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Equal-factor approach to perturbation theory

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A special application of the equal-factor method is used to reformulate perturbation theory. We derive formulas for determining the mth-order equal factors $\{f_n^{(m)}\}$ and the corresponding mth-order energy corrections $\{E_n^{(m)}\}$. A set of the mth-order perturbation energy levels $\{E_n^{(m)}\}$ thus may be calculated to arbitrarily high order by self-consistent equations. We have applied this so-called equal-factor perturbation to hydrogenlike ions in a potential field $-\delta/r^2$. Our results illustrate important advantages in aspects both of practice and theory. Work is presently underway to introduce the equal-factor assumption to perturbation theory for reformulation of the principle of the first and second kind of balance theory. [S1050-2947(99)01808-9]

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I. INTRODUCTION

Before describing the problem, we first summarize some basic ideas of PFSKB (principle of the first and second kind of balance) theory. As isolated subsystem H_0 and potential H' move closely; a perturbing potential H' imposes a force on the unperturbed subsystem. The subsystem then may vary its structure to balance this external force and, after a very short period of time, the total system stabilizes at the energy minimum position. This picture illustrates the possible metastable process of formation of H_0 and H' in passing from an unperturbed to a perturbed system [1,2] in a possible metastable time period, and also indicates that the phenomenon mentioned above is similar to a deformation of a real body in classical mechanics. Here and throughout, the terms ''possible metastable process'' and ''possible metastable time period'' refer to a helpful thought process we have employed in working out the mathematical formalism; in certain cases and under certain circumstances, it is conceivable that this process may actually have physical significance.

We begin with the time-independent Schrödinger equation, which traditionally is given by

$$H\Psi_n(\vec{x})=E_n\Psi_n(\vec{x}), \tag{1}$$

where E_n is the energy eigenvalue. As is well known, one is interested in an entire energy level $\{E_{n\beta}\}$, rather than an individual energy level in PFSKB theory. Thus we assume this entire energy level is characterized by some common eigenvalue β.

According to perturbation theory, one divides the total Hamiltonian H into two parts: H_0+H'. One is treated as an unperturbed part H_0, the other as a perturbation H'. We suppose the stable total system H in Eq. (1) is formed from two subsystems H_0 and H'. Then there is a possible metastable process which goes from an unperturbed to a perturbed system in a very short period of time t, and the total system obeys the extended Schrödinger equation [1,2]:

$$(H_0+H')\Psi_n(\vec{x},\alpha)=E_n(\alpha)\Psi_n(\vec{x},\alpha), \quad t_i\leqslant t\leqslant t_f, \tag{2}$$

where α is a parameter varying in the possible metastable period of time $t_i<t<t_f$.

Clearly, at the end of the assumed metastable process, the varying energy acquires its minimum value at the balance point α^* [1,2] and so the minimum energy can be identified with the energy eigenvalue of the Schrödinger equation (1):

$$E_n=\min\{E_n(\alpha)\}_{\alpha=\alpha^*}. \tag{3}$$

We find to our surprise that the minimization principle Eq. (3) extends the use of the variational principle to excited states as well.

II. THEORY

Suppose the exact eigenfunction set $\{\Psi_{n\beta}(\vec{x},\alpha)\}$ corresponds to the energy set $\{E_{n\beta}(\alpha)\}$. Both of them respond to the same common eigenvalue β. We assume that no eigenvalue of the operator $H_0(\alpha)$ is degenerate. Thus the exact eigenfunction and energy eigenvalue of the extended Schrödinger equation (2) can be expanded in powers of λ,

$$\Psi_{n\beta}(\vec{x},\alpha)=\Psi_{n\beta}^{(0)}(\vec{x},\alpha)+\lambda\Psi_{n\beta}^{(1)}(\vec{x},\alpha)+\cdots+\lambda^m\Psi_{n\beta}^{(m)}(\vec{x},\alpha)+\cdots \tag{4}$$

and

$$E_{n\beta}(\alpha)=E_{n\beta}^{\langle 0\rangle}(\alpha)+\lambda E_{n\beta}^{(1)}(\alpha)+\cdots+\lambda^m E_{n\beta}^{(m)}(\alpha)+\cdots, \tag{5}$$

where λ is a dummy argument. Terms $\Psi_{n\beta}^{(m)}$ and $E_{n\beta}^{(m)}$ are the mth-order perturbation wave function and mth-order perturbation energy, which is defined as

$$E_{n\beta}^{(m)}(\alpha)=E_{n\beta}^{\langle m\rangle}(\alpha)-E_{n\beta}^{\langle m-1\rangle}(\alpha), \tag{6}$$

where $E_{n\beta}^{\langle m\rangle}$ and $E_{n\beta}^{\langle m-1\rangle}$ are the mth and $(m-1)$th-order approximations to the energy, respectively.

In PFSKB theory, the unperturbed Schrödinger equation with varying parameter α is given by

$$H_0(\alpha)\phi_{n\beta}^{(0)}(\vec{x},\alpha)=E_{n\beta}^{(0)}(\alpha)\phi_{n\beta}^{(0)}(\vec{x},\alpha), \tag{7}$$

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where β is some common eigenvalue. The set $\{\phi_{n\beta}^{(0)}(\vec{x},\alpha)\}$ creates a subspace and, therefore, is chosen as a complete orthonormal function basis.

We ignore the index β as a convention in the remainder of this paper. Now, suppose the mth-order perturbation wave can be expanded in term of the unperturbed eigenfunction set $\{\phi_j^{(0)}(\vec{x},\alpha)\}$

$$\Psi_n^{(m)}(\vec{x},\alpha)=\sum_{j\neq n} C_{nj}^{(m)}\phi_j^{(0)}(\vec{x},\alpha). \tag{8}$$

Applying the extended equal-factor assumption to coefficients $C_{nj}^{(m)}$ in Eq. (8), it is straightforward to write [2]

$$C_{nj}^{(m)}=f_n^{(m)}(\alpha)E_i^{(m)}(\alpha) \quad \text{if } j<n,\ i=j,\ j>n,\ i=j-1, \tag{9}$$

where we separated integer variables of n and j for coefficient $C_{nj}^{(m)}$, and $E_i^{(m)}(\alpha)$ is the corresponding mth-order correction of the energy levels of the extended Schrödinger equation (2) and $f_n^{(m)}(\alpha)$ is the mth-order equal factor [2].

It is useful to note that coefficient $C_{nj}^{(m)}$ in Eq. (9) is independent of varying parameter α, that is, the product of $f_n^{(m)}(\alpha)E_i^{(m)}(\alpha)$ remains invariant. In particular, when α takes a value of a balance position α^*, we have

$$f_n^{(m)}(\alpha)E_i^{(m)}(\alpha)=f_n^{(m)}(\alpha^*)E_i^{(m)}(\alpha^*), \tag{10}$$

where α varies in the interval $(\alpha^*-\Delta\alpha\leqslant\alpha^*+\Delta\alpha)$.

Hence, the perturbation expansion (4) of the exact eigenfunction is reformulated:

$$\Psi_n(\vec{x},\alpha)=\psi_n^{(0)}(\vec{x},\alpha)+\lambda f_n^{(1)}(\alpha)\psi_n^{(1)}(\vec{x},\alpha)+\cdots+\lambda^{(m)}f_n^{(m)}\times(\alpha)\psi_n^{(m)}(\vec{x},\alpha)+\cdots. \tag{11}$$

According to the equal-factor assumption (9), we have

$$\psi_n^{(m)}(\vec{x},\alpha)=\sum_{j\neq n} E_i^{(m)}(\alpha)\phi_j^{(0)}(\vec{x},\alpha), \tag{12}$$

where $E_i^{(m)}(\alpha)$ is defined in expression (6), the index i is a convention in Eq. (9), and $\psi_n^{(0)}(\vec{x},\alpha)=\phi_n^{(0)}(\vec{x},\alpha)$.

Here we assume that the equal-factor relation (9) between $f_n^{(m)}(\alpha)$ and $E_i^{(m)}(\alpha)$ can be satisfied in a possible metastable process for a varying parameter α in a near-neighbor of the balance position α^* up to the mth order.

