experimental results of Hall, Hanson, and Jamnik[16] 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 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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ACKNOWLEDGMENTS

The authors wish to thank Dr. Johnson for suggesting this problem and for many useful discussions during its completion.

PHYSICAL REVIEW VOLUME 132, NUMBER 6 15 DECEMBER 1963

Nature of the Quantum Corrections to the Statistical Model

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(Received 22 July 1963)

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 Borowitz[4] lead to a common expression (for independent particles), a power series in $\hbar$, whose first term is the Fermi-Thomas density. Alfred[5] 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.,

$$V=ax. \tag{1}$$

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 Zalewski[6] 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

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

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

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

It can be shown[7] that the form of the right side of Eq. (2) is invariant with respect to an orthogonal

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transformation in Hilbert space, i.e.,

$$\rho(\epsilon;x',x)=\sum_{n=1}^{\infty}\phi_n^*(x')f(\epsilon,H)\phi_n(x),$$

where the ϕ_n constitute a second complete orthonormal system satisfying the same boundary conditions as the ψ_n. Assuming the eigenfunctions of the momentum can serve as the ϕ_n, such that

$$\psi_n(x)=(2\pi\hbar^2)^{-1/2}\int_{-\infty}^{+\infty}g_n(p)\exp(ipx/\hbar)dp,$$

gives for the particle density

$$\rho(\epsilon,x)\equiv\rho(\epsilon;x,x)$$
$$=h^{-1}\int_{-\infty}^{+\infty}\exp(-ipx/\hbar)f(\epsilon,H)\exp(ipx/\hbar)dp. \quad (3)$$

For the potential of Eq. (1) let

$$\exp(-zH)\exp(ipx/\hbar)$$
$$=\exp(ipx/\hbar)\exp[-((p^2/2m)+ax)z+v(z,p,x)], \quad (4)$$

upon defining

$$f(\epsilon,H)\equiv\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{dz}{z}e^{z(\epsilon-H)}, \quad (5)$$

where

$$e^{-zH}\equiv\sum_{m=0}^{\infty}\frac{(-1)^m z^m}{m!}H^m.$$

Taking the partial derivative of both sides of Eq. (4) with respect to z and observing the effect of the operation of H upon the right side reveal

$$\frac{\partial v}{\partial z}=\frac{i\hbar p}{m}\left(\frac{\partial v}{\partial x}-az\right)+\frac{\hbar^2}{2m}\left[\frac{\partial^2 v}{\partial x^2}+\left(\frac{\partial v}{\partial x}-az\right)^2\right].$$

The solution that satisfies the condition $v\to 0$ as $z\to 0$ is

$$v=-(i\hbar a/2m)pz^2+4\mu z^3, \quad (6)$$

where $\mu\equiv\hbar^2a^2/24m$.

Combining Eqs. (3), (4), (5), and (6) gives

$$h\rho(\epsilon,x)=\frac{1}{2\pi i}\int_{-\infty}^{+\infty}dp\int_{\sigma-i\infty}^{\sigma+i\infty}\frac{dz}{z}\exp\left[\left(\epsilon-ax-\frac{p^2}{2m}\right)z-\frac{i\hbar ap}{2m}z^2+4\mu z^3\right]$$
$$=\int_{-\infty}^{+\infty}dp\left\{\tfrac{1}{2}+\frac{1}{\pi}\int_0^{\infty}\frac{dy}{y}\exp\left(\frac{i\hbar ap}{2m}y^2\right)\sin\left[\left(\epsilon-ax-\frac{p^2}{2m}\right)y-4\mu y^3\right]\right\}$$
$$=\frac{1}{\pi}\int_{-\infty}^{+\infty}dp\int_0^{\infty}\frac{dy}{y}\left\{\sin\left(\frac{p^2}{2m}y\right)+\tfrac{1}{2}\sin[(\epsilon-ax)y-\mu y^3](\cos Q_+ +\cos Q_-)\right.$$
$$\left.-\tfrac{1}{2}\cos[(\epsilon-ax)y-\mu y^3](\sin Q_+ +\sin Q_-)\right\},$$

where $Q_\pm\equiv(p\pm\frac{1}{2}\hbar ay)^2y/2m$. An inversion in the order of integration may be justified on the basis of the Moore-Osgood theorem. The integration over p leaves

$$h\rho(\epsilon,x)=\left(\frac{m}{\pi}\right)^{1/2}\int_0^{\infty}\frac{dy}{y^{3/2}}\{1-\cos[(\epsilon-ax)y-\mu y^3]$$
$$+\sin[(\epsilon-ax)y-\mu y^3]\}. \quad (7)$$

By applying Cauchy's theorem to the expression for $\partial h\rho/\partial\mu$ from Eq. (7) one may obtain for $\mu\neq 0$

$$\frac{\partial h\rho}{\partial\mu}=\frac{\partial^3 h\rho}{\partial\epsilon^3}=-\left(\frac{2m}{\pi}\right)^{1/2}\int_0^{\infty}r^{3/2}\exp[\tfrac{1}{2}(\epsilon-ax)r-\mu r^3]$$
$$\times\cos\left[\frac{\sqrt{3}}{2}(\epsilon-ax)r-\frac{2\pi}{3}\right]dr,$$

which is differentiable to all orders in μ and ϵ. Thus, one may show that

$$\frac{\partial^n h\rho}{\partial\mu^n}=\frac{\partial^{3n}h\rho}{\partial\epsilon^{3n}}\quad\text{for}\quad\hbar\neq 0. \quad (8)$$

It is not evident that $h\rho$, which is analytic in $\hbar$ everywhere else on the real axis, is so for $\hbar=0$. If, for the moment, one assumes that it is and that Eq. (8) is valid there, the Taylor expansion in $\hbar$ becomes

$$\rho=\rho_0+\mu\frac{\partial^3\rho_0}{\partial\epsilon^3}+\frac{\mu^2}{2!}\frac{\partial^6\rho_0}{\partial\epsilon^6}+\cdots,$$

where ρ_0, the Fermi-Thomas density, is given by Eq. (7) for $\mu=0$,

$$\rho_0=[(8m/h^2)(\epsilon-ax)]^{1/2}.$$

Thus, one obtains

$$\rho(\epsilon,x)=[(8m/h^2)(\epsilon-ax)]^{1/2}[1+(\hbar^2a^2/64m(\epsilon-ax)^3)$$
$$-(105\hbar^4a^4/8192m^2(\epsilon-ax)^6)+\cdots], \quad (9)$$

as the proposed series stipulates for the linear potential.

