

Third-Order Coulomb Wave Function and Single Quantum Annihilation*

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An expression for the third-order Coulomb wave function, correct to order $(\alpha Z)^3$ for all momenta and energies, is derived. Using this wave function the total cross section for single-photon emission resulting from a positron annihilating with a K -shell electron (single quantum annihilation), valid to relative order $(\alpha Z)^2$, is calculated numerically. The results for lead are compared to the exact answer of Jaeger and Hulme, and the results for silver are also given graphically. The effect of the third-order term in the cross section is found to be significant, especially for low and intermediate positron energies. The cross section for lead is found to be qualitatively correct while that for silver is essentially exact. The question of how to treat the normalization factors of the various wave functions is also discussed.

I. INTRODUCTION

JOHNSON and Mullin¹ have derived a modification to the Sommerfeld-Maue²⁻⁴ (SM) wave function valid to order $(\alpha Z)^2$. However, when using this modified SM wave function, one is able, in general, to obtain the cross section only to relative order αZ . Since in many problems one is interested in applying the result to heavy elements, one may expect a significant contribution from the third-order term (and possibly higher order terms also) in the cross section. For this reason, it is desirable to obtain a further modification to the SM wave function.

The third-order Coulomb wave function, valid to order $(\alpha Z)^3$ for all values of β , is derived in Sec. II. In Sec. III we make use of the third-order wave function to calculate the total cross section for single-photon emission resulting from a positron annihilating with a K -shell electron (single quantum annihilation). The second- and third-order cross sections for lead are compared with each other and with the exact numerical calculation of Jaeger and Hulme.⁵ Graphical results for silver are also presented. Section IV contains a discussion of the results obtained.

II. CALCULATION OF THE THIRD-ORDER COULOMB WAVE FUNCTION

The solution of the Dirac equation in momentum space which behaves asymptotically like a plane wave plus an outgoing spherical wave is given by

$$\phi(\mathbf{k}) = \delta(\mathbf{q}_{kp})u(\mathbf{p}) + \frac{\delta H(\mathbf{k})}{k^2 - p^2 - i\epsilon} \int \frac{\phi(\mathbf{s})d\mathbf{s}}{q_{ks}^2 + \lambda^2}, \quad (1)$$

where

$$\mathbf{q}_{ab} = \mathbf{a} - \mathbf{b}, \quad H(\mathbf{k}) = \boldsymbol{\alpha} \cdot \mathbf{k} + m\gamma_4 + W, \quad \text{and} \quad \delta = (\alpha Z/2\pi^2).$$

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¹ W. R. Johnson and C. J. Mullin, *Phys. Rev.* **119**, 1270 (1960).

² A. Sommerfeld and A. W. Maue, *Ann. Physik* **22**, 629 (1935).

³ H. A. Bethe and L. C. Maximon, *Phys. Rev.* **93**, 768 (1954).

⁴ A. Sommerfeld, *Atombau und Spektrallinien* (Friedrich Vieweg und Sohn, Braunschweig, 1951), 2nd ed., Vol. 2, p. 408.

⁵ J. C. Jaeger and H. R. Hulme, *Proc. Cambridge Phil. Soc.* **32**, 158 (1936).

The screening parameter λ is set equal to zero every where except where divergences or ambiguities in choosing phases may arise. The radial wave function $\psi(\mathbf{r})$ is given by

$$\psi(\mathbf{r}) = \int \phi(\mathbf{k}) \exp(i\mathbf{k} \cdot \mathbf{r}) d\mathbf{k}. \quad (2)$$

The solution of Eq. (1) is given by⁶

$$\phi(\mathbf{k}) = \sum_{n=0}^{\infty} (\alpha Z)^n \phi_n(\mathbf{k}), \quad (3)$$

where

$$\phi_1(\mathbf{k}) = \frac{1}{2p\nu} \tilde{q}_{kp} \phi_0(\mathbf{k}), \quad (4a)$$

and

$$\phi_n(\mathbf{k}) = \frac{1}{2\pi^2} \frac{H(\mathbf{k})}{k^2 - p^2 - i\epsilon} \int \frac{\phi_{n-1}(\mathbf{s})d\mathbf{s}}{q_{ks}^2 + \lambda^2}, \quad n \geq 2, \quad (4b)$$

$$\nu = \alpha Z W / p, \quad \text{and} \quad \tilde{q} = \boldsymbol{\alpha} \cdot \mathbf{q}.$$

