follows when the electrons are fixed in a space-fixed coordinate system. For a diatomic, one may use confocal ellipsodial coordinates, in which interparticle distances are proportional to the internuclear distance R for fixed values of these coordinates. The volume element is *explicitly* proportional to R^3, ρ to R^{-3}, the potential-energy operators to R^{-1}. Taking $P=R$, we note that the potential-energy terms V are explicitly proportional to R^{-1} and the kinetic energy T (proportional to $\int\rho^{5/3}d\tau$) to R^{-2}. Then our theorem gives

$$dE/dR = -R^{-1}V - 2R^{-1}T \ , \qquad (2)$$

which is the virial theorem. This proof is well known for the quantum mechanical case.[8] The atom is the special case where one nuclear charge is zero; E then does not depend on R.

As a final example, the change in energy in going from the TF to the TFD theory is due to the additional term $-\kappa_a\int\rho^{4/3}d\tau$ in the energy functional, with $\kappa_a \sim 0.74e^2$. The energy change could be estimated from the TF function without computing the TFD function by considering E as a function of κ_a, with $\kappa_a = 0$ corresponding to TF and $\kappa_a \sim 0.74e^2$ to TFD. Imagine $E(\kappa_a)$ to be expanded in a power series about $\kappa_a = 0$. If the linear term suffices, the energy change is $\kappa_a\, dE/d\kappa_a = -\kappa_a\int\rho^{4/3}d\tau$, where ρ is the TF density. We obtain then

$$E_{\mathrm{TFD}} - E_{\mathrm{TF}} = -0.363\,Z^{5/3}\int\varphi^2 dx\, e^2/a_0 \ , \qquad (3)$$

where φ is the solution to the TF equation.[3] Evaluating the integral numerically for the tabulated φ gives 0.640, and the energy difference is $-0.232 \times Z^{5/3}\, e^2/a_0$, as compared to $-0.23Z^{5/3}e^2/a_0$, as calculated directly by Gombas[9] [If the expansion of $E(\kappa_a)$ were made around $\kappa_a = 0.74e^2$ instead of 0, the same reasoning would show the energy difference could be calculated from $\kappa_a\int\rho^{4/3}d\tau$ where ρ is the TFD density.]

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Padé Approximants and Inner Projections in the Brillouin-Wigner Perturbation Scheme for He-like Ions*

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The continued-fraction expansions in terms of Brillouin-Wigner perturbation energies are evaluated for the He-like series. They show remarkable convergence and stability properties. Both Padé approximants and perturbation energies are computed with formulas derived by the inner-projection technique.

INTRODUCTION

The Brillouin-Wigner (BW) perturbation series[1] suffers from convergence problems which, in addition to computational difficulties, made its use relatively infrequent. Modifications of the scheme, which cast it into a continued fraction expansion were made by Feenberg and others.[2-4] It is possible to derive the bounding properties of the alternate energy approximants of Young *et al.*[3] by showing that they can be obtained by inner projections of the reaction operator in the way suggested by Löwdin,[5] provided one chooses the linear manifold considered in a specific way.[6] It can be seen that the upper- and lower-bound approximants can be identified as Padé approximants[7] to the BW series.[8] In the Rayleigh-Schrödinger (RS) case, the analogous Padé approximants showed remarkable convergence even though one could

neither prove nor verify any bounding properties.[9] The fact that the same construction, but within the BW scheme, yields bounds, prompted the present study.

BRILLOUIN-WIGNER-PADÉ EXPANSIONS

Given the splitting of the Hamiltonian

$$\mathcal{H}=\mathcal{H}^0+V, \quad \mathcal{H}\Psi_n=E\Psi_n \tag{1}$$

with $$\mathcal{H}^0\varphi_n^0=E_n^0\varphi_n^0 \ , \tag{2}$$

one can write the bracketing function[10] $\mathcal{E}_1(\mathcal{E})$ in the form (from now on we consider the ground state only)

$$\mathcal{E}_1(\mathcal{E})=E_0^0+\langle\varphi_0^0|t(\mathcal{E})|\varphi_0^0\rangle \ , \tag{3}$$

where the reaction operator $t(\mathcal{E})$ has the form

$$t=(V^{-1}-T_0)^{-1} \tag{4}$$

with $$T_0=P(\mathcal{E}-\mathcal{H}^0)^{-1}, \quad P=1-|\varphi_0^0\rangle\langle\varphi_0^0| \ . \tag{5}$$