We notice this reformulated mth-order perturbation wave satisfies an orthogonal condition with an unperturbed wave for varying parameter α in the possible metastable time period,

$$\langle\psi_n^{(m)}(\vec{x},\alpha)|\psi_n^{(0)}(\vec{x},\alpha)\rangle=0, \quad m=1,2,\ldots. \tag{13}$$

Consider the extended Schrödinger equation (2) by the perturbation expansion in terms of λ, which is given by

$$\begin{aligned}&[H_0(\alpha)+h(\alpha)+\lambda H'][\psi_n^{(0)}(\alpha)+\lambda f_n^{(1)}(\alpha)\psi_n^{(1)}(\alpha)+\cdots+\lambda^m f_n^{(m)}(\alpha)\psi_n^{(m)}(\alpha)+\cdots]\\&\quad=[E_n^{\langle 0\rangle}(\alpha)+\lambda E_n^{(1)}(\alpha)+\cdots)(\psi_n^{(0)}(\alpha)+\lambda f_n^{(1)}(\alpha)\psi_n^{(1)}(\alpha)+\cdots],\end{aligned} \tag{14}$$

where $h(\alpha)$ is equal to $H_0-H_0(\alpha)$, which represents changes in subsystem H_0 under perturbation H' in the possible metastable process.

Expanding the above equation and regrouping according to ascending powers of λ, the reformulated perturbation expansions are obtained:

$$[H_0(\alpha)+h(\alpha)]\psi_n^{(0)}(\alpha)=E_n^{\langle 0\rangle}(\alpha)\psi_n^{(0)}(\alpha), \tag{15}$$

$$[H_0(\alpha)+h(\alpha)]f_n^{(1)}(\alpha)\psi_n^{(1)}(\alpha)+H'\psi_n^{(0)}(\alpha)=E_n^{\langle 0\rangle}(\alpha)f_n^{(1)}(\alpha)\psi_n^{(1)}(\alpha)+E_n^{(1)}(\alpha)\psi_n^{(0)}(\alpha), \tag{16}$$

$$\begin{aligned}&[H_0(\alpha)+h(\alpha)]f_n^{(m)}(\alpha)\psi_n^{(m)}(\alpha)+H'f_n^{(m-1)}(\alpha)\psi_n^{(m-1)}(\alpha)\\&\quad=E_n^{\langle 0\rangle}(\alpha)f_n^{(m)}(\alpha)\psi_n^{(m)}(\alpha)+E_n^{(1)}(\alpha)f_n^{(m-1)}(\alpha)\psi_n^{(m-1)}(\alpha)+\cdots+E_n^{(m)}(\alpha)\psi_n^{(0)}(\alpha).\end{aligned} \tag{17}$$

Multiplying both sides of Eqs. (15)–(17) on the left by $\langle\psi_n^{(0)}(\alpha)|$ and integrating, we have

$$E_n^{\langle 0\rangle}(\alpha)=E_n^{(0)}(\alpha)+\langle\psi_n^{(0)}(\alpha)|h(\alpha)|\psi_n^{(0)}(\alpha)\rangle, \tag{18}$$

$$E_n^{(1)}(\alpha)=\langle\psi_n^{(0)}(\alpha)|h(\alpha)|\psi_n^{(1)}(\alpha)\rangle f_n^{(1)}(\alpha)+\langle\psi_n^{(0)}(\alpha)|H'|\psi_n^{(0)}(\alpha)\rangle, \tag{19}$$

$$\vdots$$

$$E_n^{(m)}(\alpha)=\langle\psi_n^{(0)}(\alpha)|h(\alpha)|\psi_n^{(m)}(\alpha)\rangle f_n^{(m)}(\alpha)+\langle\psi_n^{(0)}(\alpha)|H'|\psi_n^{(m-1)}(\alpha)\rangle f_n^{(m-1)}(\alpha). \tag{20}$$

Furthermore, the mth-order approximation to the energy is

$$E_n^{\langle m\rangle}(\alpha)=E_n^{\langle 0\rangle}(\alpha)+\sum_{k=1}^{m} E_n^{(k)}(\alpha), \quad n=1,2,\ldots. \tag{21}$$

Recalling the second kind of balance condition in PFSKB theory [1], we obtain

$$\frac{d}{d\alpha}E_n^{\langle m\rangle}(\alpha)|_{\alpha=\alpha_n^{(m)}}=0, \quad n=1,2,\ldots. \tag{22}$$

Then the minimal energy for the mth-order approximation is

TABLE I. Coefficients a_{jn} and b_{nj} are given in triangle below and up the diagonal positions for $n=1$ to 13; $j=1$ to 13, respectively. The accuracy is estimated to be ±1 in the last digit (in a.u.). Numbers in square brackets indicate powers of 10.

n j	1*s*	2*s*	3*s*	4*s*	5*s*	6*s*	7*s*	8*s*	9*s*	10*s*	11*s*	12*s*	13*s*
1*s*		0.628540[+0]	0.336787[+0]	0.217600[+0]	0.155328[+0]	0.118009[+0]	0.935748[−1]	0.765513[−1]	0.641320[−1]	0.547434[−1]	0.474421[−1]	0.416314[−1]	0.369174[−1]
2*s*	0.209517[+0]		0.127156[+0]	0.814767[−1]	0.579767[−1]	0.439779[−1]	0.348404[−1]	0.284857[−1]	0.238551[−1]	0.203573[−1]	0.176387[−1]	0.154759[−1]	0.137220[−1]
3*s*	0.108243[+0]	0.721162[−1]		0.458699[−1]	0.324450[−1]	0.245549[−1]	0.194301[−1]	0.158750[−1]	0.132883[−1]	0.113363[−1]	0.982013[−2]	0.861459[−2]	0.763725[−2]
4*s*	0.691152[−1]	0.426630[−1]	0.364365[−1]		0.215544[−1]	0.162306[−1]	0.128203[−1]	0.104652[−1]	0.875522[−2]	0.746640[−2]	0.646616[−2]	0.567129[−2]	0.502714[−2]
5*s*	0.490743[−1]	0.294434[−1]	0.229434[−1]	0.220875[−1]		0.118113[−1]	0.929395[−2]	0.757450[−2]	0.633110[−2]	0.539599[−2]	0.467127[−2]	0.409588[−2]	0.362993[−2]
6*s*	0.371774[−1]	0.219917[−1]	0.166407[−1]	0.142362[−1]	0.146282[−1]		0.716415[−2]	0.581915[−2]	0.485829[−2]	0.413805[−2]	0.358071[−2]	0.313868[−2]	0.278096[−2]
7*s*	0.294292[−1]	0.172668[−1]	0.128784[−1]	0.106997[−1]	0.996462[−2]	0.104943[−1]		0.466928[−2]	0.388624[−2]	0.330678[−2]	0.285978[−2]	0.250575[−2]	0.221950[−2]
8*s*	0.240487[−1]	0.140373[−1]	0.103805[−1]	0.852466[−2]	0.764648[−2]	0.720167[−2]	0.788725[−2]		0.321110[−2]	0.272488[−2]	0.235436[−2]	0.206178[−2]	0.182559[−2]
9*s*	0.201319[−1]	0.117102[−1]	0.861130[−2]	0.702555[−2]	0.615720[−2]	0.568285[−2]	0.547076[−2]	0.612419[−2]		0.230246[−2]	0.198440[−2]	0.173657[−2]	0.153698[−2]
10*s*	0.171755[−1]	0.996600[−2]	0.730012[−2]	0.592944[−2]	0.511567[−2]	0.466787[−2]	0.440317[−2]	0.433566[−2]	0.491421[−2]		0.170675[−2]	0.149027[−2]	0.131800[−2]
11*s*	0.148788[−1]	0.861780[−2]	0.629464[−2]	0.509629[−2]	0.434877[−2]	0.392800[−2]	0.366278[−2]	0.352152[−2]	0.347872[−2]	0.400581[−2]		0.130015[−2]	0.114759[−2]
12*s*	0.130525[−1]	0.754971[−2]	0.550270[−2]	0.444398[−2]	0.376217[−2]	0.336908[−2]	0.310671[−2]	0.293845[−2]	0.287972[−2]	0.290407[−2]	0.334220[−2]		0.101311[−2]
13*s*	0.115718[−1]	0.668621[−2]	0.486527[−2]	0.392141[−2]	0.330085[−2]	0.293488[−2]	0.267839[−2]	0.250010[−2]	0.243312[−2]	0.239471[−2]	0.243012[−2]	0.281849[−2]	

$$E_n^{\langle m\rangle}(\alpha_n^{(m)})=\min\{E_n^{\langle m\rangle}(\alpha)\}. \tag{23}$$

