(3) In the sixth line after Eq. (II.9), read (II.2) for (II.7).

(4) For the fractional power occurring in the denominator of the unnumbered equation preceding (II.18), read  $\frac{5}{2}$  instead of  $\frac{7}{3}$ .

(5) For the fractional power appearing in the denominator at the end of Eq. (II.19), read  $\frac{1}{2}$  instead of  $\frac{1}{3}$ .

(6) In Eq. (II.20), insert

$$\frac{\Gamma(\frac{1}{3})}{2} \left(\frac{\omega}{2\omega_c}\right)^{2/3} \text{ instead of } \frac{\Gamma(\frac{2}{3})}{2} \left(\frac{\omega}{2\omega_c}\right)^{1/3}.$$
(7) In Eq. (II.37), read  $\frac{\pi^2}{8}$  instead of  $\frac{\pi^2}{4}$ .  
(8) In Eq. (III.31), read  $\frac{n}{2n_c}$  instead of  $\frac{n}{n_c}$ 

(9) The denominator of Eq. (III.32) should contain  $\pi^3$  instead of  $\pi^2$ .

<sup>3</sup>This procedure resembles that introduced in an

but is here applied to the system of charged particle

<sup>4</sup>Retaining u here gives the essence of the first

Ternov (Pergamon, New York, 1968)].

quantum correction [J. Schwinger, Proc. Nat. Acad. Sci. U. S.  $\underline{40}$ , 132 (1954), and the Russian literature

cited in Synchrotron Radiation, A. A. Sokolov and I. M.

earlier paper [J. Schwinger, Phys. Rev. 82, 664 (1951)],

 $\ast \mbox{Work}$  supported in part by the National Science Foundation.

<sup>1</sup>J. Schwinger, Phys. Rev. <u>75</u>, 1912 (1949), referred to as paper I.

<sup>2</sup>A systematic development of this new approach to particle theory is described in J. Schwinger, *Particles*, *Sources*, and *Fields I* (Addison-Wesley, Reading, Mass., 1970) and Particles, Sources, and Fields II (to be published).

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Anharmonic Oscillator

P. Lu and S. S. Wald

Department of Physics, Arizona State University, Tempe, Arizona 85281

and

B.-L. Young Ames Laboratory USAEC and Department of Physics, Iowa State University, Ames, Iowa 50010 (Received 30 October 1972)

We solve the anharmonic-oscillator problem as given by Bender and Wu to include the  $\hbar^4$  terms for the energy eignevalues and the  $\hbar^2$  terms for the eigenfunctions by means of the Miller and Good modified WKB method. This is done by accepting the harmonic oscillator as a solved problem. We see that in doing so, not only can we get better energy eigenvalues, but also we can get improved eigenfunctions.

## I. INTRODUCTION

We will discuss the familiar anharmonic-oscillator problem. We are concerned here with the simple one-dimensional oscillator with real and positive oscillator strengths (k > 0, a > 0) as given by the potential

$$V(x) = \frac{1}{2}kx^{2} + ax^{4}, \quad k > 0 \quad \text{and} \quad a > 0.$$
 (1)

When perturbation theory is used to solve the anharmonic-oscillator problem based on the solved problem of the harmonic oscillator, the perturbation series for the energy diverges and even changes sign. A clear account of this is illustrated by Chan, Stelman, and Thompson<sup>1</sup> in their Table III.

Such a simple but important problem has attracted the attention of both the field theorists and the chemists. The former are interested in it because they desire to build a model field theory on it. The latter are interested mainly due to the anharmonic bonding problem. The reader is referred to Bender and  $Wu^2$  as well as the references listed there for the detailed reason why the field theorists are interested in the problem. As for the chemists, Chen, Stelman, and Thompson<sup>1</sup> have given a good account.

