Solutions of the Schrödinger equation for an attractive $1/r^6$ potential

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Mathematical methods are presented that give pairs of linearly independent solutions for an attractive $1/r^6$ potential. These solutions represent a different class of special functions that are important to the understanding of molecular vibration spectra near the dissociation threshold and slow atomic collisions. [S1050-2947(98)04809-4]

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I. INTRODUCTION

The knowledge of Coulomb functions has played a key role in our understanding of atomic spectra and electron-ion collisions. It is the cornerstone of quantum defect theory (QDT), which provides a systematic understanding of atomic spectra near thresholds and relate properties of bound or quasibound states to properties of electron-ion scattering [1,2]. The availability of Coulomb functions also greatly reduces the configuration space that has to be treated numerically and leads to powerful computational methods such as the eigenchannel R-matrix method [3]. The solutions of the Schrödinger equation for an attractive $1/r^6$ potential, to be presented in this paper, play a similarly important role for molecular vibration spectra and atom-atom collisions [4].

Consider the radial Schrödinger equation for a $-C_n/r^n$ potential:

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+\frac{\beta_n^{n-2}}{r^n}+\bar{\epsilon}\right]u_l(r)=0, \tag{1}$$

where $\beta_n \equiv (2\mu C_n/\hbar^2)^{1/(n-2)}$ and $\bar{\epsilon}=2\mu\epsilon/\hbar^2$. The solutions of this equation are well known for $n=1,2$. They are also easily obtained for arbitrary n at $\epsilon=0$. In all these cases, Eq. (1) has only a single irregular singularity. What makes the cases of $n>2$ and $\epsilon\neq 0$ fundamentally different is the existence of two irregular singularities, one at zero and the other at infinity. For $n=4$, the solutions can be expressed in terms of Mathieu functions [5,6]. For $n=6$, however, Eq. (1) cannot be transformed into one that is satisfied by any known special function and different mathematical methods are required.

II. SUMMARY OF THE SOLUTION

Motivated by an observation of Cavagnero [7], we have found for an attractive $1/r^6$ potential that a pair of linearly independent solutions with energy-independent normalization near the origin can be written as

$$f^0_{\epsilon l}(r)=(\alpha^2_{\epsilon l}+\beta^2_{\epsilon l})^{-1}[\alpha_{\epsilon l}\bar{f}_{\epsilon l}(r)-\beta_{\epsilon l}\bar{g}_{\epsilon l}(r)], \tag{2}$$

$$g^0_{\epsilon l}(r)=(\alpha^2_{\epsilon l}+\beta^2_{\epsilon l})^{-1}[\beta_{\epsilon l}\bar{f}_{\epsilon l}(r)+\alpha_{\epsilon l}\bar{g}_{\epsilon l}(r)], \tag{3}$$

where $\bar{f}$ and $\bar{g}$ are another pair of linearly independent solutions given by

$$\bar{f}_{\epsilon l}(r)=\sum_{m=-\infty}^{\infty} b_m r^{1/2} J_{\nu+m}\left(\frac{1}{2}(r/\beta_6)^{-2}\right), \tag{4}$$

$$\bar{g}_{\epsilon l}(r)=\sum_{m=-\infty}^{\infty} b_m r^{1/2} Y_{\nu+m}\left(\frac{1}{2}(r/\beta_6)^{-2}\right), \tag{5}$$

and

$$\alpha_{\epsilon l}=\cos[\pi(\nu-\nu_0)/2]X_{\epsilon l}-\sin[\pi(\nu-\nu_0)/2]Y_{\epsilon l}, \tag{6}$$

$$\beta_{\epsilon l}=\sin[\pi(\nu-\nu_0)/2]X_{\epsilon l}+\cos[\pi(\nu-\nu_0)/2]Y_{\epsilon l}, \tag{7}$$

