Smooth transformations of Kratzer's potential in *N* dimensions

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We study smooth transformations $V(r)=g(-1/r)+f(1/r^2)$ of Kratzer's potential $-a/r+b/r^2$ in $N\geqslant 2$ spatial dimensions. Eigenvalue approximation formulas are obtained which provide lower or upper energy bounds for all the discrete energy eigenvalues E_{nl} and all $N\geqslant 2$, corresponding, respectively, to the two cases that the transformation functions g and f are either both convex ($g''\geqslant 0$) and $f''\geqslant 0$) or both concave ($g''\leqslant 0$ and $f''\leqslant 0$). Detailed results are presented for $V(r)=-a/r+b/r^{\beta}$ and $V(r)=-(v/r)[1-ar/(1+r)]+b/r^2$. © *1998 American Institute of Physics*. [S0021-9606(98)00332-8]

I. INTRODUCTION AND MAIN RESULT

Considerable interest has recently been shown in Kratzer's potential[1,2] as a model to describe internuclear vibration.[3–6] This potential can be expressed in the form

$$U(r)=-\frac{a}{r}+\frac{b}{r^2},\quad a,b>0. \tag{1}$$

It was also introduced[7–11] because it had some very general features of a molecular potential, and it was exactly soluble. In this paper we study smooth transformations $V(r)$ of Kratzer's potential with the general form

$$V(r)=f\left(-\frac{1}{r}\right)+g\left(\frac{1}{r^2}\right), \tag{2}$$

where the transformation functions f and g are smooth. This wider family of potentials includes examples of more physical significance such as

$$V(r)=-\frac{a}{r}+\frac{b}{r^{\beta}},\quad b>0, \tag{3}$$

which have been studied recently[12–15] as Coulomb problems with singular perturbations. The advantages of our approach are: (a) Our analytical expressions, which are obtained by a simple extremization over one or two variables, indicate approximately how the eigenvalues depend on all the parameters of the potential; (b) whenever the transformation functions f and g are either both convex or both concave (in the sense that f'' and $g''$are both positive or are both negative), the approximations provide, respectively, lower and upper energy *bounds* on all the discrete eigenvalues; (c) from the point of view of energy levels, the method selects a ''best'' Kratzer potential to approximate the problem studied which in turn leads to a ''best set'' of Kratzer wave functions that can be used as a basis set for closer approximations;[3–9] (d) in all the eigenvalue formulas the number $N\geqslant 2$ of spatial dimensions is a free parameter. This last feature, although usually not important for ''real'' applications, may be useful indirectly as a generator of test problems for the so-called large-N approximation.

The existence of bound states for Eq. (1) depends[16] on the presence of the term $-a/r$ which has an infinite discrete spectrum bounded above by zero for any $a>0$. The exact solutions of Schrödinger's equation with Kratzer's potential are given in terms of confluent hypergeometric functions.[17–19] Landau and Lifshitz,[19] for example, showed that the discrete energy spectrum for Kratzer potential is given (in units $\hbar=2m=1$) by

$$\epsilon_{nl}=-\frac{a^2}{(2n+1+\sqrt{(2l+1)^2+4b})^2},\quad n,l=0,1,2,\ldots. \tag{4}$$

It is interesting to extend these exact solutions to the N-dimensional case, which can be done[20] by replacing l in Eq. (4) with $l+N/2-3/2$. Indeed, these exact solutions could be generated from the well-known solutions of Coulomb potential by the following two simple transformations: First replace the angular momentum l in the Coulomb energy expression by $-\frac{1}{2}+\sqrt{(l+\frac{1}{2})^2+b}$, then replace l with $l+N/2-3/2$. Thus the exact eigenvalues of the N-dimensional Schrödinger equation with the Kratzer's potential are

$$\epsilon_{nl}=-\frac{a^2}{4(n+\frac{1}{2}+\sqrt{(l+N/2-1)^2+b})^2},\quad n,l=0,1,2,\ldots. \tag{5}$$