Of course an evaluation of the energy eigenvalues

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is important, since the validity of the method used can be tested. It is even more important to obtain the corresponding eigenfunctions, since, as an example, the transition matrix elements could then be determined. What we work out in this paper are the energy eigenvalues to terms of the order of  $\hbar^4$  based on the known values of the harmonic oscillator, namely,  $E = (n + \frac{1}{2})\hbar\omega$ , n = 0, 1,  $2, \ldots$ , and we also work out the corresponding wave functions. We use the Miller and Good<sup>3</sup> modified WKB method which was extended to include higher-order terms of the bound state by Lu.<sup>4</sup> We will see that by including higher-order terms, the energy eigenvalues converge faster than the ordinary WKB result<sup>5</sup> and improve the previous results reported.<sup>6</sup> The eigenfunctions are better than those given by Bender and Wu in the sense that there is no need to divide the boundaries into several regions so that the problem is less complicated and much easier to handle.

The essence of the Miller and Good method is that instead of starting with the free-particle wave function, the exact solution of a known potential that is as similar as possible to the unknown potential is used as the trial wave function. In this case, the known potential is chosen as the harmonic-oscillator potential. The result of Miller and Good using the zeroth-order terms in  $\hbar^2$  only indicates that this choice gives the same answer as the ordinary WKB method. This situation becomes greatly improved if we include the  $\hbar^2$  terms. Here the approximation includes the  $\hbar^4$  terms. By including the  $\hbar^4$  terms, the results obtained in the modified WKB method are better than those of both the modified WKB method to order  $\hbar^2$  and the ordinary WKB method.

The method for obtaining the eigenfunctions is illustrated to order  $\hbar^2$  only. The technique developed is quite general and there is no difficulty in going to higher orders in  $\hbar^2$ . Throughout we discuss the case where the coupling constant a is real and positive. We feel that it is easy to generalize it to complex values but it is not necessary to do so here.

### II. EIGENVALUES TO THE ORDER $\hbar^2$

We are going to use the notations of Chan. Stelman, and Thompson by defining the following relations:

$$S = (4mk'/\hbar^2)^{1/4} x, \qquad (2a)$$

$$k' = k + (a^2 \hbar^2 / m)^{1/3}$$
 (2b)

The Schrödinger equation under consideration is

$$\frac{d^2}{dx^2}\psi + \frac{2m}{\hbar^2}(E - \frac{1}{2}kx^2 - ax^4)\psi = 0.$$
 (3)

By substitution, we can rewrite Eq. (3) to be

$$\frac{d^2}{dS^2}\psi + \frac{1}{4}[\lambda - (1-\alpha)S - \alpha^{3/2}S^4]\psi = 0, \qquad (4)$$

where

$$\lambda = 4Em^{1/2}/(k'^{1/2}\hbar)$$
 (5a)

and

$$\alpha = \frac{(a^2 \hbar^2 / m)^{1/2}}{k + (a^2 \hbar^2 / m)^{1/3}}.$$
 (5b)

To the order  $\hbar^2$ , we see from previous work<sup>4</sup> that the following formula holds:

$$\oint p_1 dx - \frac{1}{8} \hbar^2 \oint p_1'^2 p_1^{-3} dx$$

$$= \oint p_2 dx - \frac{1}{8} \hbar^2 \oint p_2'^2 p_2^{-3} dx,$$
(6)

where  $p_1$  and  $p_2$  are defined in the equations

$$\left[ \left( d^2 / dx^2 \right) + p_1^2 / \bar{h}^2 \right] \psi(x) = 0 , \qquad (7a)$$

$$\left[ \left( d^2 / dx^2 \right) + p_2^2 / \hbar^2 \right] \phi(x) = 0.$$
 (7b)

Here the unknown part is represented by  $p_1^2$  $= 2m(E - \frac{1}{2}kx^2 - ax^4)$  and the known part is represented by  $p_2^2 = 2m(E_{H,O} - \frac{1}{2}kx^2)$ , where  $E_{H,O} = (n + \frac{1}{2})$  $\times \hbar (k/m)^{1/2}$  with  $n = 0, 1, 2, \ldots$  are the energy eigenvalues of (7b). The contour integration is around the two turning points in both cases. Now it is easy to see from (5a) that for a pure harmonic oscillator,

$$\lambda' \equiv \lambda_{\rm H,O} = 4n + 2$$
 with  $n = 0, 1, 2, \dots$  (8)