Form (4) is appropriate if V^{-1} exists, which is the case when, e.g., $V>0$ in an operator sense. We restrict ourselves to that case. The BW series follows from expanding (4) and substituting into (3). The usual definition

$$\epsilon_k=\epsilon_k(\mathcal{E})=\langle\varphi_0^0|V(T_0V)^{k-1}|\varphi_0^0\rangle \tag{6}$$

leads to the linear series

$$\mathcal{E}_1(\mathcal{E})\sim\mathcal{E}_s^p(\mathcal{E})=E_0^0+\sum_{k=1}^{p}\epsilon_k \tag{7}$$

and the ground-state energy E_0^0 is approximated by

$$\mathcal{E}=\mathcal{E}_s^p(\mathcal{E}) \ . \tag{8}$$

The convergence properties of (7) and (8) can be rather disappointing. One can construct better approximants in terms of the $\{\epsilon_k\}$ by considering the linear variation functional in terms of the functions $\{(T_0V)^k\varphi_0^0\}$.[2,4] A continued fraction expansion was obtained also.[3] A simple derivation of a compact form for those expressions can be given[6]: Partitioning of the eigenvalue problem of H in terms of the basis $\{(T_0V)^{k-1}\varphi_0^0\}$, $k=1,2,\ldots,n+1$ leads to a bracketing function

$$\mathcal{E}_U^N(\mathcal{E})=E_0^0+\epsilon_1+\underline{\epsilon}^\dagger\underline{E}^{-1}\underline{\epsilon} \ , \tag{9}$$

where ϵ is a column vector with elements ϵ_{k+1} and $\underline{E}$ is a square matrix with elements $E_{kl}=\epsilon_{k+l}-\epsilon_{k+l+1}$. An upper bound to the ground state can be found by solving

$$\mathcal{E}=\mathcal{E}_U^N(\mathcal{E}) \ . \tag{10}$$

Lower bounds can be obtained by a Bazley projection of the reaction operator, if t is a non-negative operator.[5] One obtains[6]:

$$\mathcal{E}_L^N=E_0^0+\epsilon_1+\epsilon_2+\underline{\bar{\epsilon}}^\dagger\underline{\bar{E}}^{-1}\underline{\bar{\epsilon}} \ , \tag{11}$$

where $\underline{\bar{\epsilon}}$ is a column vector with elements ϵ_{k+2} and $\underline{\bar{E}}$ a matrix with elements $\bar{E}_{kl}=\epsilon_{k+l+1}-\epsilon_{k+l+2}$. A lower bound to the ground-state energy is given by

$$\mathcal{E}=\mathcal{E}_L^N(\mathcal{E}) \ . \tag{12}$$

It can be seen[8] that one can express (9) and (10) in terms of Padé approximants to the series

$$\sum_{k=2}^{\infty}\epsilon_k\mu^k \tag{13}$$

or better, to the function

$$\Theta(\mathcal{E},\mu)=\langle\varphi_0^0|(V^{-1}-\mu T_0)^{-1}|\varphi_0^0\rangle-\epsilon_1 \ , \tag{14}$$

which verifies

$$\Theta(\mathcal{E},1)=\mathcal{E}_1(\mathcal{E})-E_0^0-\epsilon_1 \ . \tag{15}$$

We have, in the notation of Baker for the Padé approximants[7,11]

$$\mathcal{E}_U^N(\mathcal{E})=E_0^0+\epsilon_1-[N,N-1](\mathcal{E},1) \tag{16}$$

and $$\mathcal{E}_L^N(\mathcal{E})=E_0^0+\epsilon_1-[N,N](\mathcal{E},1) \ , \tag{17}$$

where $[N,N-1](\mathcal{E},1)$ and $[N,N](\mathcal{E},1)$ are Padé approximants to $\Theta(\mathcal{E},\mu)$ for $\mu=1$.[11] It is easily seen that in the case of $V>0$ and $T_0<0$ the series $\mathcal{E}_s^\infty$ given by (7) is of Stieltjes type provided that $\{(T_0V)^k\varphi_0^0\}$ is linearly independent. Defining

