unidirectional invisibility, etc. In fact, these unique features together with the occurrence of exceptional points in the discrete spectrum and spectral singularities in the continuous spectrum are characteristic of $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians, unknown to Hermitian ones. A lasing medium embedded in the spatial region $|z| < a_0$ where the dielectric constant satisfies the $\mathcal{PT}$-symmetry condition $\epsilon(-\vec{r}) = \epsilon^*(\vec{r})$, behaves as a laser oscillator (LO) for positive $\text{Im} \epsilon(\vec{r})$ signifying gain or as a coherent perfect absorber (CPA) for negative $\text{Im} \epsilon(\vec{r})$ signifying loss, provided the dielectric constant is real-valued and constant, $\epsilon(\vec{r}) = \epsilon_0$ (say), outside i.e. for $|z| > a_0$. While a LO can emit outgoing coherent waves, a CPA can fully absorb incoming coherent waves [18]. The interesting part of non-Hermitian Hamiltonians is that even a single $\mathcal{PT}$ cell can exhibit unconventional features [11].

On the other hand, the study of quantum mechanical systems with position-dependent effective mass (pdem) has received a boost in recent times with major developments in nanofabrication techniques of semiconductor devices [19–26]. The spatial dependence on the effective mass of the particle arises due to its interaction with an ensemble of particles within the device, as the particle propagates from left to right. For example, in Al$_x$Ga$_{1-x}$As, as the mole fraction $x$ varies along the $z$-axis, so does the effective mass of the charge carrier (electron or hole). Pdem formalism is extremely important in describing the electronic and transport properties of quantum wells and quantum dots, impurities in crystals, He-clusters, quantum liquids, semiconductor heterostructures, etc. In a recent work, we obtained the exact analytical scattering solutions of a particle (electron or hole) in a semiconductor double heterojunction—potential well/barrier—where the effective mass of the particle varies with position inside the heterojunctions [27]. It was observed that the spatial dependence on mass within the well/barrier introduces a nonlinear component in the plane wave solutions of the continuum states. Additionally, the transmission coefficient increases with increasing energy, finally approaching unity, whereas the reflection coefficient follows the reverse trend, going to zero.

This study is presented as a sequel to the work done in [27], in an attempt to extend the pdem formalism further into the complex domain. Instances of such attempts are found in other works as well—e.g. the problem of relativistic fermions subject to a $\mathcal{PT}$-symmetric potential in the presence of a position-dependent mass was studied in [28], while exact solutions of the Schrödinger equation for $\mathcal{PT}$/non-$\mathcal{PT}$ symmetric and non-Hermitian Morse and Pöschl–Teller potentials were obtained with pdem by applying a point canonical transformation method in [29]. In the present work, the main emphasis will be given on the scattering phenomenon in a $\mathcal{PT}$-symmetric double heterojunction with pdem—a special form of semiconductor device consisting of a thin layer of $\mathcal{PT}$-symmetric material sandwiched between two normal semiconductors, such that the mass of the charge carrier (electron or hole) varies with the doping concentration (and hence position) within the heterojunctions, but is constant outside. In particular, we shall see what new properties (if any) can be expected from $\mathcal{PT}$-symmetric heterojunctions with pdem, with special emphasis on the behaviour of the reflection and transmission coefficients

(i) with respect to the direction of incidence of the particle and
(ii) at the spectral singularity.

Additionally, we shall also derive explicit relations for current and charge densities, to see whether these are conserved in such a device.
Figure 1. Plot showing $m(z)$ and $V(z)$ w.r.t. $z$.

For this purpose, we shall consider a double heterojunction with the potential function in the intermediate region satisfying the $\mathcal{PT}$-symmetry condition $V(-z) = V^*(z)$, but assuming a real-valued constant outside:

$$V = \begin{cases} 
V_R(z) + iV_I(z), & a_1 < z < a_2, \\
V_{01} = V_R(a_1), & -\infty < z < a_1, \\
V_{02} = V_R(a_2), & a_2 < z < \infty,
\end{cases}$$

(1)

where $a_1, a_2$ represent the heterojunctions. The mass of the charge carrier is assumed to be of the form

$$m = \begin{cases} 
m(z), & a_1 < z < a_2, \\
m_1 = m(a_1), & -\infty < z < a_1, \\
m_2 = m(a_2), & a_2 < z < \infty.
\end{cases}$$

(2)

Thus, the mass $m(z)$ and the real part of the potential function, namely $V_R(z)$ are considered to be continuous throughout the semiconductor device. We shall mainly concentrate on obtaining the exact analytical solutions of the scattering states of a particle with pdem inside a $\mathcal{PT}$-symmetric double heterojunction, which is essential to study the nature of the reflection and the transmission coefficients.