The modified WKB method, as used by Miller and Good, coincides with the ordinary WKB method so far as the lowest-order eigenvalues are concerned. We see that the discrepancy is immediately compensated for by including the next-higher-order terms. Now Eq. (6) is rewritten as

$$\oint \left[ (\lambda' - S^2)^{1/2} + \frac{1}{6} (\lambda' - S^2)^{-3/2} \right] dS = \oint \left[ \lambda - (1 - \alpha)S^2 - \alpha^{3/2}S^4 \right]^{1/2} dS + \frac{1}{6} (1 - \alpha) \oint dS / \left[ \lambda - (1 - \alpha)S^2 - \alpha^{3/2}S^4 \right]^{3/2} + \alpha^{3/2} \oint S^2 dS / \left[ \lambda - (1 - \alpha)S^2 - \alpha^{3/2}S^4 \right]^{3/2}$$

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and

TABLE I. Reduced energy levels of the anharmonic oscillator. (a) The exact result as given by Chan, Stelman, and
Thompson. (b) The modified WKB result to second order in $\hbar$ . (c) The modified WKB result to fourth order in $\hbar$ .
(d) The WKB result as given by Handelsman and Lew to second order in $\hbar$ . Notice that (b) and (c) are given to five
decimal points mainly because the improvement can only be seen there.

n	(a)	(b)	(c)	(d)	n	(a)	(b)	(c)	
	$\alpha = 0.2$					$\alpha = 0.8$			
0	2.042 70	2.03411	2.037 20	1.98957	0	2.51648	2.361 65	2.341 45	
1	6.51050	6.510326	6.51057	6.47373	1	8.880 62	8.900 00	8.89818	
2	11.6292	11.62915	11.62918	11.6011	2	17.2430	17.24336	17.242 85	
3	17.2332	17.23317	17.23317	17.2103	3	26.7955	26.79596	26.795 75	
4	23,2391	23.23907	23.23907	23.2196	4	37.3022	37.30246	37.302 34	
5	29.5930	29.59303	29.59303	29.5760	5	48.6119	48.61208	48.612 01	
6	36.2567	36.25669	26.25669	36.2414	6	60.6228	60.62291	60.622 87	
7	43.2010	43.200 98	43.20098	43.1871	7	73.2604	73.26049	73.26046	
8	50.4029	50.40293	50.40293	50.3902	8	86.4675	86.467 53	86.467 51	
9	57.8438	57.84384	57.84384	57.8321	9	100.1983	100.19833	100.19832	
	$\alpha = 0.4$					$\alpha = 1.0$			
0	2.192 03	2.141136	2.14586	2.15181	0	2.671 95	2.47138	2,43585	
1	7.33824	7.34251	7.34222	7.33983	1	9.574 58	9.60143	9.59897	
2	13.6919	13.69217	13.692 01	13.6897	2	18.7872	18.78743	18,78678	
3	20.8389	20.83906	20.83898	20.8370	3	29.3429	29.34354	29.34327	
4	28.6242	28,624 37	28.624 32	28.6226	4	40.9773	40.97751	40.97738	
5	36.9519	36.95198	36.951 95	36.9504	5	53.5174	53.51751	53.51743	
6	45.7558	45.755 <b>91</b>	45.75589	45.7546	6	66.8476	66.84766	66.84761	
7	54.9874	54.98742	54 <i>.</i> 987 41	54.9862	7	80.8835	80.88347	80.88343	
8	64.6087	64.60874	64.60873	64.6076	8	95.5600	95.56003	95.560 00	
9	74.5895	74.589 54	74.58953	74.5885	9	110.8256	110.82561	110.82559	
$\alpha = 0.6$									
0	2.35526	2.251 10	2.24564						
1	8.13648	8.14809	8.14700						
2	15.5569	15.55736	15.55701						
3	23.9899	23.990 31	23.99016						
4	33.2344	33.234 62	33.23454						
5	43.1639	43.164 01	43.16395						
6	53.6926	53.69268	53.69265						
7	64.7577	64.75776	64.75774						
8	76.3107	76.31076	76.31074						
9	88.3128	88.312 91	88.312 89						

$$\oint (\lambda - S^2)^{-3/2} dS = 0.$$

(9′)

The numerical values in Table I indicate the importance of the terms to  $\hbar^2$  in Eq. (6).