$$e_k\equiv(-1)^{k+1}\epsilon_k \tag{18}$$

we have

$$\mathcal{E}_s^\infty=E_0^0+\sum_{k=1}^{\infty}e_k(-1)^{k+1} \ . \tag{19}$$

Consider then the formal expansion of (14):

$$\Theta(\mathcal{E},\mu)=-\sum_{k=2}^{\infty}e_k(-\mu)^k \ . \tag{20}$$

The coefficients e_k satisfy the inequalities

$$D(m,n)>0, \quad m=2,3,\ldots;\ n=0,1,\ldots \tag{21}$$

with $$D(m,n)=\begin{vmatrix} e_m & e_{m+1} & \cdots & e_{m+n} \\ \cdots & & & \\ e_{m+n} & e_{m+n+1} & \cdots & e_{m+2n} \end{vmatrix} \ . \tag{22}$$

This implies that (20) is a Stieltjes series and hence the following properties of Padé approximants to functions which admit a Stieltjes series expansion hold[7]:

$$[N,N](\mathcal{E},\mu)\leq\Theta(\mathcal{E},\mu)\leq[N,N-1](\mathcal{E},\mu) \ . \tag{23}$$

These inequalities are consistent with (9), (10), (16) and (17).

One could consider (16) and (17) and replace the BW energies by their RS counterparts. No bounding properties should be expected, but an improvement over the corresponding linear series is obtained.[9]

APPLICATIONS TO He-LIKE IONS

It is clear that the BW perturbation energies cannot be computed exactly except in trivial cases. Variational techniques have been devised.[12] The He-like series is the simplest problem where the techniques can be tested. We resort to the inner-projection technique, and for $\mathcal{E} < E_1^0$ we have

$$T_0 \leq |\underline{h}\rangle \langle \underline{h}| \mathcal{E} - \mathcal{H}^0 |\underline{h}\rangle^{-1} \langle \underline{h}| \equiv \tilde{T}_0 \leq 0, \qquad (24)$$

where $|\underline{h}\rangle = \{|h_1\rangle, \ldots, |h_m\rangle\}$ is a linear manifold such that $P|\underline{h}\rangle = |\underline{h}\rangle$. This procedure was used extensively in a number of problems.[13] From the relation between the spectrum of H^0 and H one knows that the "interesting" values of $\mathcal{E}$ satisfy $\mathcal{E} > E_1^0$ in the case of H^-. One can still use $\tilde{T}_0$ as defined in (24) but the inequality is not fulfilled and one has to make sure that $\mathcal{E}$ is not equal to any eigenvalue of H^0 in the space spanned by $|\underline{h}\rangle \langle \underline{h}|\underline{h}\rangle \langle \underline{h}|$. One could circumvent this problem altogether by introducing a multidimensional reference function,[14] but this would be of no interest in connection with conventional BW perturbation theory.

The consequences of replacing T_0 by $\tilde{T}_0$ are quite interesting. Formally, one can retain the same formulas as before, and hence ϵ_k is to be replaced by $\tilde{\epsilon}_k$. Equations (9), (10), and (16) still yield upper bounds, regardless of the character of V and $\tilde{T}_0$, provided the $\{\tilde{\epsilon}_k\}$ exist. On the other hand (11), (12), and (17) do yield lower bounds, not to the exact ground-state energy, but to the solution of

$$\mathcal{E} = \tilde{\mathcal{E}}_1(\mathcal{E}) = E_0^0 + \langle \varphi_0^0 | (V^{-1} - \tilde{T}_0(\mathcal{E}))^{-1} | \varphi_0^0 \rangle \qquad (25)$$

which is itself an upper bound to the exact ground-state energy if inequality (24) is fulfilled.

