On the bound states of the generalized inverse-power potentials in N-dimensions

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Abstract : We have presented bound state solutions to the Schrödinger equation for general inverse-power potentials, $V(r) = \sum_{\nu=1}^{2L} A_{\nu} r^{-\nu}$ in N-dimensions. By using a simple algebraic method, it is shown that bound states of these potentials exist when the paremeters A_{ν} satisfy certain constraints

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1. Introduction

The problem of quantum inverse-power potentials has been the subject of many discussion. for decades, both from an analytical and numerical points of view, because of its important applications in molecular physics [1], atomic physics [2], solid-state physics [3] and scattering theory [4]. Some special forms of the inverse-power potential describe intermolecular short and long-range interactions [1], and also, the spin-orbit and spin-spin interactions [5]. The induction energy for the interaction between a molecule with a permanent dipole moment and a non-polar molecule can be described with inverse-power potentials. The dipole-dipole dispersion energy for two molecules in their ground states is therefore attractive and inversely proportional to the sixth power of the intermolecular separation. Also, the dispersion energy arising from dipole-quadrupole interactions, quadrupole-quadrupole interactions, etc., is in a more complete form if it includes the terms of inversely proportional to higher power of the internuclear separation [1]. On the other hand, the inverse-power potentials can be used for the short and long-range interactions between two colliding particles [4]. Also, the various forms of the inverse-power potential for the short-range repulsive energy have been adopted in order to study the crystalline properties of alkali halides and other ionic solids [3].

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It should be noted that, nonrelativistic quantum mechanics with local interactions loses its general properties. Therefore, there are a number of cases where use of singular potentials is of interest. Recently, solutions to the Schrödinger equation for particular cases of inverse-power potentials have been studied by several authors [5–8] in one- and three-dimensions. In this paper we have extended the method [7,9] to use the solutions of the radial Schrödinger equation for the general inverse-power singular potentials,

$$V(r) = \sum_{\nu=1}^{2L} A_{\nu} r^{-\nu}.$$
 (1)

This potential can be reduced to well known potential by choosing appropriate A_v and L. For example, for L = 4 it reduced to eighth-order inverse power potential (EPP). EPP models to the induction energy for the interaction between a molecule with a permanent dipole moment and a non-polar molecule, or the induction energy for identical neutral molecules, including terms of upto quadrupole-induced dipole interaction which is proportional to r^{-8} [1]. Also, the crystal properties for ionic crystals have been calculated using special types of EPP. Thus, the potential $V(r) = \frac{A}{r^n} + \frac{A_1}{r} + \frac{A_6}{r^6} + \frac{A_8}{r^8}$ mas been used to calculate crystal properties of alkali halides and other ionic solids, where A and n are potential parameters, A_1 is the Madelung constant, A_6 and A_8 are van der Walls constants for dipole-dipole and dipole-quadrupole interaction, respectively [3]. On the other hand, the EPP can be used as the interaction potential in the scattering of charged particles by neutral targets or in collisions between neutral particles [4]. The long-range pairs of the interaction potential includes higher power of r, namely, $\frac{A_4}{r^4} + \frac{A_6}{r^6} + \frac{A_8}{r^8} + \dots, [4]$

For L = 2, the eq. (1) turns to fourth-order inverse power potential (FIP) [6–8], $V(r) = \frac{A_4}{r^4} + \frac{A_1}{r^4} + \frac{A_2}{r^2} + \frac{A_1}{r}$ describes zeroth moment, dipole moment, dipole-dipole and dipole-quadrupole interactions of two molecules [2]. For $A_1 = 0$, the FIP reduces to the potential $V(r) = \frac{A_1}{r^4} + \frac{A_1}{r^3} + \frac{A_2}{r^2}$, which contains magnetic spin-spin and spin-orbit interactions between two spin $-\frac{1}{2}$ particles [5]. For $A_4 = 0$ and $A_3 = 0$, the FIP reduces to the Kratzer [10], atomic Fues [11] or a Mie-type [12] potential of the form $V(r) = \frac{A_2}{r^2} + \frac{A_1}{r}$. It can be used to investigate the rotation-vibration spectrum of a diatomic molecule [10,12]. Also, for $A_4 = 0$, $A_3 = 0$ and $A_2 = 0$, the potential in eq. (1) turns to the Coulomb potential.

