$\mathcal{PT}$-symmetry and Non-Central Potentials

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We present a general procedure by which solvable non-central potentials can be obtained in 2 and 3 dimensions by the separation of the angular and radial variables. The method is applied to generate solvable non-central $\mathcal{PT}$-symmetric potentials in polar coordinates. General considerations are presented concerning the $\mathcal{PT}$ transformation properties of the eigenfunctions, their pseudo-norm and the nature of the energy eigenvalues. It is shown that within the present framework the spontaneous breakdown of $\mathcal{PT}$ symmetry can be implemented only in two dimensions.

Keywords: $\mathcal{PT}$ symmetry, angular and radial variables, non-central potentials

1 Introduction

The most widely studied quantum mechanical potentials are formulated as one-dimensional problems. These include potentials defined on a finite domain (e.g. the infinite square well) or on the full x axis (e.g. the Pöschl-Teller potential). Potentials defined on the positive semi-axis also occur as radial problems obtained after the separation of the angular variables in centrally symmetric potentials. Potentials in higher dimensions are less frequently discussed, and mainly in cases when they can be reduced to one-dimensional problems by the separation of the variables in some coordinates (Cartesian, polar, etc.). These potentials differ from the one-dimensional ones in several respects: their spectrum can be richer due to the more degrees of freedom, and this can be manifested in the occurrence of degeneracies, for example.

An interesting recent development in quantum mechanics was the introduction of $\mathcal{PT}$ symmetry [1]. Quantum systems with this symmetry are invariant under the simultaneous action of the $\mathcal{P}$ space and $\mathcal{T}$ time inversion operations, where the latter is represented by complex conjugation. It has been found that although these $\mathcal{PT}$-symmetric problems are manifestly non-Hermitian, as they possess an imaginary potential component too, they have several features in common with traditional self-adjoint systems. The most striking of these is the presence of real energy eigenvalues in the spectrum, but the orthogonality of the energy eigenstates and the time-independence of their norm is also non-typical for complex potentials. There are, however, important differences too, with respect to conventional problems. The energy spectrum can turn into complex conjugate pairs as the non-Hermiticity increases, and this 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 then. Also, the pseudo-norm defined by the modified inner product $\langle\psi|\phi\rangle_{\mathcal{PT}} \equiv \langle\psi|\mathcal{P}\phi\rangle$ turned out to have indefinite sign. $\mathcal{PT}$ symmetry was later identified as the special case of pseudo-Hermiticity, and this explained much of the unusual results. The proceedings volumes of recent workshops [2], [3] give a comprehensive account of the status of $\mathcal{PT}$-symmetric quantum mechanics and related fields.

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 $V^*(-x) = V(x)$. Here we extend the scope of these investigations by considering $\mathcal{PT}$-symmetric problems in higher spatial dimensions. In particular, we employ a simple method of generating solvable non-central potentials by the separation of the variables and combine it with the requirements of $\mathcal{PT}$ symmetry [4].

2 Non-central potentials in polar coordinates

Let us consider the Schrödinger equation with constant mass

$$\left(\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right)\psi(\mathbf{r}) = \frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}), \qquad (1)$$

where the potential $V(\mathbf{r})$ is a general function of the position $\mathbf{r}$. Although in this section we implicitly assume that V($\mathbf{r}$) is real, so the Hamiltonian describing the quantum system is self-adjoint, the procedure we follow here can be applied to complex potentials too. In what follows we choose the units as $2m = \hbar = 1$. Specifying (1) for $d = 3$ dimensions and using polar coordinates we obtain

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

Assuming that the separation of the variables is possible, we search for the solution as

$$\psi(r,\theta,\varphi) = r^{-1}\,\phi(r)\,\chi(\theta)\,\tau(\varphi), \tag{3}$$

where $r \in [0,\infty)$, $\theta \in [0,\pi]$ and $\varphi \in [0,2\pi]$. Then (2) turns into

$$\phi''\,\chi\,\tau + \frac{1}{r^2}(\chi'' + \cot(\theta)\chi')\varphi\tau + \frac{1}{r^2\sin^2\theta}\phi\,\chi\,\tau'' - \big(V(r,\theta,\varphi) - E\big)\phi\,\chi\,\tau = 0, \tag{4}$$

where prime denotes the derivative with respect to the appropriate variable.