Thus, the scheme discussed leads to rigorous upper bounds even with approximate values of the perturbation energies. One could obtain rigorous lower bounds also, but at the cost of laborious computations.[13] The procedure employed here should be compared with RS calculations[15] which were carried out to a larger degree of accuracy. Since the BW scheme is less practical in connection with the study of an isoelectronic series, we considered a medium size basis to be adequate for this pilot calculation, and 40 functions involving Hylleraas coordinates[16]: $h_i = P\varphi_i$, $\varphi_i = e^{-ns} \times s^{l_i} t^{m_i} u^{n_i}$ with integers l_i, m_i, n_i, $l_i + m_i + n_i \geq 0$ and m_i even and larger than zero. The scale factor η was chosen so as to minimize $\tilde{\epsilon}_2$, except in H^-, where a special situation arises as we will discuss later. The set is in fact identical to the one used by Kinoshita[17] plus one function more which contributed significantly to $\tilde{\epsilon}_2$: the one which has $l = -2$, $m = 4$, and $n = 2$.

About the calculations themselves it is sufficient to say that there are four steps: (a) generation of the matrices $\underline{A}$, $\underline{V}$ and $\underline{a}$ for a fixed value of $\mathcal{E}$

$$\underline{A} = \langle \underline{h} | \mathcal{E} - \mathcal{H}^0 | \underline{h} \rangle ; \ \underline{V} = \langle \underline{h} | V | \underline{h} \rangle ; \ \underline{a}^\dagger = \langle \varphi_0^0 | V | \underline{h} \rangle ; \qquad (26)$$

(b) computation of the $\tilde{\epsilon}_k$

$$\tilde{\epsilon}_k = \underline{a}^\dagger \underline{A}^{-1} (\underline{V}\underline{A}^{-1})^{k-2} \underline{a} \quad (k = 2, \ldots); \qquad (27)$$

(c) computation of (9) or (16) and (11) or (17) with the approximate $\tilde{\epsilon}_k$; (d) iteration of the preceding steps until (10) and (12) are satisfied. Step (b) is to be done with great care since the matrix $\underline{A}$ proves to be ill conditioned for inversion. It is not advisable to invert it, and a procedure based upon a Schmidt-type orthogonalization of the set $\{h_i\}$, but with the metric $\mathcal{H}^0 - \mathcal{E}$, was employed. Apparently it goes back to Hylleraas and it belongs to the computational folklore of perturbation theory.[18]

It is quite clear that the $\tilde{\epsilon}_k$ for increasing k may be rather inaccurate, and thus the approximations to the total energy are more meaningful than the individual values of the $\tilde{\epsilon}_k$ reported.

It should be noted also that step (c), which involves the computation of the Padé approximants can also involve a rather ill-conditioned matrix $\underline{E}$ or $\overline{E}$. In fact, formulas (9) and (10) are valid as they stand provided the ϵ_k (or the $\tilde{\epsilon}_k$) do not form a geometric series. Not only the numerical computations indicate that for sufficiently large k they do, but this is a consequence of the definition of the ϵ_k themselves, as it will be discussed later. In any case the computational technique employed took account of this fact, and in this respect $\underline{\epsilon}^\dagger \underline{E}^{-1} \underline{\epsilon}$ is treated in the same way as $\underline{a}^\dagger \underline{A}^{-1} \underline{a}$.

NUMERICAL RESULTS

The computations were carried in the CDC computer of the University of Uppsala, using double length arithmetic. In order to test the convergence properties economically we set a convergence threshold for the satisfaction of (10) and (12) of 10^{-5} a.u. In fact, the convergence of the iteration procedure $\mathcal{E}^{(k+1)} = \tilde{\mathcal{E}}_1(\mathcal{E}^{(k)})$ is very fast in this problem due to the desirable properties of $d\tilde{\mathcal{E}}_1(\mathcal{E})/d\mathcal{E}$.[10] In Table I we show results for He (upper bounds). They are independent of the scale factor η to the accuracy presented in the range $1.92 \leq \eta \leq 1.98$. The sequence of $[N, N-1]$ Padé approximants is seen to converge very rapidly. The linear series appears to diverge. Examination of the individual $\tilde{\epsilon}_k(\mathcal{E})$, for values of $\mathcal{E}$ near -2.90 indicate that they form an alternating diverging series.

In Table II, we present results for the $[N, N]$ Padé approximants. They are not lower bounds to E_0, but to the lowest solution of (25). The agree-

TABLE I. $[N, N-1]$ approximants for the He atom and values for the BW linear series involving the same $\tilde{\epsilon}_K(\eta=1.94)$ (exact[a]: $E_0=-2.903\,724$).