Gorshkov⁶ shows that the nonrelativistic wave function is given by

$$\psi_0(\mathbf{r}) = NM \exp(i\mathbf{p} \cdot \mathbf{r}) {}_1F_1(i\nu; 1; i\mathbf{p}r - i\mathbf{p} \cdot \mathbf{r}) u(\mathbf{p}), \quad (5)$$

where

$$N = \exp(\pi\nu/2) \Gamma(1 - i\nu),$$

$$M = \exp[i\nu \ln(2p/\lambda)] \exp[-i\nu C],$$

and C is Euler's constant. From Eq. (2):

$$\phi_0(\mathbf{k}) = \frac{1}{(2\pi)^3} \int \psi_0(\mathbf{r}) \exp(-i\mathbf{k} \cdot \mathbf{r}) d\mathbf{r}. \quad (6)$$

Thus, all screening divergences in the nonrelativistic wave function are isolated in the form of a phase factor M . From the convergence of the integrals (4b) as $\lambda \rightarrow 0$ it follows that no other divergences will

⁶ V. G. Gorshkov, *Zh. Eksperim. i Teor. Fiz.* **40**, 1481 (1961) [translation: *Soviet Phys.—JETP* **13**, 1037 (1961)].

appear. Hence it follows that the only screening divergence in the exact Coulomb wave function will be contained in the phase factor M . It is easily shown that the quantity

$$\phi_0(\mathbf{k}) + \alpha Z \phi_1(\mathbf{k}) + \alpha^2 Z^2 \phi_2(\mathbf{k}),$$

apart from an over-all phase factor, is just the Fourier transform of the modified SM wave function.¹ From Eq. (4b) we have

$$\phi_3(\mathbf{k}) = \frac{1}{8\pi^4 \nu \tilde{p}} \frac{H(\mathbf{k})}{k^2 - p^2 - i\epsilon} \int \frac{d\mathbf{s} H(\mathbf{s})}{(q_{ks}^2 + \lambda^2)(s^2 + \mu_2^2)} \times \int \frac{\tilde{q}_{s1p} \phi_0(\mathbf{s}_1) d\mathbf{s}_1}{(q_{s1s}^2 + \lambda^2)}, \quad (7)$$

where

$$\mu_2 = \epsilon - i\tilde{p}.$$

Using the contour integral representation for the confluent hypergeometric function⁷

$${}_1F_1(ia; 1; z) = \frac{1}{2\pi i} \int^{(0,1^+)} \frac{dx}{x} \left(\frac{-x}{1-x}\right)^{ia} e^{zx}, \quad (8)$$

we obtain

$$\phi_0(\mathbf{s}_1) = \frac{NM}{2\pi i} \int^{(0,1^+)} \frac{dx}{x} \left(\frac{-x}{1-x}\right)^{i\nu} \frac{1}{2\pi^2 i} \times \frac{\partial}{\partial B} \frac{1}{[(\mathbf{q}_{s1p} + \mathbf{p}x)^2 - (B + i\epsilon)^2]} u(\mathbf{p}), \quad (9)$$

where

$$\mathbf{B} = \mathbf{p}x.$$

Setting

$$\mathbf{J} = \frac{1}{2\pi^2 i} \frac{\partial}{\partial B} \int \frac{\mathbf{q}_{s1p} d\mathbf{s}_1}{(q_{s1s}^2 + \lambda^2)[(\mathbf{q}_{s1p} + \mathbf{p}x)^2 - (B + i\epsilon)^2]}, \quad (10)$$

and using the identity

$$\frac{i}{2P_s} \ln\left(\frac{P_s + B + i\lambda}{-P_s + B + i\lambda}\right) = \int_{\lambda}^{\infty} \frac{d\lambda'}{P_s^2 - (B + i\lambda')^2}, \quad (11)$$

we find that

$$\mathbf{J} = i\tilde{p} \nabla_B \int_{\lambda}^{\infty} \frac{d\lambda'}{P_s^2 - (B + i\lambda')^2}, \quad (12)$$

