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Solvable $\mathcal{PT}$-symmetric potentials in higher dimensions

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Abstract

$\mathcal{PT}$-symmetric, non-relativistic quantum mechanical potentials are discussed in two and three spatial dimensions. Conditions are formulated under which these potentials are $\mathcal{PT}$-symmetric and can be solved exactly by the separation of the radial and angular variables. It is found that the angular variables play an essential role in introducing non-Hermiticity via the imaginary potential terms. A simple partially exactly solvable potential is used to demonstrate various aspects of $\mathcal{PT}$ symmetry in both two and three dimensions. Possible generalizations of the results are outlined.

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1. Introduction

Quantum mechanical Hamiltonians invariant under the simultaneous action of the $\mathcal{P}$ space and $\mathcal{T}$ time inversion operations possess several unusual features. Despite being non-Hermitian, the discrete energy spectrum of these $\mathcal{PT}$-symmetric systems can be partly or completely real [1]. Typically the transition from the fully real energy spectrum to the complex one occurs when the non-Hermitian component of the Hamiltonian exceeds a certain critical limit, and it can be interpreted as the spontaneous breakdown of $\mathcal{PT}$ symmetry in that the energy eigenstates cease to be eigenstates of the $\mathcal{PT}$ operator. Another important feature of these systems is that the orthogonality of the energy eigenstates and the time-independence of their norm can be guaranteed if the inner product is redefined in a suitable way, $\langle\psi|\phi\rangle_{\mathcal{PT}} \equiv \langle\psi|\mathcal{P}\phi\rangle$, however, the pseudo-norm defined this way turned out to have indefinite sign. Much effort has been devoted to restoring the probabilistic interpretation of $\mathcal{PT}$-symmetric [2], and in general, pseudo-Hermitian [3] systems by constructing equivalent Hermitian Hamiltonians. For this a positive definite metric operator had to be constructed, by which a consistent treatment of physical operators (not only that of the Hamiltonian) could be done. This task has been carried out recently by various systematic methods [4]. It is notable that the question of the consistent

description of non-Hermitian Hamiltonians in terms of a modified metric has been discussed well before [5] the introduction of $\mathcal{PT}$-symmetric quantum mechanics within the framework of quasi-Hermiticity.

With only a few exceptions the study of $\mathcal{PT}$-symmetric systems has been restricted to the bound states of one-dimensional non-relativistic problems, where $\mathcal{PT}$ symmetry amounts to the requirement $V^*(-x) = V(x)$ imposed on the potential. Recently, various generalizations of this problem have been proposed, and the investigation of systems with scattering solutions [6, 7], periodic structure [8–10], coupled channels [11], more particles [12] and relativistic wave equations [13] has been started.

Here we propose another generalization by extending the study of $\mathcal{PT}$-symmetric problems to higher spatial dimensions. Some investigations focusing on specific aspects of such $\mathcal{PT}$-symmetric systems have been performed already: in [14] various 2- and 3-dimensional generalizations of the imaginary cubic potential have been discussed in Cartesian coordinates, while [15] dealt with some cyclic potentials as the angular component of potentials in $d = 2$. Motivated by the question to what extent the unusual features of $\mathcal{PT}$-symmetric systems persist in $d > 1$ dimensions, we perform systematic analysis of potentials that can be solved exactly in polar coordinates for $d = 2$ and 3. Although this task seems more complicated than the study of non-central real potentials [16, 17], one might expect that the special constraints imposed on the potential function $V(\mathbf{r})$ by $\mathcal{PT}$ symmetry might facilitate the handling of this problem.