N	$\mathcal{E}_N=E_0^0+\epsilon_1+[N,N-1](\mathcal{E}_N,1)$	$E_0^0+\epsilon_1+\sum_{K=2}^{2N+1}\tilde{\epsilon}_K(\mathcal{E}_N)$
1	−2.897 61	−2.639 72
2	−2.903 70	−2.360 86
3	−2.903 72	−1.738 59
4	−2.903 723	−0.398 73

[a]Reference 15.

TABLE II. $[N, N]$ approximants for the He atom and values for the BW linear series involving the same $\tilde{\epsilon}_K(\eta=1.94)$ (exact[a]: $E_0=-2.903\,724$).

N	$\mathcal{E}_N=E_0^0+\epsilon_1+[N,N](\mathcal{E}_N,1)$	$E_0^0+\epsilon_1+\sum_{K=2}^{2N+2}\tilde{\epsilon}_K(\mathcal{E}_N)$
1	−2.906 07	−3.269 82
2	−2.903 73	−3.698 49
3	−2.903 73	−4.611 75

[a]Reference 15.

ment between the results of Tables I and II indicate that within an accuracy of 10^{-5} a.u. we have solved the eigenvalue problem (1) by a modified Brillouin-Wigner-Padé expansion.

In order to study how convergence depends on the nuclear charge we compare in Table III results obtained for H^-, He, Li^+, and Be^{++}, which suffice as illustration. All the perturbation energies $\tilde{\epsilon}_k$ in each column are computed with the scale factor and energy value given on top. In each case the value of $\mathcal{E}$ is very near the solution, and thus the convergence of the BW series can be examined meaningfully. Several features are revealed by this table. The series of $\tilde{\epsilon}_k$ for H^- is not alternating and not particularly convergent. The series for He does not converge either but is alternating. For Li^+ and Be^{++}, the series are alternating and apparently convergent. That the Padé approximants and the linear series coincide for Be^{++}, and almost coincide for Li^+ is not too surprising. That for He and even for H^- the Padé approximants manage to sum the series is quite remarkable.

One may doubt, as we did, the accuracy or even the relevancy of calculations of this type for H^-. The procedure to compute (9) is very sensitive to round off errors in the individual $\tilde{\epsilon}_k$ for H^-. Any attempt of changing slightly the values of the $\tilde{\epsilon}_k$ (for $\mathcal{E}$ in neighborhood of −0.527), i.e., by going from double into single precision was catastrophic: The Padé approximant would vary enormously. On the other hand confidence in the results obtained with double-precision arithmetic is established by varying the scale factor in the basis set. Since $\tilde{T}_0$ is not definite we do not have a variational principle for $\tilde{\epsilon}_2$. The $\tilde{\epsilon}_k$ change a great deal but the Padé approximants are very stable, as it can be seen in Table IV for $E_0^0+\epsilon_1+[10,9]$. In all other cases the accuracy of the individual $\tilde{\epsilon}_k$ is not so critical and the results obtained using $\tilde{\epsilon}_k$ given to 10 decimal digits do not differ appreciably when they are given to 25 decimal digits (differences of the order 10^{-7} in He and less in Li^+ and Be^{++}).

The computations indicate that the ratios $\tilde{\epsilon}_{k+1}/\tilde{\epsilon}_k$, for a given value of $\mathcal{E}$ rapidly approach a constant value, i.e., the series becomes geometric. In fact, the ratio gives the largest eigenvalue of the operator T_0V, which is one of the poles of the function $\underline{\Theta}(\mathcal{E},\mu)$ defined in (14). The problem of determining the other poles is a classical one,[19] and they can be obtained by the QD algorithm.[20] We obtained for the largest eigenvalues (in absolute value) of T_0V, which determines the conver-

TABLE III. Values of selected $\tilde{\epsilon}_K(\mathcal{E})$, $[N, N-1]$ Padé approximants and linear series for specific choices of η and $\mathcal{E}$.