where

$$P_s = \mathbf{q}_{sp} + \mathbf{B}.$$

From Eqs. (9) and (12) we obtain, after interchanging

the order of integration,

$$\int \frac{\mathbf{q}_{s1p} \phi_0(\mathbf{s}_1) d\mathbf{s}_1}{q_{s1s}^2 + \lambda^2} = 2\nu NM \int_{\lambda}^{\infty} \frac{d\lambda' (p\mathbf{q}_{sp} - i\lambda'\mathbf{p})}{(q_{sp}^2 + \lambda'^2)(s^2 + \mu_1'^2)} u(\mathbf{p}), \quad (13)$$

where

$$\mu_1 = \lambda' - i\tilde{p}.$$

From Eqs. (7) and (13) we obtain

$$\phi_3(\mathbf{k}) = \frac{NM}{4\pi^4 \tilde{p}} \frac{H(\mathbf{k})}{k^2 - p^2 - i\epsilon} \int_{\lambda}^{\infty} d\lambda' \times \int \frac{d\mathbf{s} H(\mathbf{s}) (p\tilde{q}_{sp} - i\lambda'\tilde{p})}{(q_{ks}^2 + \lambda^2)(s^2 + \mu_1'^2)(s^2 + \mu_2'^2)(q_{sp}^2 + \lambda'^2)} u(\mathbf{p}). \quad (14)$$

Since there are 2 scalar factors in the denominators of Eq. (14), we see that the most complicated integrals encountered are vector and scalar 3-denominator integrals, whose solutions are well known.^{8,9} Using partial fractions and performing the volume integration we finally obtain

$$\phi_3(\mathbf{k}) = \frac{NM}{2\pi^2} \frac{H(\mathbf{k})}{k^2 - p^2 - i\epsilon} \int_{\lambda}^{\infty} \frac{Id\lambda'}{\lambda' - 2i\tilde{p}} u(\mathbf{p}), \quad (15a)$$

where

$$I = \Delta I + [W(W - \gamma_4 m)\mathcal{J}_2 + m(W\gamma_4 - m)\mathcal{J}_3]/p^2, \quad (15b)$$

$$\Delta I = \frac{-i\tilde{p}}{4\Delta} [12\Delta + (k^2 - p^2)^2 - 3q^2(k^2 + p^2)$$

$$+ 2q^2(k^2 - 2\mathbf{p} \cdot \mathbf{k}) + 2\lambda'^2(k^2 + \mathbf{p} \cdot \mathbf{k})] \frac{J}{2\pi^2} - \frac{1}{2}\mathcal{J}_3 + (\boldsymbol{\alpha} \cdot \mathbf{k} + m\gamma_4 - W)(W - m\gamma_4)(\mathcal{J}_2 - \mathcal{J}_3) - \frac{i\tilde{p}}{2\Delta} (k^2 + \mathbf{p} \cdot \mathbf{k}) \frac{\Delta K_2}{2\pi^2}, \quad (15c)$$

$$\mathcal{J}_2 = \frac{1}{\Delta} \left[i\tilde{p} \mathbf{p} \cdot \mathbf{k} \frac{\Delta K_2}{2\pi^2} - i\tilde{p} (p^2 q^2 - \mathbf{p} \cdot \mathbf{k} \lambda'^2) \frac{J}{2\pi^2} \right] + \frac{\mathbf{p} \cdot \mathbf{k}}{p^2 + \mathbf{p} \cdot \mathbf{k}} \mathcal{J}_3, \quad (15d)$$

$$\mathcal{J}_3 = \frac{(p^2 + \mathbf{p} \cdot \mathbf{k})}{2\Delta} \left[\ln\left(\frac{q^2 + \lambda'^2}{\lambda'^2}\right) + \ln\left(\frac{\mu_1'^2 + p^2}{\mu_1'^2 + k^2}\right) \right], \quad (15e)$$

$$\Delta = (\mathbf{p} \times \mathbf{k})^2, \quad \Delta K_2 = K_{21} - K_{22}, \quad \mathbf{q} = \mathbf{k} - \mathbf{p}, \quad (15f)$$

⁷ A. Erdelyi et al., *Higher Transcendental Functions*, Bateman Manuscript Project (McGraw-Hill Publishing Company, Inc., New York, 1953), Vol. 1, p. 272, Sec. 6.11.1, Eq. (3).