We note that deriving formula (22) with equal-factor relations (9) yields

$$f_n^{(m)}(\alpha)\sum_{j\neq n} E_i^{(m)}(\alpha)\phi_j^{(0)}(\vec{x},\alpha)=f_n^{(m)}(\alpha_n^{(m)})\sum_{j\neq n} E_i^{(m)} \times(\alpha_n^{(m)})\phi_j^{(0)}(\vec{x},\alpha). \tag{24}$$

Therefore, a series of mth-order self-consistent perturbation equations can be obtained [3]. If $m=1$,

$$E_n^{(1)}(\alpha_n^{(1)})=f_n^{(1)}(\alpha_n^{(1)})\langle\psi_n^{(0)}(\alpha)|h(\alpha)|\psi_n^{(1)}(\alpha)\rangle|_{\alpha=\alpha_n^{(1)}} +\langle\psi_n^{(0)}(\alpha)|H'|\psi_n^{(0)}(\alpha)\rangle|_{\alpha=\alpha_n^{(1)}}. \tag{25}$$

If $m\geqslant 2$,

$$\begin{aligned}E_n^{(m)}(\alpha_n^{(m)})&=f_n^{(m)}(\alpha_n^{(m)})\langle\psi_n^{(0)}(\alpha)|h(\alpha)|\psi_n^{(m)}(\alpha)\rangle|_{\alpha=\alpha_n^{(m)}}\\&\quad+f_n^{(m-1)}(\alpha_n^{(m-1)})\\&\quad\times\langle\psi_n^{(0)}(\alpha)|H'|\psi_n^{(m-1)}(\alpha)\rangle|_{\alpha=\alpha_n^{(m)}},\end{aligned} \tag{26}$$

where $\alpha_n^{(m)}$ is the balance position at the end of the metastable process.

Next, we shall seek the values of the equal-factor $f_n^{(m)}(\alpha_n^{(m)})$ corresponding to the mth-order energy corrections $E_n^{(m)}(\alpha_n^{(m)})$. Let us now turn to Eqs. (15)–(17). Multiplying both sides of Eqs. (15)–(17) on the left by the perturbing function $\langle\psi_n^{(m)}|$ and integrating, we have

$$f_n^{(1)}(\alpha_n^{(1)})=\left\{\frac{-\langle\psi_n^{(1)}|H'|\psi_n^{(0)}\rangle}{\langle\psi_n^{(1)}|H_0(\alpha)+h(\alpha)-E_n^{\langle 0\rangle}(\alpha)|\psi_n^{(1)}\rangle}\right\}_{\alpha=\alpha_n^{(1)}}, \tag{27}$$

$$f_n^{(2)}(\alpha_n^{(2)})=\left\{\frac{\langle\psi_n^{(2)}|E_n^{(1)}-H'|\psi_n^{(1)}\rangle f_n^{(1)}(\alpha_n^{(1)})}{\langle\psi_n^{(2)}|H_0(\alpha)+h(\alpha)-E_n^{\langle 0\rangle}(\alpha)|\psi_n^{(2)}\rangle}\right\}_{\alpha=\alpha_n^{(2)}}, \tag{28}$$

and

TABLE II. Demonstration of the possible metastable process for a hydrogen atom in a potential field $-\delta/r^2$, $\delta=-10^6$ by an iterative procedure. The integer k is the index of the repeated process and $\Delta E_n^{(1)}=E_n^{(1),k+1}-E_n^{(1),k}$. Numbers in square brackets indicate powers of 10.

	$k=1$					$k=3$				
ns	$\Delta E_n^{(1)}$	$E_n^{(1)}$	$E_n^{\langle 1\rangle}$	$f_n^{(1)}$	$\alpha_n^{(1)}$	$\Delta E_n^{(1)}$	$E_n^{(1)}$	$E_n^{\langle 1\rangle}$	$f_n^{(1)}$	$\alpha_n^{(1)}$
1s	0.20[+07]	0.20[+07]	0.20[+07]	0.00[+00]	0.10[+01]	0.11[+00]	0.11[+00]	−0.12[−06]	0.59[−04]	0.23[−03]
2s	0.25[+06]	0.25[+06]	0.25[+06]	0.00[+00]	0.10[+01]	0.55[−04]	0.10[−06]	−0.30[−07]	0.42[−02]	0.50[−06]
3s	0.74[+05]	0.74[+05]	0.74[+05]	0.00[+00]	0.10[+01]	0.68[−02]	0.22[−08]	−0.47[−07]	−0.55[−03]	0.23[−06]
4s	0.31[+05]	0.31[+05]	0.31[+05]	0.00[+00]	0.10[+01]	0.33[+00]	0.18[−07]	−0.54[−07]	−0.17[−02]	0.11[−05]
5s	0.16[+05]	0.16[+05]	0.16[+05]	0.00[+00]	0.10[+01]	0.11[+02]	0.17[−07]	−0.57[−07]	−0.21[−02]	0.19[−05]
6s	0.93[+04]	0.93[+04]	0.93[+04]	0.00[+00]	0.10[+01]	0.16[+03]	0.83[−08]	−0.64[−07]	−0.22[−02]	0.26[−05]
7s	0.58[+04]	0.58[+04]	0.58[+04]	0.00[+00]	0.10[+01]	0.42[+03]	−0.11[−07]	−0.83[−07]	−0.25[−02]	0.35[−05]
8s	0.39[+04]	0.39[+04]	0.39[+04]	0.00[+00]	0.10[+01]	0.34[+03]	−0.37[−07]	−0.12[−06]	−0.30[−02]	0.50[−05]
9s	0.27[+04]	0.27[+04]	0.27[+04]	0.00[+00]	0.10[+01]	0.24[+03]	−0.52[−07]	−0.14[−06]	−0.35[−02]	0.72[−05]
10s	0.20[+04]	0.20[+04]	0.20[+04]	0.00[+00]	0.10[+01]	0.17[+03]	−0.55[−07]	−0.15[−06]	−0.37[−02]	0.92[−05]
11s	0.15[+04]	0.15[+04]	0.15[+04]	0.00[+00]	0.10[+01]	0.13[+03]	−0.47[−07]	−0.14[−06]	−0.37[−02]	0.11[−04]
12s	0.12[+04]	0.12[+04]	0.12[+04]	0.00[+00]	0.10[+01]	0.99[+02]	−0.34[−07]	−0.12[−06]	−0.35[−02]	0.12[−04]
	$k=6$					$k=10$				
ns	$\Delta E_n^{(1)}$	$E_n^{(1)}$	$E_n^{\langle 1\rangle}$	$f_n^{(1)}$	$\alpha_n^{(1)}$	$\Delta E_n^{(1)}$	$E_n^{(1)}$	$E_n^{\langle 1\rangle}$	$f_n^{(1)}$	$\alpha_n^{(1)}$
1s	−0.27[−08]	0.13[−06]	−0.12[−06]	−0.37[+04]	0.25[−06]	−0.26[−09]	0.13[−06]	−0.12[−06]	−0.24[+05]	0.25[−06]
2s	0.10[−05]	0.65[−07]	−0.59[−07]	−0.14[+05]	0.49[−06]	0.12[−08]	0.65[−07]	0.58[−07]	−0.12[+06]	0.50[−06]
3s	−0.15[−04]	0.14[−06]	−0.62[−08]	−0.32[+06]	0.70[−06]	0.85[−09]	0.45[−07]	−0.32[−07]	−0.28[+06]	0.69[−06]
4s	0.20[−07]	0.15[−06]	−0.12[−06]	0.12[+06]	−0.15[−05]	0.18[−06]	0.40[−07]	−0.11[−07]	−0.72[+06]	0.78[−06]
5s	0.66[−07]	0.96[−07]	−0.54[−07]	0.59[+05]	0.31[−05]	−0.18[−05]	−0.95[−08]	−0.75[−07]	0.88[+06]	0.43[−06]
6s	0.58[−08]	0.32[−07]	−0.40[−07]	0.46[+05]	0.25[−05]	0.20[−05]	0.21[−05]	−0.10[−04]	−0.20[+08]	0.31[−05]
7s	0.25[−08]	0.23[−07]	−0.32[−07]	0.38[+05]	0.27[−05]	0.16[−04]	0.16[−04]	−0.70[−08]	−0.33[+06]	−0.54[−04]
8s	0.14[−08]	0.19[−07]	−0.27[−07]	0.33[+05]	0.29[−05]	0.88[−08]	0.25[−08]	−0.19[−07]	0.90[+05]	0.10[−05]
9s	0.15[−08]	0.16[−07]	−0.23[−07]	0.30[+05]	0.31[−05]	0.13[−06]	−0.68[−08]	−0.44[−07]	0.68[+06]	0.25[−05]
10s	0.16[−08]	0.13[−07]	−0.21[−07]	0.28[+05]	0.34[−05]	−0.20[−06]	−0.22[−07]	−0.74[−07]	0.12[+07]	0.49[−05]
11s	0.11[−08]	0.12[−07]	−0.19[−07]	0.27[+05]	0.37[−05]	0.80[−08]	0.32[−07]	−0.39[−07]	0.67[+06]	0.75[−05]
12s	0.78[−09]	0.11[−07]	−0.17[−07]	0.26[+05]	0.40[−05]	0.31[−08]	0.16[−07]	−0.28[−07]	0.48[+06]	0.60[−05]
	$k=12$					$k=25$				
ns	$\Delta E_n^{(1)}$	$E_n^{(1)}$	$E_n^{\langle 1\rangle}$	$f_n^{(1)}$	$\alpha_n^{(1)}$	$\Delta E_n^{(1)}$	$E_n^{(1)}$	$E_n^{\langle 1\rangle}$	$f_n^{(1)}$	$\alpha_n^{(1)}$
1s	0.14[−07]	0.14[−06]	−0.11[−06]	−0.13[+07]	0.25[−06]	−0.24[−13]	0.14[−06]	−0.11[−06]	−0.15[+07]	0.25[−06]
2s	−0.72[−07]	−0.88[−08]	−0.14[−06]	0.33[+07]	0.39[−06]	0.85[−14]	0.58[−08]	−0.11[−06]	0.23[+07]	0.38[−06]
3s	0.52[−07]	0.94[−07]	−0.94[−07]	0.25[+07]	0.16[−05]	0.22[−13]	0.37[−07]	−0.11[−06]	0.34[+07]	0.13[−05]
4s	0.26[−07]	0.57[−07]	−0.66[−07]	0.19[+07]	0.19[−05]	0.37[−15]	0.41[−07]	−0.92[−07]	0.33[+07]	0.21[−05]
5s	0.13[−07]	0.37[−07]	−0.51[−07]	0.15[+07]	0.21[−05]	−0.26[−13]	0.34[−07]	−0.76[−07]	0.30[+07]	0.27[−05]
6s	−0.40[−07]	0.26[−07]	−0.42[−07]	0.14[+07]	0.24[−05]	−0.24[−13]	0.27[−07]	−0.62[−07]	0.26[+07]	0.31[−05]
7s	0.10[−06]	0.72[−07]	−0.47[−08]	−0.14[+07]	0.28[−05]	−0.94[−13]	0.21[−07]	−0.51[−07]	0.23[+07]	0.35[−05]
8s	−0.77[−07]	−0.28[−07]	−0.21[−06]	0.73[+07]	0.72[−06]	−0.59[−13]	0.17[−07]	−0.43[−07]	0.20[+07]	0.38[−05]
9s	0.88[−07]	0.13[−06]	−0.62[−07]	0.29[+07]	0.98[−05]	−0.11[−12]	0.15[−07]	−0.37[−07]	0.18[+07]	0.41[−05]
10s	0.18[−07]	0.25[−07]	−0.39[−07]	0.19[+07]	0.60[−05]	−0.98[−14]	0.12[−07]	−0.32[−07]	0.17[+07]	0.44[−05]
11s	0.50[−08]	0.99[−08]	−0.34[−07]	0.18[+07]	0.53[−05]	0.60[−13]	0.11[−07]	−0.29[−07]	0.16[+07]	0.48[−05]
12s	−0.93[−08]	0.74[−08]	−0.32[−07]	0.17[+07]	0.56[−05]	0.56[−13]	0.98[−08]	−0.26[−07]	0.15[+07]	0.51[−05]