$$X_{\epsilon l}=\sum_{m=-\infty}^{\infty}(-1)^m b_{2m}, \tag{8}$$

$$Y_{\epsilon l}=\sum_{m=-\infty}^{\infty}(-1)^m b_{2m+1}, \tag{9}$$

$$b_j=(-\Delta)^j\frac{\Gamma(\nu)\Gamma(\nu-\nu_0+1)\Gamma(\nu+\nu_0+1)}{\Gamma(\nu+j)\Gamma(\nu-\nu_0+j+1)\Gamma(\nu+\nu_0+j+1)}c_j(\nu), \tag{10}$$

$$b_{-j}=(-\Delta)^j\frac{\Gamma(\nu-j+1)\Gamma(\nu-\nu_0-j)\Gamma(\nu+\nu_0-j)}{\Gamma(\nu+1)\Gamma(\nu-\nu_0)\Gamma(\nu+\nu_0)}c_j(-\nu). \tag{11}$$

In Eqs. (10) and (11), j is a positive integer, Δ is a scaled energy defined by

$$\Delta\equiv\bar{\epsilon}\beta_6^2/16=\frac{1}{16}\frac{\epsilon}{(\hbar^2/2\mu)(1/\beta_6)^2}, \tag{12}$$

ν_0 is related to angular momentum l by $\nu_0=(2l+1)/4$, and

$$c_j(\nu)=b_0 Q(\nu)Q(\nu+1)\cdots Q(\nu+j-1). \tag{13}$$

The coefficient b_0 is a normalization constant that can be set to 1 and $Q(\nu)$ is given by a continued fraction

$$Q(\nu)=\frac{1}{1-\Delta^2\dfrac{1}{(\nu+1)[(\nu+1)^2-\nu_0^2](\nu+2)[(\nu+2)^2-\nu_0^2]}Q(\nu+1)}. \tag{14}$$

Finally, ν is a root, which can be complex, of a characteristic function

$$\Lambda_l(\nu;\Delta^2)\equiv(\nu^2-\nu_0^2)-(\Delta^2/\nu)[\bar{Q}(\nu)-\bar{Q}(-\nu)], \tag{15}$$

in which

$$\bar{Q}(\nu)\equiv\{(\nu+1)[(\nu+1)^2-\nu_0^2]\}^{-1}Q(\nu). \tag{16}$$

The pair of solutions f^0 and g^0 have been defined in such a way that they have energy-independent normalization near the origin with asymptotic behaviors given by

$$f^0_{\epsilon l}(r)\underset{r\to 0}{\to}\sqrt{\frac{4}{\pi}}(r/\beta_6)r^{1/2}\cos\left(\frac{1}{2}(r/\beta_6)^{-2}-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right), \tag{17}$$

$$g^0_{\epsilon l}(r)\underset{r\to 0}{\to}\sqrt{\frac{4}{\pi}}(r/\beta_6)r^{1/2}\sin\left(\frac{1}{2}(r/\beta_6)^{-2}-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right) \tag{18}$$

for both positive and negative energies. Their asymptotic behaviors at large r are given for $\epsilon>0$ by

$$f^0_{\epsilon l}(r)\underset{r\to\infty}{\to}\sqrt{\frac{2}{\pi k}}\left[Z_{ff}\sin\left(kr-\frac{l\pi}{2}\right)-Z_{fg}\cos\left(kr-\frac{l\pi}{2}\right)\right], \tag{19}$$

$$g^0_{\epsilon l}(r)\underset{r\to\infty}{\to}\sqrt{\frac{2}{\pi k}}\left[Z_{gf}\sin\left(kr-\frac{l\pi}{2}\right)-Z_{gg}\cos\left(kr-\frac{l\pi}{2}\right)\right], \tag{20}$$

where $k=(2\mu\epsilon/\hbar^2)^{1/2}$ and

$$Z_{ff}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin(\pi\nu)]^{-1}\{-(-1)^l[\alpha_{\epsilon l}\sin(\pi\nu)-\beta_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)\sin(\pi\nu-l\pi/2-\pi/4)$$
$$+\beta_{\epsilon l}G_{\epsilon l}(\nu)\cos(\pi\nu-l\pi/2-\pi/4)\}, \tag{21}$$

