International Journal of Theoretical Physics, Vol. 36, No. 1, 1997

Vibrational-Rotational Analysis of Supersingular plus Quadratic $A/r^4 + r^2$ Potential

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Received March 11, 1996

Most work on supersingular potentials has focused on the study of the ground state. In this paper, a global analysis of the ground and excited states for the successive values of the orbital angular momentum of the supersingular plus quadratic potential is carried out, making use of centrifugal plus quadratic potential eigenfunction bases. First, the radially nodeless states are variationally analyzed for each value of the orbital angular momentum using the corresponding functions of the bases; the output includes the centrifugal and frequency parameters of the auxiliary potentials and their eigenfunction bases. In the second stage, these bases are used to construct the matrix representation of the Hamiltonian of the system, and from its diagonalization the energy eigenvalues and eigenvectors of the successive states are obtained. The systematics of the accuracy and convergence of the overall results are discussed with emphasis on the dependence on the intensity of the supersingular part of the potential and on the orbital angular momentum.

1. INTRODUCTION

Since the papers by Klauder (1973), Ezawa *et al.* (1975), and Detwiler and Klauder (1975) singular potentials have been receiving increased interest (Harrell, 1977; Klauder, 1978; de Llano, 1981; Znojil, 1982, 1992; Killingbeck, 1982; Ullah, 1986; Aguilera-Navarro *et al.*, 1990, 1992; Aguilera-Navarro and Guardiola, 1991; Aguilera-Navarro and Ullah 1994; Fernández, 1991; Guardiola and Ros, 1992; Solano-Torres *et al.*, 1992). These potentials are present in a number of situations which are mathematically challenging and physically interesting. The analysis of the supersingular plus quadratic potential $A/r^4 + r^2$ carried out in Aguilera-Navarro and Ullah (1994) was

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0020-7748/97/0100-0157$12.50/0

restricted to the study of the ground state as a function of the intensity parameter A. The same restriction is shared by other studies of supersingular potentials (Aguilera-Navarro *et al.*, 1990, 1992; Aguilera-Navarro and Guardiola, 1991; Aguilera-Navarro and Ullah, 1994; Fernández, 1991; Guardiola and Ros, 1992; Solano-Torres *et al.*, 1992; Znojil, 1992). In order to have a better understanding of the effects of the presence of the supersingular components of the potential in such systems, it is necessary to investigate not only the ground state, but also the radially and rotationally excited states.

In this paper a global analysis of the supersingular plus quadratic potential is formulated by using the bases of eigenfunctions of centrifugal plus quadratic potentials, leading to a reliable description of the vibrational-rotational energy spectra of the quantum system. In Section 2 the variational analysis of the radially nodeless states for successive values of the orbital angular momentum is carried out using a trial function which is the product of a power of the radial coordinate and a Gaussian function. In Section 3 the general solution is formulated in matrix form using the bases of eigenfunctions of the centrifugal plus quadratic potentials with intensity parameters provided by the analysis of the previous section. Section 4 consists of a discussion of the specific results of this work and also of possible ways of extending the present method to the study of other systems with supersingular potentials.

2. VARIATIONAL ANALYSIS OF RADIALLY NODELESS STATES FOR SUCCESSIVE VALUES OF ORBITAL ANGULAR MOMENTUM

The radial Schrödinger equation for the supersingular plus quadratic potential

$$\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+\frac{l(l+1)}{r^2}+\frac{A}{r^4}+r^2\right]\psi(r)=E\psi(r) \tag{1}$$

for the successive values $l = 0, 1, 2, \ldots$ of the orbital angular momentum is the subject of analysis in this section and the next one. Here the variational analysis is restricted to the radially nodeless states by using trial functions of the form

$$\psi_{\text{trial}}(r) = Nr^{\lambda}e^{-\omega r^2/2} \tag{2}$$

where λ and ω are identified as the centrifugal and harmonic variational parameters, respectively. The normalization factor N is determined by the condition

$$1 = \int_0^\infty dr\, r^2 |\psi_{\text{trial}}(r)|^2 = \frac{N^2\Gamma(\lambda + 3/2)}{2\omega^{\lambda+3/2}} \tag{3}$$