2. $\mathcal{PT}$-symmetric Hamiltonians in various dimensions

Let us consider non-relativistic quantum mechanical potential problems with constant mass. These are described by the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) = -\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}). \tag{1}$$

The kinetic term is obviously $\mathcal{PT}$-symmetric, so it is the potential term $V(\mathbf{r})$ that decides whether (1) is $\mathcal{PT}$-symmetric or not. In what follows we formulate the $\mathcal{PT}$ symmetry requirement in $d = 2$ and 3 dimensions using polar coordinates. Considering that $\mathcal{P} : \mathbf{r} \to -\mathbf{r}$, we obtain

$$V(\rho, \varphi) = V^*(\rho, \varphi + \pi) \tag{2}$$

for $d = 2$ and

$$V(r, \theta, \varphi) = V^*(r, \pi - \theta, \varphi + \pi) \tag{3}$$

for $d = 3$. It is obvious, that central potentials $V(\mathbf{r}) = V(|\mathbf{r}|) \equiv V(r)$ can be $\mathcal{PT}$-symmetric only if they are real: $V(r) = V^*(r)$, so the angular variables play an essential role in introducing an imaginary potential component.

Although real central potentials are uninteresting from the point of view of $\mathcal{PT}$ symmetry, it is worthwhile to inspect the transformation property of the angular component of the corresponding wavefunctions, i.e. that of the exponential and spherical harmonic functions. It turns out that these get transformed in a characteristic way: $\mathcal{PT}\exp(\mathrm{i}m\varphi) = (-1)^m \exp(-\mathrm{i}m\varphi)$, $\mathcal{PT}Y_{lm}(\theta, \varphi) = (-1)^{l+m}Y_{l-m}(\theta, -\varphi)$, therefore it is reasonable to expect that the angular wavefunctions of the $\mathcal{PT}$-symmetric problems will appear as the generalization of these functions.

In what follows we focus on two- and three-dimensional $\mathcal{PT}$-symmetric problems and attempt to find potentials that are exactly solvable by means of the separation of the variables. For the sake of simplicity we use the units $\hbar = 2m = 1$.

2.1. The case of $d = 2$

The Schrödinger equation corresponding to (1) is

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right)+\frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2}-V(\rho,\varphi)\psi+E\psi=0. \tag{4}$$

Factorizing $\psi\equiv\psi(\rho,\varphi)$ as

$$\psi(\rho,\varphi)=\rho^{-1/2}\phi(\rho)\tau(\varphi) \tag{5}$$

we obtain the equation

$$\phi''\tau+\frac{1}{\rho^2}\phi\tau''-\left(V(\rho,\varphi)-\frac{1}{4\rho^2}-E\right)\phi\tau=0, \tag{6}$$

where prime denotes derivation with respect to the corresponding single variable. Let us assume that $\tau(\varphi)$ satisfies the equation

$$\tau''=(K(\varphi)-k)\tau \tag{7}$$

such that

$$V(\rho,\varphi)=V_0(\rho)+\frac{1}{\rho^2}K(\varphi) \tag{8}$$

holds. Then (2) requires $V_0(\rho)$ to be real and $K(\varphi)\mathcal{PT}$-symmetric

$$K^*(\varphi+\pi)=K(\varphi). \tag{9}$$

In this case a radial Schrödinger equation can be separated as

$$-\phi''+\left[V_0(\rho)+\left(k-\frac{1}{4}\right)\frac{1}{\rho^2}\right]\phi-E\phi=0. \tag{10}$$

Equation (10) is similar to the radial Schrödinger equation obtained for real potentials, and its solution can be done similarly. Exact solutions are known for the harmonic oscillator, Coulomb and square well for arbitrary value of k, while for $k=1/4$, (10) is solvable for many more potentials. Some solutions can also be obtained for arbitrary k for quasi-exactly solvable (QES) potentials [18] in the sense that the first few solutions (up to a given principal quantum number) can be determined exactly then. It has to be noted that in principle, (2) does not restrict k to real values. This is because (7) can be considered a $\mathcal{PT}$-symmetric Schrödinger equation in itself, where $K(\varphi)$ and k plays the role of the potential and the energy eigenvalue, and the latter one can be complex too in the case of the spontaneous breakdown of $\mathcal{PT}$ symmetry. k then does not appear in the potential (8) itself, only in the term equivalent with the centrifugal term of the Hermitian problems. If k is complex, then (10) has to be solved formally for complex angular momenta. In this case the energy eigenvalues E can also become complex, in principle, corresponding to the spontaneous breakdown of $\mathcal{PT}$ symmetry.