$$Z_{fg}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin(\pi\nu)]^{-1}\{-(-1)^l[\alpha_{\epsilon l}\sin(\pi\nu)-\beta_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)\cos(\pi\nu-l\pi/2-\pi/4)$$
$$+\beta_{\epsilon l}G_{\epsilon l}(\nu)\sin(\pi\nu-l\pi/2-\pi/4)\}, \tag{22}$$

$$Z_{gf}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin(\pi\nu)]^{-1}\{-(-1)^l[\beta_{\epsilon l}\sin(\pi\nu)+\alpha_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)\sin(\pi\nu-l\pi/2-\pi/4)$$
$$-\alpha_{\epsilon l}G_{\epsilon l}(\nu)\cos(\pi\nu-l\pi/2-\pi/4)\}, \tag{23}$$

$$Z_{gg}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin(\pi\nu)]^{-1}\{-(-1)^l[\beta_{\epsilon l}\sin(\pi\nu)+\alpha_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)\cos(\pi\nu-l\pi/2-\pi/4)$$
$$-\alpha_{\epsilon l}G_{\epsilon l}(\nu)\sin(\pi\nu-l\pi/2-\pi/4)\}, \tag{24}$$

in which

$$G_{\epsilon l}(\nu)=|\Delta|^{-\nu}\frac{\Gamma(1+\nu_0+\nu)\Gamma(1-\nu_0+\nu)}{\Gamma(1-\nu)}C(\nu) \tag{25}$$

and $C(\nu)=\lim_{j\to\infty}c_j(\nu)$.

For $\epsilon<0$, f^0 and g^0 have asymptotic behaviors given by

$$f^0_{\epsilon l}\underset{r\to\infty}{\to}r^{1/2}\lim_{r\to\infty}\left[W_{fI}I_{2\nu}(\kappa r)+W_{fK}\frac{1}{\pi}K_{2\nu}(\kappa r)\right], \tag{26}$$

$$g^0_{\epsilon l} \underset{r\to\infty}{\to} r^{1/2} \lim_{r\to\infty}\left[W_{gI} I_{2\nu}(\kappa r) + W_{gK}\frac{1}{\pi}K_{2\nu}(\kappa r)\right], \tag{27}$$

where $\kappa=(2\mu|\epsilon|/\hbar^2)^{1/2}$ and

$$W_{fI}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin(\pi\nu)]^{-1}\{[\alpha_{\epsilon l}\sin(\pi\nu)-\beta_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)+\beta_{\epsilon l}G_{\epsilon l}(\nu)\}, \tag{28}$$

$$W_{fK}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})]^{-1}2[\alpha_{\epsilon l}\sin(2\pi\nu)-\beta_{\epsilon l}\cos(2\pi\nu)-\beta_{\epsilon l}]G_{\epsilon l}(-\nu), \tag{29}$$

$$W_{gI}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})\sin(\pi\nu)]^{-1}\{[\beta_{\epsilon l}\sin(\pi\nu)+\alpha_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)-\alpha_{\epsilon l}G_{\epsilon l}(\nu)\}, \tag{30}$$

$$W_{gK}=[(X^2_{\epsilon l}+Y^2_{\epsilon l})]^{-1}2[\beta_{\epsilon l}\sin(2\pi\nu)+\alpha_{\epsilon l}\cos(2\pi\nu)+\alpha_{\epsilon l}]G_{\epsilon l}(-\nu). \tag{31}$$

It is important to note that both the Z and the W matrices for a specific l are universal functions of Δ that are independent of the specific value of C_6. Different C_6 coefficients only scale the energy differently according to Eq. (12).

III. DERIVATION OF THE SOLUTION

The key steps in arriving at this solution can be summarized as follows. First, express the solution as a generalized Neumann expansion with proper argument so that the coefficients satisfy a three-term recurrence relation. Second, solve the recurrence relation using continued fractions. Third, sum a corresponding Laurent-type expansion to obtain the asymptotic behavior at infinity.