2. Solutions in N-dimensional space

The radial Schrödinger wave equation for a spherically-symmetric potential V(r) in Ndimensional space is

$$\frac{\hbar^2}{2\mu} \left[\frac{\partial^2}{\partial r^2} + \frac{N-1}{r} \frac{\partial}{\partial r} + \frac{l(l+N-1)}{r} \right] R(r) = (E-V(r))R(r).$$
(2)

The transformation $\phi(r) = r^{\frac{(N-1)}{2}}R(r)$ reduces eq. (2) to the form

$$-\frac{\bar{h}^2}{2\mu} \left[\frac{\partial^2}{\partial r^2} - \frac{(M-1)(M-3)}{4r^2} \right] \phi(r) = (E - V(r))\phi(r)$$
(3)

where M = N + 2l. Choosing the following factorized form for $\phi(r)$

$$\phi(r) = f(r) \exp[g(r)] \tag{4}$$

and substituting it in eq. (3), one can obtain

$$\phi''(r) = \left[g''(r) + g'(r)^2 + \frac{f''(r) + 2f'(r)g'(r)}{f(r)}\right]\phi(r).$$
(5)

Comparing eq. (3) and eq. (5) we obtain

$$U(r) + \frac{(M-1)(M-3)}{4r^2} - \varepsilon = g''(r) + g'(r)^2 + \frac{f''(r) + 2f'(r)g'(r)}{f(r)}$$
(6)

where $U(r) = \frac{2\mu}{\hbar^2} V(r)$ and $\epsilon = \frac{2\mu}{\hbar^2} E$. Eq. (6) for f(r) = constant is one of the forms of the Riccati equation. Our purpose is to find the fraction of right hand side of eq. (6) corresponding to the potential and energy. Exponential part of wave function, g(r), and other part f(r), which is a polynomial in r must ensure the normalizability of $\phi(r) [\phi(r \rightarrow \infty) \rightarrow 0]$ and $\phi(r \rightarrow 0) \rightarrow 0]$.

Eq. (6) in N-dimensional space for the reduced radial wave function ϕ (r) has the structure of the one-dimensional Schrödinger equation for a spherically symmetric potential V(r). To solve the transformed Schrödinger equation, eq. (6), for V(r) in eq. (1) we choose f(r) in the nodal form,

$$f_n(r) = \prod_{i=1}^n \left[r - \alpha_i^{(n)} \right], \ n = 1, 2, ..., f_0(r) = 1$$
(7)

and g(r) in the polynomial form as,

$$g(r) = a_0 r + \sum_{k=2}^{L} \frac{a_k r^{1-k}}{1-k} + b \ln r,$$
(8)

where $\alpha_{i}^{(n)}$ values correspond to the nodes of the wave function $\phi(r)$ that are determined by roots of f(r). We can rewrite eq. (6) by substituting g(r) and $f_n(r)$ for ground and excited states respectively, as given below.

$$U_{\text{eff}} - \varepsilon_0 = a_0^2 + \frac{2a_0b}{r} + \frac{b(b-1)}{r^2} + \sum_{j=2}^{L} \frac{a_j}{r^j} \left(2a_0 + \frac{2b-j}{r} \right) + \sum_{j=2}^{L} \left(\sum_{k=2}^{L} \frac{a_ja_k}{r^{j+k}} \right)$$
(9)

the first term of the right-hand side in eq. (9) is the equivalent energy ($\varepsilon = -a_0^2$), others corresponding to the parametric inverse-power potential U_{eff} , and

$$U_{\text{eff}} - \varepsilon_n = a_0^2 + \frac{2a_0b}{r} + \frac{b(b-1)}{r^2} + \sum_{j=2}^{L} \frac{a_j}{r^j} \left(2a_0 + \frac{2b-j}{r} \right) \\ + \sum_{j=2}^{L} \left(\sum_{k=2}^{L} \frac{a_j a_k}{r^{j+k}} \right) \times \left(2a_0 + \frac{2b}{r} \right) \left(\sum_{i=1}^{n} \frac{1}{r - \alpha_i^{(n)}} \right) \\ + \sum_{k=2}^{L} \frac{2a_k}{r^k} \left(\sum_{i=1}^{n} \frac{1}{r - \alpha_i^{(n)}} \right) + \sum_{i(10)$$