It has to be noted that appropriate boundary conditions have to be applied to both the radial and the angular wavefunctions. In the former case the situation is similar to the standard Hermitian setting, while in the latter case the conditions $\tau(\varphi)=\tau(\varphi+2\pi)$ and $\tau'(\varphi)=\tau'(\varphi+2\pi)$ apply. These are formally similar to the boundary conditions of 2π-periodic problems, so it is worthwhile to consider periodic potentials in (7).

Rather than searching for fully solvable examples of the radial and angular equations (10) and (7), here we consider a specific choice for $\tau(\varphi)$ and use it to demonstrate some important aspects of $\mathcal{PT}$ symmetry in two spatial dimensions. Let us consider

$$\tau(\varphi)=c_\varphi\exp(\mathrm{i}D(\varphi)),\qquad D(\varphi)\ \text{real}, \tag{11}$$

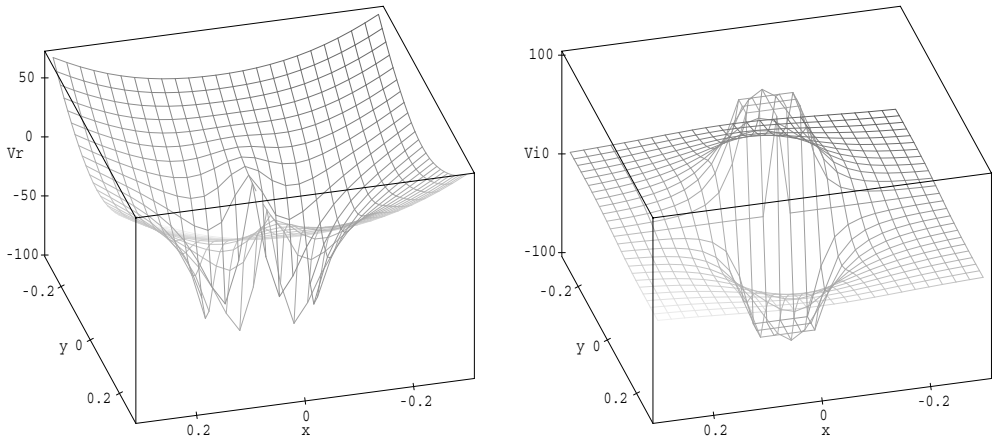

Figure 1. The real (left panel) and imaginary (right panel) components of $V(\rho, \varphi)$ in (15) displayed in Cartesian coordinates, where $p = 1$ and the real central potential component is an harmonic oscillator $V_0(\rho) = \omega^2\rho^2$ with $\omega = 20$. Singularities are cut.

which corresponds to $K(\varphi) = \mathrm{i}D''(\varphi) - (D'(\varphi))^2$ and $k = 0$. Then (8) turns into

$$V(\rho, \varphi) = V_0(\rho) + \frac{1}{\rho^2}[\mathrm{i}D''(\varphi) - (D'(\varphi))^2], \tag{12}$$

which is $\mathcal{PT}$-symmetric if

$$D''(\varphi + \pi) = -D''(\varphi), \qquad D'(\varphi + \pi) = \pm D'(\varphi) \tag{13}$$

holds. Note that $D(\varphi) = m\varphi$, i.e. searching for the solution $\tau(\varphi)$ in the simplest possible form leads to a real $V(\rho, \varphi)$, since in this case $D'' = 0$. Actually, this choice corresponds to a special case of $\mathcal{PT}$ symmetry: real central potentials.