⁸ H. Mitter and P. Urban, *Acta Phys. Austriaca* 7, 311 (1953).

⁹ R. R. Lewis, *Phys. Rev.* 102, 537 (1956).

$$K_{21} = \frac{\pi^2}{ik} \ln \left(\frac{\mu_1 + ik}{\mu_1 - ik} \right), \quad K_{22} = \frac{\pi^2}{ik} \ln \left(\frac{\lambda + i(k-p)}{\lambda - i(k+p)} \right), \quad (15g)$$

$$J = \frac{\pi^2}{R} \ln \left[\frac{S+R}{S-R+\lambda(\mu_1^2+p^2)} \right], \quad (15h)$$

$$S = -i\dot{p}(q^2+\lambda'^2) + \lambda'(k^2-p^2), \quad (15i)$$

$$R = [S^2 - (q^2+\lambda'^2)(k^2-p^2)(\mu_1^2+p^2)]^{1/2}. \quad (15j)$$

The λ term is left in Eq. (15g) so that one may choose the proper phase. For k unequal to p one may drop the λ terms in Eq. (15h). There is also a contribution to the third order from $\phi_2(\mathbf{k})$. Denoting this contribution by $\phi_2^3(\mathbf{k})$ we find

$$\phi_2^3(\mathbf{k}) = \frac{NM}{2\pi^2} \frac{H(\mathbf{k})}{k^2-p^2-i\epsilon} \frac{W}{p^2} (W-mr\gamma_4) g_2 u(\mathbf{p}), \quad (16a)$$

where

$$g_2 = \int_{\lambda}^{\infty} \frac{\lambda' d\lambda'}{(q^2+\lambda'^2)(\mu_1^2+k^2)} \ln \left(\frac{q^2+\lambda'^2}{\mu_1^2+k^2} \right). \quad (16b)$$

Thus, we may write the third-order Coulomb wave function as

$$\phi_{3r}(\mathbf{k}) = \phi_3(\mathbf{k}) + \phi_2^3(\mathbf{k}). \quad (17)$$

The asymptotic form of the Coulomb scattering wave function, correct to order $\alpha^3 Z^3$, may be written¹⁰

$$\psi(\mathbf{r}) \rightarrow \exp \left[i\mathbf{p} \cdot \mathbf{r} - i\nu \ln \left(2pr \sin^2 \frac{\theta}{2} \right) \right] u(\mathbf{p}) + \frac{f(\theta)}{r} \exp [i\dot{p}r + i\nu \ln(2pr)] u(\mathbf{p}), \quad (18)$$

where

$$\cos \theta = \mathbf{p}' \cdot \mathbf{p} / p^2, \quad \text{and} \quad \mathbf{p}' = \dot{p}\mathbf{r}/r.$$

It is easily shown that¹

$$f(\theta) = 2\pi^2 \lim_{\mathbf{k} \rightarrow \mathbf{p}'} (k^2 - p^2) \phi(\mathbf{k}), \quad (19)$$

where $\phi(\mathbf{k})$ is given by Eq. (1). We find that our result for $f(\theta)$ agrees with that of Johnson and Mullin¹⁰ except for an over-all phase factor.

III. CROSS SECTION FOR SINGLE QUANTUM ANNIHILATION

The matrix element for a positron annihilating with a K -shell electron with the subsequent emission of a single photon of momentum \mathbf{k} is given by

$$M = - \left(\frac{2\pi\alpha}{k} \right)^{1/2} [\psi_2, \alpha \cdot \boldsymbol{\epsilon} \exp(-i\mathbf{k} \cdot \mathbf{r}) \psi_1], \quad (20)$$

¹⁰ W. R. Johnson, T. A. Weber, and C. J. Mullin, Phys. Rev. **121**, 933 (1961).

