N93-27315

WAVE PACKET MOTION IN HARMONIC POTENTIAL AND COMPUTER VISUALIZATION

Hideo TSURU
Institute of Computational Fluid Dynamics
1-22-3 Haramachi, Meguroku, Tokyo 152, Japan

Takeshi KOBAYASHI
12-104, Kounandai 5-1, Kounanku
Yokohama, Kanagawa 233, Japan

Abstract

Wave packet motions of a single electron in harmonic potentials or a magnetic field are obtained analytically. The phase of the wave function which depends on both time and space is also presented explicitly. The probability density of the electron changes its width and central position periodically. These results are visualized using computer animation techniques.

1 Introduction

We investigate a time evolution of the electron wave packet through analytical methods. The time evolutions of restricted initial wave packets were obtained [1]-[3]. Here, we consider a general initial wave packet and obtain a classical harmonic oscillation of the center of mass of the probability density and an oscillation of its variance. We have also obtained the analytic form of the phase of the wave packet.

2 One-dimensional harmonic potential

We consider the Schrödinger equation for the one-dimensional harmonic potential

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\psi + \frac{k}{2}x^2\psi. \tag{1}$$

The stationary solution is

$$\varphi_n(x,t) = u_n(x)\exp(-i\omega(n+\frac{1}{2})t), \tag{2}$$

where $\omega = \sqrt{\frac{k}{m}}$ and $u_n(x)$ is expressed using the Hermite polynominal $H_n(x)$

$$u_n(x) = N_n H_n(\alpha x)\exp(-\frac{1}{2}\alpha^2 x^2) \tag{3}$$

with $\alpha = \sqrt[4]{\frac{mk}{\hbar^2}}$ and the normalization factor $N_n(x) = \sqrt{\frac{\alpha}{\sqrt{\pi}2^n n!}}$.

Next, we shall expand an initial wave function by these functions and trace its time evolution. Hereafter, the unit length $\alpha = 1$ is used. Without loss of generality, we choose the initial wave packet as

$$\psi(x,0) = \sqrt{\frac{1}{\sqrt{2\pi}\sigma}}\exp(-\frac{(x-z)^2}{4\sigma^2})\exp(-\frac{z_1^2}{4\sigma^2}), \tag{4}$$

where z is a complex number $z = z_0 + iz_1$. We shall expand this wave packet in terms of the stationary solutions

$$\psi(x,0) = \sum_{n=0}^{\infty} C_n u_n(x). \tag{5}$$

We calculate a expansion coefficient C_n, with the help of the generating function of the Hermite polynominal and obtain the following expression.

$$C_n = \sqrt{\frac{4\sigma n!}{\sqrt{2\pi}2^n(1+2\sigma^2)}}\exp(-\frac{z^2}{2(1+2\sigma^2)} - \frac{z_1^2}{4\sigma^2})\sum_{m=0}^{[\frac{n}{2}]}\frac{(-\frac{1-2\sigma^2}{1+2\sigma^2})^m(\frac{2z}{1+2\sigma^2})^{n-2m}}{m!(n-2m)!}. \tag{6}$$

Thus we obtain the time evolution of the wave packet by the following infinite series

$$\psi(x,t) = \sqrt{\frac{4\sigma}{\sqrt{2\pi}(1+2\sigma^2)}}\exp(-\frac{z^2}{2(1+2\sigma^2)} - \frac{z_1^2}{4\sigma^2})\exp(-\frac{x^2}{2})\exp(-\frac{i\omega t}{2})$$
$$\times\sum_{n=0}^{\infty} H_n(x)(\frac{\exp(-i\omega t)}{2})^n\sum_{m=0}^{[\frac{n}{2}]}\frac{(-\frac{1-2\sigma^2}{1+2\sigma^2})^m(\frac{2z}{1+2\sigma^2})^{n-2m}}{m!(n-2m)!}. \tag{7}$$

When σ^2 equals $\frac{1}{2}$, this summation is evaluated easily.

$$\psi(x,t) = \sqrt[4]{\frac{1}{\pi}}\exp(-\frac{z^2}{4} - \frac{z_1^2}{2} - \frac{x^2}{2})\exp(-\frac{i\omega t}{2})\exp(-\frac{z^2}{4}\exp(-2i\omega t) + zx\exp(-i\omega t)). \tag{8}$$

The center of mass of the probability density of the wave packet oscillates sinusoidally. On the other hand, the variance of the probability density is constant during the motion.