This paper is organized as follows. For the sake of completeness, the position-dependent mass Schrödinger equation is introduced in section 2, and the method of obtaining the solutions is discussed briefly. To give a better insight into the physical nature of the problem, we shall study an explicit model in section 3, and plot the potential and mass functions as a function of $z$ in figure 1 and the scattering solutions in figure 2. The transmission and reflection coefficients are also calculated, and their behaviour is discussed with respect to the relative strengths of the coupling parameters of the potential (both real and imaginary parts) and the mass functions. Since non-Hermitian Hamiltonians (with constant mass) are known to show peculiar behaviour at spectral singularities and also exhibit left–right asymmetry, the transmission and reflection coefficients are plotted in figures 3–6, to check whether similar phenomena are observed in
Figure 2. A plot of $\text{Re} \psi(z)$ versus $z$; dashed (black) lines show the abrupt heterojunctions.

Figure 3. Plot of $|T|^2$ versus $E$—same for left and right incidence.

Figure 4. Plot of $|R|^2$ versus $E$ for left incidence.
the presence of pdem as well. Section 4 is devoted to the conservation of charge and current densities for non-Hermitian \( \mathcal{P}\mathcal{T} \) systems with pdem. Finally, section 5 is kept for conclusions and discussions.

2. Theory

We start with the basic assumption that the one-dimensional time-independent Schrödinger equation associated with a particle endowed with pdem is the same for Hermitian and non-Hermitian systems, and is given by

\[
H_{\text{EM}}(z)\psi(z) = \left[ T_{\text{EM}}(z) + V(z) \right] \psi(z) = E \psi(z),
\]

\[
V(z) = V_R(z) + iV_I(z),
\]

(3)
in the intermediate region within the heterojunctions. $T_{EM}$ is the kinetic energy term given by [22, 24]

$$T_{EM} = \frac{1}{4} (m'^2 p^n m' p^n + m'^2 p^n m' p^n) = \frac{1}{2} p \left( \frac{1}{m} \right) p,$$

(4)

where $p = -i \hbar \frac{d}{dz}$ is the momentum operator. It is to be noted here that the kinetic energy term is considered to be Hermitian. The non-Hermiticity is introduced through the potential term $V(z)$, with an even real part $V_R(z)$ and an odd imaginary part $V_I(z)$. The ambiguity parameters $\alpha$, $\beta$, $\gamma$ obey the von Roos constraint [22]

$$\alpha + \beta + \gamma = -1.$$  

(5)

In the absence of a unique or universal choice for the ambiguity parameters, several suggestions exist in literature [30–33], etc. However, for continuity conditions at the abrupt interfaces, and well-behaved ground state energy [34, 35], we shall restrict ourselves to the BenDaniel–Duke choice, namely $\alpha = \gamma = 0, \beta = -1$. Incidentally, this particular choice consistently produces the best fit to experimental results [36]. Furthermore, we shall work in units $\hbar = c = 1$ and use prime to denote differentiation w.r.t. $z$. Thus, inside the potential well $a_1 < z < a_2$, the Hamiltonian for the particle with pdem reduces to [37]

$$H = -\frac{1}{2m(z)} \frac{d^2}{dz^2} - \left( \frac{1}{2m(z)} \right)' \frac{d}{dz} + V_R(z) + i V_I(z),$$

(6)

whereas, outside the well, $z < a_1$ and $z > a_2$, the particle obeys the conventional Schrödinger equation

$$\left\{ -\frac{1}{2m_{1,2}} \frac{d^2}{dz^2} + V_{01,02} \right\} \psi(z) = E \psi(z),$$

(7)

having plane wave solutions. In case we consider a wave incident from left, the solutions in the two regions are

$$\psi_L(z) = e^{ik_1 z} + R e^{-ik_1 z}, \quad -\infty < z < a_1$$

$$\psi_R(z) = T e^{ik_2 z}, \quad a_2 < z < \infty,$$

(8)

where $R$ and $T$ denote the reflection and transmission amplitudes, and

$$k_{1,2} = \sqrt{2m_{1,2}(E - V_{01,02})}.$$  

(9)

To find the solution in the region $a_1 < z < a_2$, we make use of the following transformations [38]

$$\psi_m(z) = (2m(z))^{1/4} \phi(\rho), \quad \rho = \int \sqrt{2m(z)} dz,$$

(10)

which reduce the Schrödinger equation for pdem to one for constant mass, namely

$$- \frac{d^2 \phi}{d\rho^2} + [\tilde{V}(\rho) - E] \phi = 0,$$

(11)

with

$$\tilde{V}(\rho) = V(z) + \frac{7}{32} \frac{m'}{m^2} - \frac{m''}{8m^2}.$$  

(12)