where¹¹

$$\psi_1 = N_1 r^{\gamma-1} \exp(-m\alpha Zr) \left[1 + i \left(\frac{1-\gamma}{1+\gamma} \right)^{1/2} \frac{\boldsymbol{\alpha} \cdot \mathbf{r}}{r} \right] u(\mathbf{p}_1) \quad (21)$$

describes the K -shell electron,

$$N_1 = \left[\frac{(1+\gamma)(2m\alpha Z)^{2\gamma+1}}{8\pi\Gamma(2\gamma+1)} \right]^{1/2}, \quad \gamma = (1-\alpha^2 Z^2)^{1/2},$$

and $u(\mathbf{p}_1)$ is the Dirac plane-wave spinor for a particle of momentum \mathbf{p}_1 which we take to be zero. The polarization of the photon is given by the unit vector $\boldsymbol{\epsilon}$, and ψ_2 is the positron wave function which behaves asymptotically like a plane wave plus an outgoing spherical wave. The charge conjugate wave function ψ_+ is defined by¹²

$$\psi_+ = (B\gamma_4\gamma_5\psi(-\alpha))^{c.c.}, \quad (22)$$

where c.c. denotes complex conjugate, $\psi(-\alpha)$ is an electron wave function with the sign of the Coulomb interaction reversed, and B is a unitary matrix satisfying

$$B\gamma_\mu B^{-1} = \gamma_\mu^{c.c.}, \quad \mu = 1, \dots, 4, \quad (23a)$$

and

$$B^T = -B^{-1}. \quad (23b)$$

Thus, using

$$(B\gamma_4\gamma_5\boldsymbol{\alpha}u(\mathbf{p}))^{c.c.} = \boldsymbol{\alpha}u_+(\mathbf{p}), \quad (24a)$$

and

$$(B\gamma_4\gamma_5\gamma_4u(\mathbf{p}))^{c.c.} = -\gamma_4u_+(\mathbf{p}), \quad (24b)$$

we see from Eq. (22) that we may obtain the positron wave function from the corresponding electron wave function by making the replacements

$$\alpha \rightarrow -\alpha, \quad (25a)$$

$$\gamma_4 \rightarrow -\gamma_4, \quad (25b)$$

$$i \rightarrow -i, \quad (25c)$$

and interpreting the spinor as being that for a positron. Setting

$$\psi_2 = \psi_{SM} + \chi_2 + \chi_3, \quad (26)$$

then¹³

$$\psi_{SM} = N_2 \exp(-i\mathbf{p} \cdot \mathbf{r}) \left(1 - \frac{\boldsymbol{\alpha} \cdot \nabla}{2iW} \right) \times {}_1F_1(i\nu; 1; -; pr + i\mathbf{p} \cdot \mathbf{r}) u(\mathbf{p}), \quad (27)$$

and

$$\chi_2 = - \frac{N_2\alpha^2 Z^2}{2\pi^2} \int \frac{d\mathbf{k} \exp(-i\mathbf{k} \cdot \mathbf{r})}{k^2 - p^2 + i\epsilon} \times \int_0^\infty \frac{d\mu [-i\mu A(\mathbf{p}, \mathbf{k}) + p^2 - k^2]}{(\mu^2 + q^2)(\mu^2 + 2i\dot{p}\mu + k^2 - p^2)} u(\mathbf{p}), \quad (28)$$

¹¹ H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer-Verlag, Berlin, 1957), p. 69.

¹² S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Row, Peterson and Company, New York, 1961), pp. 205-6.

¹³ See Ref. 1. When one makes the transformations (25) on the given electron wave functions, one obtains Eqs. (27) and (28).

where

$$N_2 = \exp(-\pi\nu/2)\Gamma(1-i\nu), \quad \nu = aZW/p,$$

and

$$A(\mathbf{p}, \mathbf{k}) = p(1 + \tilde{k}\tilde{p}/p^2).$$

From Eqs. (2) and (17) we have

$$\chi_3 = -\alpha^2 Z^3 \int \phi_{3r}'(\mathbf{k}) \exp(-i\mathbf{k}\cdot\mathbf{r}) d\mathbf{k}, \quad (29)$$

where $\phi_{3r}'(\mathbf{k})$ is related to $\phi_{3r}(\mathbf{k})$ by the transformations (25b) and (25c). The third-order term in the matrix element cannot be obtained in closed form and thus one must resort to numerical methods.