The evaluation of the first integral on the right-hand side of Eq. (9) is easily done by use of the elliptic integrals with the following results:

$$\oint \left[\lambda - (1 - \alpha)S^{2} - \alpha^{3^{\prime}2}S^{4}\right]^{1^{\prime}2}dS = \alpha^{3^{\prime}4}\oint \left[\frac{\lambda}{\alpha^{3^{\prime}2}} - \frac{1 - \alpha}{\alpha^{3^{\prime}2}}S^{2} - S^{4}\right]^{1^{\prime}2}dS$$

$$= \alpha^{3^{\prime}4}\oint \left[(b^{2} - S^{2})(a^{2} + S^{2})^{1^{\prime}2}dS\right]$$

$$= \alpha^{3^{\prime}4}\frac{4}{3}(a^{2} + b^{2})^{1^{\prime}2}\left[b^{2}F\left(\frac{a}{(a^{2} + b^{2})^{1^{\prime}2}}\right) + (b^{2} - a^{2})E\left(\frac{a}{(a^{2} + b^{2})^{1^{\prime}2}}\right)\right], \quad (10)$$

with

$$a^{2} = \frac{1}{2} \left[ \frac{1-\alpha}{\alpha^{3/2}} + \left( \frac{(1-\alpha)^{2}}{\alpha^{3}} + \frac{4\lambda}{\alpha^{3/2}} \right)^{1/2} \right]$$
(11a)

and

$$b^{2} = \frac{1}{2} \left[ -\frac{1-\alpha}{\alpha^{3/2}} + \left( \frac{(1-\alpha)^{2}}{\alpha^{3}} + \frac{4\lambda}{\alpha^{3/2}} \right)^{1/2} \right].$$
(11b)

The F and E are the complete elliptic integrals of the first and second kind. They can be approximated by the polynomial approximation to within an error of  $10^{-8}$  by the formulas given on p. 591 of Ref. 7.

We will make use of the fact that the integrals involved are contour integrals. The evaluation of them is greatly facilitated by the use of the external differentiation method. The same result can also be obtained by using a table of integrals. We illustrate the former method by performing differentiation on both sides of

$$\oint \frac{dx}{\left[(a^2+x^2)(b^2-x^2)\right]^{1/2}} = \frac{4}{(a^2+b^2)^{1/2}} F(\frac{1}{2}\pi, K)$$

with respect to  $b^2$  and using the relations

$$\frac{dF}{dK} = \frac{E - (1 - K^2)F}{K(1 - K^2)} \quad \text{and} \quad \frac{dE}{dK} = \frac{E - F}{K}$$

with  $K = b / [a^2 + b^2]^{1/2}$ . We then obtain

$$\oint \frac{dx}{(a^2 + x^2)^{1/2}(b^2 - x^2)^{3/2}} = \frac{4(F - E)}{b^2(a^2 + b^2)^{1/2}}.$$
(12)

The table of integrals<sup>8</sup> gives

$$\int_{0}^{u} \frac{dx}{(a^{2} + x^{2})^{1/2}(b^{2} - x^{2})^{3/2}} = \frac{4(F - E)}{b^{2}(a^{2} + b^{2})^{1/2}} \left[F(\gamma, K) - E(\gamma, K)\right] + \frac{u}{b^{2}\left[(a^{2} + u^{2})(b^{2} - u^{2})\right]^{1/2}},$$
(13)

with

$$\gamma = \sin^{-1} \left( \frac{(a^2 + b^2)^{1/2}}{(a^2 + u^2)^{1/2}} \frac{u}{6} \right).$$