In determining the exact wave-mechanical expression for $\rho(\epsilon,x)$, one is permitted to substitute in Eq. (2) an integration over n for the summation over states since $E(n+1)-E(n)\to 0$ as $d^rV/dx^r\to 0$, for $r=2, 3, 4, \cdots$.

With the boundary condition $\psi_n(x)\to 0$ as $x\to\infty$, it may be shown that[8]

$$\pi\rho(\epsilon,x)=P(\epsilon,x)+S(\epsilon,x)[1-\cos K(\epsilon,x)]+R(\epsilon,x)\sin K(\epsilon,x), \quad (10)$$

where P is the solution of the equation

$$P^2+\left(\frac{1}{2P}\right)\left(\frac{\partial^2 P}{\partial x^2}\right)-\frac{3}{4}\left(\frac{1}{P}\frac{\partial P}{\partial x}\right)^2=\frac{2m}{\hbar^2}(\epsilon-ax)\equiv\left(\frac{3ma}{\hbar^2}u\right)^{2/3}$$

conforming to

$$P\sim(3mau/\hbar^2)^{1/3}(1+5/72u^2-\cdots),$$

for large u,

$$K(\epsilon,x)\equiv 2\int_x^\infty P(\epsilon,x')dx', \quad R\equiv-(\partial K/\partial\epsilon)^{-1}\partial P/\partial\epsilon,$$

and

$$S\equiv-(\partial K/\partial\epsilon)^{-1}\partial R/\partial\epsilon.$$

One finds

$$P=(\partial/\partial x)\tan^{-1}\{[J_{\frac{1}{3}}(u)+J_{-\frac{1}{3}}(u)]/\sqrt{3}[J_{\frac{1}{3}}(u)-J_{-\frac{1}{3}}(u)]\}, \quad (11)$$

where J_s is the Bessel function of order s.

Letting ρ_a represent the nonoscillatory portion of the particle density, i.e., $\pi\rho_a=P+S$, one obtains[8]

$$\pi\frac{\partial\rho_a}{\partial\epsilon}=\frac{\partial P}{\partial\epsilon}+\frac{\partial}{\partial\epsilon}\left\{\left(\frac{\partial K}{\partial\epsilon}\right)^{-1}\frac{\partial}{\partial\epsilon}\left[\left(\frac{\partial K}{\partial\epsilon}\right)^{-1}\frac{\partial P}{\partial\epsilon}\right]\right\}=\frac{m}{\hbar^2 P},$$

or, upon application of Eq. (11),

$$\partial\rho_a/\partial\epsilon=(mau^4/9\hbar^2)^{1/3}\times[J_{\frac{1}{3}}^2(u)-J_{\frac{1}{3}}(u)J_{-\frac{1}{3}}(u)+J_{-\frac{1}{3}}^2(u)].$$

Integrating both sides of this equation with respect to ϵ after employing the asymptotic expansion of $J_s(u)$ in terms of u^{-1} gives

$$\rho_a\sim[(8m/h^2)(\epsilon-ax)]^{1/2}[1+(\hbar^2a^2/64m(\epsilon-ax)^3)-(105\hbar^4a^4/8192m^2(\epsilon-ax)^6)+\cdots].$$

Since asymptotic expansions can be multiplied and integrated unconditionally, this expression, which is apparently identical to that of relation (9), constitutes such an expansion.

Letting ρ_b represent the oscillatory part of the particle density according to Eq. (10), i.e., $\pi\rho_b=R\sin K-S\cos K$, one finds

$$\rho_b\sim-(a/4\pi(\epsilon-ax))\times\{[1-(1225\hbar^2a^2/2304m(\epsilon-ax)^3)+\cdots]\cos 2u+(\hbar a/24(2m)^{1/2}(\epsilon-ax)^{3/2})\times[17-(199115\hbar^2a^2/6912m(\epsilon-ax)^3)+\cdots]\sin 2u\}.$$

It should be noted that in the region where $\epsilon-ax$ is large, these terms may very well transcend those beyond the first in relation (9), the quantum corrections.

It is seen that, as u is proportional to $\hbar^{-1}$, $\hbar=0$ is a singularity of $h\rho_b$ due to the sine and cosine. Since it may be verified that Eqs. (7) and (10) are in agreement, the premise upon which Eq. (9) depends—that $h\rho$, as given by Eq. (7), is analytic in $\hbar$ at $\hbar=0$—is false.

In the application of the quantum corrected statistical model to the atom, Golden's results for C^{++} and O do not display the wavelike features of the corresponding results from self-consistent field calculations.

For a physical quantity, such as the total energy of a system, which is represented by the integral of a product of the particle density over the space occupied by the system, the use of the usual quantum corrections may indeed give a marked improvement in the computed value, as has been reported for the total energy of the atom. The effect of the oscillatory terms tends to vanish through integration, while the contribution from the region where the particle density is small may be unimportant.

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