A. Change of variable and Neumann expansion

Through a change of variable defined by

$$x=(r/L)^{\alpha}, \tag{32}$$

$$u_l(r)=r^{1/2}f(x), \tag{33}$$

with $\alpha=-2$ and $L=(1/2)^{1/2}\beta_6$, Eq. (1) can be written as

$$\left[x^2\frac{d^2}{dx^2}+x\frac{d}{dx}+x^2-\nu_0^2\right]f(x)=-2\Delta\frac{1}{x}f(x), \tag{34}$$

in which Δ is the scaled energy defined by Eq. (12). Expanding $f(x)$ in a Neumann expansion [7,8]

$$f(x)=\sum_{m=-\infty}^{\infty} b_m \mathcal{J}_{\nu+m}(x), \tag{35}$$

where $\mathcal{J}$ can be either J or Y, and making use of the property of Bessel functions [8]

$$x^{-1}\mathcal{J}_{\nu+m}(x)=[2(\nu+m)]^{-1}[\mathcal{J}_{\nu+m+1}(x)+\mathcal{J}_{\nu+m-1}(x)], \tag{36}$$

one can easily show that the coefficients b_m satisfy a three-term recurrence relation

$$\Delta(\nu+m+1)^{-1}b_{m+1}+[(\nu+m)^2-\nu_0^2]b_m + \Delta(\nu+m-1)^{-1}b_{m-1}=0. \tag{37}$$

B. Solution of the recurrence relation

The three-term recurrence relations for $m\geqslant 1$ are solved by defining

$$b_j=(-\Delta)^j\frac{\Gamma(\nu)\Gamma(\nu-\nu_0+1)\Gamma(\nu+\nu_0+1)}{\Gamma(\nu+j)\Gamma(\nu-\nu_0+j+1)\Gamma(\nu+\nu_0+j+1)}c_j^+ \tag{38}$$

for $j\geqslant 0$ and

$$Q_j^+=c_{j+1}^+/c_j^+ . \tag{39}$$

It is then easily shown that Q_j^+ is given by a continued fraction

$$Q_j^+=\cfrac{1}{1-\Delta^2\dfrac{1}{(\nu+j+1)[(\nu+j+1)^2-\nu_0^2](\nu+j+2)[(\nu+j+2)^2-\nu_0^2]}Q_{j+1}^+} \tag{40}$$

and

$$c_j^+(\nu)=Q_{j-1}^+Q_{j-2}^+\cdots Q_0^+b_0. \tag{41}$$

The recurrence relations for $m\leqslant -1$ are solved in terms of b_0 by defining

$$b_{-j}=(-\Delta)^j\frac{\Gamma(\nu-j+1)\Gamma(\nu-\nu_0-j)\Gamma(\nu+\nu_0-j)}{\Gamma(\nu+1)\Gamma(\nu-\nu_0)\Gamma(\nu+\nu_0)}c_j^- \tag{42}$$

for $j\geqslant 0$ and

$$Q_j^-=c_{j+1}^-/c_j^- . \tag{43}$$

Q_j^- is then given by a continued fraction

$$Q_j^-=\frac{1}{1-\Delta^2\dfrac{1}{(\nu-j-1)[(\nu-j-1)^2-\nu_0^2](\nu-j-2)[(\nu-j-2)^2-\nu_0^2]}Q_{j+1}^-} \tag{44}$$

and

$$c_j^-(\nu)=Q_{j-1}^-Q_{j-2}^-\cdots Q_0^-b_0. \tag{45}$$

From Eqs. (40) and (44), Q_j^+ and Q_j^- have the properties

$$Q_j^+(\nu)\underset{j\to\infty}{\longrightarrow}1, \tag{46}$$

$$Q_j^-(\nu)\underset{j\to\infty}{\longrightarrow}1, \tag{47}$$

$$Q_j^+(\nu)=Q_0^+(\nu+j), \tag{48}$$

$$Q_j^-(\nu)=Q_0^-(\nu-j), \tag{49}$$

$$Q_j^-(\nu)=Q_j^+(-\nu). \tag{50}$$

By defining

$$Q(\nu)\equiv Q_0^+(\nu), \tag{51}$$

one can write Q_j^+ and Q_j^- in terms of a single function $Q(\nu)$ as

$$Q_j^+(\nu)=Q(\nu+j), \tag{52}$$

$$Q_j^-(\nu)=Q(-\nu+j), \tag{53}$$

where function Q is given by the continued fraction (14). By defining c_j as in Eq. (13), c_j^+ and c_j^- can be written as