For the first node, parametric potential and energy are obtained from eq. (10) for n = 1 as

$$U_{\rm eff}(r) - \varepsilon_1 = a_0^2 + \frac{2a_0b}{r} + \frac{b(b-1)}{r^2} + \sum_{j=2}^L \frac{a_j}{r^j} \left(2a_0 + \frac{2b-j}{r} \right) + \sum_{j=2}^L \left(\sum_{k=2}^L \frac{a_ja_k}{r^{j+k}} \right) + \sum_{k=0}^{L-1} \left(\sum_{j=k}^{L-1} \frac{2a_k\alpha_1^{(1)^{j+k}}}{r^{j+1}} \right), \tag{11}$$

where $\varepsilon_1 = -a_0^2$, $a_1 = b$ and

$$\sum_{k=0}^{l} a_k \alpha_1^{(1)^{l-k}} = 0.$$
 (12)

In general case, parametric potential can be written as

$$U_{\text{eff}}(r) = \frac{2a_0b}{r} + \frac{b(b-1)}{r^2} + \sum_{j=2}^{L} \frac{a_j}{r^j} \left(2a_0 + \frac{2b-j}{r} \right) + \sum_{j=2}^{L} \left(\sum_{k=2}^{L} \frac{a_ja_k}{r^{j+k}} \right) + \sum_{k=0}^{L-1} \left(\sum_{j=k}^{L-1} \frac{2a_k}{r^{j+1}} \right) \left(\sum_{i=1}^{n} \alpha_i^{(n)^{i-1}} \right) + \sum_{k=0}^{L-2} \left(\sum_{j=k}^{L-2} \frac{2}{r^{j+2}} \right) \left(\sum_{i(13)$$

$$\varepsilon_n = -a_0^2, \left(\varepsilon_n = \frac{2\mu}{\hbar^2} E_n\right). \tag{14}$$

On comparing eq. (13) and eq. (1) we find the relations between the corresponding potential parameters and wave function coefficients $(a_k, \alpha_i^{(n)})$ as

$$\frac{2\mu}{\hbar^2} A_{\nu} = \sum_{j=0}^{\nu} a_j a_{\nu-j} + a_{\nu-1}(2n-\nu+1) + 2\sum_{j=0}^{\nu-2} a_j \left(\sum_{i=1}^n \alpha_i^{(n)^{\nu-j-1}}\right)$$

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+
$$2\sum_{m=0}^{\nu-2}\left(\sum_{i\leq j}^{n}\alpha_{i}^{(n)^{m}}\alpha_{j}^{(n)^{1-m-2}}\right), \nu = 1, 2, 3, ..., L;$$
 (15a)

$$\frac{2\mu}{\hbar^2} A_{\nu} = (1-\nu)a_{\nu-1} + \sum_{j=\nu-L}^{L} a_j a_{\nu-j}, \quad \nu = L+1;$$
(15b)

$$\frac{2\mu}{\hbar^2} A_{\nu} = \sum_{j=\nu-L}^{L} a_j a_{\nu-j}, \quad \nu = L+2, L+3, ..., 2L;$$
(15c)

where $a_1 = b$ (2b = 2l + N - 1). Note that for v = 2, $\frac{1}{4}(M - 1)(M - 3)$ is second contributor to the parameter $\frac{2\mu}{\hbar^2} A_2$. There are the relations between the wave function parameters a_k and $a_i^{(n)}$ (for the first three sets) as

$$\sum_{k=0}^{L} a_{k} \left(\sum_{i=1}^{n} \alpha_{i}^{(n)^{L-k}} \right) + \sum_{k=0}^{L-1} \left(\sum_{i

$$\sum_{k=0}^{L} a_{k} \left(\sum_{i\neq j}^{n} \alpha_{i}^{(n)^{k-1}} \alpha_{j}^{(n)} \right) + \sum_{k=0}^{L-2} \left(\sum_{i

