line of length L, i.e.,

$$\frac{1}{n_j!}\int_L\cdots\int\prod_{K=1}^{n_j} dZ_K e^{-\beta U'}=\frac{1}{n_j!}[L-(n_j-1)a]^{n_j}, \tag{IIIA-2}$$

and

$$Q_N(V)\leqslant\sum_{\{n_j\}}{}'\prod_{j=1}^{N_0^2}\frac{a^{2n_j}}{n_j!}[L-(n_j-1)a]^{n_j}. \tag{IIIA-3}$$

It is easily shown that the largest term in the sum is the term with all n_j equal (i.e., $n_j=N_0$ for all j). Then

$$Q_N(V)\leqslant\mathfrak{N}\left\{\frac{a^{2N_0}}{N_0!}[L-(N_0-1)a]^{N_0}\right\}^{N_0^2}, \tag{IIIA-1}$$

where $\mathfrak{N}$ is the number of terms in the sum and is equal to the number of ways of placing N_0^3 indistinguishable particles in N_0^2 boxes; therefore

$$Q_N(V)\leqslant\frac{[N_0^3+N_0^2-1]!}{N_0^3![N_0^2-1]!}\left\{\frac{a^{2N_0}}{N_0!}[L-(N_0-1)a]^{N_0}\right\}^{N_0^2}. \tag{IIIA-5}$$

With $L\equiv(N_0-1)l$, we then have

$$f(v)=\lim_{N_0\to\infty}\frac{1}{N_0^3}\ln Q_N(V)\leqslant\ln(la^2-a^3)+1 \tag{IIIA-6}$$

or

$$f(v)\leqslant\ln(v-v_{\min})+1. \tag{IIIA-7}$$

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Refinement of the Brillouin-Wigner Perturbation Method*

PAUL GOLDHAMMER† AND EUGENE FEENBERG
Wayman Crow Laboratory, Washington University, St. Louis, Missouri

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New variational parameters are introduced into the wave function employed in the Brillouin-Wigner perturbation method, and determined to minimize the total energy. The original and modified procedures are illustrated by a numerical example.

THE variational perturbation method for bound states generated by the operator $H+V$ can be developed in terms of the complete set of functions ψ_l generated by the eigenvalue equation

$$H\psi_l=E_l\psi_l,\quad E_0\leqq E_l\leqq E_{l+1}\cdots. \tag{1}$$

The prescription[1–3]

$$\psi^{(n)}=\frac{1}{N}\left[\psi_0+\sum{}'\psi_a\frac{V_{a0}}{E-E_a}+\sum{}'\psi_b\frac{V_{ba}V_{a0}}{(E-E_b)(E-E_a)}+\cdots+\sum{}'\psi_l\frac{V_{lk}\cdots V_{a0}}{(E-E_l)(E-E_k)\cdots(E-E_a)}\right], \tag{2}$$

inserted into the variational integral for the energy,

$$E=(\psi|H+V|\psi)/(\psi|1|\psi), \tag{3}$$

yields

$$E=E_0+V_{00}+\epsilon_2+\epsilon_3+\cdots+\epsilon_{2n+1}, \tag{4}$$

in which

$$\epsilon_2=\sum_a{}'\frac{V_{0a}V_{a0}}{E-E_a},\qquad \epsilon_3=\sum_{a,b}{}'\frac{V_{0a}V_{ab}V_{b0}}{(E-E_a)(E-E_b)}, \tag{5}$$

and so on. Here E in the energy denominator is identified with the approximate value of the energy given by the variational integral. The prime on the summation symbols in Eqs. (2), (4), and (5) signifies that the value 0 is excluded; the variable indices range through the values 1, 2, $\cdots l$, $\cdots\infty$ independently. Because the indices are independent, repetitions occur; i.e., two or more indices may take on the same value in a single product of V matrix elements. The proof that $\epsilon_{2l}<0$ for $E<E_0$ is fairly immediate.

The Brillouin-Wigner perturbation procedure just described can be improved in accuracy and rapidity of convergence by a simple modification of the wave function which entails no additional complications in the actual calculations. The wave function of Eq. (2) is replaced by

$$\psi^{(n)}=\frac{1}{N}\left[\psi_0+G_1\sum{}'\psi_a\frac{V_{0a}}{E-E_a}+G_2\sum{}'\psi_b\frac{V_{ba}V_{a0}}{(E-E_b)(E-E_a)}+\cdots+G_n\sum{}'\psi_l\frac{V_{lk}\cdots V_{a0}}{(E-E_l)(E-E_k)\cdots(E-E_a)}\right]. \tag{6}$$

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† University Fellow.
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TABLE I. Comparison of numerical results for the Mathieu equation.

