JOURNAL OF COMPUTATIONAL PHYSICS 33, 382–396 (1979)

Monte Carlo Solution of Schrödinger's Equation for the Hydrogen Atom in a Magnetic Field

YASUO TOMISHIMA AND JIRO OZAKI

Department of Physics, Okayama University, Okayama, Japan

Received May 31, 1978; revised February 6, 1979

The analytical expressions suitable for the Monte Carlo calculation to obtain the solution of Schrödinger's equation of the hydrogen atom in a magnetic field are developed. The energy values and the wavefunctions for the even states of $m = 0$ and 1 are obtained numerically and compared with other results based on the variational method. The agreement between them is rather good.

1. INTRODUCTION

In a recent paper [1] we reported a remark on the Monte Carlo solution of Schrödinger's equation for molecular systems, in which the advantage of the technique developed by Grimm and Storer [2] was emphasized. Here we will apply this method to the problem of the hydrogen atom in a magnetic field.

The solution of Schrödinger's equation for the hydrogen atom in a magnetic field is very important in many branches of physics, i.e., atomic physics, astrophysics, solid state physics, etc. Unfortunately its exact solution is not available at present, so we have to be content with approximate solutions. For weak magnetic fields the perturbation method is usually applied and for very intense magnetic fields the adiabatic method based on the solution of free electrons in magnetic field is known to be efficient. For intermediate strength magnetic fields, however, there is no efficient method, the only available one is a variational method using some special analytic form of wavefunction. These aspects are fully explained in the review article by Garstang [3], where many important papers are cited. Since the Monte Carlo method does not need to assume a special form of wavefunction, it is appropriate to check the solution based on the variational method by the comparison with the results obtained by the Monte Carlo method.

In Section 2, the analytical expressions which are necessary for the Monte Carlo calculation are derived. In Section 3, the method of calculation is explained, and Section 4 is devoted to the discussion of numerical results.

0021-9991/79/120382-15$02.00/0

2. Analytical Expressions

The Hamiltonian for a hydrogenic atom in a constant magnetic field H along the z-axis can be written as

$$\mathscr{H} = \mathscr{H}_0 + \mathscr{H}', \tag{2.1}$$

$$\mathscr{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + \frac{e\hbar H}{2imc}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{e^2H^2}{8m^2c^2}(x^2 + y^2), \tag{2.2}$$

$$\mathscr{H}' = -Ze^2/r, \tag{2.3}$$

in the gauge where the vector potential $\mathbf{A} = \mathbf{H} \times \mathbf{r}/2$.

If we adopt the atomic unit $e = m = \hbar = 1$, and a parameter γ in place of H ($\mu_0 H/Ry = \gamma$, μ_0: Bohr magneton), Eqs. (2.2) and (2.3) are transformed into

$$\mathscr{H}_0 = -\frac{1}{2}\nabla^2 + \frac{\gamma}{2i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{\gamma^2}{8}(x^2 + y^2), \tag{2.4}$$

$$\mathscr{H}' = -Z/r. \tag{2.5}$$

The problem of solving the Schrödinger equation for the lowest energy state can be replaced by the following iteration process. (See Grimm and Storer [2], Tomishima and Ozaki [1]) That is, starting from an arbitrary function $\Psi^{(0)}(\mathbf{r})$, we define a series of functions $\Psi^{(N)}(\mathbf{r})$;

$$\Psi^{(N)}(\mathbf{r}) = \int \langle \mathbf{r} \mid e^{-\beta(\mathscr{H}-C)} \mid \mathbf{r}' \rangle \, \Psi^{(N-1)}(\mathbf{r}')\, d\mathbf{r}', \tag{2.6}$$

where β is a small parameter and C is a constant selected for convenience of numerical calculation. Then in the limit of $N \to \infty$,

$$\lim_{N\to\infty} \Psi^{(N)}(\mathbf{r}) = e^{-\beta(E_0 - C)}\Psi^{(N-1)}(\mathbf{r}), \tag{2.7}$$

$$\lim_{N\to\infty} \Psi^{(N)}(\mathbf{r}) = \text{const. } \psi_0(\mathbf{r}), \tag{2.8}$$

where E_0 and $\psi_0(\mathbf{r})$ are the eigenvalue and the eigenfunction for the ground state of the given Hamiltonian.

The density matrix $\langle \mathbf{r} \mid \exp(-\beta(\mathscr{H} - C)) \mid \mathbf{r}' \rangle$ in Eq. (2.6) can be approximated up to the order of β^2 as follows:

$$\langle \mathbf{r} \mid \exp(-\beta(\mathscr{H} - C)) \mid \mathbf{r}' \rangle = e^{-(1/2)\beta(\mathscr{H}'(\mathbf{r})-C)} \langle \mathbf{r} \mid e^{-\beta\mathscr{H}_0} \mid \mathbf{r}' \rangle \, e^{-(1/2)\beta(\mathscr{H}'(\mathbf{r}')-C)}, \tag{2.9}$$

and Sondheimer and Wilson [4] has given the exact expression

$$\langle \mathbf{r} \mid e^{-\beta \mathscr{H}_0} \mid \mathbf{r}' \rangle = f(\beta) \exp \left[\frac{i\gamma}{2} (xy' - yx') - g(\beta)\{(x - x')^2 + (y - y')^2\} - \pi\nu(z - z')^2 \right], \quad (2.10)$$

where

$$\nu \equiv 1/2\pi\beta,$$
$$g(\beta) \equiv \frac{\gamma}{4} \coth \left(\frac{\gamma}{2} \beta \right), \quad (2.11)$$
$$f(\beta) \equiv \nu^{1/2} \frac{\gamma}{4\pi} \operatorname{cosech} \left(\frac{\gamma}{2} \beta \right).$$

Let us define a function $\chi^{(N)}$ in place of $\Psi^{(N)}$,

$$\chi^{(N)}(\mathbf{r}) = e^{(1/2)\beta(\mathscr{H}'(\mathbf{r}) - C)} \Psi^{(N)}(\mathbf{r}). \quad (2.12)$$