$$+ \sum_{k=0}^{L-1} \left(\sum_{i\neq j\neq l}^{n} \alpha_{i}^{(n)^{k}} \alpha_{j}^{(n)^{L-k-1}} \alpha_{l}^{(n)} \right) = 0, \quad (16b)$$

$$\sum_{k=0}^{L} a_{k} \left(\sum_{i\neq j\neq l}^{n} \alpha_{i}^{(n)} \alpha_{l}^{(n)} \alpha_{l}^{(n)^{k-k}} \right) + 2 \sum_{k=0}^{L-2} \left(\sum_{i\neq j\neq l}^{n} \alpha_{i}^{(n)^{k+1}} \alpha_{l}^{(n)^{L-k-1}} \alpha_{l}^{(n)} \right)$$

$$+ \sum_{k=0}^{L-1} \left(\sum_{i\neq j\neq l\neq m}^{n} \alpha_{i}^{(n)^{i}} \alpha_{j}^{(n)^{k-k-1}} \alpha_{l}^{(n)} \alpha_{m}^{(n)} \right) = 0. \quad (16c)$$$$$$

Hence, the unnormalized wave functions are given by

$$\phi_n(r) = \prod_{i=1}^n \left(r - \alpha_i^{(n)}\right) r^{(2i+N-1)/2} \exp\left[a_0 r + \sum_{k=2}^L \frac{a_k r^{1-k}}{1-k}\right].$$
 (17)

The index *n* denotes the number of nodes of the wave function in $0 < r < \infty$. The eqs. (15ac) contain the relations between the potential parameters A_v and wave function parameters a_k and $\alpha_i^{(n)}$. From eqs. (15a-c) and eqs. (16a-c) it is possible to obtain the coefficients a_k as a function of A_v . Hence, for the potential in eq. (1), the exact energy and the corresponding wave functions in N-dimensional space can be determine from eq. (14) and eq. (17), respectively.

The general results obtained above can be simplified for special cases of L:

For L = 4, the potential in eq. (1) reduces to EPP as

$$V(r) = \frac{A_8}{r^8} + \frac{A_7}{r^7} + \frac{A_6}{r^6} + \frac{A_5}{r^5} + \frac{A_4}{r^4} + \frac{A_3}{r^3} + \frac{A_2}{r^2} + \frac{A_1}{r}$$
(18)

From eqs. (15a-c), relations between potential parameters and wave function coefficients can be obtained as $(\hbar = 2\mu = 1)$

$$A_{1} = 2a_{0}(b+n);$$

$$A_{2} = b(b+2n-1)+2a_{0}(a_{2} + \sum_{i=1}^{n} \alpha_{i}^{(n)}) + n(n-1) - \frac{1}{4}(M-1)(M-3);$$

$$A_{3} = 2a_{0}a_{3} + 2a_{2}(b+n-1) + (2b+2n-2) \sum_{i=1}^{n} \alpha_{i}^{(n)} + 2a_{0} \sum_{i=1}^{n} \alpha_{i}^{(n)^{2}}; \quad (19)$$

$$A_{4} = 2a_{0}a_{4} + a_{3}(2b+2n-3) + a_{2}^{2} + 2a_{0} \sum_{i=1}^{n} \alpha_{i}^{(n)^{3}} + (2b+2n-2) \sum_{i=1}^{n} \alpha_{i}^{(n)^{2}};$$

$$+ 2a_{2} \sum_{i=1}^{n} \alpha_{i}^{(n)} + 2 \sum_{i < j}^{n} \alpha_{i}^{(n)} \alpha_{j}^{(n)};$$

$$A_{5} = 2a_{2}a_{3} + 2a_{4}(b-2); \quad A_{6} = a_{3}^{2} + 2a_{2}a_{4}; \quad A_{7} = 2a_{3}a_{4}; \quad A_{8} = a_{4}^{2}.$$