When the variance σ^2 is not $\frac{1}{2}$, we shall eliminate the time dependent phase factor in eq.(7) by the following transformations.

$$\frac{1-2\sigma^2}{1+2\sigma^2}\exp(-2i\omega t) = \frac{1-2\delta}{1+2\delta}, \tag{9}$$

$$\frac{z^2}{1-4\sigma^4} = \frac{w^2}{1-4\delta^2}. \tag{10}$$

From eqs.(9) and (10) we obtain

$$\delta = \delta_0 + i\delta_1 = \frac{4\sigma^2 + i(1 - 4\sigma^4 \sin(2\omega t))}{2((1+4\sigma^4) + (1-4\sigma^4)\cos(2\omega t))}, \tag{11}$$

$$w = w_0 + iw_1 = \frac{2(z_0\cos(\omega t) + 2z_1\sigma^2\sin(\omega t)) + 2i(z_1\cos(\omega t) - 2z_0\sigma^2\sin(\omega t))}{(1+4\sigma^4) + (1-4\sigma^4)\cos(2\omega t)}. \tag{12}$$

Inserting these values into the expression (7), we have

$$\psi(x,t) = \sqrt{\frac{4\sigma}{\sqrt{2\pi}(1+2\sigma^2)}}\exp\left(-\frac{z^2}{2(1+2\sigma^2)} - \frac{z_1^2}{4\sigma^2}\right)\exp\left(-\frac{x^2}{2}\right)\exp\left(-\frac{i\omega t}{2}\right)$$
$$\times \sum_{n=0}^{\infty} H_n(x)\frac{1}{2^n}\sum_{m=0}^{[\frac{n}{2}]}\frac{\left(-\frac{1-2\delta}{1+2\delta}\right)^m\left(\frac{2w}{1+2\delta}\right)^{n-2m}}{m!(n-2m)!}. \tag{13}$$

Comparing this and the expression (7) at $t=0$, we see that this is also the expansion formula of a Gaussian wave packet. After a straight forward but lengthy calculation we obtain

$$\psi(x,t) = \exp(i\gamma)\sqrt{\frac{\sqrt{\delta_0}}{\sqrt{2\pi}\mid\delta\mid}}\exp\left(-\frac{(x-w)^2}{4\delta}\right)\exp\left(-\frac{w_1^2}{4\delta_0}\right), \tag{14}$$

where $\exp(i\gamma)$ is a phase factor which depends only on time

$$\gamma = \frac{-(z_0^2 - z_1^2)\sin(2\omega t) + 4z_0z_1\sigma^2(\cos(2\omega t) - 1)}{2(\cos(2\omega t)(1-4\sigma^4) + 1 + 4\sigma^4)} - \frac{1}{2}\arctan\left(\frac{\tan(\omega t)}{2\sigma^2}\right). \tag{15}$$

The center of mass of the wave packet oscillates sinusoidally between $-\frac{\sqrt{4z_0^2\sigma^4+z_1^2}}{2\sigma^2}$ and $\frac{\sqrt{4z_0^2\sigma^4+z_1^2}}{2\sigma^2}$. The variance of the probability density changes periodically in the range between $\frac{1}{4\sigma^2}$ and σ^2 ($\sigma^2 > \frac{1}{2}$) or between σ^2 and $\frac{1}{4\sigma^2}$ ($\sigma^2 < \frac{1}{2}$). The period of its change is half of that of the oscillatory motion of the center of mass[5]. The motion of the probability density function is presented in FIG. 1.

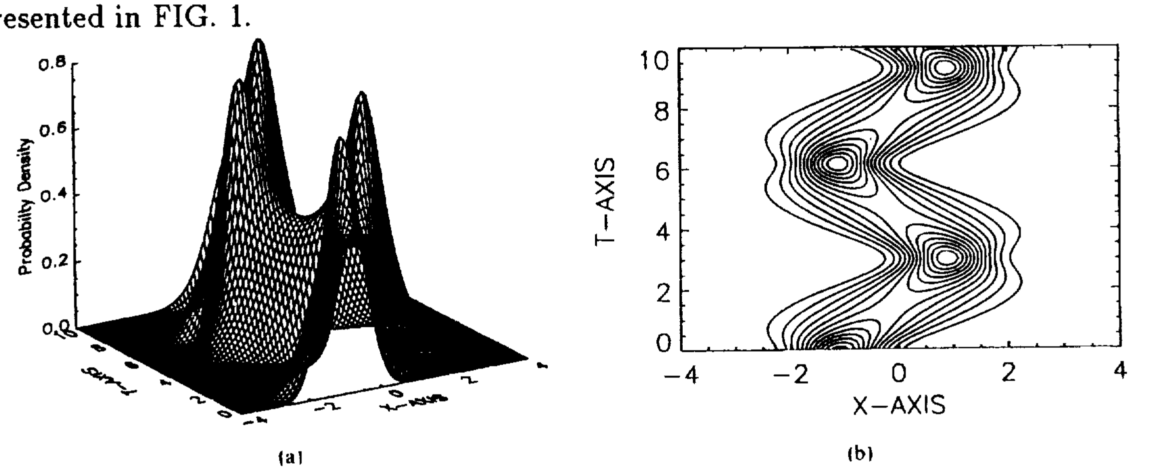

FIG. 1. The motion of the probability density function. Here, we choose the variance of the probability density of the initial wave packet as $\frac{1}{4}$. (a) bird's-eye view. (b) contour line.