Upon substitution of Eqs. (2.9), (2.10), and (2.12) into (2.6), we have

$$\chi^{(N)}(\mathbf{r}) = f(\beta) \int \exp \left[\frac{i\gamma}{2} (xy' - yx') - g(\beta)\{(x - x')^2 + (y - y')^2\} - \pi\nu(z - z')^2 \right] \cdot e^{-\beta(\mathscr{H}'(\mathbf{r}') - C)} \chi^{(N-1)}(\mathbf{r}') \, d\mathbf{r}'. \quad (2.13)$$

Since it is clear from the structure of the Hamiltonian $\mathscr{H}$ that the parity and the magnetic quantum number m are good quantum numbers, $\chi^{(N)}$ can be written in cylindrical coordinate system by the form

$$\chi^{(N)}(\mathbf{r}) = \frac{1}{(2\pi)^{1/2}} e^{-im\varphi} R_m^{(N)}(\rho, z). \quad (2.14)^1$$

Substituting Eq. (2.14) in (2.13) and performing the integration with respect to φ', we get finally the equation for $R_m^{(N)}$;

$$R_m^{(N)}(\rho, z) = 2\pi f(\beta) \, e^{(1/2)m\gamma\beta} \int I_{|m|} \left[\frac{\gamma}{2} \rho\rho' \operatorname{cosech} \left(\frac{\gamma}{2} \beta \right) \right] \times \exp[-g(\beta)(\rho^2 + \rho'^2) - \pi\nu(z - z')^2] \times \exp \left[\beta \left(\frac{Z}{(\rho'^2 + z'^2)^{1/2}} + C \right) \right] R_m^{(N-1)}(\rho', z') \, \rho' \, d\rho' \, dz', \quad (2.15)$$

where $I_{|m|}$ is the modified Bessel function of the first kind.

[1] As will be stated in Section 3, we have to express the value of the wave function as the density of psips in Monte Carlo method. Therefore the transform from complex χ to real R is necessary for the present purpose.

Here we define the probability function $P_{|m|}(\rho, \rho')$ and $P(z, z')$ for the purpose of Monte Carlo calculation in such a way as

$$\int_0^\infty P_{|m|}(\rho, \rho')\, d\rho = \int_{-\infty}^{\infty} P(z, z')\, dz = 1. \tag{2.16}$$

That is

$$P_{|m|}(\rho, \rho') = \frac{2^{|m|+1} g^{(2+|m|)/2} \Gamma(|m|+1)}{\Gamma((2+|m|)/2)\, K^{|m|} F((2+|m|)/2; |m|+1; K^2/4g)}\, \rho e^{-g\rho^2} I_{|m|}(K\rho), \tag{2.17}$$

where F is a confluent hypergeometric function and

$$K = \frac{\gamma}{2}\rho' \cdot \operatorname{cosech}\left(\frac{\gamma}{2}\beta\right), \tag{2.18}$$

and

$$P(z, z') = \nu^{1/2} \exp[-\pi\nu(z - z')^2]. \tag{2.19}$$

Then Eq. (2.15) can be rewritten as

$$\begin{aligned} \rho R_m^{(N)}(\rho, z) = \int & P_{|m|}(\rho, \rho')\, P(z, z')\, \Omega_{|m|}(\rho') \\ & \times \exp\left[-\frac{\gamma}{4}\tanh\left(\frac{\gamma}{2}\beta\right)\rho'^2 + \beta\left(\frac{Z}{(\rho'^2 + z'^2)^{1/2}} + C + \frac{1}{2}m\gamma\right)\right] \\ & \times \rho' R_m^{(N-1)}(\rho', z')\, d\rho'\, dz', \end{aligned} \tag{2.20}$$

where

$$\Omega_{|m|}(\rho') = \operatorname{sech}\left(\frac{\gamma}{2}\beta\right) \tilde{F}\left(\frac{|m|}{2}; |m|+1; -\frac{\gamma}{2}\operatorname{cosech}(\gamma\beta)\, \rho'^2\right), \tag{2.21}$$

and

$$\tilde{F}(\alpha, \delta, -z) = \frac{\Gamma(\delta - \alpha)}{\Gamma(\delta)} z^\alpha F(\alpha, \delta, -z). \tag{2.22}$$

If we write the wavefunction corresponding to the lowest energy for given magnetic quantum number m in the form

$$\psi_{m,0}(\mathbf{r}) = \frac{1}{(2\pi)^{1/2}} e^{-im\varphi} \phi_{m,0}(\rho, z), \tag{2.23}$$

$$\phi_{m,0}(\rho, z) = \exp\left(\frac{1}{2}\beta\left(\frac{Z}{(\rho^2 + z^2)^{1/2}} + C\right)\right) R_{m,0}(\rho, z), \tag{2.24}$$

then from Eq. (2.8) $R_m^{(N)}$ obtained by Eq. (2.20) tends to $R_{m,0}$ in the limit of $N \to \infty$. Moreover, from Eq. (2.7) in the limit of $N \to \infty$, Eq. (2.20) can be written as

$$\begin{aligned} & e^{-\beta(E_{m0}-C)} \rho R_{m,0}(\rho, z) \\ & \quad = \int P_{|m|}(\rho, \rho')\, P(z, z')\, \Omega_{|m|}(\rho') \\ & \qquad \times \exp\left[-\frac{\gamma}{4} \tanh\left(\frac{\gamma}{2}\beta\right) \rho'^2 + \beta\left(\frac{Z}{(\rho'^2 + z'^2)^{1/2}} + C + \frac{1}{2} m\gamma\right)\right] \\ & \qquad \times \rho' R_{m,0}(\rho', z')\, d\rho'\, dz', \end{aligned} \tag{2.25}$$

where E_{m0} is the lowest energy eigenvalue corresponding to magnetic quantum number m.