The energy expectation value from equations (1) and (2) can be evaluated immediately and reduced to

$$E(\omega, \lambda) = \left(\frac{1}{\omega} + \omega\right)\left(\lambda + \frac{3}{2}\right) - \frac{\lambda(\lambda + 1) - l(l + 1)}{\lambda + 1/2}\omega + \frac{A\omega^2}{\lambda^2 - 1/4} \tag{4}$$

Its minimization with respect to the parameters ω and λ leads to the two simultaneous equations

$$\frac{\partial E}{\partial \omega} = 0 = \left(-\frac{1}{\omega^2} + 1\right)\left(\lambda + \frac{3}{2}\right) - \frac{\lambda(\lambda + 1) - l(l + 1)}{\lambda + 1/2} + \frac{2A\omega}{\lambda^2 - 1/4} \tag{5}$$

and

$$\frac{\partial E}{\partial \lambda} = 0 = \frac{1}{\omega} - \omega + \frac{\lambda(\lambda + 1) - l(l + 1)}{(\lambda + 1/2)^2}\omega - \frac{2A\omega^2\lambda}{(\lambda^2 - 1/4)^2} \tag{6}$$

The elimination of the terms in A from equations (5) and (6) leads in turn to the following relationship between the variational parameters:

$$\omega = \sqrt{\frac{12\lambda^2 + 8\lambda + 1}{8\lambda^2 + 4\lambda + 4l(l + 1) + 1}} \tag{7}$$

which will prove to be very useful in interpreting the highly rotationally excited states of the system. In general, the numerical solution of equations (5) and (6) for chosen values of the supersingular potential intensity A and the orbital angular momentum l is readily accomplished, giving the values of ω and λ and the corresponding variational energy, equation (4), for the respective radially nodeless states. Table I presents a sample of such values for $A = 0.001, 0.01, 0.1, 1, 10, 100, 1000$ and the lowest successive values of l. Certain general trends can be identified in the variations of the potential parameters A and l of equation (1) and of the variational parameters λ and ω of equation (2). For a given value of A, the values of λ are larger than the corresponding values of l, reflecting that in the trial function of equation (2) the takeoff for $r \to 0$ is slower than the usual r^l, due to the dominance at small distances of the supersingular potential over the centrifugal potential associated with the rotational contribution to the kinetic energy. For small enough values of l, the values of λ are substantially different from them, and

Table I. Supersingular Potential Intensity A, Orbital Angular Momentum l, Centrifugal Parameter λ, Frequency Parameter ω, and Variational Energy of Radially Nodeless States $E(\omega, \lambda)$, Equation (4)

A	l	λ	ω	$E(\omega, \lambda)$
0.001	0	0.55635609067	1.26785711749	3.21682779558
	1	1.00459902364	1.00130941428	5.00132691491
	2	2.00057747164	1.00008881969	7.00026660823
	3	3.00021711826	1.00002285306	9.00011427982
	4	4.00011337402	1.00000906968	11.0000634908
	5	5.00006958338	1.00000448919	13.0000404037
0.01	0	0.66893658381	1.27101542953	3.33111301651
	1	1.04115007402	1.01139689904	5.01276501609
	2	2.00574742837	1.00088203464	7.00266085302
	3	3.00216897323	1.00022816411	9.00114226825
	4	4.00113332150	1.00009064198	11.0006347955
	5	5.00069571314	1.00004487886	13.0004040018
0.1	0	0.97543301926	1.27119792653	3.66428055431
	1	1.24757267867	1.05906902541	5.10280260830
	2	2.05497948090	1.00826157071	7.02611295409
	3	3.02147315822	1.00224580616	9.01137032809
	4	4.01129160365	1.00090097563	11.0063367394
	5	5.00694509280	1.00044748703	13.0040365464
1	0	1.73245599570	1.26207150656	4.54354754654
	1	1.91370184920	1.14510778231	5.57795364854
	2	2.41194071070	1.05348925198	7.22729215901
	3	3.19657363650	1.01952166851	9.10901325038
	4	4.10903189307	1.00850691627	11.0622931434
	5	5.06828604990	1.00434963869	13.0400254838
	50	50.0006081338	1.00000404071	103.000400037
10	0	3.46483253803	1.24818957799	6.62988715565
	1	3.57318766034	1.20719477639	7.24071018439
	2	3.82286404480	1.14736889950	8.36190509563
	3	4.24931380470	1.09356485978	9.84321738516
	4	4.85239544035	1.05656402987	11.5454312668
	5	5.59416818222	1.03440084229	13.3718186570
	50	50.0060805430	1.00004039740	103.004000075
100	0	7.27421543241	1.23732934528	11.2754389358
	1	7.33312772605	1.22663095873	11.5911786351
	2	7.45582321997	1.20697279756	12.2076838419
	3	7.65067105680	1.18135394107	13.0973086041
	4	7.92699881655	1.15323730733	14.2237964169
	5	8.29200840238	1.12571751989	15.5471338767
	50	50.0607266241	1.00040301280	103.039971557
1000	0	15.5278820747	1.23099105958	21.3740874828
	1	15.5577070076	1.22852456861	21.5273970556
	2	15.6179197156	1.22369033849	21.8322499808
	3	15.7096047927	1.21667910763	22.2851808516
	4	15.8342877126	1.20776058997	22.8811554541
	5	15.9938173908	1.19726525746	23.6137572037
	50	50.5995738825	1.00393685865	103.396842644