	H^-	He	Li^+	Be^{++}
η	0.73	1.96	3.099	4.2
$\mathcal{E}$	−0.527 75	−2.903 72	−7.279 9	−13.655
E_0^0	−1.000 00	−4.000 00	−9.000 00	−16.000 00
ϵ_1	0.625 00	+1.250 00	1.875 00	2.500 00
$\tilde{\epsilon}_2(\mathcal{E})$	$0.775\,99\times10^{1}$	−0.339 55	−0.238 08	−0.209 98
$\tilde{\epsilon}_3(\mathcal{E})$	$1.033\,14\times10^{3}$	0.443 40	0.131 83	$0.748\,59\times10^{-1}$
$\tilde{\epsilon}_4(\mathcal{E})$	$1.367\,43\times10^{5}$	−0.629 32	−0.078 136	$-0.283\,92\times10^{-1}$
$\tilde{\epsilon}_{21}(\mathcal{E})$	$1.216\,12\times10^{39}$	$2.838\,963\times10^{2}$	$-3.620\,17\times10^{-5}$	$-1.117\,51\times10^{-9}$
$E_0^0+\epsilon_1+[1,0]$	−0.433 73	−2.897 26	−7.278 24	−13.654 79
$E_0^0+\epsilon_1+\tilde{\epsilon}_2+\tilde{\epsilon}_3$	1.04×10^{3}	−2.646 16	−7.231 26	−13.635 13
$E_0^0+\epsilon_1+[10,9]$	−0.527 56	−2.903 72	−7.279 91	−13.655 57
$E_0^0+\epsilon_1+\sum_{K=2}^{21}\tilde{\epsilon}_K$	1.2×10^{39}	-1.7×10^{2}	−7.279 93	−13.655 57
Exact[a]	−0.527 751	−2.903 724	−7.279 93	−13.655 57

[a]Reference 21.

TABLE IV. Variation of $\tilde{\epsilon}_K(\mathcal{E})$ and $E_0^0+\epsilon_1+[N,N-1]$ with change of the scale factor η in the case of H^- ($\mathcal{E}$ fixed at 0.527 75 a.u.). In order to facilitate comparison we give only three significant figures for the individual $\tilde{\epsilon}_K$.

η	0.71	0.72	0.73	0.74	0.75	0.76
$\tilde{\epsilon}_2(\mathcal{E})$	3.24×10^{0}	4.61×10^{0}	7.76×10^{0}	2.26×10^{1}	-2.66×10^{1}	-8.56×10^{0}
$\tilde{\epsilon}_3(\mathcal{E})$	1.85×10^{2}	3.69×10^{2}	1.03×10^{3}	8.71×10^{3}	1.19×10^{4}	1.22×10^{3}
$\tilde{\epsilon}_4(\mathcal{E})$	1.04×10^{4}	2.93×10^{4}	1.37×10^{5}	3.34×10^{6}	-5.33×10^{6}	-1.76×10^{5}
$\tilde{\epsilon}_5(\mathcal{E})$	5.85×10^{5}	2.32×10^{6}	1.81×10^{7}	1.28×10^{9}	2.39×10^{9}	2.53×10^{7}
$\tilde{\epsilon}_{20}(\mathcal{E})$	1.03×10^{32}	7.10×10^{34}	1.22×10^{39}	7.44×10^{47}	-1.41×10^{49}	-5.83×10^{39}
$\tilde{\epsilon}_{21}(\mathcal{E})$	5.79×10^{33}	5.63×10^{36}	1.61×10^{41}	2.86×10^{50}	6.32×10^{51}	8.38×10^{41}
$E_0^0+\epsilon_1+[10,9]$	−0.527 592	−0.527 572	−0.527 557	−0.527 359	−0.527 525	−0.527 513
$E_0^0+\epsilon_1+[1,0]$	−0.432 945	−0.433 369	−0.433 726	−0.434 020	−0.434 522	−0.435 282

gence of the linear series,[5] the values 1.3058, 0.6200, and 0.3988 for He, Li^+, and Be^{++}. These numbers justify the results of Table III. For H^-, the ratio is very sensitive to the value of the scale factor (and hence to the location of the singularity of T_0) and varies from 10^2 to 10^3.

DISCUSSION

The preceding results indicate the remarkable convergence properties of the Padé approximants in conjunction with the BW quantities. The formulas given for both the approximants themselves and the perturbation coefficients entering in them are compact and efficient computationally. They show the usefulness of the projection technique and remove the need for the formulation of *ad hoc* variational principles, for which they give explicit solutions directly.