Integration with respect to ρ and z of Eq. (2.25) gives the equation for determining the energy values E_{m0} ;

$$\begin{aligned} & e^{-\beta E_{m0}} \int \rho R_{m,0}(\rho, z)\, d\rho\, dz \\ & \quad = \int \Omega_{|m|}(\rho) \exp\left[-\frac{\gamma}{4} \tanh\left(\frac{\gamma}{2}\beta\right) \rho^2 + \beta\left(\frac{Z}{(\rho^2 + z^2)^{1/2}} + \frac{1}{2} m\gamma\right)\right] \\ & \qquad \times \rho R_{m,0}(\rho, z)\, d\rho\, dz. \end{aligned} \tag{2.26}$$

The numerical calculation is to be carried out on the basis of Eqs. (2.20) and (2.26). Referring to Eqs. (2.17) and (2.18), one will see that the probability function $P_{|m|}(\rho, \rho')$ depends on both β and γ, and this will be rather inconvenient for numerical calculation. Therefore we will adopt the following change of scale:

$$\begin{aligned} \rho &= \gamma^{-1/2}\bar{\rho}, \qquad z = \gamma^{-1/2}\bar{z}, \qquad \beta = \gamma^{-1}\bar{\beta}, \\ E_{m0} &= \gamma \bar{E}_{m0}, \qquad C = \gamma \bar{C}, \qquad Z = \gamma^{1/2}\bar{Z}. \end{aligned} \tag{2.27}$$

Then Eqs. (2.20) and (2.26) become

$$\begin{aligned} & \bar{\rho} R_m^{(N)}(\bar{\rho}, \bar{z}) \\ & \quad = \int \bar{P}_{|m|}(\bar{\rho}, \bar{\rho}')\, \bar{P}(\bar{z}, \bar{z}')\, \Omega_{|m|}(\bar{\rho}') \\ & \qquad \times \exp\left[-\frac{1}{4} \tanh\left(\frac{\bar{\beta}}{2}\right) \bar{\rho}'^2 + \bar{\beta}\left(\frac{\bar{Z}}{(\bar{\rho}'^2 + \bar{z}'^2)^{1/2}} + \bar{C} + \frac{1}{2} m\right)\right] \\ & \qquad \times \bar{\rho}' R_m^{(N-1)}(\bar{\rho}', \bar{z}')\, d\bar{\rho}'\, d\bar{z}', \end{aligned} \tag{2.28}$$

$$\begin{aligned} & e^{-\bar{\beta}\bar{E}_{m0}} \int \bar{\rho} R_{m,0}(\bar{\rho}, \bar{z})\, d\bar{\rho}\, d\bar{z} \\ & \quad = \int \Omega_{|m|}(\bar{\rho}) \exp\left[-\frac{1}{4} \tanh\left(\frac{\bar{\beta}}{2}\right) \bar{\rho}^2 + \bar{\beta}\left(\frac{\bar{Z}}{(\bar{\rho}^2 + \bar{z}^2)^{1/2}} + \frac{1}{2} m\right)\right] \\ & \qquad \times \bar{\rho} R_{m,0}(\bar{\rho}, \bar{z})\, d\bar{\rho}\, d\bar{z}, \end{aligned} \tag{2.29}$$

where

$$\begin{aligned}\bar{P}_{|m|}(\bar{\rho}, \bar{\rho}') &= \gamma^{-1/2} P_{|m|}(\gamma^{-1/2}\bar{\rho}, \gamma^{-1/2}\bar{\rho}') \\ &= \frac{1}{(4\pi)^{1/2}} \cosh\left(\frac{\bar{\beta}}{2}\right) \cdot \left[\operatorname{cosech}\left(\frac{\bar{\beta}}{2}\right)\right]^{1/2} (\bar{\rho}/\bar{\rho}')^{1/2} \\ &\quad \times \frac{\tilde{I}_{|m|}(\frac{1}{2}\bar{\rho}\bar{\rho}' \operatorname{cosech}(\bar{\beta}/2))}{\tilde{F}(|m|/2; |m| + 1; -\frac{1}{2}\operatorname{cosech}(\bar{\beta}) \cdot \bar{\rho}'^2)} \\ &\quad \times \exp\left[-\frac{1}{4}\coth\left(\frac{\bar{\beta}}{2}\right)\left(\bar{\rho} - \operatorname{sech}\left(\frac{\bar{\beta}}{2}\right)\bar{\rho}'\right)^2\right], \end{aligned} \tag{2.30}$$

$$\begin{aligned}\bar{P}(\bar{z}, \bar{z}') &= \gamma^{-1/2} P(\gamma^{-1/2}\bar{z}, \gamma^{-1/2}\bar{z}') \\ &= \frac{1}{(2\pi\bar{\beta})^{1/2}} \exp\left(-\frac{(\bar{z} - \bar{z}')^2}{2\bar{\beta}}\right), \end{aligned} \tag{2.31}$$

$$\Omega_{|m|}(\bar{\rho}') = \operatorname{sech}\left(\frac{\bar{\beta}}{2}\right) \tilde{F}\left(\frac{|m|}{2}; |m| + 1; -\frac{1}{2}\operatorname{cosech}\bar{\beta} \cdot \bar{\rho}'^2\right), \tag{2.32}$$

$$\tilde{I}_{|m|}(z) = (2\pi z)^{1/2} e^{-z} I_{|m|}(z). \tag{2.33}$$

3. Monte Carlo Method

As stated in the preceeding section, z-parity of the wavefunction is a good quantum number, therefore we can predetermine the z-parity of the function $R_m^{(N)}(\bar{\rho}, \bar{z})$ in the process of iteration (2.28). For simplicity we restrict ourselves to the case of parity even, then the function $R_m^{(N)}(\bar{\rho}, \bar{z})$ may be taken as always positive since the iteration process gives only the lowest energy state for given magnetic quantum number m and even parity, and the function is necessarily nodeless in $(\bar{\rho}, \bar{z})$-plane.

Now the Monte Carlo method which simulates the iteration process can be described as follows.

(i) First, we select $M^{(0)}$ *psips* (the name comes from Anderson [5]) in the $(\bar{\rho}, \bar{z})$-plane which are distributed according to an arbitrarily selected density function $\bar{\rho}R_m^{(0)}(\bar{\rho}, \bar{z})$.