Next we assume that $\chi(\theta)$ and $\tau(\varphi)$ satisfy the second-order differential equations

$$\chi'' + \cot(\theta)\chi' = \big(Q(\theta) - q\big)\chi, \tag{5}$$

$$\tau'' = \big(K(\varphi) - k\big)\tau. \tag{6}$$

It is seen that (6) can be considered a one-dimensional Schrödinger equation defined in the finite domain $[0,2\pi]$ with periodic boundary conditions $\tau(0) = \tau(2\pi)$ and $\tau'(0) = \tau'(2\pi)$. Note that in the case of one-dimensional potentials defined within a finite domain the wavefunction is usually required to vanish at the boundaries, however, considering periodic boundary conditions, this is not a necessary requirement: it can also be finite there.

Equation (5) is solvable for the choice

$$Q(\theta) = \mu^2\sin^{-2}(\theta), \quad q = \nu(\nu+1), \tag{7}$$

when the solutions are given by the associated Legendre functions $P_\nu^\mu\big(\cos(\theta)\big)$ [5]. Normalizability requires μ and ν to be non-negative integers such that $\nu = l$, $\mu = m \le l$. Then

$$\chi_{lm}(\theta) = i^m\left[\left(l+\frac{1}{2}\right)\frac{(l-m)!}{(l+m)!}\right]^{\frac{1}{2}} P_l^m\big(\cos(\theta)\big). \tag{8}$$

Substituting (6), (5) and (7) in (4) the angular part can be separated, and a radial Schrödinger equation is obtained

$$-\phi'' + \left[V_0(r) + \frac{l(l+1)}{r^2}\right]\phi - E\phi = 0, \tag{9}$$

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

$$V(r,\theta,\varphi) = V_0(r) + \frac{1}{r^2\sin^2(\theta)}\Big(K(\varphi) - k + m^2\Big). \tag{10}$$

In its most general form, (10) is a non-central potential that depends on the states through k and m. In order to eliminate the state-dependence one can apply the prescription $k = m^2 + a$, where a is a constant. Since m has to be an integer, this prescription represents a restriction on the solutions of equation (6). A special case occurs for $K(\varphi) = a$, i.e. for the free motion on a circle (or an infinite square well with periodic boundary conditions), which reduces (10) to a central potential, and takes the angular wavefunctions $\chi(\theta)\tau(\varphi)$ into spherical harmonics $Y_{lm}(\theta,\varphi)$ [5].

Exact solutions of the radial Schrödinger equation (9) are known for the harmonic oscillator, Coulomb and square well potentials for arbitrary value of l, while for $l = 0$ (i.e. for s waves), it is solvable for many more potentials. Some solutions can also be obtained for arbitrary l for quasi-exactly solvable (QES) potentials [6] in the sense that the first few solutions (up to a given principal quantum number) can be determined exactly then.

Specifying (1) to $d = 2$ dimensions the whole procedure can essentially be repeated. The equivalents of equations (2) and (3) are then

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}\left(\rho\frac{\partial\psi}{\partial\rho}\right) + \frac{1}{\rho^2}\frac{\partial^2\psi}{\partial\varphi^2} - V(\rho,\varphi)\psi + E\psi = 0 \tag{11}$$

and

$$\psi(\rho,\varphi) = \rho^{-\frac{1}{2}}\phi(\rho)\,\tau(\varphi) \tag{12}$$

The separation of the angular variable φ is again possible if (6) holds, and the solutions are required to satisfy periodic boundary conditions. The radial Schrödinger equation is now

$$-\phi'' + \left[V_0(\rho) + \left(k - \frac{1}{4}\right)\frac{1}{\rho^2}\right]\phi - E\phi = 0, \tag{13}$$

where

$$V(\rho,\varphi) = V_0(\rho) + \frac{1}{\rho^2}K(\varphi). \tag{14}$$

Equation (13) can be solved exactly for the same potentials as in three dimensions.

3 Non-central $\mathcal{PT}$-symmetric potentials

Let us now specify the procedure outlined in the previous section to $\mathcal{PT}$-symmetric potentials. Since the kinetic term in (1) is $\mathcal{PT}$-symmetric, we have to take care separately only of the $\mathcal{PT}$ symmetry of the potential term. The effect of the $\mathcal{P}$ operation is $\mathcal{P}:\mathbf{r} \to -\mathbf{r}$, so the condition for the $\mathcal{PT}$ symmetry of a general potential in $d = 3$ dimensions is

$$V(r,\theta,\varphi) = V^*(r,\pi-\theta,\varphi+\pi). \tag{15}$$

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.

Applying condition (15) to the general potential form (10), the prescriptions

$$V_0^*(r) = V_0(r), \quad K^*(\varphi+\pi) = K(\varphi), \quad k^* = k \tag{16}$$

are obtained, i.e. $V_0(\rho)$ is real, $K(\varphi)$ is $\mathcal{PT}$-symmetric and the eigenvalue of equation (6) is real. Note that the reality of the potential $V_0(r)$ implies that (9) has the same form as the radial Schrödinger equation of a centrally symmetric self-adjoint quantum system, therefore the eigenvalues E also have to come out real. This means that the spontaneous breakdown

of $\mathcal{PT}$ symmetry cannot be implemented in the present approach for non-central potentials in $d = 3$ dimensions.