3 Two-dimensional Harmonic Potential

Next, we consider the two dimensional Schrödinger equation for an isotropic harmonic potential

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2\nabla^2}{2m}\psi + \frac{k^2(x^2+y^2)}{2}\psi. \tag{16}$$

We choose the initial wave packet as

$$\psi(x,y,0) = N\exp(-\xi(x-x_0)^2+ik_{x0}(x-x_0)-\eta(y-y_0)^2+ik_{y0}(y-y_0)+\lambda(x-x_0)(y-y_0)), \tag{17}$$

where ξ, η and λ are complex constants,

$$\xi = \xi_0 + i\xi_1, \quad \eta = \eta_0 + i\eta_1, \quad \lambda = \lambda_0 + i\lambda_1, \tag{18}$$

which satisfy the following inequalities

$$\xi_0 > 0, \quad \eta_0 > 0, \quad 4\xi_0\eta_0 - \lambda_0^2 > 0, \tag{19}$$

and N is a normalization constant

$$N = \sqrt{\frac{\sqrt{4\xi_0\eta_0 - \lambda_0^2}}{\pi}}, \tag{20}$$

Using the same techniques and procedure in the one-dimensional case, we obtain the time evolution of the wave packet in terms of an infinite series.

$$\psi(x,y,t) = \sum_{n=0}^{\infty}[u_n(y)\sum_{m=0}^{\infty}C_{m,n}u_m(x)\exp(-i\omega(m+n+1)t)], \tag{21}$$

The expansion coefficients $C_{m,n}$ are also calculated explicitly.

For an uncorrelated initial condition

$$\psi(x,y,0) = \sqrt{\frac{\sqrt{4\xi_0\eta_0}}{\pi}}\exp(-\xi(x-x_0)^2+ik_{x0}(x-x_0)-\eta(y-y_0)^2+ik_{y0}(y-y_0)), \tag{22}$$

we can evaluate the infinite series

$$\begin{aligned}\psi(x,y,t) = &\sqrt{\frac{1}{2\pi\sigma_{xt}\sigma_{yt}}}\exp(-\frac{(x-x_t)^2}{4\sigma_{xt}^2} - \frac{(y-y_t)^2}{4\sigma_{yt}^2})\exp(ik_{xt}x + ik_{yt}y) \\ &\times\exp(i\frac{(1-4\sigma_x^4)\sin(2\omega t+2\gamma_x)(x-x_t)^2}{16\sigma_x^2\sigma_{xt}^2} + i\frac{(1-4\sigma_y^4)\sin(2\omega t+2\gamma_y)(y-y_t)^2}{16\sigma_y^2\sigma_{yt}^2}) \\ &\times\exp(-i\frac{k_{xt}x_t}{2} - i\frac{k_{x0}x_0}{2} - i\frac{1}{2}\arctan(\frac{\tan(\omega t)}{2\sigma_x^2}) + i\theta_x) \\ &\times\exp(-i\frac{k_{yt}y_t}{2} - i\frac{k_{y0}y_0}{2} - i\frac{1}{2}\arctan(\frac{\tan(\omega t)}{2\sigma_y^2}) + i\theta_y),\end{aligned} \tag{23}$$

where

$$\sigma_x^2 = \frac{(1-4(\xi_0^2+\xi_1^2))\xi_0}{(-16(\xi_0^2+\xi_1^2)^2+4(\xi_0^2-\xi_1^2))\cos^2(\gamma_x)+(1-4(\xi_0^2-\xi_1^2))\sin^2(\gamma_x)}, \tag{24}$$

$$\sigma_y^2 = \frac{(1-4(\eta_0^2+\eta_1^2))\eta_0}{(-16(\eta_0^2+\eta_1^2)^2+4(\eta_0^2-\eta_1^2))\cos^2(\gamma_y)+(1-4(\eta_0^2-\eta_1^2))\sin^2(\gamma_y)}, \tag{25}$$

$$\gamma_x = \frac{1}{2}\arctan(\frac{4\xi_1}{1-4(\xi_0^2+\xi_1^2)}) \ , \quad \gamma_y = \frac{1}{2}\arctan(\frac{4\eta_1}{1-4(\eta_0^2+\eta_1^2)}), \tag{26}$$

$$\sigma_{xt}^2 = \frac{\sin^2(\omega t+\gamma_x)+4\sigma_x^4\cos^2(\omega t+\gamma_x)}{4\sigma_x^2}, \quad \sigma_{yt}^2 = \frac{\sin^2(\omega t+\gamma_y)+4\sigma_y^4\cos^2(\omega t+\gamma_y)}{4\sigma_y^2}, \tag{27}$$