Also, there are four constraint relations on the potential parameters as follows :

$$A_{2} = n(n+2l+N-2) + \frac{A_{1}}{2n+2l+N-1} \left(\frac{4A_{6}A_{8} - A_{7}^{2}}{\pm 4A_{8}^{\frac{1}{2}}} + 2\sum_{i=1}^{n} \alpha_{i}^{(n)} \right),$$

$$A_{3} = \pm \frac{A_{1}A_{7}}{\sqrt{A_{8}}(2l+N+2n-1)} \pm \frac{4A_{6}A_{8} - A_{7}^{2}}{8A_{8}^{\frac{1}{2}}} (2l+N+2n-3)$$

$$+ \left(\frac{2A_{1}}{2n+2l+N-1} \right) \sum_{i=1}^{n} \alpha_{i}^{(n)^{2}} + (2l+N+2n-3) \sum_{i=1}^{n} \alpha_{i}^{(n)}, \quad (20b)$$

$$A_{4} = \frac{\pm 2A_{1}\sqrt{A_{8}}}{2n+2l+N-1} \pm \frac{A_{7}}{2\sqrt{A_{8}}} (2l+N+2n-4) + \frac{(4A_{6}A_{8} - A_{7}^{2})^{2}}{64A_{8}^{3}}$$

$$+ 2\sum_{i

$$+ (2l+N+2n-3) \sum_{i=1}^{n} \alpha_{i}^{(n)^{2}} \pm \frac{4A_{6}A_{8} - A_{7}^{2}}{4A_{8}^{\frac{1}{2}}} \sum_{i=1}^{n} \alpha_{i}^{(n)}, \quad (20c)$$

$$A_{5} = \frac{4A_{6}A_{8}A_{7} - A_{7}^{3}}{8A_{8}^{2}} \pm \sqrt{A_{8}} (2l+N-5). \quad (20d)$$$$

The energy for any n and l is

$$E_{nl} = -\frac{A_l^2}{(2n+2l+N-1)^2}.$$
 (21a)

Also, one can write the energy expression in different forms in terms of other potential parameters from eqs. (19-20), for example

$$E_{nl} = -16A_8^3 \left(\frac{A_2 - n(n+2l+N-2)}{4A_6A_8 - A_7^2 \pm 8A_8^{\frac{1}{2}} \sum_{i}^{n} \alpha_i^{(n)}}\right)^2.$$
 (21b)

In order to use last form of energy expressions, $\alpha_i^{(n)}$ parameters must be found from eqs. (16a-c) with above restrictions. Note that, there is no simple form of $\alpha_i^{(n)}$ as seen in eqs. (16). For the first excited state (n = 1) this parameter can be obtained from

$$\frac{2A_{1}}{(2l+N+1)} \alpha_{1}^{(1)^{4}} + (2l+N-1) \alpha_{1}^{(1)^{3}} \pm \left(\frac{4A_{6}A_{8}-A_{7}^{2}}{4A_{8}^{\frac{1}{2}}}\right) \alpha_{1}^{(1)^{2}}$$
$$\pm \frac{A_{7}}{\sqrt{A_{8}}} \alpha_{1}^{(1)} \pm 2\sqrt{A_{8}} = 0, \qquad (22)$$

and corresponding wave function is

$$\phi_{1}(r) = \left(r - \alpha_{1}^{(1)}\right) r^{(2l+N-1)/2} \exp\left[\frac{A_{1}}{(2l+N+1)}r \pm \frac{4A_{6}A_{8} - A_{7}^{2}}{8A_{8}^{\frac{1}{2}}} \frac{1}{r} + \frac{1}{\pm 4\sqrt{A_{8}}} \frac{1}{r^{2}} \pm \frac{\sqrt{A_{8}}}{3} \frac{1}{r^{3}}\right].$$
(23)

For L = 3, from eq. (1) we have

$$V(r) = \frac{A_6}{r^6} + \frac{A_5}{r^5} + \frac{A_4}{r^4} + \frac{A_3}{r^3} + \frac{A_2}{r^2} + \frac{A_1}{r}.$$
 (24)

In this case, relations between the parameters can be determined with eqs. (16, 19–20) for $a_4 = 0$ ($A_8 = A_7 = 0$). The wave functions are

$$\phi_n(r) = \prod_{i=1}^n \left(r - \alpha_i^{(n)} \right) r^{(2l+N-1)/2} \exp\left[\frac{A_1}{(2l+N+1)} r + \frac{A_5}{2\sqrt{A_6}} \frac{1}{r} \pm \frac{\sqrt{A_6}}{3} \frac{1}{r^2} \right],$$
(25)

with the consistency relations

$$A_{2} = n(n+2l+N-2) + \frac{A_{1}}{2n+2l+N-1} \left(\frac{A_{5}}{\pm \sqrt{A_{6}}} + 2 \sum_{i=1}^{n} \alpha_{i}^{(n)} \right), \quad (26a)$$