TABLE III. Comparison of various computed eigenvalues with the exact value (in a.u.) for positive coupling parameters $\delta=0.01$, 0.005, and 0.001. $E_n^{\langle 1\rangle,a}$, $E_n^{\langle 1\rangle,b}$, and $E_n^{\langle 1\rangle,RS}$ are the first-order approximation to the energy. The corresponding equal factors $f_n^{(1),a}$ and $f_n^{(1),b}$ are determined by formula (46) and by trial, respectively. The equal factors $f_n^{(1),b}$ take the value 0.05 for $0\leqslant\delta\leqslant0.125$ and $n=1$ to 12 states. Numbers in square brackets indicate powers of 10.

$\delta=0.01,\ f_n^{(1),b}=0.05$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1*s*	−0.52106[+00]	−0.52065[+00]	−0.89865[+00]	−0.52084[+00]	−0.52000[+00]
2*s*	−0.12759[+00]	−0.12766[+00]	0.81037[+00]	−0.12756[+00]	−0.12750[+00]
3*s*	−0.56320[−01]	−0.56326[−01]	0.41377[+00]	−0.56308[−01]	−0.56296[−01]
4*s*	−0.31571[−01]	−0.31571[−01]	0.24114[+00]	−0.31567[−01]	−0.31562[−01]
5*s*	−0.20164[−01]	−0.20163[−01]	0.16464[+00]	−0.20162[−01]	−0.20160[−01]
6*s*	−0.13984[−01]	−0.13983[−01]	0.12230[+00]	−0.13982[−01]	−0.13981[−01]
7*s*	−0.10264[−01]	−0.10263[−01]	0.95693[−01]	−0.10263[−01]	−0.10262[−01]
8*s*	−0.78525[−02]	−0.78520[−02]	0.77603[−01]	−0.78519[−02]	−0.78516[−02]
9*s*	−0.62009[−02]	−0.62006[−02]	0.64617[−01]	−0.62005[−02]	−0.62003[−02]
10*s*	−0.50205[−02]	−0.50202[−02]	0.54912[−01]	−0.50202[−02]	−0.50200[−02]
11*s*	−0.41476[−02]	−0.41474[−02]	0.47427[−01]	−0.41474[−02]	−0.41473[−02]
12s	−0.34841[−02]	−0.34839[−02]	0.41508[−01]	−0.34839[−02]	−0.34838[−02]

$\delta=0.005,\ f_n^{(1),b}=0.05$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1*s*	−0.51026[+00]	−0.51016[+00]	−0.89491[+00]	−0.51021[+00]	−0.51000[+00]
2*s*	−0.12627[+00]	−0.12629[+00]	0.83965[+00]	−0.12626[+00]	−0.12525[+00]
3*s*	−0.55932[−01]	−0.55933[−01]	0.40529[+00]	−0.55929[−01]	−0.55926[−01]
4*s*	−0.31408[−01]	−0.31408[−01]	0.24253[+00]	−0.31407[−01]	−0.31406[−01]
5*s*	−0.20081[−01]	−0.20081[−01]	0.16751[+00]	−0.20080[−01]	−0.20080[−01]
6*s*	−0.13936[−01]	−0.13936[−01]	0.12508[+00]	−0.13935[−01]	−0.13935[−01]
7*s*	−0.10234[−01]	−0.10233[−01]	0.98157[−01]	−0.10233[−01]	−0.10233[−01]
8*s*	−0.78323[−02]	−0.78322[−02]	0.79757[−01]	−0.78321[−02]	−0.78320[−02]
9*s*	−0.61867[−02]	−0.61866[−02]	0.66503[−01]	−0.61866[−02]	−0.61866[−02]
10*s*	−0.50101[−02]	−0.50100[−02]	0.56573[−01]	−0.50100[−02]	−0.50100[−02]
11*s*	−0.41398[−02]	−0.41398[−02]	0.48902[−01]	−0.41398[−02]	−0.41397[−02]
12*s*	−0.34781[−02]	−0.34780[−02]	0.42827[−01]	−0.34780[−02]	−0.34780[−02]