Let us now consider the periodic solution

$$\tau(\varphi) = c_\varphi \exp[\mathrm{i}\sin(p\varphi)], \tag{14}$$

where p is integer. Then

$$V(\rho, \varphi) = V_0(\rho) - \frac{p^2}{\rho^2}\left[\frac{1}{2} + \frac{1}{2}\cos(2p\varphi) + \mathrm{i}\sin(p\varphi)\right], \tag{15}$$

and $\mathcal{PT}$ symmetry requires p to be an odd integer. It is notable, that the periodicity of the real and imaginary components of the angle-dependent potential term has to be different. Also note that the coupling coefficient of these terms cannot be varied independently. Qualitatively similar results are obtained if (14) is generalized by using the complex combination $D(\varphi) = \sin(p\varphi) + \mathrm{i}\sin(q\varphi)$ in (11): then the real and imaginary components of $K(\varphi)$ have richer structure, but the difference in the periodicities remain.

The $\mathcal{PT}$ normalization constant in (14) can be expressed in terms of Bessel functions [19] as $c_\varphi = [2\pi J_0(2)]^{-1/2}$, irrespective of p. Then $\tau(\varphi)$ has the transformation property

$$\mathcal{PT}\tau(\varphi) = \tau(\varphi). \tag{16}$$

The solutions of the radial Schrödinger equation (10) do not depend on p in this case, so due to $k = 0$ the radial Schrödinger equation has to be solved with zero angular momentum in the Hermitian setting.

Figure 1 shows (15) where $V_0(\rho)$ is an harmonic oscillator. It is seen that the real component has dual well structure, while the singularities of the imaginary component have