Also notice that

 $E(m\pi\pm\phi,K)=2mE(\tfrac{1}{2}\pi,K)\pm E(\phi,K),$ 

$$F(m\pi\pm\phi,K)=2mF(\tfrac{1}{2}\pi,K)\pm F(\phi,K).$$

Here m is an integer and  $\phi = 0$  gives E(0, K) = 0 and F(0, K) = 0. Therefore, it gives

$$\oint \frac{dx}{(a^2 + x^2)^{1/2}(b^2 - x^2)^{3/2}} = \frac{4}{b^2(a^2 + b^2)^{1/2}} \left[ F(\frac{1}{2}\pi, K) - E(\frac{1}{2}\pi, K) \right].$$
(14)

Notice here that the contour integration leads from -b to 0 and 0 to b in the third and first quadrant and from b to 0 and 0 to -b in the second and fourth quadrant, respectively. This gives the number 4 in front, which is the same as before [Eq. (12)]. This external diffraction method is important in finding some of the more complicated contour integrals used in Sec. III where we just list the results obtained and do not go into details.

Similarly we get

$$\oint \frac{dx}{(a^2 + x^2)^{3/2}(b^2 - x^2)^{3/2}} = \frac{4}{a^2 b^2 (a^2 + b^2)^{3/2}} \left[ a^2 F(\frac{1}{2}\pi, K) - (a^2 - b^2) E(\frac{1}{2}\pi, K) \right]$$
(15a)

and

$$\oint \frac{x^2 dx}{(a^2 + x^2)^{3/2} (b^2 - x^2)^{3/2}} = \frac{4}{(a^2 + b^2)^{3/2}} \left[ F(\frac{1}{2}\pi, K) - 2E(\frac{1}{2}\pi, K) \right].$$
(15b)

With the identification  $a^2$  and  $b^2$  as given in Eq. (11), Eq. (9) is readily evaluated.

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### III. EIGENVALUES TO THE ORDER $\hbar^4$

Equations (3) and (4) of Ref. 4 are the equations to be used. Equation (3) of Ref. 4 reads

$$\oint p_1 dx - \frac{1}{8} \hbar^2 \oint (p_1')^2 p_1^{-3} dx - \frac{1}{32} \hbar^4 \oint (p_1'')^2 p_1^{-5} dx + \frac{15}{128} \hbar^4 \oint (p_1')^4 p_1^{-7} dx$$

$$= \oint p_2 dx - \frac{1}{8} \hbar^2 \oint (p_2')^2 p_2^{-3} dx - \frac{1}{32} \hbar^4 \oint (p_2'')^2 p_2^{-5} dx + \frac{15}{128} \hbar^4 \oint (p_2')^4 p_2^{-7} dx$$
(16)

and Eq. (4) of Ref. 4 reads

$$\oint \left(R_1 - \frac{1}{48} \frac{T_1''}{T_1^{3/2}} - \frac{7}{1536} \frac{T_1''^2}{T_1^{3/2}} + \frac{5}{1536} \frac{T_1' T_1''}{T_1^{3/2}}\right) dx = \oint \left(R_2 - \frac{1}{48} \frac{T_2''}{T_2^{3/2}} - \frac{7}{1536} \frac{T_2''^2}{T_2^{3/2}} + \frac{5}{1536} \frac{T_2' T_2'''}{T_2^{3/2}}\right) dx \tag{17}$$

with

$$p_{1,2} \equiv \hbar R_{1,2} \equiv \hbar (T_{1,2})^{1/2} .$$

Equation (17) is obtained from Eq. (16) after integrating by parts several times. Equation (16) can be directly seen as an extension of Eq. (6) by including the  $\hbar^4$  terms. Equation (17) is the equation to work with here. We list in the following the formulas used in evaluating the integrals, which are obtained by means of differentiation before the contour integrals are evaluated. In Table I we list the results and it can be seen that the contributions of the  $\hbar^4$  terms are in the right direction. They are converging and they give us a feeling that this modified WKB approximation is essentially correct, in spite of the complexity of the higher-order terms.