Method	ϵ_2	ϵ_4	ϵ_6	E
$n=1$, $G_1=1$	−0.36602	...	...	−0.36602
$n=2$, $G_1=G_2=1$	−0.36287	−0.01503	...	−0.37790
$n=2$, $G_1=G_2\neq 1$ Eq. (16)	−0.36273	−0.01502	...	−0.37839
$n=3$, $G_1=G_2=G_3=1$	−0.36273	−0.01502	−0.00071	−0.37845
$n=3$, $G_1=1$, $G_2=G_3\neq 1$ Eq. (18)	−0.36272	−0.01502	−0.00071	−0.37847

Equation (4) for the energy is then replaced by

$$E=E_0+V_{00}+(2G_1-G_1^2)\epsilon_2+(G_1^2+2G_2-2G_1G_2)\epsilon_3 +(2G_3-G_2^2+2G_1G_2-2G_1G_3)\epsilon_4 +(G_2^2+2G_4+2G_1G_3-2G_1G_4-2G_2G_3)\epsilon_5+\cdots +(2G_nG_{n-1}-G_n^2)\epsilon_{2n}+G_n^2\epsilon_{2n+1}. \quad (7)$$

Minimum energy now occurs for

$$\partial E/\partial G_l=0,\quad l=1,2\cdots n, \quad (8)$$

which yields n linear equations:

$$\epsilon_j=\sum_{i=1}^{n} G_i(\epsilon_{i+j-1}-\epsilon_{i+j}),\quad j=2,3,\cdots n+1. \quad (9)$$

The substitution $G_i=1+K_i$ in Eq. (9) reduces it to

$$\epsilon_{j+n}=\sum_{i=1}^{n} K_i(\epsilon_{i+j-1}-\epsilon_{i+j}),\quad j=2,3,\cdots n+1. \quad (10)$$

The further substitution $L_1=K_1$, $L_2=K_2-K_1$, $\cdots L_n=K_n-K_{n-1}$ transforms Eq. (10) into

$$\epsilon_{j+n}\left[1+\sum_{i=1}^{n} L_i\right]=\sum_{i=1}^{n} L_i\epsilon_{i+j-1}. \quad (11)$$

The solution of Eq. (11) can be expressed in terms of the determinant

$$\Delta=\begin{vmatrix} \epsilon_2 & \epsilon_3 & \cdots\epsilon_{n+1} \\ \vdots & & \\ \epsilon_{n+1} & \epsilon_{n+2} & \cdots\epsilon_{2n} \end{vmatrix}, \quad (12)$$

and a set of n determinants Δ_k ($k=1,\cdots n$) derived from Δ by the substitution of ϵ_{n+2}, ϵ_{n+3}, $\cdots\epsilon_{2n+1}$ for the kth column of Δ. We get

$$L_k=\Delta_k\Big/\left(\Delta-\sum_{l=1}^{n}\Delta_l\right). \quad (13)$$

For the special case $n=1$, Eqs. (7) and (9) yield directly

$$G_1(\epsilon_2-\epsilon_3)=\epsilon_2, \quad (14)$$

$$E=E_0+V_{00}+\epsilon_2+\epsilon_3/(1-\epsilon_3/\epsilon_2) \cong E_0+V_{00}+\epsilon_2+\epsilon_3+\epsilon_3^2/\epsilon_2. \quad (15)$$

Equally simple relations may be obtained in higher orders if $\epsilon_i=0$ for odd i. With this stipulation, the solution for the case $n=2$ is

$$G_1=G_2=(1-\epsilon_4/\epsilon_2)^{-1}, \quad (16)$$

$$E=E_0+V_{00}+\epsilon_2+\epsilon_4/(1-\epsilon_4/\epsilon_2) \cong E_0+V_{00}+\epsilon_2+\epsilon_4+\epsilon_4^2/\epsilon_2, \quad (17)$$

and for $n=3$

$$G_1=1,\quad G_2=G_3=(1-\epsilon_6/\epsilon_4)^{-1}, \quad (18)$$

$$E=E_0+V_{00}+\epsilon_2+\epsilon_4+\epsilon_6/(1-\epsilon_6/\epsilon_4) \cong E_0+V_{00}+\epsilon_2+\epsilon_4+\epsilon_6+\epsilon_6^2/\epsilon_4. \quad (19)$$

Wigner uses the Mathieu equation,

$$(-d^2/dx^2+\sin x)\psi=E\psi, \quad (20)$$

to illustrate the eigenvalue calculation based on Eq. (4). Identifying the $\sin x$ term with V, one has $E_0=V_{00}=0$, $\epsilon_i=0$ for i odd, and

$$\epsilon_2=\frac{1}{2}\frac{1}{E-1},$$

$$\epsilon_4=\frac{1}{8}\frac{1}{(E-1)^2(E-4)},$$

$$\epsilon_6=\frac{1}{32}\left[\frac{1}{(E-1)^3(E-4)^2}+\frac{1}{(E-1)^2(E-4)^2(E-9)}\right]. \quad (21)$$

Numerical results for the lowest eigenvalue with and without the refinement of this note are shown in Table I.

The second-order wave function with optimum values given to G_1 and G_2 is almost as good for the calculation of the energy eigenvalue as the third-order function with $G_1=G_2=G_3=1$. One additional order is needed to give five-figure accuracy.