According to (15) the $\mathcal{P}$ operator can be factorized as

$$\mathcal{P} = \mathcal{P}_r\, \mathcal{P}_\theta\, \mathcal{P}_\varphi, \text{ (where, obviously, } \mathcal{P}_r = 1),$$

so the $\mathcal{PT}$ transformation properties of the functions $\phi(r)$, $\chi(\theta)$ and $\tau(\varphi)$ can also be studied. Due to the arguments concerning (9) above, $\phi(r)$ can be chosen real, and in this case it obviously satisfies $\mathcal{P}_r\mathcal{T}\,\phi(r) = \phi(r)$. Introducing an extra phase factor i^l in (8), it is possible to make $\chi(\theta)$ the eigenfunction of the $\mathcal{P}_\theta\mathcal{T}$ operator with eigenvalue 1. A similar procedure also has to be applied to the $\tau(\varphi)$ functions and the $\mathcal{P}_\varphi$ operator, but this can be done only in the exact knowledge of the $K(\varphi)$ function. This guarantees that the full wavefunction $\psi(r, \theta, \varphi)$ (3) is also the eigenfunction of the $\mathcal{PT}$ operator with unit eigenvalue.

These phase choices are also reflected in the sign of the pseudo-norm of the eigenstates $\psi(r, \theta, \varphi)$, since $\langle\psi|\mathcal{P}\psi\rangle$ can be determined by the inner products calculated with the constituent functions $\phi(r)$, $\chi(\theta)$ and $\tau(\varphi)$, using the appropriate $\mathcal{P}_i$ $(i = r,\ \theta,\ \varphi)$ operators. Obviously, the contribution of the radial component will be 1, while it can be shown that with the phase convention described above, $\langle\chi|\mathcal{P}_\theta\,\chi\rangle = (-1)^{l+m}$ holds. Although the corresponding inner product for the $\tau(\varphi)$ functions can be evaluated only in the knowledge of K(φ), similar inner products are known to exhibit oscillatory behaviour $(-1)^n$ with respect to the principal quantum number for wide classes of $\mathcal{PT}$-symmetric potentials with infinite number of eigenstates [7], [8], [9]. (Note that for some potentials with finite number of eigenstates this is not necessarily the case [10].) The sign of the pseudo-norm is thus indefinite for three-dimensional non-central $\mathcal{PT}$-symmetric potentials too, and it depends on the quantum numbers associated with the angular component of the eigenfunctions.

Let us now discuss the conditions under which non-central potentials can be $\mathcal{PT}$-symmetric in $d = 2$ dimensions. The equivalent of (15) is now

$$V(\rho,\varphi) = V^*(\rho,\varphi + \pi), \tag{17}$$

and from (14) the conditions

$$V_0^*(\rho) = V_0(\rho),\ \ K^*(\varphi + \pi) = K(\varphi) \tag{18}$$

follow from the $\mathcal{PT}$ symmetry of the $V(\rho, \varphi)$. The arguments on the $\mathcal{PT}$ symmetry of the wavefunction and the constituent functions are the same as in the three-dimensional case, as are those concerning the sign of the pseudo-norm.

A major difference with respect to the three-dimensional case is that now k can be complex too. Since k is the eigenvalue of (6), which itself can be considered a Schrödinger equation with a $\mathcal{PT}$-symmetric potential ($K(\varphi)$), its complex eigenvalues occur in complex conjugate pairs. Substituting k and k^* into the radial Schrödinger equation (13) one finds that the two equations are each other's complex conjugate, so their energy eigenvalues will also appear as each other's complex conjugates. This indicates that similarly to the one-dimensional case, the spontaneous breakdown of $\mathcal{PT}$ symmetry leads to complex conjugate energy eigenvalues for $d = 2$ too.

4 Summary

The most important results of this work are presented in the table below.

	$d = 2$	$d = 3$
State-independent potential	always	$k = m^2 + a$
Central potential	$K(\varphi) = const.$	$K(\varphi) = a$
$\mathcal{PT}$-symmetric potential	$V_0^*(\rho) = V_0(\rho)$ $K^*(\varphi + \pi) = K(\varphi)$	$V_0^*(r) = V_0(r)$, $k = k^*$ $K^*(\varphi + \pi) = K(\varphi)$
Energy eigenvalues	real or complex conjugate pairs	real
Sign of pseudo-norm	indefinite	indefinite

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