The following formulas shown here are important:

$$\oint \frac{dx}{(a^2+x^2)^{5'2}(b^2-x^2)^{5'2}} = (-\frac{2}{3}) \frac{1}{a^4 b^2 (a^2+b^2)^{5'2}} \left[ F(\frac{1}{2}\pi, K)(-6a^4+2a^2b^2) + E(\frac{1}{2}\pi, K)(6a^4-14a^2b^2-4b^4) \right],$$
(18)  
$$\oint \frac{dx}{(a^2+x^2)^{5'2}(b^2-x^2)^{5'2}} = \frac{4}{9} \frac{1}{a^4 b^4 (a^2+b^2)^{5'2}} \left[ (6a^6+27a^4b^2-3a^4b^2)F(\frac{1}{2}\pi, K) + (-6a^6-30a^4b^2+30a^2b^4+6b^6)E(\frac{1}{2}\pi, K) \right],$$
(18)

$$\oint \frac{dx}{(a^2 + x^2)^{5'2}(b^2 - x^2)^{7'2}} = -\frac{4}{45} \frac{1}{a^4 b^6 (a^2 + b^2)^{9'2}} \left[ (-24a^8 - 117a^6 b^2 - 270a^4 b^4 + 15a^2 b^6) F(\frac{1}{2}\pi, K) + (24a^8 + 129a^6 b^2 + 324a^4 b^4 - 195a^2 b^6 - 30b^8) E(\frac{1}{2}\pi, K) \right],$$
(19)
  
(19)

-

$$\oint \frac{dx}{(a^2 + x^2)^{\frac{1}{2}}(b^2 - x^2)^{\frac{1}{2}}} = \frac{4}{225} \frac{1}{a^6 b^6 (a^2 + b^2)^{\frac{1}{2}}} [a^2 (120a^8 + 735a^6b^2 + 2250a^4b^4 - 345a^2b^2 - 60b^8)F(\frac{1}{2}\pi, K) + (-120a^{10} - 795a^8b^2 - 2595a^6b^4 + 2595a^4b^6 + 795a^2b^8 + 120b^{10})E(\frac{1}{2}\pi, K)].$$

(21)

The additional terms added to the right-hand side of Eq. (6) through Eq. (17) are

$$-\frac{7}{1536}\oint \frac{T_{1}^{"2}}{T_{1}^{"2}}dx + \frac{5}{1536}\oint \frac{T_{1}^{'}T_{1}^{"'}}{T^{"'^{2}}}dx$$

$$= \frac{-1}{1536}\left(224(1-\alpha^{2})\oint \frac{dS}{[\lambda-(1-\alpha)S^{2}-\alpha^{3'2}S^{4}]^{"2}} + 768(1-\alpha)\alpha^{3'^{2}}\oint \frac{S^{2}dS}{[\lambda-(1-\alpha)S^{2}-\alpha^{3'2}S^{4}]^{"2}} + 4224\alpha^{3}\oint \frac{S^{4}dS}{[\lambda-(1-\alpha)S^{2}-\alpha^{3'2}S^{4}]^{"2}}\right)$$

$$= \frac{1}{1536}\left[\frac{4224}{\alpha^{9'4}}\oint \frac{dS}{[\lambda^{2}-S^{2})^{5'2}(a^{2}+S^{2})^{5'2}} - \left(\frac{768(1-\alpha)}{\alpha^{15/4}} + \frac{4224(b^{2}-a^{2})}{\alpha^{9'4}}\right)\oint \frac{dS}{(b^{2}-S^{2})^{"2}(a^{2}+S^{2})^{"2}} + \left(\frac{-224(1-\alpha^{2})}{\alpha^{2^{1}/4}} + \frac{768(1-\alpha)}{\alpha^{15/4}}a^{2} - \frac{4224}{\alpha^{9'4}}a^{4}\right)\oint \frac{dS}{(b^{2}-S^{2})^{"2}(a^{2}+S^{2})^{"2}}\right], \quad (22)$$

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and the higher terms of Eq. (9) in  $\hbar^2$  are zero [e.g., Eq. (9a)]. The definitions of the parameters  $\alpha$ , a, and b are the same as in Eq. (5b), Eq. (11a), and Eq. (11b). They are easily handled by a computer. The results obtained for different  $\alpha$  values up to the order of  $\hbar^4$  are given in Table I. An important fact of this calculation is that the contribution due to  $\hbar^4$  terms above is very small but in the right direction.