the values of ω are appreciably different from 1 [which is the frequency in the harmonic potential of equation (1)]; as larger values of l are considered, the values of λ get closer to them from above, and the values of ω also approach 1 from above. The usefulness of equation (7) enters here, since it shows that in fact as $\lambda \to l$, $\omega \to 1$. The latter situation indicates that the effect of the supersingular parameter becomes less important as the centrifugal potential becomes larger. Correspondingly, the energy eigenvalues approach the corresponding values of the harmonic oscillator $2l + 3$ from above for large enough values of l. If the supersingular potential is taken as a perturbation on the harmonic potential, then for small (large) values of A the situation of the previous sentences appears for smaller (larger) values of l, as it can be checked from the entries of Table I for the successive values of A.

3. MATRIX REPRESENTATION AND SOLUTION IN CENTRIFUGAL PLUS QUADRATIC POTENTIAL EIGENFUNCTION BASES

Two questions can be asked about improving and extending the results of Section 2: Can the variational analysis of the radially nodeless states be improved? Can such an analysis be extended to states with radial excitations? Both questions are addressed in this section, and a unified affirmative answer is given. Indeed, the answer to the first question requires a trial function more flexible than the one of equation (2), the additional flexibility coming from functions orthogonal to that one; the incorporation of such functions provides simultaneously the key to answer the second question.

To wit, the Schrödinger equation for the centrifugal plus quadratic potential

$$\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr} + \frac{l(l+1)}{r^2} + \frac{B}{r^2} + \omega^2 r^2\right]\phi_{n\lambda}(r) = E^0_{n\lambda}\phi_{n\lambda}(r) \tag{8}$$

has the exact eigenfunctions

$$\phi_{n\lambda}(r) = N_{n\lambda} r^{\lambda} e^{-\omega r^2/2} M(-n, \lambda + 3/2, \omega r^2) \tag{9}$$

where

$$\lambda(\lambda + 1) = l(l + 1) + B \tag{10}$$

and M is the confluent hypergeometric function reducing to a polynomial of degree $n = 0, 1, 2, \ldots$ of its argument. In particular, the trial function of equation (2) belongs to the set of equation (9) for $n = 0$. The energy eigenvalues of equation (8) are

$$E^0_{n\lambda} = (4n + 2\lambda + 3)\omega \tag{11}$$

The solution of equation (1) for states with any radial excitation and any orbital angular momentum can be obtained by using the trial functions of the form

$$\psi_{\nu\lambda}(r) = \sum_{n=0}^{N} a_{\nu n}\phi_{n\lambda}(r) \tag{12}$$

i.e., superpositions of the orthonormal functions of equation (9). For given values of the potential parameters A and l in equation (1), the analysis of Section 2 provides the values of the corresponding variational parameters ω and λ of the basis of functions of equation (9) as well as the associated frequency and centrifugal potential intensities of equation (8), the latter via equation (10).