$$c_j^+(\nu)=c_j(\nu), \tag{54}$$

$$c_j^-(\nu)=c_j(-\nu), \tag{55}$$

which correspond to the notation used in Eqs. (10) and (11). Finally, the recurrence relation for $m=0$,

$$\Delta(\nu+1)^{-1}b_1+(\nu^2-\nu_0^2)b_0+\Delta(\nu-1)^{-1}b_{-1}=0, \tag{56}$$

requires the ν to be a root of the characteristic function defined by Eq. (15). The same set of coefficients b_m gives two linearly independent solutions corresponding to using either J or Y in Eq. (35).

C. Asymptotic behaviors

The asymptotic behaviors of $\overline{f}$ and $\overline{g}$ for small r are straightforward. From the asymptotic expansions of Bessel functions for large arguments [8] we have

$$\overline{f}_{\epsilon l}(r)\underset{r\to 0}{\longrightarrow}\sqrt{\frac{4}{\pi}}(r/\beta_6)r^{1/2}\left[\alpha_{\epsilon l}\cos\left(\frac{1}{2}(r/\beta_6)^{-2}-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)+\beta_{\epsilon l}\sin\left(\frac{1}{2}(r/\beta_6)^{-2}-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)\right], \tag{57}$$

$$\overline{g}_{\epsilon l}(r)\underset{r\to 0}{\longrightarrow}\sqrt{\frac{4}{\pi}}(r/\beta_6)r^{1/2}\left[-\beta_{\epsilon l}\cos\left(\frac{1}{2}(r/\beta_6)^{-2}-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)+\alpha_{\epsilon l}\sin\left(\frac{1}{2}(r/\beta_6)^{-2}-\frac{\nu_0\pi}{2}-\frac{\pi}{4}\right)\right], \tag{58}$$

TABLE I. Critical scaled energy for different angular momenta l.

l	Δ_c
s	9.654418×10^{-2}
p	1.473792×10^{-1}
d	4.306921×10^{-1}
f	1.580826
g	2.073296

where α and β are defined in Eqs. (6) and (7). The pair of functions f^0 and g^0 has been defined in Eqs. (2) and (3) such that each has energy-independent normalization near the origin with asymptotic behaviors characterized by Eqs. (17) and (18).

For the derivation of asymptotic behaviors at large r, it is more convenient to use the pair of functions

$$\xi_{\epsilon l}(r)=\sum_{m=-\infty}^{\infty} b_m r^{1/2} J_{\nu+m}\left(\frac{1}{2}(r/\beta_6)^{-2}\right), \tag{59}$$

$$\eta_{\epsilon l}(r)=\sum_{m=-\infty}^{\infty} (-1)^m b_m r^{1/2} J_{-\nu-m}\left(\frac{1}{2}(r/\beta_6)^{-2}\right), \tag{60}$$

which are related to $\overline{f}$ and $\overline{g}$ by

$$\overline{f}_{\epsilon l}(r)=\xi_{\epsilon l}(r), \tag{61}$$

$$\overline{g}_{\epsilon l}(r)=\frac{1}{\sin(\pi\nu)}[\xi_{\epsilon l}\cos(\pi\nu)-\eta_{\epsilon l}]. \tag{62}$$