The convergence properties of the BW series were discussed by Ahlrichs[21] who showed that $Z>5.9$ is a sufficient condition for convergence. Our results seem to indicate that even for $Z=3$ the linear series converges. In a recent paper Amos discussed the improvement of perturbation expansions by a scale transformation.[22] He considers the RS case and sets

$$\tilde{\mathcal{H}}^0=\mu\mathcal{H}^0+E^0(1-\mu)\ ,$$
$$\tilde{V}=(1-\mu)\mathcal{H}^0+E^0(\mu-1)+V\ , \tag{28}$$

and proceeds to optimize μ. It is interesting to point out that a similar transformation in the BW *leaves* $E_0^0+\epsilon_1+[N,N-1]$ *invariant*, as shown by Feenberg.[3,23] This optimal property of the $[N,N-1]$ Padé approximant accounts partially for its remarkable stability and makes it preferable to the linear series. Furthermore, it should be noted that whereas the exact expression (3) has singularities at the eigenvalues of PHP, the linear series has poles when $\mathcal{E}$ is equal to the eigenvalues of PH^0P. This incorrect analytic behavior disappears when one employs the Padé approximants, e.g.:

$$\lim_{\mathcal{E}\to E_k^0}\epsilon_2+\epsilon_3=\infty\ ,$$
$$\lim_{\mathcal{E}\to E_k^0}\epsilon_2^2/(\epsilon_2-\epsilon_3)=|\langle\varphi_0^0|V|\varphi_k^0\rangle|^2/\langle\varphi_k^0|V|\varphi_k^0\rangle\ . \tag{29}$$

This explains why one obtains reasonable results in H^-, even though the energy E_0^0 is quite near an excited state of H^0.

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Range-Energy Relation in Helium†

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The mean excitation potential of helium has been determined to be 42.7±0.6 eV by measuring the ranges of monoenergetic particles in a helium bubble chamber. Special care was taken to minimize systematic errors in the measurement of track lengths. The result obtained is independent of assumed corrections to the Bethe-Bloch equation at low velocity, but a discussion of such corrections is presented. Two existing theoretical estimates of 41.5 and 41.8 eV are in fair agreement with the measured value.

I. INTRODUCTION

The study of penetration of charged particles in matter has been of interest since the earliest experiments in nuclear physics. Such studies are still important, since precise information on stopping power can be used in the measurement of fundamental quantities such as particle masses.

In the present experiment, we have obtained accurate data on particle ranges in a liquid-helium bubble chamber, which are used to deduce the value of I, the mean excitation energy, in the Bethe-Bloch equation.[1] This determination of I is of interest for practical application of the helium range-energy relation, and also provides an accurate experimental value for comparison with values of I that have been computed[2,3] for helium from first principles.

From an experimental point of view, liquid helium is advantageous in several respects. Its thermodynamic properties are very accurately known, its small refractive index (1.02) allows precise photography of events, multiple Coulomb scattering is small, and there are frequent reactions which produce monoenergetic secondary particles when the initiating particle is at rest.

The basic range measurements of this experiment were performed with the following reactions, selecting those cases with zero kinetic energy in the initial state:

$$\pi^- + \mathrm{He}^4 \rightarrow \mathrm{H}^3 + n\,, \tag{1}$$

$$K^- + \mathrm{He}^4 \rightarrow {}_\Lambda\mathrm{H}^4 + \pi^0\,, \tag{2}$$

$$\pi^+ \rightarrow \mu^+ + \nu_\mu\,, \tag{3}$$

$$\pi^- \rightarrow \mu^- + \bar{\nu}_\mu\,. \tag{4}$$

II. THEORY

A basic expression for energy loss per unit path length is given by the Bethe-Bloch equation,[1]

$$-\left(\frac{\partial E}{\partial X}\right) = \frac{2\pi z^2 e^4 NZ}{mc^2\beta^2 A}\left(\ln\frac{2mc^2\gamma^2\beta^2 Q_{\max}}{I^2} - 2\beta^2 - \frac{2C}{Z} - \delta\right), \tag{5}$$