Here θ_x and θ_y are time independent phase factors

$$\theta_x = -(\frac{(1-4\sigma_x^4)\sin(2\gamma_x)}{4(\sin^2(\gamma_x)+4\sigma_x^4\cos^2(\gamma_x))}+\xi_1)x_0^2+\frac{1}{2}\arctan(\frac{\tan(\gamma_x)}{2\sigma_x^2}), \tag{28}$$

$$\theta_y = -(\frac{(1-4\sigma_y^4)\sin(2\gamma_y)}{4(\sin^2(\gamma_y)+4\sigma_y^4\cos^2(\gamma_y))}+\eta_1)y_0^2+\frac{1}{2}\arctan(\frac{\tan(\gamma_y)}{2\sigma_y^2}). \tag{29}$$

We obtain the explicit time dependence of the following parameters

$$x_t = x_0\cos(\omega t)+k_{x0}\sin(\omega t)\ , \quad y_t = y_0\cos(\omega t)+k_{y0}\sin(\omega t), \tag{30}$$

$$k_{xt} = k_{x0}\cos(\omega t)-x_0\sin(\omega t)\ , \quad k_{yt} = k_{y0}\cos(\omega t)-y_0\sin(\omega t)\ . \tag{31}$$

The trajectory of the center of mass of the probability density function is an elliptic motion around the origin with an angular frequency ω.

4 Uniform magnetic field

The Schrödinger equation for a single electron in a uniform magnetic field perpendicular to the two dimensional flat plane is

$$i\hbar\frac{\partial}{\partial t}\psi = \frac{1}{2m}(-i\hbar\nabla+\frac{e\boldsymbol{A}}{c})^2\psi, \tag{32}$$

where the vector potential $\boldsymbol{A}$ in Landau gauge is

$$\boldsymbol{A} = (-By, 0) \tag{33}$$

We separate a special solution of the wave equation as

$$\psi(x,y,t) = \exp(ikx)f(k,y,t) \tag{34}$$

The wave equation for $f(k,y,t)$ becomes

$$i\hbar\frac{\partial}{\partial t}f(k,y,t) = \frac{\hbar^2}{2m}(-\frac{\partial^2}{\partial y^2}+\alpha^2(y-\frac{k}{\alpha})^2)f(k,y,t), \tag{35}$$

where

$$\alpha = \frac{eB}{c\hbar} \tag{36}$$

This is the one dimensional Schrödinger equation for the harmonic potential centered at $y = k/\alpha$. Thus above techniques and procedures can be applied in order to obtain the time evolution of the wave packet [6]. We choose the initial wave packet eq.(17). The comlete descriptions are presented in the literatutre [6]. The major difference between two dimensional isotropic harmonic potential and magnetic field is the period of the change of the variance. The former is the half of the latter. This fact is also interpreted by the pass integration technique [6], [8].

For the following initial condition

$$\xi = \eta \ , \ \ \lambda = \frac{i}{2}. \tag{37}$$

the shape of the contour lines of the probability density function remains circular during the motion.

For the following initial condition

$$\xi = \eta = \frac{1}{4} \ , \ \ \lambda = \frac{i}{2}, \tag{38}$$

the shape of the probability density remains unchanged.

5 Conclusion

Using a frame buffer NVS2000 and video recorder BVW-75, we have made CG animations which can give us an intuitive understanding of the wave packet motions.

The potentials are simple but due to the quantum mecanical property the analytic form of the wave packet motions are very complicated.

References

[1] E. Schrödinger: Naturwiss. **14** 664 (1926).

[2] L. I. Schiff: *Quantum Mechanics* 3rd ed. (McGraw-Hill, New York, 1968).

[3] I. Fujiwara and K. Miyoshi : Prog. Theor. Phys. **64** 715 (1980).

[4] S. Brandt and H. D. Dahmen : *Quantum Mechanics on the Personal Computer* (Springer, Berlin, 1989).

[5] H. Tsuru : J. Phys. Soc. Japan. **60** 3657 (1991).

[6] H. Tsuru : J. Phys. Soc. Japan. **61** 2246 (1991).

[7] H. Tsuru : J. Phys. Soc. Japan. **61** 2595 (1991).

[8] R. P. Feynmann and A. R. Hibbs: *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).