$\delta=0.001,\ f_n^{(1),b}=0.05$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1*s*	−0.50201[+00]	−0.50201[+00]	−0.89270[+00]	−0.50201[+00]	−0.50200[+00]
2*s*	−0.12525[+00]	−0.12525[+00]	0.86263[+00]	−0.12525[+00]	−0.12525[+00]
3*s*	−0.55630[−01]	−0.55630[−01]	0.39993[+00]	−0.55630[−01]	−0.55630[−01]
4*s*	−0.31281[−01]	−0.31281[−01]	0.24417[+00]	−0.31281[−01]	−0.31281[−01]
5*s*	−0.20016[−01]	−0.20016[−01]	0.16993[+00]	−0.20016[−01]	−0.20016[−01]
6*s*	−0.13898[−01]	−0.13898[−01]	0.12735[+00]	−0.13898[−01]	−0.13898[−01]
7*s*	−0.10210[−01]	−0.10210[−01]	0.10016[+00]	−0.10210[−01]	−0.10210[−01]
8*s*	−0.78164[−02]	−0.78164[−02]	0.81507[−01]	−0.78164[−02]	−0.78164[−02]
9*s*	−0.61756[−02]	−0.61756[−02]	0.68035[−01]	−0.61756[−02]	−0.61756[−02]
10*s*	−0.50020[−02]	−0.50020[−02]	0.57924[−01]	−0.50020[−02]	−0.50020[−02]
11*s*	−0.41337[−02]	−0.41337[−02]	0.50101[−01]	−0.41337[−02]	−0.41337[−02]
12*s*	−0.34734[−02]	−0.34734[−02]	0.43899[−01]	−0.34734[−02]	−0.34734[−02]

TABLE IV. Comparison of various computed eigenvalues with the exact value (in a.u.) for negative coupling parameters $\delta=-0.1$, -0.01, and -0.001. $E_n^{\langle 1\rangle,a}$, $E_n^{\langle 1\rangle,b}$, and $E_n^{\langle 1\rangle,RS}$ are the first-order approximation to the energy. The corresponding equal factors $f_n^{(1),a}$ and $f_n^{(1),b}$ are determined by formula (46) and by trial, respectively. The equal factors $f_n^{(1),b}$ take the value 0.125 for $-0.10\leqslant\delta\leqslant 0$ and $n=1$ to 12 states. Numbers in square brackets indicate powers of 10.

$\delta=-0.10,\ f_n^{(1),b}=0.125$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1s	−0.36475[+00]	−0.35241[+00]	−0.94833[+00]	−0.35775[+00]	−0.30000[+00]
2s	−0.10610[+00]	−0.10912[+00]	0.13130[+01]	−0.10457[+00]	−0.10000[+00]
3s	−0.49731[−01]	−0.49688[−01]	0.44328[+00]	−0.49187[−01]	−0.48148[−01]
4s	−0.28743[−01]	−0.28674[−01]	0.33493[+00]	−0.28496[−01]	−0.28125[−01]
5s	−0.18700[−01]	−0.18635[−01]	0.24755[+00]	−0.18571[−01]	−0.18400[−01]
6s	−0.13131[−01]	−0.13081[−01]	0.19427[+00]	−0.13056[−01]	−0.12963[−01]
7s	−0.97237[−02]	−0.96863[−02]	0.15773[+00]	−0.96774[−02]	−0.96210[−02]
8s	−0.74893[−02]	−0.74610[−02]	0.13143[+00]	−0.74590[−02]	−0.74219[−02]
9s	−0.59450[−02]	−0.59234[−02]	0.11174[+00]	−0.59246[−02]	−0.58985[−02]
10s	−0.48335[−02]	−0.48166[−02]	0.96538[−01]	−0.48192[−02]	−0.48000[−02]
11s	−0.40068[−02]	−0.39934[−02]	0.84507[−01]	−0.39967[−02]	−0.39820[−02]
12s	−0.33754[−02]	−0.33647[−02]	0.74791[−01]	−0.33681[−02]	−0.33565[−02]

$\delta=-0.01,\ f_n^{(1),b}=0.125$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1s	−0.48095[+00]	−0.48064[+00]	−0.88966[+00]	−0.48079[+00]	−0.48000[+00]
2s	−0.12258[+00]	−0.12265[+00]	0.92372[+00]	−0.12256[+00]	−0.12250[+00]
3s	−0.54836[−01]	−0.54839[−01]	0.39037[+00]	−0.54828[−01]	−0.54815[−01]
4s	−0.30946[−01]	−0.30945[−01]	0.25039[+00]	−0.30943[−01]	−0.30938[−01]
5s	−0.19844[−01]	−0.19843[−01]	0.17702[+00]	−0.19842[−01]	−0.19840[−01]
6s	−0.13799[−01]	−0.13798[−01]	0.13382[+00]	−0.13798[−01]	−0.13796[−01]
7s	−0.10147[−01]	−0.10147[−01]	0.10582[+00]	−0.10147[−01]	−0.10146[−01]
8s	−0.77743[−02]	−0.77739[−02]	0.86434[−01]	−0.77741[−02]	−0.77734[−02]
9s	−0.61460[−02]	−0.61457[−02]	0.72346[−01]	−0.61459[−02]	−0.61454[−02]
10s	−0.49804[−02]	−0.49802[−02]	0.61723[−01]	−0.49803[−02]	−0.49800[−02]
11s	−0.41175[−02]	−0.41173[−02]	0.53476[−01]	−0.41175[−02]	−0.41172[−02]
12s	−0.34609[−02]	−0.34607[−02]	0.46921[−01]	−0.34609[−02]	−0.34606[−02]

$\delta=-0.001,\ f_n^{(1),b}=0.125$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1s	−0.49801[+00]	−0.49801[+00]	−0.89184[+00]	−0.49801[+00]	−0.49800[+00]
2s	−0.12475[+00]	−0.12475[+00]	0.87397[+00]	−0.12475[+00]	−0.12475[+00]
3s	−0.55482[−01]	−0.55482[−01]	0.39766[+00]	−0.55482[−01]	−0.55481[−01]
4s	−0.31219[−01]	−0.31219[−01]	0.24513[+00]	−0.31219[−01]	−0.31219[−01]
5s	−0.19984[−01]	−0.19984[−01]	0.17117[+00]	−0.19984[−01]	−0.19984[−01]
6s	−0.13880[−01]	−0.13880[−01]	0.12851[+00]	−0.13880[−01]	−0.13880[−01]
7s	−0.10198[−01]	−0.10198[−01]	0.10118[+00]	−0.10198[−01]	−0.10198[−01]
8s	−0.78086[−02]	−0.78086[−02]	0.82391[−01]	−0.78086[−02]	−0.78086[−02]
9s	−0.61701[−02]	−0.61701[−02]	0.68809[−01]	−0.61701[−02]	−0.61701[−02]
10s	−0.49980[−02]	−0.49980[−02]	0.58605[−01]	−0.49980[−02]	−0.49980[−02]
11s	−0.41307[−02]	−0.41307[−02]	0.50706[−01]	−0.41307[−02]	−0.41307[−02]
12s	−0.34711[−02]	−0.34711[−02]	0.44441[−01]	−0.34711[−02]	−0.34711[−02]

$$f_n^{(m)}(\alpha_n^{(m)})=\left\{\frac{\langle\psi_n^{(m)}|\{[-H+E_n^{(1)}]|\psi_n^{(m-1)}\rangle f_n^{(m-1)}+E_n^{(2)}f_n^{(m-2)}|\psi_n^{(m-2)}\rangle+\cdots+E_n^{(m-1)}f_n^{(1)}|\psi_n^{(1)}\rangle\}}{\langle\psi_n^{(m)}|H_0(\alpha)+h(\alpha)-E_n^{\langle 0\rangle}(\alpha)|\psi_n^{(m)}\rangle}\right\}_{\alpha=\alpha_n^{(m)}}. \tag{29}$$

As expected, we have the mth-order self-consistent associated equations (22), (26), and (29). To be explicit, we choose $m=1$. Then we have

$$\frac{d}{d\alpha}E_n^{\langle 1\rangle}(\alpha)|_{\alpha=\alpha_n^{(1)}}=0, \tag{30}$$

$$E_n^{(1)}(\alpha_n^{(1)})=f_n^{(1)}(\alpha_n^{(1)})\langle\psi_n^{(0)}|h(\alpha)|\psi_n^{(1)}\rangle|_{\alpha=\alpha_n^{(1)}}+\langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle|_{\alpha=\alpha_n^{(1)}}, \tag{31}$$

and

$$f_n^{(1)}(\alpha_n^{(1)})=\left\{\frac{-\langle\psi_n^{(1)}(\alpha)|H'|\psi_n^{(0)}(\alpha)\rangle}{\langle\psi_n^{(1)}|H_0(\alpha)+h(\alpha)-E_n^{\langle 0\rangle}(\alpha)|\psi_n^{(1)}\rangle}\right\}_{\alpha=\alpha_n^{(1)}}. \tag{32}$$

We then seek to find a solution by using iterative techniques as in the previous work [2]. We shall illustrate this in a simple example in the next section.