The substitution of the trial function of equation (12) in equation (1) followed by the projection on the successive states of the basis of equation (9) leads to the matrix representation of equation (1). In fact, the functions of the basis of equation (9) are normalized to unity,

$$1 = (\phi_{n\lambda}, \phi_{n\lambda}) = \frac{N^2 n!\,\Gamma^2(\lambda + 3/2)}{2\omega^{\lambda+3/2}\Gamma(n + \lambda + 3/2)} \tag{13}$$

The Hamiltonian H of equation (1) can be written as the Hamiltonian H_0 of equation (8) plus the difference between the two Hamiltonians

$$H = H_0 + (1 - \omega^2)r^2 - \frac{\lambda(\lambda + 1) - l(l + 1)}{r^2} + \frac{A}{r^4} \tag{14}$$

Then the matrix form of equation (1) becomes ($n, m = 0, 1, 2,\ldots$)

$$\left\|(E^0_{n\lambda} - E)\delta_{nm} + (1 - \omega^2)\langle n|r^2|m\rangle - [\lambda(\lambda + 1) - l(l + 1)] \times \left\langle n\left|\frac{1}{r^2}\right|m\right\rangle + A\left\langle n\left|\frac{1}{r^4}\right|m\right\rangle\right\| = 0 \tag{15}$$

where

$$\langle n|r^2|n\rangle = (2n + \lambda + 3/2)/\omega \tag{16}$$

$$\left\langle n\left|\frac{1}{r^2}\right|n\right\rangle = \frac{\omega}{\lambda + 1/2} \tag{17}$$

$$\left\langle n\left|\frac{1}{r^4}\right|n\right\rangle = \frac{(2n + \lambda + 3/2)\omega^2}{(\lambda + 3/2)(\lambda^2 - 1/4)} \tag{18}$$

are the diagonal matrix elements, and

$$\langle n|r^2|m\rangle = -\frac{1}{\omega}\sqrt{m(n+\lambda+3/2)}\,\delta_{n,m-1} \tag{19}$$

$$\left\langle n\left|\frac{1}{r^2}\right|m\right\rangle = \sqrt{\frac{m!\,\Gamma(n+\lambda+3/2)}{n!\,\Gamma(m+\lambda+3/2)}}\,\frac{\omega}{\lambda+1/2} \tag{20}$$

$$\left\langle n\left|\frac{1}{r^4}\right|m\right\rangle = \sqrt{\frac{m!\,\Gamma(n+\lambda+3/2)}{n!\,\Gamma(m+\lambda+3/2)}}\,\frac{(m-n+1)(\lambda+3/2)+2n}{(\lambda+3/2)(\lambda^2-1/4)}\,\omega^2 \tag{21}$$

give the values of the nondiagonal ones for $m > n$. The matrix elements with $m < n$ are incorporated by using the symmetry property of the matrix.

The solution of equation (15) as a secular equation for an $N \times N$ matrix gives upper limits to the energy eigenvalues of the lowest N states for the chosen orbital angular momentum. The larger the matrix, the closer one can expect such limiting values to be to the exact energy eigenvalues, especially for the states with lower radial excitations. The diagonalization of such matrices also provides the corresponding eigenvectors, i.e., the coefficients a_{vn} in equation (12).

The numerical results presented through Table II illustrate the convergence and accuracy of the variational energies for the lowest vibrational rotational states, as obtained for different sizes $N \times N$ of the diagonalized matrices, and for different values of the intensity A of the supersingular potential. It can be seen that the convergence is faster (slower) for larger (smaller) values of A, as indicated by the smaller (larger) values of N needed to obtain the lowest energy eigenvalues with a certain number of significant digits (we worked out the numerical calculations with 12 significant digits; however, for the sake of space, Table II displays only seven). The energy eigenvalues of the ground state $v = 0$, $l = 0$ can be compared with those of Aguilera-Navarro and Ullah (1994) and seen to coincide, admitting that the convergence in that work is faster. The advantage of the present work consists in the simultaneous determination of the vibrationally $v = 1, 2, 3, \ldots$ and rotationally $l = 0, 1, 2, \ldots$ excited states. For the sake of space, Table II illustrates only the states with $l = 0, 1, 2, 3$ for $A = 0.1, 1, 10, 100, 1000$. However, our method and programs can obviously give the energies of the corresponding states for other values of A. In particular, for $A = 1$ and $l = 4, 5, \ldots$ and also $A = 1000$ and $l = 1000, \ldots$ it can be verified that the energy levels are slightly shifted upward from their harmonic oscillator values $4v + 2l + 3$, illustrating that the effect of the supersingular potential on so high angular momentum states is very small; the fast convergence in the evaluation of such states can also be contrasted with the slower convergence for the lower angular momentum states. These trends are directly connected