(ii) Then we multiply each $M^{(0)}$ *psips* by a factor

$$W(\bar{\rho}, \bar{z}) = \Omega_{|m|}(\bar{\rho}) \exp\left[-\frac{1}{4}\tanh\left(\frac{\bar{\beta}}{2}\right)\bar{\rho}^2 + \bar{\beta}\left(\frac{\bar{Z}}{(\bar{\rho}^2 + \bar{z}^2)^{1/2}} + \bar{C} + \frac{1}{2}m\right)\right]. \tag{3.1}$$

This is done by replacing each *psips* $(\bar{\rho}_i, \bar{z}_i)$ $(i = 1, 2, \ldots, M^{(0)})$ by m_i *psips* at the same position. The integer m_i is chosen so that

$$m_i = [W(\bar{\rho}_i, \bar{z}_i)] + 1 \tag{3.2}$$

if the fractional part of $W(\bar{\rho}_i, \bar{z}_i)$ is greater than a uniform random number between 0 and 1, and

$$m_i = [W(\bar{\rho}_i, \bar{z}_i)] \tag{3.3}$$

otherwise. The square bracket means the greatest integer not exceeding its content. By this process we have now $M^{(1)}$ *psips*,

$$M^{(1)} = \sum_{i=1}^{M^{(0)}} m_i . \tag{3.4}$$

(iii) Each *psips* is executed a random walk by which the position of each *psips* $(\bar{\rho}, \bar{z})$ is displaced to a position $(\bar{\rho} + \Delta\bar{\rho}, \bar{z} + \Delta\bar{z})$. The step size $\Delta\bar{z}$ is governed by the probability function (cf. Eq. (2.31))

$$\bar{P}(\bar{z} + \Delta\bar{z}, \bar{z}) = \frac{1}{(2\pi\beta)^{1/2}} \exp\left[-\frac{\Delta\bar{z}^2}{2\beta}\right], \tag{3.5}$$

therefore $\Delta\bar{z}$ is a random number of normal distribution with zero mean and variance β. While the step size $\Delta\bar{\rho}$ is governed by the probability function $\bar{P}_{|m|}(\bar{\rho} + \Delta\bar{\rho}, \bar{\rho})$ defined by Eq. (2.30). Corresponding to a uniform random number s between 0 and 1, we determine the displacement $\Delta\bar{\rho}$ by the equation

$$s = \int_0^{\bar{\rho}+\Delta\bar{\rho}} \bar{P}_{|m|}(t, \bar{\rho})\, dt. \tag{3.6}$$

The probabililty function $\bar{P}_{|m|}(\bar{\rho} + \Delta\bar{\rho}, \bar{\rho})$ depends on both $\bar{\rho}$ and $\Delta\bar{\rho}$ whose behavior is illustrated in the Appendix.

To facilitate the computation, we have made a table of $\Delta\bar{\rho}$ for s ranging from 0 to 1 by the step 0.005 and $\bar{\rho}$ ranging from 0 to 2 by the step 0.1. $\Delta\bar{\rho}$ is obtained by the four-point interpolation for given s and $\bar{\rho}$ if $\bar{\rho} < 2.0$, and for the case of $\bar{\rho} \geqslant 2.0$ $\Delta\bar{\rho}$ is calculated by using the table for $\bar{\rho} = 2.0$, because $\Delta\bar{\rho}$ is approximately independent on $\bar{\rho}$ for $\bar{\rho} > 2.0$ (see Figs. A1 and A2 in the Appendix). The accuracy of the calculation of $\Delta\bar{\rho}$ seriously affects the results obtained, so one has to calculate $\Delta\bar{\rho}$ as accurate as possible.

One additional remark should be stated on the random walk. Since we are seeking the even parity solution, we may restrict our attention to the *psips* distribution on the half plane $(z > 0)$. $\bar{\rho} + \Delta\bar{\rho}$ is always positive owing to the nature of the probability function $\bar{P}_{|m|}(\bar{\rho} + \Delta\bar{\rho}, \bar{\rho})$. While $\bar{z} + \Delta\bar{z}$ happens to be negative, if this happens, we may replace it by its absolute value.

(iv) It is clear that the new $M^{(1)}$ *psips* obtained after step (iii) are distributed according to the density function $\bar{\rho}R_m^{(1)}(\bar{\rho}, \bar{z})$. Then repeating the process (ii) and (iii) where new $M^{(1)}$ *psips* are substituted in place of old $M^{(0)}$ *psips*, we have the Monte Carlo simulation of the iteration process (2.28).

Energy Values

Equation (2.29) may be transformed as

$$e^{-\beta \bar{E}_{m0}} = \frac{1}{M^{(1)}} \sum_{i=1}^{M^{(1)}} \Omega_{|m|}(\bar{\rho}_i) \exp\left[-\frac{1}{4}\tanh\left(\frac{\bar{\beta}}{2}\right)\bar{\rho}_i^2 + \bar{\beta}\left(\frac{\bar{Z}}{(\bar{\rho}_i^2 + \bar{z}_i^2)^{1/2}} + \frac{m}{2}\right)\right], \tag{3.7}$$

where $\bar{\rho}_i$ and $\bar{z}_i$ stand for the coordinate of the ith *psips*. Therefore at each end of step (iii) stated above, we calculate the right-hand side of Eq. (3.7) and get the value of $\bar{E}_{m0}$. As will be shown in the next section, the variation of $\bar{E}_{m0}$ evaluated during the iteration process gives a measure of the convergence.

Wavefunctions

The (ρ, z)-dependent part of the wavefunction with a given magnetic quantum number m, $\phi_{m,0}(\rho, z)$, Eq. (2.23), is related to the distribution function $\rho R_{m,0}(\rho, z)$ of the *psips* in (ρ, z)-plane by Eq. (2.24). Therefore by making a histogram of *psips* distribution in (ρ, z)-plane with the weight $\exp(\frac{1}{2}\beta Z/(\rho^2 + z^2)^{1/2})$ after the convergence of the iteration process is reached, we will have the wavefunction $\phi_{m,0}(\rho, z)$.

4. Numerical Results

By the method described in the preceeding section, the energy values and the wavefunctions of the hydrogen atom ($Z = 1$) are calculated for the magnetic quantum number $m = 0$, 1, and the magnetic field strength $\gamma = 0.1$, 1.0, 10.0.