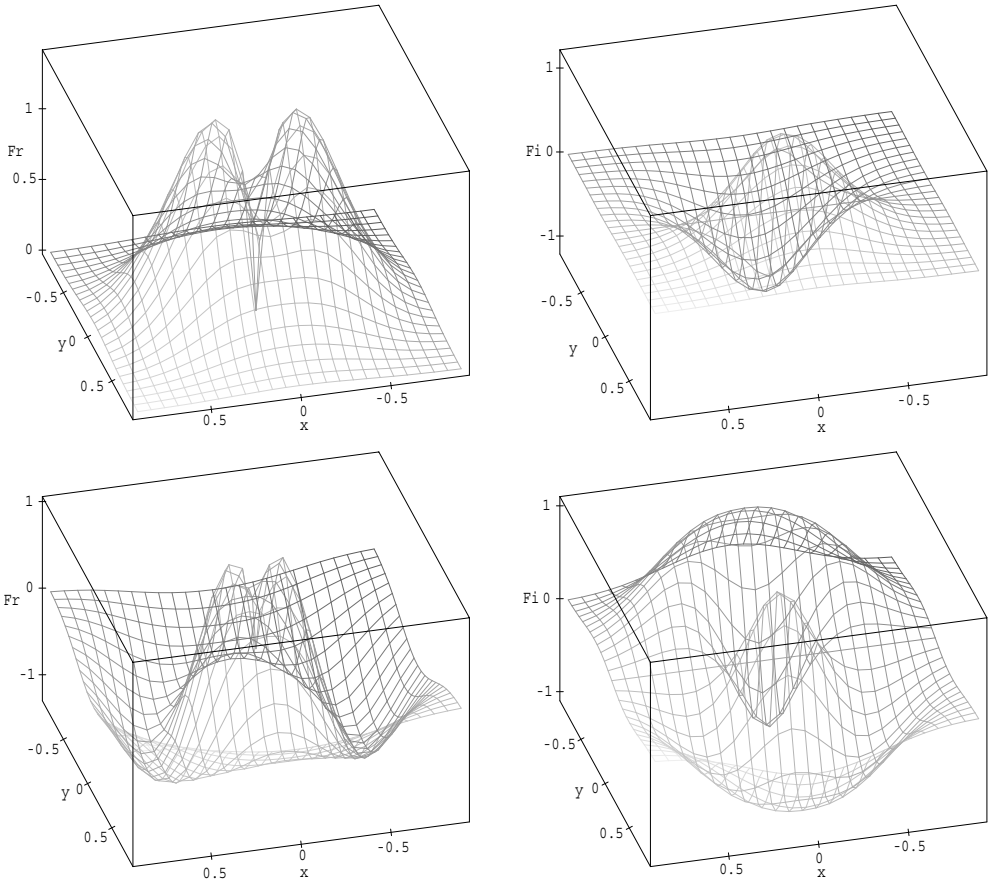

Figure 2. The real (left panel) and imaginary (right panel) components of wavefunctions corresponding to the potential in figure 1. The wavefunctions belonging to $n = 0$ with $E_0 = \omega = 20$ and $n = 1$ with $E_1 = 3\omega = 60$ are presented in the first and the second row, respectively. Note the length scale different from that in figure 1.

opposite sign. This latter finding is similar to one-dimensional $\mathcal{PT}$-symmetric potentials, which are also characterized by a fine balance of absorptive and emissive imaginary potential terms. The corresponding wavefunctions are displayed in figure 2 for principal quantum number $n = 0$ and 1. The structure of the wavefunctions reflect $\mathcal{PT}$ symmetry, as in (16). The difference in the radial structure is also seen.

In a more general and complete approach $K(\varphi)$ and k can be chosen a $\mathcal{PT}$-symmetric potential and its energy eigenvalue, considered together with periodic boundary conditions. Possible candidates could be the periodic ones from the list of shape-invariant $\mathcal{PT}$-symmetric potentials [20], such as the Scarf I potential [21], $\mathcal{PT}$-symmetric Lamé type potentials [9], or periodic potentials constructed from delta [8, 10] or step functions [15].

2.2. The case of $d = 3$

The Schrödinger equation is now

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2} + \frac{1}{r^2}\cot(\theta)\frac{\partial\psi}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2} - V(r,\theta,\varphi)\psi + E\psi = 0. \qquad (17)$$

With the substitution $\psi \equiv \psi(r, \theta, \varphi)$

$$\psi(r, \theta, \varphi) = r^{-1}\phi(r)\chi(\theta)\tau(\varphi) \tag{18}$$

the equation

$$\phi''\chi\tau + \frac{1}{r^2}(\chi'' + \cot(\theta)\chi') + \frac{1}{r^2\sin^2\theta}\phi\chi\tau'' - (V(r, \theta, \varphi) - E)\phi\chi\tau = 0 \tag{19}$$

is obtained. Following the procedure applied to the $d = 2$ case, next we eliminate the derivatives of $\chi(\theta)$ and $\tau(\varphi)$ by assuming that these functions satisfy some ordinary second-order differential equation. In particular, besides prescribing (7) for $\tau(\varphi)$, we assume that $\chi(\theta)$ satisfies

$$\chi'' + \cot(\theta)\chi' = (Q(\theta) - q)\chi. \tag{20}$$

This equation is known to be solvable for

$$Q(\theta) = \mu^2\sin^{-2}(\theta), \qquad q = \nu(\nu + 1), \tag{21}$$

when the solutions are given by the associated Legendre functions $P_\nu^\mu(\cos(\theta))$ [19]. It can be shown that $\mathcal{PT}$-normalization of these functions is possible if the μ and ν parameters are non-negative integers such that $\nu = n$, $\mu = m \leqslant n$. Then

$$\chi_{nm}(\theta) = \mathrm{i}^{n+m}\left[\left(n + \frac{1}{2}\right)\frac{(n-m)!}{(n+m)!}\right]^{1/2} P_n^m(\cos(\theta)) \tag{22}$$

transforms under $\mathcal{PT}$ as $\mathcal{PT}\chi_{nm}(\theta) = \chi_{nm}(\theta)$, and its $\mathcal{PT}$-norm is indefinite

$$\langle\chi_{nm}|\mathcal{P}|\chi_{nm}\rangle = (-1)^{n+m}. \tag{23}$$

With the prescriptions (7), (20) and (21) a radial Schrödinger equation

$$-\phi'' + \left[V_0(r) + \frac{n(n+1)}{r^2}\right]\phi - E\phi = 0 \tag{24}$$

is obtained for $\phi(r)$, where the central potential $V_0(r)$ is related to $V(r, \theta, \varphi)$ as

$$V(r, \theta, \varphi) = V_0(r) + \frac{1}{r^2\sin^2(\theta)}(K(\varphi) - k + m^2). \tag{25}$$