Some definite practical forms of $V(z)$ and $m(z)$ give exact analytical solutions of (11). An explicit example in the next section illustrates our purpose.
3. Explicit model: $P\mathcal{T}$-symmetric potential well with position-dependent mass

We consider the following ansatz for the potential, whose real part describes a diffused quantum well

$$V(z) = \begin{cases} 
-\frac{\mu_1}{1+z^2} + i \frac{\mu_2}{1+z^2}, & |z| < a_0, \\
-\frac{\mu_1}{1+a_0^2} = V_0, & |z| > a_0.
\end{cases}$$

(13)

Let the mass of the particle be

$$m(z) = \begin{cases} 
\beta^2 \left(1 + \frac{z^2}{2(1+z^2)}\right), & |z| < a_0, \\
\frac{\beta^2}{2(1+a_0^2)} = m_0, & |z| > a_0,
\end{cases}$$

(14)

where $\mu_1$, $\mu_2$ and $\beta$ are some constant parameters.

For a better understanding of the mass dependence and the potential in the semiconductor device, we plot $m(z)$ and the real and imaginary parts of $V(z)$ as a function of $z$ in figure 1, for a suitable set of parameter values, namely $\beta = 4$, $\mu = 3$, $a_0 = 4$.

For the spatial mass dependence given by equation (14), equation (10) transforms the coordinate $z$ to

$$\rho = \beta \sinh^{-1} z,$$

(15)

so that after some straightforward algebra $\tilde{V}(\rho)$ in equation (12) reduces to

$$\tilde{V}(\rho) = \frac{1}{4\beta^2} - \frac{V_1}{\beta^2} \tanh^{2} \frac{\rho}{\beta} + i \frac{V_2}{\beta^2} \tanh \frac{\rho}{\beta}.$$

(16)

Thus, equation (11) may be written as

$$\frac{d^2\phi}{d\rho^2} + \left(\kappa^2 + V_1 \tanh^2 \tilde{\rho} - i V_2 \tanh \tilde{\rho}\right)\phi = 0,$$

(17)

where

$$\kappa^2 = E\beta^2 - \frac{1}{4}, \quad \tilde{\rho} = \frac{\rho}{\beta}$$

(18)

and the parameters $V_1, V_2$ depend on the constants $\mu_1, \mu_2$ and $\beta$ through the equations

$$V_1 = \mu_1 \beta^2 + \frac{1}{4}, \quad V_2 = \mu_2 \beta^2.$$

(19)

Let us introduce a new variable

$$y = \frac{1 + i \sinh \tilde{\rho}}{2},$$

(20)

and write the solutions of (17) as

$$\phi = y^p (1-y)^q u(y).$$

(21)

In terms of the new variable $y$, equation (17) reduces to the hypergeometric equation

$$y(1-y) \frac{d^2 u}{dy^2} + \left\{ \left(2p + \frac{1}{2} - (2p+2q+1) y \right) \frac{du}{dy} - \left(\kappa^2 - (p+q)^2\right) u \right\} = 0,$$

(22)

where

$$p = \frac{1}{2} \pm \frac{i}{2} \sqrt{\frac{1}{4} + V_1 - V_2},$$

$$q = \frac{1}{2} \pm \frac{i}{2} \sqrt{\frac{1}{4} + V_1 + V_2}.$$
Now, \( (22) \) has complete solution \([39]\)
\[
u = P \, _2F_1 (a, b, c; y) + Q y^{1-c} \, _2F_1 (1 + a - c, 1 + b - c, 2 - c; y),
\]
where \( P \) and \( Q \) are constants, and the parameters \( a \) and \( b \) are as defined below
\[
a = p + q - i \kappa, \quad b = p + q + i \kappa.
\]
After some straightforward algebra, the final solution to the pdem Schrödinger equation \((3)\), within the potential well \( |z| < a_0 \), is obtained as
\[
\psi_n(z) = \frac{\rho^{1/2}}{2^{p+q}} (1 + i z)^{p-1/4} (1 - i z)^{-p+1/4} \left\{ P \, _2F_1 (a, b, c; y) \
+ Q \left( \frac{1 - i z}{2} \right)^{1-c} \, _2F_1 (1 + a - c, 1 + b - c, 2 - c; y) \right\},
\]
where \( \gamma = (1 + i z)/2 \). Outside the well \( (|z| > a_0) \), the solutions are given by equation \((8)\), with \( k_1 = k_2 \). The solution in the entire region is plotted in figure 2 for the same set of parameter values as in figure 1, namely \( \beta = 4 \), \( \mu = 3 \), \( a_0 = 4 \). With the help of Mathematica, the constants \( P, Q \) and the reflection and transmission amplitudes \( |R| \) and \( |T| \), respectively, are determined using modified boundary conditions for pdem systems \([30, 40]\)—the functions \( \psi(z) \) and \( \frac{1}{|z|} \frac{d\psi(z)}{dz} \) should be continuous at each heterojunction \( \pm a_0 \). That the effect of pdem is to introduce a nonlinear component in the solution is obvious from the figure. This finding is analogous to the Hermitian model with pdem \([27]\).