Starting from a uniform distribution of 2,000 *psips* in the $(\bar{\rho}, \bar{z})$-plane, 400 iterations are performed for each m and γ value. In these iteration processes, $\bar{\beta}$ is fixed to be 0.05 during 1 to 100 iterations and 0.02 during 101 to 400 iterations. Only for the

TABLE I

The Energy Values of the Hydrogen Atom E_{m0} [a]

m	γ	E_{m0} (AU)	$2E_{m0} - \gamma$
0	0.1	-0.4963 ± 0.0194	-1.0926
	1.0	-0.3344 ± 0.0130	-1.6688
	10.0	3.3197 ± 0.0739	-3.3606
1	0.1	-0.1532 ± 0.0028	-0.4064
	1.0	0.0564 ± 0.0120	-0.8872
	10.0	3.8618 ± 0.0748	-2.2764

[a] Last column shows the energy measured from the lowest Landau level in Rydbergs.

$m = 0$, $\gamma = 0.1$ case, the first value of β is taken to be 0.02 and the second one 0.01. The convergence is almost reached by the first 100 iterations. Therefore the *psips* distribution during iterations from 101 to 400 is used to make a histogram of the wavefunction.

The energy values thus obtained, E_{m0}, are listed in Table I and compared with other

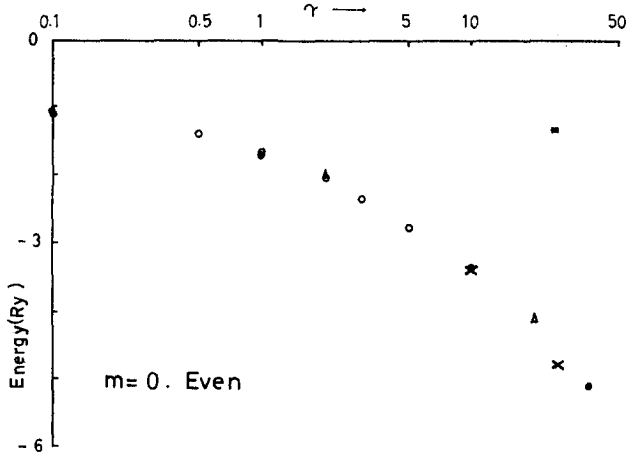

FIG. 1. The energy of the $m = 0$ even state measured from the lowest Landau level is plotted against the magnetic field strength γ in Rydbergs. ●, Present results; ○, Cabib *et al.* [7]; △, Rau and Spruch [8]; ×, Smith *et al.* [9]; ◎, Wallis and Bowlden [10]; ■, dos Santos and Brandi [11].

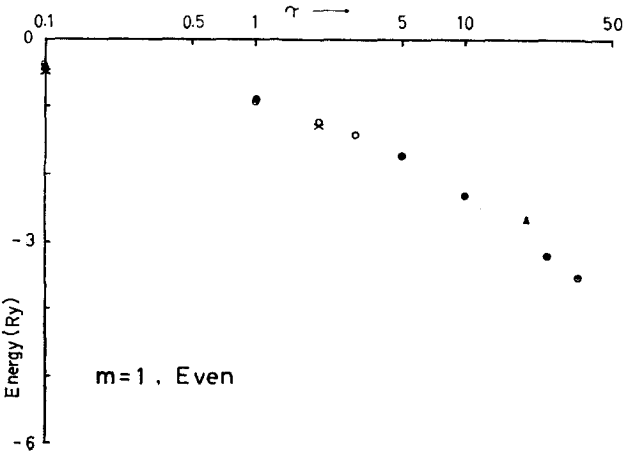

FIG. 2. The energy of the $m = 1$ even state measured from the Lowest Landau level is plotted against the magnetic field strength γ in Rydbergs. ●, Present results; ○, dos Santos and Brandi [11]; ⊕, Larsen [12]; △, Rau and Spruch [8]; ◎, Wallis and Bowlden [10]; ×, Praddaude [13].

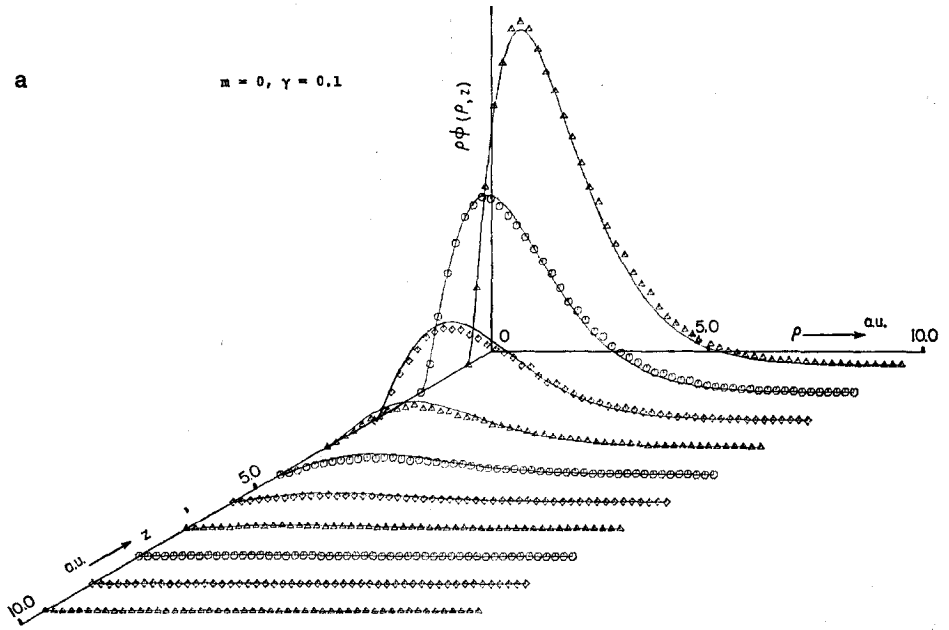

FIG. 3. (a, b, c) Wavefunction $\phi_{0,0}(\rho, z)$, Eq. (2.24), in arbitrary scale: Marks show the histogram obtained by Monte Carlo calculation and solid lines show the analytical form Eq. (4.1) fitted by the least-squares method.

results due to variational method in Figs. 1 and 2, where the energy measured from the lowest Landau level, $\gamma - 2E_{m0}(Ry)$, is plotted against the magnetic field strength γ.