### IV. EIGENFUNCTIONS TO THE ORDER OF $\hbar^2$

Assume that r is the one-dimensional space coordinate of the anharmonic oscillator. Since we know that

$$\oint u dv = -\oint v du,$$

then by several integrations by parts, Eq. (6) can be written as

$$\oint \left[ R_1 - \frac{1}{24T_1^{1/2}} \left( \frac{T_1'''}{T_1'} - \frac{T_1''^2}{T_1'^2} \right) \right] dr$$
$$= \oint \left[ R_2 - \frac{1}{24T_2^{1/2}} \left( \frac{T_2'''}{T_2'} - \frac{T_2''^2}{T_2'^2} \right) \right] dr , \qquad (23)$$

where as before

 $R_{1,2} \equiv T_{1,2}^{1/2} \equiv p_{1,2}/\hbar$  .

Because there is no longer any apparent divergence in the second-order term in  $\hbar^2$ , we can evaluate this contour integral as follows:

$$\int_{r_{1}}^{r} \left[ R_{1} - \frac{1}{24} \frac{1}{T_{1}^{1/2}} \left( \frac{T_{1}^{\prime\prime\prime}}{T_{1}^{\prime}} - \frac{T_{1}^{\prime\prime2}}{T_{1}^{\prime/2}} \right) \right] dr$$
$$= \int_{x_{1}}^{x} \left[ R_{2} - \frac{1}{24} \frac{1}{T_{2}^{1/2}} \left( \frac{T_{2}^{\prime\prime\prime}}{T_{2}^{\prime}} - \frac{T_{2}^{\prime\prime2}}{T_{2}^{\prime/2}} \right) \right] dx ,$$
(24)

where  $r_1$  and  $x_1$  are the corresponding turning points. We see that the above gives us the relation

$$x = x(r) , \qquad (25)$$

where x is the one-dimensional space coordinate of the harmonic oscillator. The wave function of the harmonic oscillator is already known and given by

$$\phi_n(x) = H_n(\xi) e^{-\xi^2/2} \tag{26}$$

with  $\xi = (mk/\hbar^2)^{1/4} x$  and  $H_n$  being the Hermite polynomials. Therefore, the wave function of the anharmonic oscillator is<sup>3</sup>

$$\psi_n(r) = [x'(r)]^{-1/2} \phi(x(r)) .$$
(27)

Of course we see that for  $x \ge |x_1|$  and  $x \le -|x_1|$ mapping to  $r \ge |r_1|$  and  $r \le -|r_1|$ , there is one-toone correspondence. But both  $R_1$  and  $R_2$  simultaneously turn from real values to imaginary values. The equation is still valid outside of the turningpoint regions. We just have to multiply by i to transform both sides into real quantities. There appears to be a divergence at first glance in the place where  $T_1' = T_2' = 0$ . There are important conditions used in deriving Eq. (23), simply  $T_1'$  $\neq 0$  and  $T_2' \neq 0$ . Or we have to return back to the earlier Eq. (6), where, as r and x are close to zero, only the zeroth-order terms contribute. Or we can approximate the case by choosing a finite distance around both  $r_{\min}$  and  $x_{\min}$  such that only the zeroth-order terms contribute there and with adequate connections outside. Thus the eigenfunction obtained is valid throughout.

In so doing, we think that we get a better eigenfunction than Bender and Wu, for then we have avoided the necessity of dividing the space into many regions where each of the regions has its own form of valid wave function.

# V. REMARKS

As we look at the results in Table I. several interesting things can be seen. First, the modified WKB method gives better over-all results than the ordinary WKB results to second order in  $\hbar$  already and this leaves very little room for improvement to fourth order in  $\hbar$ . Although the terms of fourth order in h are messy, the contribution to the overall values is small. Here we begin to consider the accuracy of the exact result which is obtained by the method of diagonalization. It could be possible that there are some errors to the fourth or fifth decimal points due to roundoff. Second, we see that the modified WKB method cannot give the eigenvalues for n=0 and n=1. However, the results indicate that the eigenvalues for n=2 or above are already good. We see that this statement is true too even if we include the  $\hbar^4$  terms. This seems contrary to our anticipation, namely, the improvement obtained with the  $\hbar^4$  terms is not drastic. However, it is in the right direction.