III. CALCULATIONS

The excited hydrogenlike ion in a potential field $-\delta/r^2$ is an excellent system for testing the accuracy of the equal-factor approach because the coupling parameter δ in this case varies from $-\infty$ to 0.125 over a wide range, and the exact eigenvalues can be obtained easily by an analytic approach. To explicitly demonstrate the equal-factor approach, we investigate this simple case in S-wave states which have common l eigenvalues $l=0$. Application of the screened hydrogenic partitioning scheme of Dalgarno *et al.* (see, for example, [4]) yields

$$H_0(\alpha)=-\tfrac{1}{2}\nabla^2-\alpha/r, \tag{33}$$

$$h(\alpha)=-\frac{Z-\alpha}{r}, \tag{34}$$

$$H'=-\delta/r^2, \tag{35}$$

where the potential $h(\alpha)=H_0-H_0(\alpha)$ represents changes in an initial system of the hydrogenlike ion under the potential field $-\delta/r^2$ in a very short period of time T.

It is well known that the exact energy level is given as follows:

$$E_n^{\text{exc}}=-Z^2/2n'^2, \quad n'=n+\Delta l \tag{36}$$

and Δl is the root of a quadratic equation [1],

$$\Delta l^2+\Delta l+2\delta=0.$$

Now the mth-order perturbation equation for hydrogenlike ions in a $-\delta/r^2$ field is given explicitly. If $m=1$,

$$E_n^{(1)}(\alpha)=\alpha^2\{f_n^{(1)}(\alpha)P_n^{(1)}(\alpha)-2\delta/n^3\}-Z\alpha f_n^{(1)}(\alpha)P_n^{(1)}(\alpha). \tag{37}$$

If $m\geqslant 2$,

$$E_n^{(m)}(\alpha)=\alpha^2\{f_n^{(m)}(\alpha)P_n^{(m)}(\alpha)-\delta f_n^{(m-1)}(\alpha)Q_n^{(m-1)}(\alpha)\}-Z\alpha f_n^{(m)}(\alpha)P_n^{(m)}(\alpha), \tag{38}$$

so that the mth-order approximation to the energy is

$$E_n^{\langle m\rangle}(\alpha)=\alpha^2\left\{\frac{1}{2n^2}+\sum_{k=1}^{m}f_n^{(k)}P_n^{(k)}-\delta\left(\frac{2}{n^3}+\sum_{k=1}^{m-1}f_n^{(k)}Q_n^{(k)}\right)\right\}-\alpha Z\left(\frac{1}{n^2}+\sum_{k=1}^{m}f_n^{(k)}P_n^{(k)}\right), \quad n=1,2,\ldots, \tag{39}$$

where we have the convention $\Sigma_{k=1}^{m-1}f_n^{(k)}Q_n^{(k)}=0$ if $m=1$.

According to the condition of the second kind of balance, the balance principle now yields

$$\frac{d}{d\alpha}E_n^{\langle m\rangle}(\alpha)=2\alpha\left\{\frac{1}{2n^2}+\sum_{k=1}^{m}f_n^{(k)}P_n^{(k)}-\delta\left(\frac{2}{n^3}+\sum_{k=1}^{m-1}f_n^{(k)}Q_n^{(k)}\right)\right\}-Z\left(\frac{1}{n^2}+\sum_{k=1}^{m}f_n^{(k)}P_n^{(k)}\right)=0. \tag{40}$$

By using the fact that

$$f_n^{(m)}(\alpha)\sum_{j\neq n}E_i^{(m)}(\alpha)\phi_j^{(0)}(\vec{x},\alpha)=f_n^{(m)}(\alpha_n^{(m)})\sum_{j\neq n}E_i^{(m)}(\alpha_n^{(m)})\phi_j^{(0)}(\vec{x},\alpha), \tag{41}$$

hence the parameter $\alpha_n^{(m)}$ is chosen as the corresponding mth-order balance point

$$\alpha_n^{(m)}=\frac{Z\left(1+n^2\sum_{k=1}^{m}f_n^{(k)}P_n^{(k)}\right)}{1+2n^2\sum_{k=1}^{m}f_n^{(k)}P_n^{(k)}-2n^2\delta\left(\frac{2}{n^3}+\sum_{k=1}^{m-1}f_n^{(k)}Q_n^{(k)}\right)}, \tag{42}$$

so the mth-order approximation of minimum energy may be expressed as

TABLE V. Comparison of various computed eigenvalues with the exact value (in a.u.) for extremely large negative coupling parameters $\delta=-10^2$, -10^4, and -10^6. $E_n^{\langle 1\rangle,a}$, $E_n^{\langle 1\rangle,b}$, and $E_n^{\langle 1\rangle,RS}$ are the first-order approximation to the energy for $n=1$ to 12 states of a perturbed hydrogen atom. The corresponding equal factors $f_n^{(1),a}$ and $f_n^{(1),b}$ are determined by formula (46) and by trial, respectively. Numbers in square brackets indicate powers of 10.

$\delta=-10^2$ $f_n^{(1),b}=600$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1s	−0.23294[−02]	−0.11038[−02]	−0.15693[+03]	−0.17104[−02]	0.19950[+03]
2s	−0.20412[−02]	−0.10750[−02]	0.23005[+03]	−0.17050[−02]	0.24875[+02]
3s	−0.18034[−02]	−0.10326[−02]	0.33843[+03]	−0.13742[−02]	0.73519[+01]
4s	−0.16048[−02]	−0.87221[−03]	0.32351[+03]	−0.11468[−02]	0.30937[+01]
5s	−0.14374[−02]	−0.70226[−03]	0.28357[+03]	−0.99026[−03]	0.15800[+01]
6s	−0.12948[−02]	−0.56289[−03]	0.24516[+03]	−0.87746[−03]	0.91204[+00]
7s	−0.11724[−02]	−0.45998[−03]	0.21368[+03]	−0.79265[−03]	0.57289[+00]
8s	−0.10666[−02]	−0.38506[−03]	0.18956[+03]	−0.72664[−03]	0.38281[+00]
9s	−0.97453[−03]	−0.32976[−03]	0.17114[+03]	−0.67382[−03]	0.26818[+00]
10s	−0.89387[−03]	−0.28786[−03]	0.15686[+03]	−0.63071[−03]	0.19500[+00]
11s	−0.82281[−03]	−0.25502[−03]	0.14551[+03]	−0.59554[−03]	0.14613[+00]
12s	−0.75991[−03]	−0.22860[−03]	0.13622[+03]	−0.56651[−03]	0.11227[+00]

$\delta=-10^4$ $f_n^{(1),b}=50\,000$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1s	−0.24824[−04]	−0.11073[−04]	−0.15348[+05]	−0.16683[−04]	0.19999[+05]
2s	−0.24478[−04]	−0.10910[−04]	0.23070[+05]	−0.15674[−04]	0.24999[+04]
3s	−0.24139[−04]	−0.10691[−04]	0.34256[+05]	−0.12820[−04]	0.74069[+03]
4s	−0.23807[−04]	−0.92390[−05]	0.33201[+05]	−0.10870[−04]	0.31247[+03]
5s	−0.23482[−04]	−0.75892[−05]	0.29493[+05]	−0.95235[−05]	0.15998[+03]
6s	−0.23163[−04]	−0.61699[−05]	0.25765[+05]	−0.85484[−05]	0.92579[+02]
7s	−0.22851[−04]	−0.50877[−05]	0.22606[+05]	−0.78196[−05]	0.58299[+02]
8s	−0.22545[−04]	−0.42837[−05]	0.20129[+05]	−0.72534[−05]	0.39055[+02]
9s	−0.22245[−04]	−0.36841[−05]	0.18211[+05]	−0.68026[−05]	0.27429[+02]
10s	−0.21951[−04]	−0.32284[−05]	0.16715[+05]	−0.64377[−05]	0.19995[+02]
11s	−0.21663[−04]	−0.28713[−05]	0.15528[+05]	−0.61420[−05]	0.15022[+02]
12s	−0.21381[−04]	−0.25841[−05]	0.14558[+05]	−0.59009[−05]	0.11571[+02]