For $\epsilon>0$, $\Delta=k^2\beta_6^2/16$ and one can rewrite ξ function as a Laurent-type expansion

$$\xi_{\epsilon l}(r)=r^{1/2}(kr/2)^{-2\nu}\sum_{m=-\infty}^{\infty} p_m (kr/2)^{2m}, \tag{63}$$

where

$$p_m=\Delta^{\nu}\sum_{s=0}^{\infty}\frac{(-1)^s}{s!\Gamma(\nu-m-s+1)}\Delta^{2s}[\Delta^{-(m+2s)}b_{-(m+2s)}]. \tag{64}$$

The key to deriving the asymptotic behavior at large r is to recognize that the asymptotic behavior of a Laurent-type expansion, such as the one in Eq. (63), depends only on the m dependence of p_m for large m [9]. Making use of the properties of the Γ function for large arguments [8] and the properties of b_{-j} for large j as embedded in Eq. (47), one can show that

$$p_m \underset{m\to\infty}{\longrightarrow} G_{\epsilon l}(-\nu)(-1)^m\frac{1}{m!\Gamma(-2\nu+m+1)}, \tag{65}$$

where $G_{\epsilon l}(\nu)$ is defined by Eq. (25). Comparing the m dependence of p_m with the coefficients of the Bessel function, we have

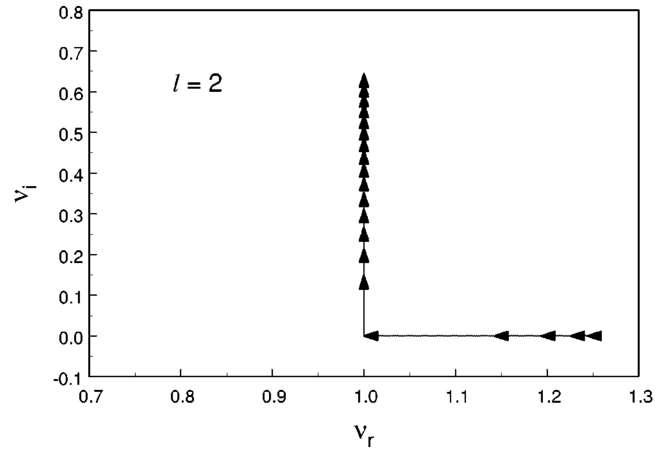

FIG. 1. Movement of the root of the characteristic function for $l=2$. ν_r and ν_i represent the real and imaginary parts of ν, respectively. The root becomes complex beyond Δ_c.

$$\xi_{\epsilon l}(r)\underset{r\to\infty}{\longrightarrow} G_{\epsilon l}(-\nu)r^{1/2}\lim_{r\to\infty}J_{-2\nu}(kr)\to\sqrt{\frac{2}{\pi k}}(-1)^l G_{\epsilon l}(-\nu)\times\left[-\sin\left(\pi\nu-\frac{l\pi}{2}-\frac{\pi}{4}\right)\sin\left(kr-\frac{l\pi}{2}\right)+\cos\left(\pi\nu-\frac{l\pi}{2}-\frac{\pi}{4}\right)\cos\left(kr-\frac{l\pi}{2}\right)\right]. \tag{66}$$

Similarly for the η function, we have

$$\eta_{\epsilon l}(r)\underset{r\to\infty}{\longrightarrow} G_{\epsilon l}(\nu)r^{1/2}\lim_{r\to\infty}J_{2\nu}(kr)\to\sqrt{\frac{2}{\pi k}}G_{\epsilon l}(\nu)\left[\cos\left(\pi\nu-\frac{l\pi}{2}-\frac{\pi}{4}\right)\sin\left(kr-\frac{l\pi}{2}\right)-\sin\left(\pi\nu-\frac{l\pi}{2}-\frac{\pi}{4}\right)\cos\left(kr-\frac{l\pi}{2}\right)\right]. \tag{67}$$

For $\epsilon<0$, $\Delta=-\kappa^2\beta_6^2/16$ and a similar procedure leads to

$$\xi_{\epsilon l}\underset{r\to\infty}{\longrightarrow} G_{\epsilon l}(-\nu)r^{1/2}\lim_{r\to\infty}I_{-2\nu}(\kappa r)$$