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<sup>1</sup>S. I. Chan, D. Stelman, and L. E. Thompson, J. Chem. Phys. 41, 2828 (1964).

<sup>2</sup>C. M. Bender and T. T. Wu, Phys. Rev. 184, 1231 (1969).

<sup>3</sup>S. C. Miller and R. H. Good, Jr., Phys. Rev. 91, M4 (1953).

<sup>4</sup>P. Lu. J. Chem. Phys. 51, 1524 (1969).

<sup>5</sup>R. A. Handelsman and J. S. Lew, J. Chem. Phys. <u>50</u>, 3342 (1969).

<sup>6</sup>P. Lu, J. Chem. Phys. 53, 845 (1970).

<sup>1</sup>Handbook of Mathematical Functions, edited by

M. Abramowitz and I. A. Stegun, National Bureau of Standards Applied Mathematics Series, No. 55

(U.S.G.P.O., Washington, D. C., 1964).

<sup>8</sup>J. S. Gradshteyn and I. M. Ryzhik, Tables of Integrals, Series and Products (Academic, New York, 1965), p. 252.

PHYSICAL REVIEW D

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# Lorentz-Invariant Localization for Elementary Systems. V. General Transformations

A. J. Kálnay

Departamento de Física Atómica y Molecular, Instituto Venezolano de Investigaciones Científicas, Apartado 1827, Caracas, Venezuela

and

### P. L. Torres

Departamento de Física, Facultad de Ciencias, Universidad Central de Venezuela, Caracas, Venezuela (Received 25 July 1972)

In parts II and III of the present series of papers, the localization problem was studied for the cases of relativistic nonzero mass (spin 0,  $\frac{1}{2}$ ) and zero mass (spin 0,  $\frac{1}{2}$ , and 1). With a set of postulates, of which the basic one is the imposition of Lorentz invariance of localization (LIL) (which is a self-consistency requirement), it was possible to define the position operator uniquely (except for a constant in the spin- $\frac{1}{2}$ , nonzero-mass case). For the determination of the position operators it was enough to consider only very special cases of homogeneous Lorentz transformations. One of the purposes of the present paper is to consider the effect of arbitrary inhomogeneous continuous Lorentz transformations in order to obtain general Poincaré-invariant localization (GPIL). Our main result will be that localization is LIL if and only if it is GPIL. In II and III, LIL was obtained in spite of the fact that the position operators were not 4-vector operators but only 3-vector operators. In this paper, following Fleming, we construct formally covariant position operators from the 3-vector operators. We prove that their eigenfunctions are just the localized states defined in the GPIL sense.

# I. INTRODUCTION

#### A. General

In papers II (Ref. 1) and III (Ref. 2) of the present series, the problem of localizability of elementary systems in relativistic quantum mechanics was considered by requiring the consistency of the description of localization from different inertial frames as the only basic assumption; the position operators were uniquely defined (except for a constant in the spin- $\frac{1}{2}$ , nonzero-mass case<sup>3</sup>), and their form was found explicitly. In II the nonzeromass systems of spin 0 and  $\frac{1}{2}$  were considered, and in III the zero-mass systems of spin 0,  $\frac{1}{2}$ , and 1 were considered.

The basic assumption (Postulate 4 of II) is a self-consistency one: If a state is a 1-localized state<sup>1</sup> (i.e., an eigenstate of only one component of the position operator  $\mathbf{X}$ ) in a two-dimensional plane, e.g.,  $X^3 = 0$  at t = 0, then, making a homogeneous continuous Lorentz transformation such that the region of localization remains invariant, the transformed state is again a localized state in the same region. This is what was called Lorentz*invariant localization* (LIL). It is clear that only very special cases of homogeneous Lorentz transformations leave invariant those two-dimensional planes.

One of the purposes of the present paper is to consider the effect of arbitrary inhomogeneous continuous Lerentz transformations on states