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$$A_{1} = \frac{\pm 2A_{1}\sqrt{A_{6}}}{2l+N+2n-1} \pm \frac{A_{5}}{2\sqrt{A_{6}}} (2l+N+2n-3) \\ + \left(\frac{2A_{1}}{2n+2l+N-1}\right) \sum_{i=1}^{n} \alpha_{i}^{(n)^{2}} + (2l+N+2n-3) \sum_{i=1}^{n} \alpha_{i}^{(n)}, \quad (26b)$$

$$A_{4} = \pm \sqrt{A_{6}} (2n+2l+N-4) + \frac{A_{5}^{2}}{4A_{6}} + \left(\frac{2A_{1}}{2n+2l+N-1}\right) \sum_{i=1}^{n} \alpha_{i}^{(n)^{3}} \\ + (2n+2l+N-3) \sum_{i=1}^{n} \alpha_{i}^{(n)^{2}} \pm \frac{A_{5}}{\sqrt{A_{6}}} \sum_{i=1}^{n} \alpha_{i}^{(n)} + 2 \sum_{i$$

The energies are of same form as in eq. (21) with restrictions in eqs. (26a, b, c). Also, parameters $\alpha_{\perp}^{(n)}$ can be found from eqs. (16a–c) for several values of *n*.

We note that, if the potentials in eq. (18) and eq. (24) do not consist of the Coulomb term (*i.e.* $A_1 = 0$ or b = -n), the energy $(\epsilon = -a_0^{-1})$ is determined in terms of other potential parameters, from eq. (19). Also, the potential in eq. (24) for $A_6 = A_5 = 0$ (or $a_3 = 0$) reduces to the FIP which can be obtained from eq. (1) for L = 2. In this case, there are two restrictions between potential parameters : $A_2 = \frac{2A_1}{2n+2l+N-1}$ ($\sqrt{A_4} + \sum_{i=1}^n \alpha_i^{(n)}$) + n(n + 2l + N - 2) and $A_3 = (2l + N - 3)\sqrt{A_4}$. These results are identical with the previous works [6–8] in three-dimensional (N = 3) spaces. This potential for several values of A_1 turns to some special potentials, *i.e.*, for $A_1 = 0$, the FIP can be reduced to the potential $\frac{A_1}{r} + \frac{A_4}{r^4}$ that includes only Coulombic interaction and interaction of an ion with a neutral atom or polarization term of atom or molecule, where $E_n = a_0^2$, b = 1, $A_1 = 2a_0$ (n + 1) and $2a_0$ ($\sqrt{A_4} + \sum_{i=1}^n \alpha_i^{(n)}$) + $n(n + 1) + \frac{1}{4}(2l + N - 1)(2l + N - 3) = 0$. Moreover, one can obtain Kratzer and atomic Fues (or a Mie-type) potentials for L = 1 (*i.e.* $A_6 = A_5 = A_4 = A_3 = 0$ in eq. (24) or $a_3 = a_2 = 0$) by the same way. For this potential, there is no constraint on the potential parameters.

3. Conclusions

A large area of mathematical physics is concerned with exact solutions of singular systems from the viewpoint of quantum mechanics. We have given solutions to the Schrödinger equation (eqs. (2)-(6)) for general inverse-power potentials, eq. (1), in N-dimensions. We take all the solutions in the form $\phi(r) = f(r) \exp [g(r)]$, which suitably restricts f(r) and g(r)to incorporate the boundary conditions. The wave functions and energies of different forms of the inverse-power potentials can be determined by using this algorithm for several values of L. Our solutions have involved some restrictions between the potential parameters. The number of restrictions on the 2L potential parameters are L except L = 1. We note that, the solutions of general inverse-power potentials can be reduced to some molecular, atomic and

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spin systems. Thus, the difference between the present work and the previous works [6–9] is that the previous works are the special solutions of the general solution derived in this work, and its attempt to extend the class of quasiexactly solvable potentials from polynomial towards essentially singular potentials.

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