IV. DISCUSSION OF RESULTS

The total cross section for single quantum annihilation was computed numerically on the IBM-1620 computer at Notre Dame. Figure 1 shows a comparison between the exact answer of Jaeger and Hulme and our second- and third-order cross sections for lead. In Fig. 2 the second- and third-order cross sections are compared for silver. One sees from Figs. 1 and 2 that the third-order term in the cross section has a significant effect, being most pronounced for low and intermediate positron energies. The third-order results for lead are qualitatively correct, i.e., they give the right order of magnitude and the general shape of the cross section. The ratio of the fourth-order term for silver to that for lead is (excluding all normalization factors) $[Z(\text{Ag})/Z(\text{Pb})]^3 \approx 0.2$. Thus, we expect that the third-order result for silver gives good quantitative agreement with the exact answer. On the basis of these results and the third-order calculations of Johnson, Weber, and Mullin¹⁰ for the Coulomb scattering of polarized electrons, it would seem that for large Z one gets qualitative agreement with the exact answer, while for intermediate or low Z one essentially reproduces the exact answer when retaining only the first three terms in an αZ expansion.

It is seen that the difference between our second- and third-order result (approximately 20%) is less than the difference between our third-order result and the exact answer (approximately 70%) for $W/m = 2.8$,

FIG. 1. The second- and third-order cross sections and the exact answer of Jaeger and Hulme for lead ($Z=82$).

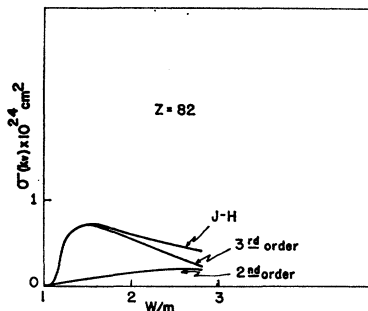
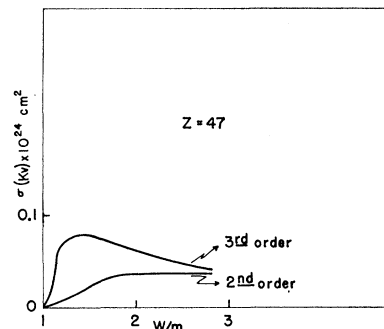


FIG. 2. The second- and third-order cross sections for silver ($Z=47$).



while as W/m becomes smaller this latter difference decreases rapidly. Since we cannot determine the specific structure of the terms which we have neglected without actually calculating them, it is difficult to determine their effect on the cross section. However, in view of the large discrepancy at high energies between our third-order result and the exact answer it would be desirable to have a more exact treatment of the problem in this region.

On purely physical grounds we would expect that for extremely relativistic positrons we may neglect the binding energy of the K -shell electron. Mathematically this is equivalent to setting $\gamma=1$. For such energies the positron is described [with an error proportional to $(1-\beta^2)^{1/2} \rightarrow 0$] by $\psi_0(\mathbf{r})$ which asymptotically approaches a distorted plane wave. Subject to the above approximation for very high energies we may obtain an exact answer.

Since the cross section we have calculated is explicitly an expansion in the parameter αZ , and since the normalization factors associated with the wave functions contain αZ , the question of how to treat these factors naturally arises. One possible answer is that since the result is an expansion in αZ , consistency demands that the normalization factors be expanded also. However, this approach leads to negative results for the cross section for low energies because of the factor $e^{-\pi\nu}$. Pratt¹⁴ performs two different partial expansions of the normalization factors. The one finally chosen is that which apparently makes the series converge most rapidly. However, this approach assumes one knows something about the effect of the expansion on the terms neglected. The criterion used by Deck¹⁵ is whether the first three terms in an expansion adequately represent the function. In our calculation various partial expansions were tried in an attempt to get a best fit to the exact answer of Jaeger and Hulme. It was found that when all factors were retained except the term $\pi\nu/\sinh\pi\nu$, a best fit was obtained. This result is in agreement with the conclusions presented by Deck, though differing slightly from the results of Pratt. The

¹⁴ R. H. Pratt, Phys. Rev. **117**, 1017 (1960).