For real and discrete spectrum, \( |V_2| < V_1 + 1/4 \) implying
\[
|\mu_2| < \mu_1 + \frac{1}{2 \beta^2}.
\]
However, in this work we are interested in the scattering states only, i.e. positive \( \kappa^2 \). Hence,
\[
E > \frac{1}{4 \beta^2}.
\]

The transmission and reflection amplitudes \( T \) and \( R \), respectively, are plotted in figures 3–5, for both left and right incidence, with the help of Mathematica. While \( |T| \) comes out to be the same for either case, the reflection coefficient depends on whether the particle enters from the left or right. \(|R|\) is normal \( (|R| < 1) \) when the particle enters from the left—the absorptive side \( \text{Im} \, V(z) < 0 \), and anomalous \( (|R| > 1) \) when the particle enters from the right—the emissive side \( \text{Im} \, V(z) > 0 \). Thus, this phenomenon of left–right asymmetry, characteristic of non-Hermitian pdem potentials with constant mass particles \([41–43]\), remains unaltered even when the particle mass has a spatial dependence.

Another interesting feature worth discussing here is when the well is replaced by a barrier—i.e. \( \mu_1 < 0 \), so that
\[
\tilde{V} (\tilde{\rho}) = \frac{1}{4} + \left( \mu_1 \beta^2 - \frac{1}{4} \right) \frac{\text{sech}^2 \tilde{\rho}}{\text{sech} \tilde{\rho} \, \tanh \tilde{\rho}} + i \mu_2 \beta^2 \text{sech} \tilde{\rho} \, \tanh \tilde{\rho}.
\]
For particles with constant mass, the potential in \((28)\) is known to admit a spectral singularity, with the reflection and transmission coefficients blowing up at the positive energy \([44, 45]\)
\[
E_r = \frac{1}{4} \left[ |V_2| - \left( \frac{1}{4} + V_1 \right) \right]
\]
when
\[
|V_2| > |V_1| + \frac{\text{sign of } V_1}{4}.
\]
For the pdem non-Hermitian heterojunction considered here, (30) condition becomes
\[ \mu_2 > \mu_1 + \frac{1}{2\beta^2}, \]  
(31)
so that the spectral singularity occurs at
\[ E_s = \frac{1}{4}(\mu_2 - \mu_1)\beta^2 - \frac{1}{8}. \]  
(32)
Interestingly, even in a \( \mathcal{PT} \)-symmetric double heterojunction, with a spatially varying mass, both \(|R|^2\) and \(|T|^2\) blow up at the value of \( E_s \) given in equation (32), as observed in figure 6.