The purpose of this article is to use such solutions to investigate the discrete spectrum of the N-dimensional Schrödinger equation

$$[-\Delta+V(r)]\psi=E_{nl}\psi, \tag{6}$$

where $V(r)$ is given by Eq. (2). We shall show in Sec. II that E_{nl} can be approximated by the expression

$$\epsilon_{nl}(s,t)=g\left(-\frac{1}{s}\right)+\frac{g'(-1/s)}{s}+f\left(\frac{1}{t^2}\right)-\frac{f'(1/t^2)}{t^2}-\frac{[g'(-1/s)]^2}{4(n+\frac{1}{2}+\sqrt{(l+N/2)-1)^2+f'(1/t^2))^2}}, \tag{7}$$

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where the extreme value (min or max) of $\epsilon_{nl}(s,t)$ provides a lower bound or an upper bound to the corresponding exact eigenvalue when the transformation functions g and f are, respectively, either both convex or both concave (that is to say, g'' and f'' are both positive or both negative). This allows us, for example, to obtain simple expressions which bound the discrete spectrum of the generalized Kratzer's potential $V(r)=-(a/r)+(b/r^{\beta})$, $\beta>0$, for all dimensions $N\geqslant 2$.

II. TRANSFORMED POTENTIALS

We consider the Schrödinger equation

$$[-\Delta+V(r)]\psi=E_{nl}\psi, \tag{8}$$

$$V(r)=g\left(-\frac{1}{r}\right)+f\left(\frac{1}{r^2}\right), \tag{9}$$

in N-dimensions, where g and f are smooth transformations of $-1/r$ and $1/r^2$, respectively. For example, when g and f are identity transformations, the problem has the exact solution (5) for all n, l, and arbitrary positive values of a and b in all dimensions.

The core of our technique lies in noticing that each term of the potential (9) can be approximated by its tangential approximation. That is to say, we replace g and f in Eq. (9) by

$$\begin{aligned} g^{(s)}\left(-\frac{1}{r}\right)&=a(s)-\frac{b(s)}{r},\\ f^{(t)}\left(\frac{1}{r^2}\right)&=c(t)+\frac{d(t)}{r^2}, \end{aligned} \tag{10}$$

respectively, where s is a contact point between $g(-1/r)$ and its tangent approximation $g^{(s)}(1/r^2)$, and t plays a similar role for f. Elementary analysis implies that $V(r)$ in Eq. (9) can thus be approximated by

$$\begin{aligned} V^{(s,t)}(r)=g\left(-\frac{1}{s}\right)+\frac{g'(-1/s)}{s}+f\left(\frac{1}{t^2}\right)-\frac{f'(1/t^2)}{t^2}\\ -\frac{g'(-1/s)}{r}+\frac{f'(1/t^2)}{r^2}. \end{aligned} \tag{11}$$

This two-parameter family of ''tangent'' potentials generates the so-called ''envelope representation'' for $V(r)$ expressed by

$$V(r)=\underset{s,t>0}{\text{Envelope}}\{V^{(s,t)}(r)\}.$$

With this representation of $V(r)$, we may use the energy expression (5) for the eigenvalues of the Schrödinger equation

$$[-\Delta+V^{(s,t)}(r)]\psi=\epsilon_{nl}(s,t)\psi. \tag{12}$$

which implies that $\epsilon_{nl}(s,t)$is given by Eq. (7). Now an application of the comparison theorem in quantum mechanics allow us to conclude the following. For the eigenvalues E_{nl} of the Schrödinger Eq. (8), we have

TABLE I. Some lower bounds E_{01}^{L} and upper bounds E_{01}^{U} using Eq. (13) for $H=-\Delta-5/r+1/r^{\beta}$ in three-dimensions with $l=1$. The ''exact'' values E_{01} were obtained by direct numerical integration of Schrödinger's equation.

β	E_{01}^{L}	E_{01}	E_{01}^{U}
1.5	⋯	−1.111 34	−1.073 66
1.6	⋯	−1.127 68	−1.097 39
1.7	⋯	−1.142 44	−1.119 66
1.8	⋯	−1.155 77	−1.140 56
1.9	⋯	−1.167 79	−1.160 19
2	−1.178 63	−1.178 63	−1.178 63
2.1	−1.195 96	−1.188 38	⋯
2.2	−1.212 28	−1.197 18	⋯
2.3	−1.227 65	−1.205 08	⋯
2.4	−1.242 14	−1.212 19	⋯
2.5	−1.255 81	−1.218 58	⋯

(a) $E_{nl}\leqslant\epsilon_{nl}(s,t)$ if g'' and f'' are both positive.