$\delta=-10^6$ $f_n^{(1),b}=5\,000\,000$

ns	E_n^{exc}	$E_n^{\langle 1\rangle,a}$	$f_n^{(1),a}$	$E_n^{\langle 1\rangle,b}$	$E_n^{\langle 1\rangle,RS}$
1s	−0.24982[−06]	−0.11074[−06]	−0.15344[+07]	−0.16684[−06]	0.20000[+07]
2s	−0.24947[−06]	−0.10912[−06]	0.23071[+07]	−0.15677[−06]	0.25000[+06]
3s	−0.24912[−06]	−0.10695[−06]	0.34261[+07]	−0.12824[−06]	0.74074[+05]
4s	−0.24877[−06]	−0.92446[−07]	0.33211[+07]	−0.10874[−06]	0.31250[+05]
5s	−0.24842[−06]	−0.75955[−07]	0.29505[+07]	−0.95283[−07]	0.16000[+05]
6s	−0.24807[−06]	−0.61760[−07]	0.25779[+07]	−0.85537[−07]	0.92592[+04]
7s	−0.24772[−06]	−0.50933[−07]	0.22620[+07]	−0.78252[−07]	0.58309[+04]
8s	−0.24737[−06]	−0.42887[−07]	0.20143[+07]	−0.72594[−07]	0.39062[+04]
9s	−0.24702[−06]	−0.36886[−07]	0.18223[+07]	−0.68091[−07]	0.27435[+04]
10s	−0.24667[−06]	−0.32325[−07]	0.16727[+07]	−0.64445[−07]	0.20000[+04]
11s	−0.24633[−06]	−0.28750[−07]	0.15539[+07]	−0.61492[−07]	0.15026[+04]
12s	−0.24598[−06]	−0.25876[−07]	0.14569[+07]	−0.59086[−07]	0.11574[+04]

TABLE VI. Comparison of various computed eigenvalues with the exact value (in a.u.) for various coupling parameters δ for the ground state $(1s)$ of a perturbed hydrogen atom in a potential $-\delta/r^2$. E_{1s}^{V} denotes variational (Ref. [5]).

δ	$E_{1s}^{\langle 1\rangle ,b}$	$f_{1s}^{(1),b}$	$E_{1s}^{\langle 1\rangle ,RS}$	E_{1s}^{V}	E_{1s}^{exc}
0.1	−0.840609	0.05	−0.700000	−0.833333	−0.954915
0.01	−0.520844	0.05	−0.520000	−0.520833	−0.521060
0.005	−0.510206	0.05	−0.510000	−0.510204	−0.510257
−0.1	−0.357746	0.125	−0.300000	−0.357140	−0.364745
−0.01	−0.480789	0.125	−0.480000	−0.480770	−0.480947
−0.005	−0.490201	0.125	−0.490000	−0.490200	−0.490243
−50	−0.003444	325	99.500000	−0.002488	−0.004524
−100	−0.001710	600	199.500000	−0.001247	−0.002329

$$E_n^{\langle m\rangle}(\alpha_n^{(m)}) = -\frac{Z^2}{2n^2} \times \frac{\left(1+n^2\sum_{k=1}^{m} f_n^{(k)}P_n^{(k)}\right)^2}{1+2n^2\sum_{k=1}^{m} f_n^{(k)}P_n^{(k)} - 2n^2\delta\left(\frac{2}{n^3}+\sum_{k=1}^{m-1} f_n^{(k)}Q_n^{(k)}\right)} \tag{43}$$

if parameter α takes the value of balance point $\alpha_n^{(m)}$.

Substituting the mth-order balance point $\alpha_n^{(m)}$ in Eqs. (37) and (38), the corresponding mth-order self-consistent perturbation equation for a hydrogenlike ion in a $-\delta/r^2$ field is obtained. If $m=1$,

$$E_n^{(1)}(\alpha_n^{(1)}) = (\alpha_n^{(1)})^2\left\{ f_n^{(1)}(\alpha_n^{(1)})P_n^{(1)}(\alpha_n^{(1)}) - \frac{2\delta}{n^3}\right\} - Z\alpha_n^{(1)} f_n^{(1)} \times(\alpha_n^{(1)})P_n^{(1)}(\alpha_n^{(1)}), \quad n=1,2,\ldots,M. \tag{44}$$

If $m\geqslant 2$,

$$\begin{aligned} E_n^{(m)}(\alpha_n^{(m)}) = {} & (\alpha_n^{(m)})^2\{ f_n^{(m)}(\alpha_n^{(m)})P_n^{(m)}(\alpha_n^{(m)}) \\ & - \delta f_n^{(m-1)}(\alpha_n^{(m-1)})Q_n^{(m-1)}(\alpha_n^{(m-1)})\} \\ & - Z\alpha_n^{(m)} f_n^{(m)}(\alpha_n^{(m)})P_n^{(m)}(\alpha_n^{(m)}), \\ & n=1,2,\ldots,M. \end{aligned} \tag{45}$$

Moreover, substituting the first-order balance point $\alpha_n^{(1)}$ in Eq. (27), we have the first-order equal factor

$$f_n^{(1)}(\alpha_n^{(1)}) = \frac{\delta Q_n^{(1)}(\alpha_n^{(1)})}{\Sigma_{l\neq n}[E_i^{(1)}(\alpha_n^{(1)})]^2\left[\frac{1}{2n^2}-\frac{1}{2l^2}+\frac{Z-\alpha_n^{(1)}}{\alpha_n^{(1)}}\left(\frac{1}{n^2}-\frac{1}{l^2}\right)\right] - \frac{Z-\alpha_n^{(1)}}{\alpha_n^{(1)}}\Sigma_{l\neq n}\Sigma_{j\neq l}^{j\neq n}E_i^{(1)}(\alpha_n^{(1)})E_{i'}^{(1)}(\alpha_n^{(1)})a_{lj}}, \quad n=1,2,\ldots,M. \tag{46}$$

Now it is very clear that associated Eqs. (42), (44), and (46) are self-consistent because the unknown set $\{E_i^{(1)}(\alpha_n^{(1)})\}$ appears on both sides of Eq. (44). Therefore, this associated equation can be solved by applying the iterative technique step by step as has been shown in previous work [2].

The notations in Eqs. (37)–(46) are defined as follows:

$$P_n^{(m)}(\alpha) = \sum_{j\neq n}^{M+1} a_{nj}E_i^{(m)}(\alpha) \tag{47}$$

and

$$Q_n^{(m)}(\alpha) = \sum_{j\neq n}^{M+1} b_{nj}E_i^{(m)}(\alpha), \tag{48}$$

where

$$\left\langle \alpha ns\left|\frac{1}{r}\right|\alpha js\right\rangle = \begin{cases} \dfrac{\alpha}{n^2}, & j=n \\ a_{nj}\alpha, & j\neq n \end{cases} \tag{49}$$

and

$$\left\langle \alpha ns\left|\frac{1}{r^2}\right|\alpha js\right\rangle = \begin{cases} \dfrac{2\alpha^2}{n^3}, & j=n \\ b_{nj}\alpha^2, & j\neq n \end{cases} \tag{50}$$

and where a_{nj} and b_{nj} both are proportional coefficients and symmetric. They are listed in Table I.