4. Current and charge conservation

Since we are dealing with non-Hermitian \( \mathcal{PT} \)-symmetric systems, it would be interesting to check whether the current and charge densities are conserved in this case. The boundary conditions used in this work are
\[ \psi(z)|_L = \psi(z)|_R, \quad \frac{1}{m(z)} \frac{d\psi}{dz}|_L = \frac{1}{m(z)} \frac{d\psi}{dz}|_R, \]  
(33)
where \( L \) and \( R \) stand for left and right side of the heterojunctions. This choice of the boundary conditions ensures that current and charge densities are conserved in the Hermitian system \([30, 40]\). In this section, we explore the possibility of this choice for the non-Hermitian case discussed here. It is known from earlier works that charge density (say \( \omega \)) and current density (say \( j \)) for non-Hermitian quantum systems with constant mass obey the equation of continuity (for exact or unbroken \( \mathcal{PT} \) symmetry) \([46]\)
\[ \frac{\partial \omega}{\partial t} + \nabla \cdot j = 0, \]  
(34)
only if the current and charge densities are redefined as
\[ \omega = \phi^* \eta \phi, \quad j = i \left( \frac{d\phi^*}{d\rho} \eta \phi - \phi^* \eta \frac{d\phi}{d\rho} \right), \]  
(35)
where \( \eta \) is a linear, invertible, Hermitian operator, with respect to which the non-Hermitian Hamiltonian \( H \) is pseudo Hermitian:
\[ H^\dagger = \eta^{-1} H \eta. \]  
(36)
The interesting point to note here is that \( \eta \) does not have a unique representation \([47]\). For \( \mathcal{PT} \)-symmetric potentials consisting of an even real part \( V_R \) and an odd imaginary part \( V_I \), namely
\[ V(z) = V_R(z) + i V_I(z) \quad \text{or} \quad \tilde{V}(\rho) = V_R(\rho) + i V_I(\rho) \]  
(37)
\( \eta \) may be represented by the parity operator \( \mathcal{P} \) \([47, 48]\). For the non-Hermitian \( \mathcal{PT} \) Scarf II potential, namely \( V(\rho) = -V_R \sech^2 \rho - i V_I \sech \rho \tanh \rho \) some definite forms of \( \eta \) are given in \([49]\). With \( \eta = \mathcal{P} \), and the forms given in \([49]\), it is easy to check that for exact or unbroken \( \mathcal{PT} \) symmetry, the equation of continuity is obeyed in the transformed coordinate system \( \rho \), where the problem reduces to one with constant mass, namely equation (34). Now, if one applies the inverse transformations of those in equation (10), one can verify by straightforward algebra that equation (34) in the transformed coordinate system \( \rho \) (with constant mass) can be mapped to a similar equation of continuity in the original \( z \)-coordinate system (where the mass of the particle is dependent on its position):
\[ \frac{\partial \bar{\omega}}{\partial \bar{t}} + \nabla \cdot \bar{j} = 0. \]  
(38)
provided the charge density ($\bar{\omega}$) and current density ($\bar{j}$) in the original space are mapped to those ($\omega$ and $j$, respectively) in the transformed space by

$$\bar{\omega} = \frac{1}{\sqrt{2m(z)}} \omega = \psi^* \eta \psi,$$

$$\bar{j} = \frac{1}{\sqrt{2m(z)}} j = \frac{i}{\sqrt{2m(z)}} \left( \frac{d\psi^*}{dz} \eta \psi - \psi^* \eta \frac{d\psi}{dz} \right).$$

(39)

Thus, if the charge and current densities ($\bar{\omega}$ and $\bar{j}$, respectively) for non-Hermitian $\mathcal{PT}$-symmetric quantum systems with pdem are given a modified definition in accordance with equation (39), then the boundary conditions in equation (33) ensure conservation of current so long as $\mathcal{PT}$ symmetry is unbroken or exact. However, with the spontaneous breakdown of this space–time symmetry, the current is no longer conserved.

5. Conclusions and discussions

To conclude, in this work we studied a special form of semiconductor device consisting of a thin layer of $\mathcal{PT}$-symmetric material sandwiched between two normal semiconductors, such that the mass of the charge carrier (electron or hole) varies with position within the heterojunctions, but is constant outside. The mass $m(z)$ and the real part of the potential $V_R(z)$ are taken to be continuous throughout the device. We obtained the exact analytical solutions for the scattering states of a particle inside such a semiconductor device and also the reflection and transmission amplitudes, $R$ and $T$, respectively. Additionally, we also obtained explicit relations for current and charge densities for such a $\mathcal{PT}$-symmetric double heterojunction.

The primary aim of this work was to extend the pdem formalism into the complex domain, to see if the spatial dependence of mass introduces any new feature in case of the non-Hermitian $\mathcal{PT}$-symmetric double heterojunctions. It is observed that at least two of the general features of $\mathcal{PT}$-symmetric potentials—namely left–right asymmetry and blowing up of the reflection and transmission coefficients at a spectral singularity—are preserved even for particles with pdem. The effect of the pdem is simply to introduce a nonlinear component in the otherwise plane wave solution, within the heterojunctions. Another interesting feature we discussed here is the equation of continuity. For non-Hermitian $\mathcal{PT}$ quantum systems with pdem, a modified definition of charge and current densities as given in equation (39) renders the conservation of current for exact $\mathcal{PT}$ symmetry. To the best of our knowledge, this is a new observation.

Treating particles with position-dependent effective mass because of varying doping concentration in semiconductor devices of extremely small dimensions, is found to give better explanation to experimentally observed phenomena. On the other hand, $\mathcal{PT}$-symmetric waveguides fabricated from iron-doped LiNbO3 are also a reality [13, 50]. The time may not be far when a new generation of sophisticated, integrated devices are constructed based on the simple model discussed in this work. So our next attempt would be to see if the results of this study are typical of this particular example, or model independent.

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