¹⁵ R. T. Deck, Ph.D. thesis, University of Notre Dame (unpublished).

experimental results of Hall, Hanson, and Jamnik¹⁶ seem to provide further justification for our treatment of the normalization factors (as well as Deck's treatment). In any case a rigorous theoretical justification would involve knowledge of the terms which have been neglected. Failing this, the treatment of the normalization factors seems to be somewhat arbitrary. Because

¹⁶H. E. Hall, A. O. Hanson, and D. Jamnik, *Phys. Rev.* **129**, 2207 (1963).

of the discrepancy at high energies for lead and the arbitrary treatment of the normalization factors one of the authors (C.O.C.) has undertaken an exact calculation of single quantum annihilation.

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Nature of the Quantum Corrections to the Statistical Model

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The scheme of correcting the Fermi-Thomas particle density formula by a power series in \hbar , procedures for which have been proposed by a number of authors, is examined through its application to a one-dimensional linear potential, which yields an analytical expression for the exact wave mechanical density for comparison. It is concluded that this is an asymptotic series, valid only where the particle density is large. Furthermore, terms of an oscillatory nature, which may very well transcend the so-called quantum corrections, are missing. A reason for this is offered.

THE simplicity of the Fermi-Thomas approximation of the particle density for a fermion system in the ground state, which in the past has found its principal application to the atom, has led a number of investigators to develop procedures for systematically improving upon it; presumably approaching, when independent particles are assumed, the accurate but difficult to compute self-consistent field result from wave mechanics. The formalisms of Kompaneets and Pavlovskii,¹ Kirzhnits,² Golden,³ and Baraff and Borowitz⁴ lead to a common expression (for independent particles), a power series in \hbar , whose first term is the Fermi-Thomas density. Alfred⁵ has given a modification of Golden's method involving a Bromwich integral.

It is the purpose of this article to examine this series in \hbar through an example, namely, the one-dimensional case for which the potential energy is a linear function of the displacement, i.e.,

$$V = ax. \quad (1)$$

A comparison with the exact analytical expression from wave mechanics indicates that it is only an asymptotic expansion, valid where the particle density is large, and

that, even there, important terms of an oscillatory nature are missing. The apparent source of error is brought out in the chosen method, basically that of Alfred, for developing the series.

Stephen and Zalewski⁶ have reached similar conclusions after a study of a simple harmonic oscillator system. However, it is believed that the use of the linear potential permits a much simpler and more comprehensible analysis.

For a one-dimensional system of independent fermions in the ground state one may write

$$\begin{aligned} \rho(\epsilon; x', x) &\equiv \sum_{n=1}^N \psi_n^*(x') \psi_n(x) \\ &= \sum_{n=1}^{\infty} \psi_n^*(x') f(\epsilon, H) \psi_n(x), \quad (2) \end{aligned}$$

where $H \equiv -(\hbar^2/2m)d^2/dx^2 + V(x)$, $\psi_n(x)$ is the normalized eigenfunction of H corresponding to the eigenvalue $E(n)$, which is less than $E(n+1)$, and $E(N) < \epsilon < E(N+1)$. The operator $f(\epsilon, H)$ has the property

$$\begin{aligned} f(\epsilon, H) \psi_n(x) &= \psi_n(x) \quad \text{for } E(n) < \epsilon \\ &= 0 \quad \text{for } E(n) > \epsilon. \end{aligned}$$

It can be shown⁷ that the form of the right side of Eq. (2) is invariant with respect to an orthogonal

¹A. S. Kompaneets and E. S. Pavlovskii, *Zh. Eksperim. i Teor. Fiz.* **31**, 427 (1956) [translation: *Soviet Phys.—JETP* **4**, 328 (1957)].

²D. A. Kirzhnits, *Zh. Eksperim. i Teor. Fiz.* **32**, 115 (1957) [translation: *Soviet Phys.—JETP* **5**, 64 (1957)].

³S. Golden, *Phys. Rev.* **105**, 604 (1957); **107**, 1283 (1957).

⁴G. A. Baraff and S. Borowitz, *Phys. Rev.* **121**, 1704 (1961).

⁵L. C. R. Alfred, *Phys. Rev.* **121**, 1275 (1961).

⁶M. J. Stephen and K. Zalewski, *Proc. Roy. Soc. (London)* **A270**, 435 (1962).

⁷J. E. Mayer and W. Band, *J. Chem. Phys.* **15**, 141 (1947).