(b) $E_{nl}\geqslant\epsilon_{nl}(s,t)$ if g'' and f'' are both negative.

The proof of this claim is obtained by the following simple argument. For definiteness we consider case (a). Since g and f are convex (g'' and f'' are both positive), their graphs lie above their tangents. Consequently, we have from Eq. (11) that $V^{(s,t)}(r)\leqslant V(r)\forall s,\ t>0$. Case (a) then follows by an application of the comparison theorem. Case (b) is proved in analogous way if ''convex'' is replaced by ''concave'' (g'' and f'' are both negative). It is appropriate to mention here that the conclusions follow in the special cases that either f or g is the identity transformation. These bounds may, of course, be sharpened by optimization with respect to s and t, and moreover they are valid for the entire discrete spectrum $n,l\geqslant 0$.

III. NUMERICAL RESULTS AND CONCLUSION

One of the interesting points concerning the bounds we have obtained in the previous section is the large variety of approximations made possible by different choices of the transformations g and f. We consider, for example, the case where $g(-1/r)=-a/r$ and $f(1/r^2)=b/r^{\beta}$ yields the generalized Kratzer potential (3). From Eqs. (8) and (12) we find that

$$E_{nl}\approx\epsilon_{nl}(t),\quad \text{where}\quad \epsilon'_{nl}(\hat{t})=0$$

and from Eq. (7)

$$\begin{aligned} \epsilon_{nl}(t)=\left(1-\frac{\beta}{2}\right)\frac{b}{t^{\beta}}\\ -\frac{a^2}{4(n+\frac{1}{2}+\sqrt{(l+N/2-1)^2+\beta b/2t^{\beta-2}})^2}. \end{aligned} \tag{13}$$

This function is convex in t [$\epsilon''_{nl}(t)>0$] for $\beta>2$ the maximum providing a lower energy bound, and concave [$\epsilon''_{nl}(t)<0$] for $\beta<2$ yielding an upper energy bound. In Table I we exhibit some results of the upper and lower bounds derived from Eq. (13) for $a=5$, $b=1$, $n=0$, $l=1$, and for different values of β in three-dimensional space, along with some accurate values obtained by direct numerical integration of

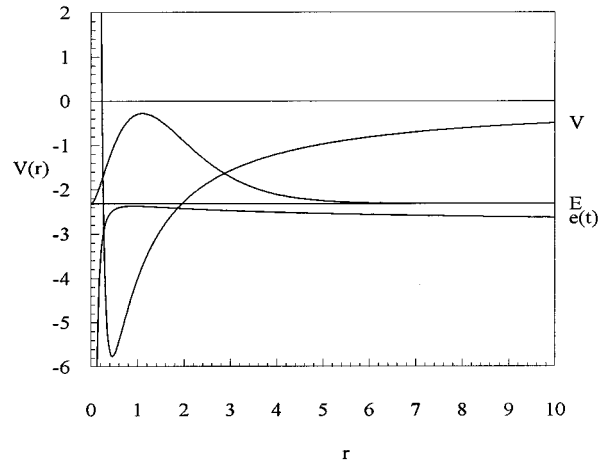

FIG. 1. Graph of $e(t)=\epsilon_{01}(t)$ along with the exact eigenvalue E and corresponding unnormalized wave function in three-dimensions.

Schrödinger's equation. The graph of $\epsilon_{01}(t)$ is displayed in Fig. 1 along with the exact eigenvalue E and corresponding unnormalized wavefunction in three-dimensions for Schrödinger's equation with $V(r)=-5/r+1/r^{2.1}$. The main advantage of an analytic approximation such as Eq. (13) is that questions to do with the dependence of the eigenvalues on the potential parameters are easy to answer. For example, in Fig. 2, we plot the lower bound obtained by Eq. (13), for $\beta=2.1$ and for $a=5$, as a function of the parameter b, along with some exact eigenvalues obtained by direct numerical integration. In Table II we exhibit the results of the lower bounds obtained by use of formula (13) for $\beta=2.1$ and for $a=5$, $b=1$ for the dimensions $N=2$ to $N=10$, along with some accurate values obtained by direct numerical integration of Schrödinger's equation.