Note that in the case of real central potentials the second term vanishes, as $K(\varphi) = 0$ and $k = m^2$ holds then, and the whole procedure reduces to separating the angular variables using spherical harmonics. The radial Schrödinger equation (24) can again be solved exactly for any n in the few standard cases discussed in the previous subsection.

There is an important difference with respect to the two-dimensional case. The $\mathcal{PT}$ symmetry of (25) requires not only the reality of $V_0(r)$ and the $\mathcal{PT}$ symmetry of $K(\varphi)$ as in (9), but also the reality of k, which appears explicitly in the expression of the three-dimensional potential. Since n is also real, the radial Schrödinger equation (24) is that of a Hermitian problem, so its energy eigenvalues might be restricted to real values. Since the E are also the energy eigenvalues of the $\mathcal{PT}$-symmetric system, it appears that unlike the 2-dimensional case, the spontaneous breakdown of $\mathcal{PT}$ symmetry cannot occur for 3-dimensional potentials derived in the present framework.

In order to generate solvable potentials in 3 dimensions, the same φ-dependent wave equations can be applied as in 2 dimensions. Using (14) corresponds to a special generalization of the spherical harmonics.

3. Summary and conclusions

We generalized the formalism of $\mathcal{PT}$-symmetric quantum mechanics to quantum potentials defined in terms of polar coordinates in two and three spatial dimenensions. We searched for potential problems that can be solved exactly by means of the separation of the variables. For this the angular dependence of the potential terms had to be tailored to the structure of the kinetic term expressed in terms of polar coordinates.

The $\mathcal{PT}$ symmetry condition had different effect on the radial and angular components of the wavefunction. The differential equation describing the radial component turned out to be essentially the same as the radial Schrödinger equation obtained for conventional (Hermitian) centrally symmetric quantum potentials, while the angular variables were found to play an essential role in introducing the imaginary potential component. In this respect the wave equation in the φ variable had a special role in both 2 and 3 dimensions, as it turned out that due to the joint effect of the boundary conditions and $\mathcal{PT}$ symmetry it has to be chosen as a Schrödinger equation defined with a 2π-periodic $\mathcal{PT}$-symmetric potential on the $\varphi \in [0, 2\pi]$ domain. It also turned out that in 3 dimensions the θ-dependent component of the wavefunction is best described by associated Legendre functions $P_n^m(\cos(\theta))$, which also appear in the case of spherically symmetric conventional potentials. These functions are $\mathcal{PT}$-symmetric, and their pseudo-norm exhibits an oscillatory behaviour $(-1)^{n+m}$.

As an example we considered a simple exponential form of a periodic function to describe the φ-dependent component of the wave function. Although the corresponding wave equation is solvable exactly only for zero eigenvalue, the resulting solution illustrated several important aspects of $\mathcal{PT}$ symmetry in higher dimensions. One of these is the difference in the φ-periodicity in the real and imaginary potential components.

In order to obtain a more complete picture, it would be worthwhile to employ exactly solvable 2π-periodic $\mathcal{PT}$-symmetric potentials to account for the φ-dependence of the potential in both 2 and 3 dimensions. With this the complete energy spectrum could be generated, furthermore, the spontaneous breakdown of $\mathcal{PT}$ symmetry could also be induced, although only in 2 dimensions. Degeneracy patterns and possible underlying symmetries could also be investigated. The presence or absence of quasi-parity in higher dimensional problems is another important question to be settled.

Further possible generalizations of these results are considering solvable problems in even higher dimensions, and searching for alternative solutions of the angular wave equations. Extending these studies to pseudo-Hermitian systems in $d > 1$ also seems worthwhile.

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