These results show that the present calculation is in fairly good agreement with those obtained by the variational method. The overestimation of the weight factor near the origin which was pointed out in our previous paper [1], is automatically cut off in the present case because of the character of the probability function $\bar{P}_{|m|}(\bar{\rho}, \bar{\rho}')$. That is, as shown in the Appendix, the probability that the *psips* happens to come very near the origin is extremely small, therefore the overestimation of the weight factor scarcely occurs. This is one of the advantages of our present formulation.

It should be noted that the energy values for $m = -1$ are higher than those for $m = 1$ exactly by γ, while the (ρ, z)-dependent part of the wavefunction $\phi_{m,0}(\rho, z)$ is the same for both states, which is easily seen from Eqs. (2.28) and (2.29).

The most significant advantage of the Monte Carlo method is in the fact that it is not necessary to assume beforehand some special analytical form of the wavefunction, that is, the distribution of the *psips* in (ρ, z)-plane gives directly the shape of the wavefunction. The form of $\rho\phi_{m,0}(\rho, z)$ is constructed by the method stated in Section 3 and plotted in Fig. 3.[2]

[2] We have prepared similar figures for $m = 1$ case and will send copies of these on request.

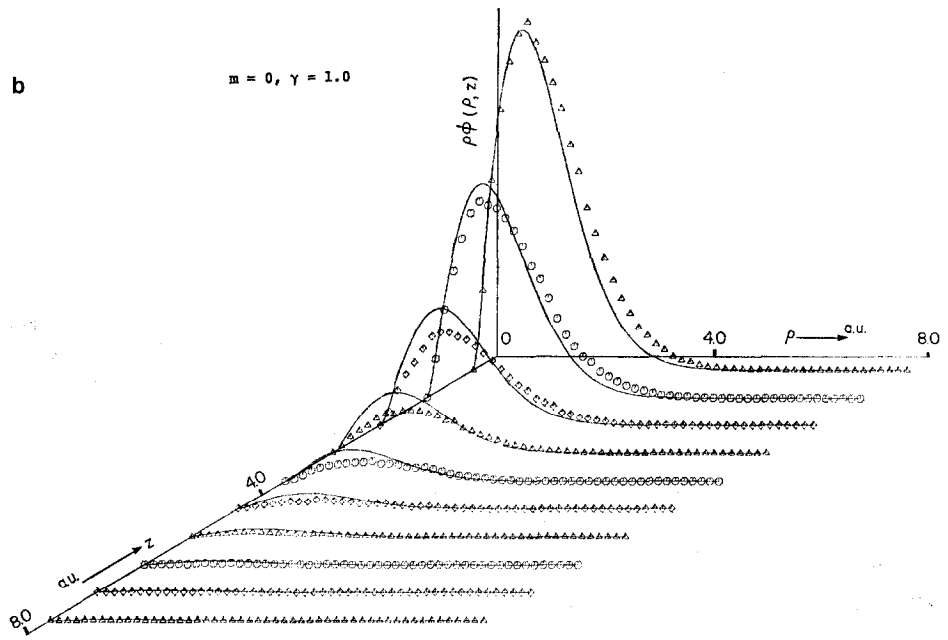

FIGURE 3b.

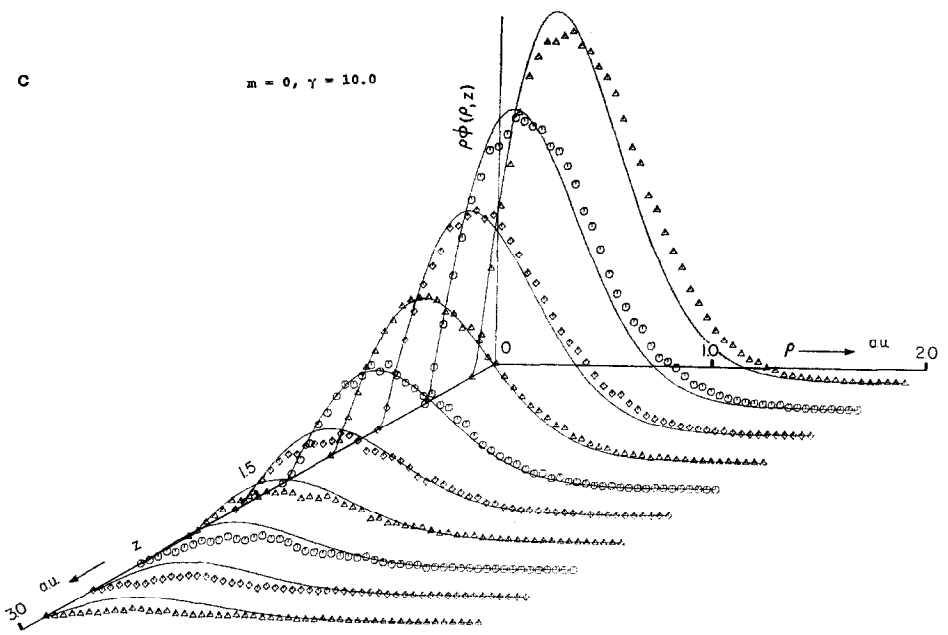

FIGURE 3c.

For comparison, the analytical form given by Rau *et al.* [6]

$$\phi_{m=0} \propto \exp\left(-\frac{\gamma}{4}\rho^2 - Z'r\right), \tag{4.1}$$

$$\phi_{m=1} \propto \rho \exp\left(-\frac{\gamma}{4}\rho^2 - Z'r\right), \tag{4.2}$$

whose variable parameter Z', giving the best fit to our histogram, is determined by the least-squares method, is also shown in this figure. The values of Z' obtained are as shown in Table II.

TABLE II

	$m = 0$			$m = 1$		
γ	0.1	1.0	10.0	0.1	1.0	10.0
Z'	0.89402	0.89577	1.1567	0.41611	0.54190	1.0817

Both the curve of analytical form and the histogram now obtained are normalized in such a way that $\int \phi\rho \, d\rho dz = 1$.

It is clearly demonstrated that the range of the electron distribution both in ρ and z directions becomes smaller as the strength of magnetic field increases. For a constant magnetic field the distribution of electron cloud not only in the ρ direction but also in the z direction are wider for $m = 1$ than for $m = 0$.