Table II. First Four Lowest Energies[a] E_{vl} Obtained from the Diagonalization of the Hamiltonian (14) in the N-Dimensional Space Spanned by the Basis Functions (9), for Some Values of the Supersingular Potential Intensity A

	$A = 0.1$				$A = 1$			
N	E_{00}	E_{10}	E_{20}	E_{30}	E_{00}	E_{10}	E_{20}	E_{30}
4	3.634708	7.863175	12.11053	16.85972	4.528807	8.915767	13.25423	18.27755
10	3.632051	7.859925	12.02653	16.16506	4.518518	8.895405	13.17149	17.40108
50	3.592018	7.793466	11.93500	16.04811	4.494356	8.846038	13.09223	17.28629
100	3.578996	7.771997	11.90575	16.01127	4.494241	8.845799	13.09184	17.28572
200	3.575799	7.766710	11.89853	16.00216	4.494184	8.845686	13.09167	17.28547
250	3.575681	7.766515	11.89827	16.00182	4.494179	8.845676	13.09165	17.28545
300	3.575665	7.766488	11.89823	16.00177	4.494178	8.845673	13.09165	17.28544
	E_{01}	E_{11}	E_{21}	E_{31}	E_{01}	E_{11}	E_{21}	E_{31}
4	5.101363	9.166384	13.22725	17.33071	5.573287	9.808259	14.01163	18.49015
10	5.101081	9.165692	13.22499	17.28114	5.568834	9.797886	13.98613	18.15295
50	5.097109	9.155956	13.20802	17.25552	5.559268	9.773711	13.94213	18.08335
100	5.095784	9.152747	13.20251	17.24735	5.559181	9.773491	13.94173	18.08271
150	5.095444	9.151924	13.20110	17.24526	5.559175	9.773476	13.94170	18.08267
200	5.095339	9.151672	13.20067	17.24462	5.559170	9.773463	13.94168	18.08263
	E_{02}	E_{12}	E_{22}	E_{32}	E_{02}	E_{12}	E_{22}	E_{32}
4	7.026096	11.04053	15.05478	19.07023	7.226741	11.33002	15.42606	19.57042
10	7.026075	11.04047	15.05466	19.06873	7.225815	11.32730	15.42069	19.50927
50	7.025991	11.04018	15.05401	19.06755	7.224316	11.32225	15.40951	19.48883
100	7.025971	11.04011	15.05386	19.06727	7.224288	11.32215	15.40929	19.48845
150	7.025965	11.04009	15.05382	19.06719	7.224288	11.32215	15.40929	19.48844
200	7.025963	11.04008	15.05380	19.06716	7.224288	11.32215	15.40929	19.48844
	E_{03}	E_{13}	E_{23}	E_{33}	E_{03}	E_{13}	E_{23}	E_{33}
4	9.011370	13.01638	17.02137	21.02645	9.108956	13.15354	17.19693	21.24754
10	9.011367	13.01637	17.02135	21.02645	9.108808	13.15302	17.19582	21.23773
50	9.011364	13.01636	17.02131	21.02624	9.108662	13.15239	17.19414	21.23417
80	9.011364	13.01635	17.02131	21.02624	9.108659	13.15237	17.19411	21.23410

	$A = 10$				$A = 100$			
N	E_{00}	E_{10}	E_{20}	E_{30}	E_{00}	E_{10}	E_{20}	E_{30}
4	6.623194	11.18473	15.64570	20.86153	11.27130	15.97551	20.57437	25.80266
10	6.609923	11.14771	15.55647	19.89742	11.26516	15.94779	20.50880	24.99076
50	6.606628	11.13752	15.53430	19.85631	11.26508	15.94731	20.50693	24.98516
100	6.606623	11.13751	15.53426	19.85625	11.26508	15.94731	20.50693	24.98516
	E_{01}	E_{11}	E_{21}	E_{31}	E_{01}	E_{11}	E_{21}	E_{31}
4	7.235960	11.71475	16.11249	21.08018	11.58738	16.26208	20.83830	25.99834
10	7.226013	11.68568	16.04723	20.35502	11.58168	16.23621	20.77767	25.24498
50	7.223524	11.67739	16.02829	20.31865	11.58162	16.23574	20.77586	25.23948
80	7.223520	11.67738	16.02827	20.31861	11.58162	16.23574	20.77586	25.23948
100	7.223520	11.67738	16.02826	20.31861	11.58162	16.23574	20.77586	25.23948

Table II. Continued.