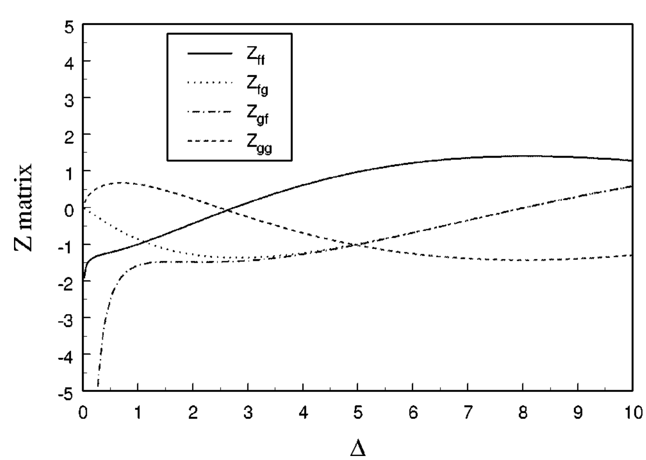

FIG. 2. Z matrix for $l=2$.

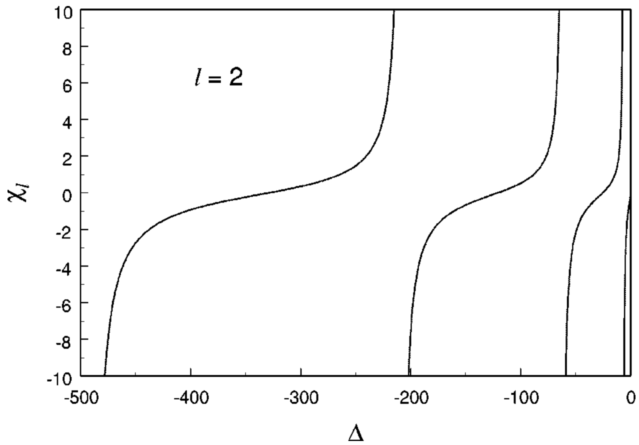

FIG. 3. $\chi_l(\Delta)$ function for $l=2$.

$$=G_{\epsilon l}(-\nu)r^{1/2}\lim_{r\to\infty}\left[I_{2\nu}(\kappa r)+\frac{2\sin(2\pi\nu)}{\pi}K_{2\nu}(\kappa r)\right], \tag{68}$$

$$\eta_{\epsilon l}\underset{r\to\infty}{\to}G_{\epsilon l}(\nu)r^{1/2}\lim_{r\to\infty}I_{2\nu}(\kappa r). \tag{69}$$

The asymptotic behaviors of other pairs of functions are easily obtained from the asymptotic behaviors of ξ and η.

IV. DISCUSSION

A. Computation

The computation is most conveniently carried by starting with $\overline{Q}$ as defined in Eq. (16). It is given by a continued fraction

$$\overline{Q}(\nu)=\frac{1}{(\nu+1)[(\nu+1)^2-\nu_0^2]-\Delta^2\overline{Q}(\nu+1)}, \tag{70}$$

which can be calculated following standard procedures [10].

B. Roots of the characteristic function

The characteristic function $\Lambda_l(\nu;\Delta^2)$ defined by Eq. (15) is a function of ν with Δ^2 as a parameter (thus independent of the sign of Δ). Consistent with the Neumann expansion, the roots of this function have the following properties: (i) If ν is a solution, $-\nu$ is also a solution; (ii) if ν is a solution, ν^* is also a solution; and (iii) if ν is a noninteger solution, $\pm\nu+n$, where n, an integer, is also a solution. To ensure continuity across the threshold, the proper root to take is the one that originates at ν_0 at $\Delta=0$. Using the property of the roots mentioned above, it can be shown that this root becomes complex beyond a critical scaled energy Δ_c determined by

$$\Lambda_l(\nu=0;\Delta^2)=-\nu_0^2-2\Delta^2\overline{Q}'(\nu=0)=0. \tag{71}$$

The critical scaled energy corresponds to the Δ at which the root that started out at ν_0 coalesces with another root (from $-\nu+n$) at

$$\nu=n_l=\begin{cases} l/2, & l \text{ even} \\ (l-1)/2+1, & l \text{ odd.}\end{cases} \tag{72}$$

This pair of roots becomes a complex pair $\nu=n_l+i\nu_i$ and ν^* for $|\Delta|>\Delta_c$ [11]. Both ν and ν^* give the same physical results and we will take the one with positive imaginary part. Table I lists Δ_c for the first few partial waves. Figure 1 illustrates the movement of this root for $l=2$.