In general the agreement of the histogram and the analytical form is rather good, but one can note that the extension in ρ direction of the histogram is slightly larger than that of the analytical form, while in the z-direction the histogram diminishes to zero faster than the analytical form. Therefore it would be better to find some simple analytical form which behaves more similarly to the histogram.

The calculation for larger values of m, even state, can be done in a very similar manner to those mentioned in this paper. However to obtain the results for odd states by the Monte Carlo method, we have to develop the technique of treating the negative value of wavefunction by the *psips* distribution, or rather of finding the probability function $P(z, z')$ suitable for odd state. This is an interesting future problem.

APPENDIX: Probability Function $\bar{P}_{|m|}(\bar{\rho}, \bar{\rho}')$

In this appendix, some additional remarks on the probability function $\bar{P}_{|m|}(\bar{\rho}, \bar{\rho}')$ defined by Eq. (2.30) are included.

Case of $m = 0$: $\bar{P}_{|m|}(\bar{\rho}, \bar{\rho}')$ can be written as

$$\bar{P}_0(\bar{\rho}, \bar{\rho}') = \frac{1}{(4\pi)^{1/2}} \cosh\left(\frac{\bar{\beta}}{2}\right)\left[\operatorname{cosech}\left(\frac{\bar{\beta}}{2}\right)\right]^{1/2} (\bar{\rho}/\bar{\rho}')^{1/2} \tilde{I}_0\left(\frac{1}{2}\bar{\rho}\bar{\rho}' \operatorname{cosech}\left(\frac{\bar{\beta}}{2}\right)\right)$$
$$\times \exp\left[-\frac{1}{4}\coth\left(\frac{\bar{\beta}}{2}\right)\left(\bar{\rho} - \operatorname{sech}\left(\frac{\bar{\beta}}{2}\right)\bar{\rho}'\right)^2\right], \tag{A:1}$$

where $\tilde{I}_0$ is defined in Eq. (2.33).

Especially for $\bar{\rho}' = 0$,

$$\bar{P}_0(\bar{\rho}, 0) = \frac{1}{2} \coth\left(\frac{\bar{\beta}}{2}\right) \bar{\rho} \exp\left[-\frac{1}{4} \coth\left(\frac{\bar{\beta}}{2}\right) \bar{\rho}^2\right]$$

$$\simeq \frac{1}{\bar{\beta}} \bar{\rho} e^{-\bar{\beta}^2/2\bar{\beta}} \qquad (\bar{\beta} \ll 1), \tag{A:2}$$

and for $\bar{\rho}' \gg 1$ and $\bar{\beta} \ll 1$,

$$\bar{P}_0(\bar{\rho}, \bar{\rho}') \simeq \frac{1}{(2\pi\bar{\beta})^{1/2}} \left(\frac{\bar{\rho}}{\bar{\rho}'}\right)^{1/2} \exp\left(-\frac{1}{2\bar{\beta}} (\bar{\rho} - \bar{\rho}')^2\right). \tag{A:3}$$

Case of $m = 1$: $\bar{P}_{|m|}(\bar{\rho}, \bar{\rho}')$ can be rewritten as

$$\bar{P}_1(\bar{\rho}, \bar{\rho}') = \frac{1}{(4\pi)^{1/2}} \cosh\left(\frac{\bar{\beta}}{2}\right)\left[\operatorname{cosech}\left(\frac{\bar{\beta}}{2}\right)\right]^{1/2} (\bar{\rho}/\bar{\rho}')^{1/2}$$

$$\times \frac{\tilde{I}_1(\frac{1}{2}\bar{\rho}\bar{\rho}' \operatorname{cosech}(\bar{\beta}/2))}{\tilde{F}(\frac{1}{2}; 2; -\frac{1}{2} \operatorname{cosech}(\bar{\beta}) \cdot \bar{\rho}'^2)}$$

$$\times \exp\left[-\frac{1}{4} \coth\left(\frac{\bar{\beta}}{2}\right) \cdot \left(\bar{\rho} - \operatorname{sech}\left(\frac{\bar{\beta}}{2}\right) \cdot \bar{\rho}'\right)^2\right], \tag{A:4}$$

where $\tilde{I}_1(z)$ is defined by Eq. (2.33) and $\tilde{F}$ by Eq. (2.22).

Especially for $\bar{\rho}' = 0$,

$$\bar{P}_1(\bar{\rho}, 0) = \frac{1}{(4\pi)^{1/2}} \left(\coth\left(\frac{\bar{\beta}}{2}\right)\right)^{3/2} \bar{\rho}^2 \exp\left(-\frac{1}{4} \coth\left(\frac{\bar{\beta}}{2}\right) \bar{\rho}^2\right)$$

$$\simeq \left(\frac{2}{\pi\bar{\beta}^3}\right)^{1/2} \bar{\rho}^2 \exp\left(-\frac{1}{2\bar{\beta}} \bar{\rho}^2\right) \qquad (\bar{\beta} \ll 1), \tag{A:5}$$

and for $\bar{\rho}' \gg 1$ and $\bar{\beta} \ll 1$

$$\bar{P}_1(\bar{\rho}, \bar{\rho}') \simeq \frac{1}{(2\pi\bar{\beta})^{1/2}} \left(\frac{\bar{\rho}}{\bar{\rho}'}\right)^{1/2} \exp\left[-\frac{1}{2\bar{\beta}} (\bar{\rho} - \bar{\rho}')^2\right]. \tag{A:6}$$

Figures A1 and A2 clearly show how dependent these probability functions are on the values of $\bar{\rho}'$ and $\bar{\rho} - \bar{\rho}'$. Equations (A3) and (A6) indicate that both P_0 and P_1 have a similar form to the Gaussian distribution function, and $\bar{\beta}$ is the variance of these functions. One can see in the figures that these functions are very similar to each other for the value of $\bar{\rho}' > 1$. On the other hand, for the small value of $\bar{\rho}'$ (<0.5), the functions P_0 and P_1 are rather different. For example, the maximum position of the functions for $\bar{\rho}' = 0$ is nearly at the position $\rho \simeq \bar{\beta}^{1/2}$ for $m = 0$ and $\rho \simeq (2\bar{\beta})^{1/2}$ for $m = 1$. This behavior also can be seen in the figures.