IV. DISCUSSION AND CONCLUSIONS

A very basic idea of PFSKB theory is that there is a possible metastable process in the short period of time that a

TABLE VII. The first-order approximate balance values $\alpha_n^{(1),a}$ corresponding to $f_n^{(1),a}$ determined by formula (46) for $n=1$ to 12 states of a perturbed hydrogen atom for various coupling parameters δ. Numbers in square brackets indicate powers of 10.

ns \ δ	0.01	0.005	0.001	-0.1	-0.01	-0.001	-10^2	-10^4	-10^6
1s	1.0417	1.0204	1.0040	0.71425	0.96153	0.99601	0.25028[−02]	0.25099[−04]	0.25100[−06]
2s	1.0025	1.0016	1.0004	0.89478	0.99504	0.99961	0.38051[−02]	0.38240[−04]	0.38243[−06]
3s	1.0522	1.0250	1.0048	0.75536	0.95599	0.99525	0.12617[−01]	0.12919[−03]	0.12922[−05]
4s	1.0282	1.0133	1.0025	0.85041	0.97695	0.99750	0.19825[−01]	0.20695[−03]	0.20704[−05]
5s	1.0184	1.0089	1.0017	0.87737	0.98350	0.99828	0.24998[−01]	0.26545[−03]	0.26562[−05]
6s	1.0138	1.0068	1.0013	0.89831	0.98714	0.99867	0.28836[−01]	0.31025[−03]	0.31050[−05]
7s	1.0112	1.0055	1.0011	0.91282	0.98943	0.99892	0.31934[−01]	0.34661[−03]	0.34692[−05]
8s	1.0094	1.0046	1.0009	0.92367	0.99102	0.99908	0.34777[−01]	0.37958[−03]	0.37994[−05]
9s	1.0081	1.0040	1.0008	0.93210	0.99218	0.99921	0.37566[−01]	0.41160[−03]	0.41201[−05]
10s	1.0071	1.0035	1.0007	0.93884	0.99308	0.99930	0.40383[−01]	0.44387[−03]	0.44434[−05]
11s	1.0064	1.0032	1.0006	0.94435	0.99378	0.99937	0.43245[−01]	0.47683[−03]	0.47734[−05]
12s	1.0058	1.0029	1.0006	0.94894	0.99436	0.99943	0.46128[−01]	0.51029[−03]	0.51086[−05]

system is passing from unperturbed to perturbed. Suppose we have a time-independent Schrödinger equation:

$$H\Psi_n(\vec{x})=E_n\Psi_n(\vec{x}), \tag{51}$$

where energy levels E_n and eigenfunction $\Psi_n(\vec{x})$ are stable. We assume this system historically may come from an isolated subsystem H_0 and a perturbing subsystem H'. After passing the possible metastable process, two subsystems are formed, yielding a stable system at the total energy minimum position. Clearly, energy levels E_n and wave functions $\Psi_n(\vec{x})$ in the traditional Schrödinger equation (51) are identical with the balance energy level and wave functions at the end of the possible metastable process. Namely,

$$E_n=\min\{E_n(\alpha)\}_{\alpha=\alpha^*}, \tag{52}$$

$$\Psi_n(\vec{x})=\Psi_n(\vec{x},\alpha)|_{\alpha=\alpha^*}. \tag{53}$$

Next we try to solve Eq. (51). First, if this equation is solvable by analytic means, the exact energy eigenvalues E_n and wave eigenfunctions $\Psi_n(\vec{x})$, can be obtained. But if we want to solve this equation using a perturbation method, some aspects may be essentially different. We notice first that the wave function has been divided into two parts: $\Psi_n^{(0)}(\vec{x},\alpha)+\phi^P(\vec{x},\alpha)$. This shows that one may artificially impose an operation to balanced wave functions and disassociate then into a possible metastable condition. So perturbation is essentially a means to solve the Schrödinger equation (51) in PFSKB theory but we cannot ignore the influence of the original wave functions on that physical operation.

Another point is that this possible metastable process not only exist theoretically, but also can be realized by simulating an iterative process. For example, in the case of a hydrogenlike ion in a potential field $-\delta/r^2$, the possible metastable process can be simulated and is shown in Table II. We can demonstrate the entire possible metastable process of varying $E_n^{(1)}(\alpha)$, $E_n^{\langle 1\rangle}(\alpha)$, and $f_n^{(1)}(\alpha)$, and eventually these converge to stable values. Setting the initial parameter $\alpha=1$ (if $\alpha=Z$ for hydrogenlike ions), we have the initial values of

$$f_n^{(1),i}=0, \tag{54}$$

$$E_n^{(1),i}=-2\delta/n^3, \tag{55}$$

$$E_n^{\langle 1\rangle,i}=-\frac{1}{2n^2}-\frac{2\delta}{n^3}, \tag{56}$$

where δ takes value of -10^6; the simulation process is then turned on. After 25 iterations of this procedure, eventually one sees convergence to balance values. Briefly, this process is shown in Table II.

In this work, the iterative processes converge rapidly for a very wide range of coupling parameters from $-\infty<\delta\leqslant 0.05$. Unfortunately, we find that convergence for states of $n=1$ to 3 is not as rapid for the coupling parameter $0.05<\delta\leqslant 0.125$. The possible reason is that the equal-factor relation (9) is not well-suited for a large positive coupling parameter δ.

In previous work [2], we used the trial method to determine the first-order equal factor $f_n^{(1)}$. We assume that $f_n^{(1)}$ is independent of principal quantum number n. For comparison, in this work we also calculate some cases using first-order equal factors which are determined by a trial process.

The comparison is made for the first-order approximation of various computed eigenvalues: (a) by equal factors determined by formula (46); (b) by equal factors determined by trial; (c) by an RSPT standard (Rayleigh-Schrödinger perturbation theory), where corresponding notations are $E_n^{\langle 1\rangle,a}$, $E_n^{\langle 1\rangle,b}$, and $E_n^{\langle 1\rangle,RS}$, respectively, in Tables III–V.

It appears that results from the trial method are only slightly better than results from the method of equal factors as determined by formula (46). The trial method requires exact eigenvalues as reference.

Various computed eigenvalues are shown in Table V. In the extremely large coupling parameter cases, we find to our surprise that both of the first-order equal-factor approximations of eigenvalues for extremely large coupling parameter δ from -10^2 to -10^6 lead to energy levels which are within 10–67 % of the exact answers. As may be seen from Tables III, IV, and VI, the calculated energy values from both standard first-order RSPT and our first-order equal-factor approach are in good agreement and yield accurate estimates of exact energies for small values of the coupling parameter δ; on the other hand, however, as is to be anticipated, first-order RSPT fails completely for the extremely large negative values of the coupling parameter shown in Tables V and VI.

We tabulate the balance points $\alpha_n^{(1)}$ of a hydrogen atom for various coupling parameters δ in Table VII. We find that if $\alpha_n^{(1)}$ is close to 1 (for the $Z=1$ case), the corresponding RSPT-computed eigenvalues are very close to the equal-factor PFSKB results. Otherwise, if $\alpha_n^{(1)}$ is close to zero, the corresponding RSPT-computed eigenvalues are inaccurate. This behavior indicates that the eigenvalues computed from RSPT can be considered as reasonable results only in those cases in which charge Z is close to the balance point of this system.

Comparison of variational [5] computed eigenvalues also is made with equal-factor and RSPT, and results are shown in Table VI for the ground state $(1s)$ of a perturbed hydrogen atom for various δ values.

All results computed in this paper are for the $(Z=1)$ hydrogen atom. Results for hydrogenlike ions $(Z>1)$ can be obtained easily by transformations:

$$E_{Zn}^{\langle 1\rangle}=Z^2E_{1n}^{\langle 1\rangle}, \tag{57}$$

$$f_{Zn}^{(1)}=f_{1n}^{(1)}/Z^2, \tag{58}$$

$$\alpha_{Zn}^{(1)}=Z\alpha_{1n}^{(1)}. \tag{59}$$

We have performed these first-order approximation calculations on a 386/DX personal computer. An infinite series of energy levels is truncated at $M=12$. Iterative processes for all calculations show stable and rapid convergence. Notation E_n^{exc} in the tables indicates the exact eigenvalue of state n, which was obtained in Eq. (36).

We have shown that reformulation of the perturbation approach can lead to a series of powerful iterative-self-consistent equations. A general procedure for obtaining a set of eigenfuctions and eigenenergies is also developed in detail. Results for an explicit example are illustrated.

Perturbation reformulation based on the equal-factor assumption can contribute to perturbation theory in its simplest form. It appears that the success of equal-factor perturbation in the case of hydrogenlike ions is a strong justification for PFSKB theory.

The numerical calculations performed in this work yielded relative errors $\leqslant 10^{-5}$, and have been carried out on a personal computer with software written by the author.

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