N	$A = 10$				$A = 100$			
	E_{02}	E_{12}	E_{22}	E_{32}	E_{02}	E_{12}	E_{22}	E_{32}
4	8.359469	12.71439	17.01900	21.64803	12.20447	16.82474	21.35907	26.39561
10	8.353878	12.69649	16.98150	21.23269	12.19960	16.80219	21.30703	25.74658
50	8.352485	12.69119	16.96827	21.20554	12.19954	16.80176	21.30532	25.74130
80	8.352484	12.69118	16.96826	21.20551	12.19954	16.80176	21.30532	25.74130
	E_{03}	E_{13}	E_{23}	E_{33}	E_{03}	E_{13}	E_{23}	E_{33}
4	9.842248	14.08045	18.29455	22.65344	13.09480	17.64362	22.12257	27.00246
10	9.839807	14.07164	18.27614	22.46330	13.09094	17.62527	22.08079	26.48231
50	9.839232	14.06906	18.26891	22.44709	13.09089	17.62489	22.07924	26.47740
80	9.839231	14.06906	18.26890	22.44708	13.09089	17.62489	22.07924	26.47740

	$A = 1000$							
N	E_{00}	E_{10}	E_{20}	E_{30}	E_{02}	E_{12}	E_{22}	E_{32}
4	21.37133	26.16834	30.88821	36.02221	21.82965	26.60243	31.30202	36.39355
10	21.36946	26.15319	30.85142	35.48293	21.82788	26.58806	31.26724	35.88294
50	21.36946	26.15318	30.85138	35.48270	21.82788	26.58805	31.26721	35.88271
80	21.36946	26.15318	30.85138	35.48270	21.82788	26.58805	31.26721	35.88271
	E_{01}	E_{11}	E_{21}	E_{31}	E_{03}	E_{13}	E_{23}	E_{33}
4	21.52469	26.31351	31.02654	36.14617	22.28273	27.03222	31.71227	36.76327
10	21.52286	26.29863	30.99044	35.61663	22.28106	27.01858	31.67938	36.27975
50	21.52286	26.29862	30.99040	35.61639	22.28106	27.01858	31.67934	36.27952
80	21.52286	26.29862	30.99040	35.61639	22.28106	27.01858	31.67934	36.27952

[a] ν is the number of radial nodes.

with the corresponding trends identified in Section 2; in the limit $\lambda \to l$, $\omega \to 1$ of equation (8), the difference between the Hamiltonians in equation (14) tends to zero.

4. DISCUSSION

The quantum mechanical solution of the supersingular plus quadratic potential was formulated in Section 3 through the construction and diagonalization of its Hamiltonian matrix, equation (15), in the bases of eigenfunctions of the appropriate centrifugal plus quadratic potentials, equation (9). The power and frequency parameters of the latter, λ and ω, were determined in Section 2 through the preliminary variational analysis of the radially nodeless states for each value of the orbital angular momentum l. Numerical results from the preliminary and more complete analysis for the energy eigenvalues of the respective states were presented through Tables I and II, illustrating

their global dependence on the intensity A of the supersingular component of the potential and on the orbital angular momentum l. Specifically, the supersingular component affects the states with lowest values of l the most; for large enough values of l the energy levels are slightly shifted upward from those of the harmonic oscillator, because the centrifugal effect practically nullifies the effect of the supersingular component. The convergence in the evaluation of the energy eigenvalues is fast (slow) for large (small) values of the intensity A, i.e., in the strong (weak) coupling regime.

The asymptotic form of the functions in the bases of equation (9) is determined by the quadratic component of the potential. The method of solution of this work can be adapted for the study of other potentials with supersingular and well-behaved components, the former determining the behavior of the wavefunction as $r \to 0$ and the latter as $r \to \infty$. Systematic work is being carried out for the investigation of other supersingular potentials.

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