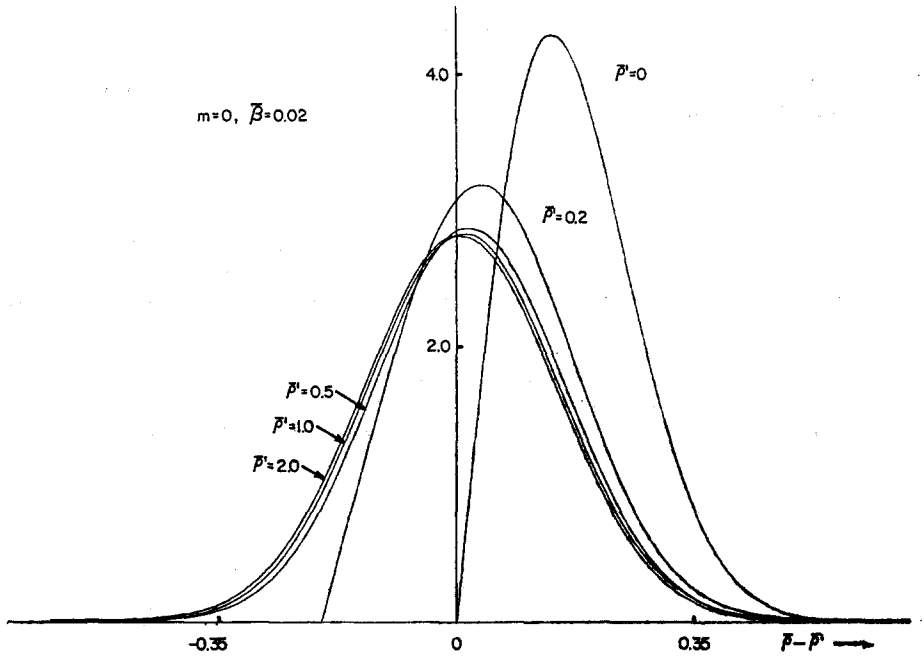

FIG. A1. Probability function $\bar{P}_0(\bar{\rho}, \bar{\rho}')$.

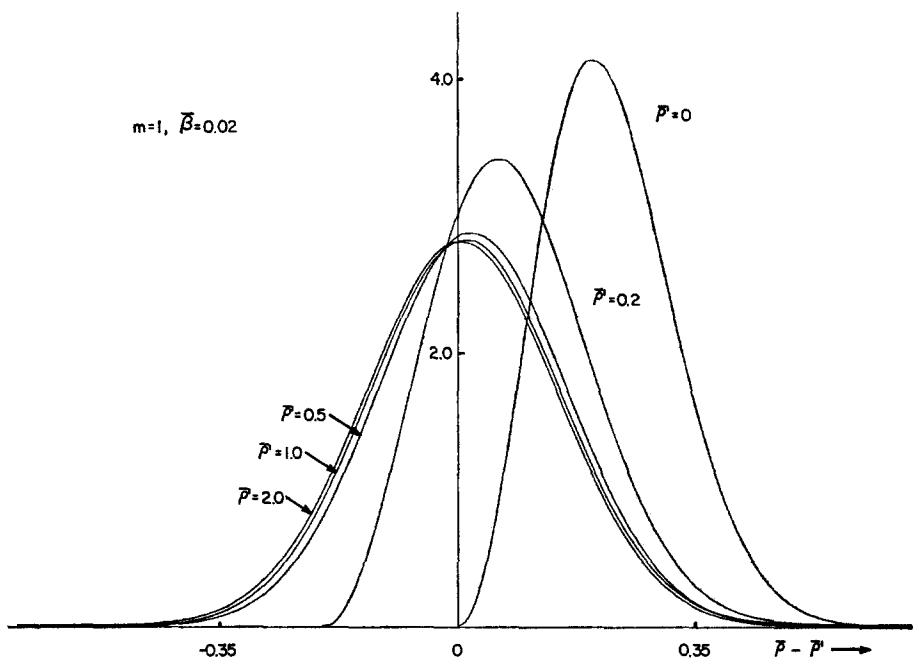

FIG. A2. Probability function $\bar{P}_1(\bar{\rho}, \bar{\rho}')$.

ACKNOWLEDGMENTS

The numerical calculation were performed by the computer system ACOS-700 of Okayama University Computer Centre.

REFERENCES

1. Y. TOMISHIMA AND J. OZAKI, *J. Phys. Soc. Japan* **44** (1978), 1323.
2. G. GRIMM AND R. G. STORER, *J. Computational Phys.* **4** (1969), 230; *J. Computational Phys.* **7** (1971), 134.
3. R. H. GARSTANG, *Rep. Progr. Phys.* **40** (1977), 105.
4. E. H. SONDHEIMER AND A. H. WILSON, *Proc. Roy. Soc. A* **210** (1951), 173.
5. J. B. ANDERSON, *J. Chem. Phys.* **63** (1975), 1499.
6. A. R. P. RAU, R. O. MUELLER, AND L. SPRUCH, *Phys. Rev. A* **11** (1975), 1865.
7. D. CABIB, E. FABRI, AND G. FIORIO, *Nuovo Cimento B* **10** (1972), 185.
8. A. R. P. RAU AND L. SPRUCH, *Astrophys. J.* **207** (1976), 671.
9. ED R. SMITH, R. J. W. HENRY, G. L. SURMELIAN, R. F. O'CONNELL, AND A. K. RAJAGOPAL, *Phys. Rev. D* **6** (1972), 3700.
10. R. F. WALLIS AND H. J. BOWLDEN, *J. Phys. Chem. Solids* **7** (1958), 78.
11. R. R. DOS SANTOS AND H. S. BRANDI, *Phys. Rev. A* **13** (1976), 1970.
12. D. M. LARSEN, *J. Phys. Chem. Solids* **29** (1968), 271.
13. H. C. PRADDAUDE, *Phys. Rev. A* **6** (1972), 1321.