As another example we consider $g(-1/r)=-v/r[1-ar/(1+r)]$ where v and $a\leqslant 1$ are positive parameters and $f(1/r^2)=b/r^2$. In this case g is the well known screened Coulomb potential[21,22] which is almost Coulombic everywhere for it is like $-v/r$ for small r and like $-v(1-a)/r$ for large r. Therefore it becomes very effective to represent the screened Coulomb potential as a smooth (concave) transformation of $-1/r$. For this choice of g and f we have from Eq. (7) that

$$\epsilon_{nl}(s)=\frac{av}{(1+s)^2}-\frac{v^2[1-as^2/(1+s)^2]^2}{4(n+\frac{1}{2}+\sqrt{(l+N/2)-1})^2+b)^2}, \tag{14}$$

which is concave in s (that is to say, it has a negative second derivative); in this case, $\epsilon_{nl}(s)$ leads to a simple upper-bound energy formula valid for all n, l, and arbitrary dimension $N\geqslant 2$. These upper bounds indicate approximately how the eigenvalues E_{nl} depend on all the potential parameters. We display some results obtained by formula (14) in Table III for $v=5$, $a=0.5$, and $b=1$ in dimension $N=2-10$. It is appropriate to mention here that in the limit as $b\to 0$ we recover the Coulomb envelopes[23] used for the special case $N=3$.

For the bottom of each angular-momentum subspace the bounds we have obtained can be improved by the use of a refined version of the comparison theorem.[24] However, the main point of the approach described in this paper is to provide a way to generate simple general approximate energy formulas to be used for exploratory purposes and for "seeding" direct numerical methods. Meanwhile, the Kratzer class of wave functions obtained are already optimally adapted to the problem at hand and, therefore, provide a best set of basis wave functions for higher-order perturbative or variational calculations.[3–9]

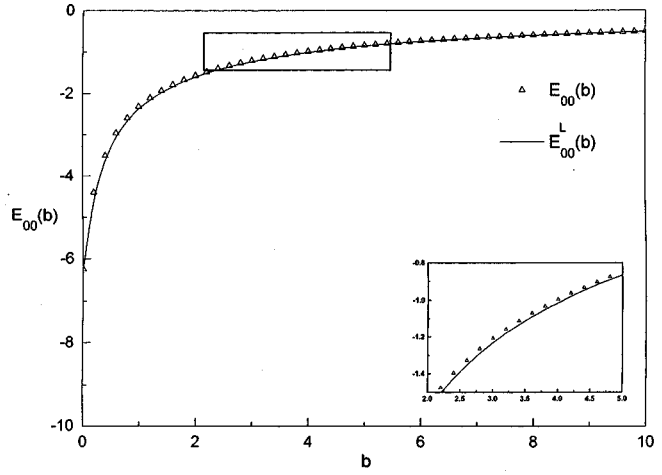

FIG. 2. The graph of the lower bound E_{00}^L obtained by Eq. (13) as a function of the parameter b, along with some exact eigenvalues E_{00} obtained by direct numerical integration.

TABLE II. Lower bounds E_{00}^L using Eq. (13) for $H=-\Delta-(5/r)+(1/r^{2.1})$ for dimension $N=2-10$. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{00}^L	E_{00}
2	−2.728 16	−2.650 75
3	−2.371 92	−2.319 71
4	−1.720 24	−1.699 15
5	−1.195 96	−1.188 39
6	−0.847 88	−0.844 98
7	−0.622 07	−0.620 84
8	−0.472 00	−0.471 43
9	−0.368 78	−0.368 49
10	−0.295 33	−0.295 17

TABLE III. Upper bounds E_{00}^U using Eq. (14) for $H=-\Delta-5/r[1-(0.5r)/(1+r)]+1/r^2$ for dimension $N=2-10$. The "exact" values E_{00} were obtained by direct numerical integration of Schrödinger's equation.

N	E_{00}	E_{00}^U
2	−1.598 63	−1.502 02
3	−1.296 02	−1.213 58
4	−0.808 11	−0.754 90
5	−0.481 10	−0.452 67
6	−0.300 88	−0.286 88
7	−0.201 54	−0.194 66
8	−0.143 49	−0.139 97
9	−0.107 23	−0.105 33
10	−0.083 20	−0.082 12

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