C. Key functions

In a quantum defect theory based on this set of solutions [4], the key functions involved above the threshold is the Z matrix, which is the transformation matrix relating the energy-normalized solution pair defined by

$$f_{\epsilon l}(r)\underset{r\to\infty}{\to}\sqrt{\frac{2}{\pi k}}\sin\left(kr-\frac{l\pi}{2}\right), \tag{73}$$

$$g_{\epsilon l}(r)\underset{r\to\infty}{\to}-\sqrt{\frac{2}{\pi k}}\cos\left(kr-\frac{l\pi}{2}\right) \tag{74}$$

to the set of solutions with energy-independent normalization near the origin. This relation in matrix form is [cf. Eqs. (19) and (20)]

$$\begin{pmatrix} f^0 \\ g^0 \end{pmatrix}=\begin{pmatrix} Z_{ff} & Z_{fg} \\ Z_{gf} & Z_{gg}\end{pmatrix}\begin{pmatrix} f \\ g\end{pmatrix}. \tag{75}$$

Figure 2 is a plot of the Z matrix for $l=2$.

Below threshold, the key function involved in a QDT formulation of bound states is

$$\chi_l\equiv W_{fI}/W_{gI}=\frac{[\alpha_{\epsilon l}\sin(\pi\nu)-\beta_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)+\beta_{\epsilon l}G_{\epsilon l}(\nu)}{[\beta_{\epsilon l}\sin(\pi\nu)+\alpha_{\epsilon l}\cos(\pi\nu)]G_{\epsilon l}(-\nu)-\alpha_{\epsilon l}G_{\epsilon l}(\nu)}. \tag{76}$$

Figure 3 is a plot of the $\chi_l(\Delta)$ function for $l=2$.

D. Wronskians

From Eqs. (17) and (18) it is easy to show that the f^0 and g^0 pair has a Wronskian given by

$$W(f^0,g^0)=-4/\pi. \tag{77}$$

Since the Wronskian is a constant that is independent of r, it is a useful check of numerical calculations. In particular, the asymptotic forms of f^0 and g^0 at large r should give the same Wronskian, which requires

$$\det(Z)=Z_{ff}Z_{gg}-Z_{gf}Z_{fg}=-2, \tag{78}$$

$$\det(W)=W_{fI}W_{gK}-W_{gI}W_{fK}=4. \tag{79}$$

These requirements have been verified in our calculations.

V. CONCLUSION

The exact solutions of the Schrödinger equation for an attractive $1/r^6$ potential have been presented. With this set of solutions, a quantum defect theory for molecular vibration spectra and slow atomic collisions can be set up in a fashion similar [4,12] to the quantum defect theories for other asymptotic potentials with known analytic solutions [1,2]. For example, in the case of a single channel, the bound states of any potential that behaves asymptotically as an attractive $1/r^6$ can be formulated as the crossing points between $\chi_l(\Delta)$ defined earlier and a short-range K matrix $K_l^0(\epsilon)$ [4]. Above the threshold, the scattering phase shift can be written in terms of the Z matrix defined earlier and the short-range K matrix K_l^0 as [4]

$$K_l\equiv\tan\delta_l=(Z_{ff}-K_l^0Z_{gf})^{-1}(K_l^0Z_{gg}-Z_{fg}), \tag{80}$$

which provides an analytic description of energy dependences, including shape resonances, of cold-atom collisions. This and other applications are discussed elsewhere [4,13].

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