CHAPTER 5

Partition Function and Free Energy of A Particle with SPP in Magnetic Field

In this Chapter, we will introduce a transverse magnetic field B in the Lagrangian from Eq. (4.1). The idea of introducing the magnetic field in a saddle point potential was given by Fertig and Halperin [2]. The presence of a magnetic field brings complications to our classical solution. However, we can solve the exact propagator of this problem by using the matrix method developed by Papadopoulos and Jones [16], [17] and applying these method by Sa-yakanit, Choosiri and Robkob [9]. We must be careful about matrix multiplication in the exponential factor terms. Then, we will transform another off-diagonal matrix to the diagonal matrix form.

5.1 The Lagrangian

The Lagrangian of the particle with SPP in magnetic field B in 2-dimensional is

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{e}{c}\mathbf{v} \cdot \mathbf{A} - \frac{m}{2}(\Omega_x^2 x^2 - \Omega_y^2 y^2)$$

where $\mathbf{v} = (\dot{x}, \dot{y}, 0)$ is a velocity of a charged particle in magnetic field, $\mathbf{A} = (A_x, A_y, A_z)$ is a vector potential, and Ω_x and Ω_y are frequencies of SPP. When we consider a uniform magnetic field along the z-axis, $\mathbf{B} = (0, 0, B)$. We set $A_z = 0$ and use $\nabla \times \mathbf{A} = \mathbf{B}$ to find the vector potential. We obtain $\mathbf{A} = (-y, x, 0)B/2$. Then the particle with SPP in a uniform magnetic field is

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) + \frac{m}{2}\omega(x\dot{y} - y\dot{x}) - \frac{m}{2}(\Omega_x^2 x^2 - \Omega_y^2 y^2) \tag{5.1}$$

where $\omega = eB/mc$, is the cyclotron frequency. From Eq. (5.1), we obtain two coupling equations of motion by variation as

$$\ddot{x} - \omega\dot{y} + \Omega_x^2 x = 0, \tag{5.2}$$

$$\ddot{y} + \omega\dot{x} - \Omega_y^2 y = 0. \tag{5.3}$$

5.2 Kernel of The Particle with SPP in Magnetic Field

We should use the method of matrices to solve the coupled equations. The matrix form for solving path integrals was developed from the paper of Papadopoulos and Jones [16], [17]. In this thesis, we want to solve this problem the particle with SPP in magnetic field in matrix form following their work. We can find the equations of motion from the Lagrangian in Eq. (5.1). We change these equations to matrix forms by defining our notation as follow:

$$\mathbf{r} = \begin{bmatrix} x \\ y \end{bmatrix}; \tilde{\mathbf{r}} = \begin{bmatrix} x & y \end{bmatrix};$$

$$\mathbf{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}; \mathbf{J} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}; \mathbf{\Omega_{xy}} = \begin{bmatrix} \Omega_x & 0 \\ 0 & i\Omega_y \end{bmatrix}.$$

The matrix $\mathbf{r}$ and its transpose $\tilde{\mathbf{r}}$ represent the variables of configuration space. The matrix $\mathbf{J}$ represents a coupled term of magnetic field. We observe that the coupling matrix $\mathbf{J}$ that $\mathbf{J}^2 = -\mathbf{I}$. Then we can find $\mathbf{J}$ in a diagonal matrix form as $i\mathbf{I}$. From these matrix, we add Eqs. (5.2) and (5.3) to one equation of motion in matrix form as

$$\ddot{\mathbf{r}} + \omega\mathbf{J}\dot{\mathbf{r}} + \mathbf{\Omega^2_{xy}}\mathbf{r} = 0. \tag{5.4}$$

We solve this equation of motion in an operator equation as

$$(D^2 + \omega\mathbf{J}D + \mathbf{\Omega^2_{xy}})\,\mathbf{r} = 0$$

where $D \equiv d/dt$. We find two roots $\mathbf{R}_1$ and $\mathbf{R}_2$ as

$$\begin{aligned} \mathbf{R}_{1,2} &= -\frac{\omega\mathbf{J}}{2} \pm \frac{\sqrt{\omega^2\mathbf{J}^2 - 4\mathbf{\Omega_{xy}}^2}}{2} \\ &= -i\frac{\omega}{2}\mathbf{I} \pm \sqrt{-\frac{\omega^2}{4}\mathbf{I} - \mathbf{\Omega_{xy}}^2} \\ &= -i\frac{\omega}{2}\mathbf{I} \pm i\begin{bmatrix} \sqrt{\omega^2/4 + \Omega_x^2} & 0 \\ 0 & \sqrt{\omega^2/4 - \Omega_y^2} \end{bmatrix}\mathbf{I} \end{aligned}$$

$$
\begin{aligned}
&= -i\frac{\omega}{2}\mathbf{I} \pm i \begin{bmatrix} \Omega_1 & 0 \\ 0 & \Omega_2 \end{bmatrix} \mathbf{I} \\
&= -i\frac{\omega}{2}\mathbf{I} \pm i\mathbf{\Omega}\mathbf{I} \qquad (5.5)
\end{aligned}
$$

where $\Omega_1 = \sqrt{\omega^2/4 + \Omega_x^2}$, $\Omega_2 = \sqrt{\omega^2/4 - \Omega_y^2}$ and $\mathbf{\Omega} = \begin{bmatrix} \Omega_1 & 0 \\ 0 & \Omega_2 \end{bmatrix}$. From Eq. (5.5), we observe that we can arrange to another form as $(\omega\mathbf{I}/2 \pm \mathbf{\Omega})\mathbf{J}$. This is an off-diagonal matrix. It is an improper form to solve this problem. Thus, the matrix in the exponential of this equation have two cases. In the first case, the argument of matrix of exponential has only a matrix **J** multiplying scalar quantity. We prove that

$$
e^{\omega\mathbf{J}\tau/2} = \mathbf{I}\cos\frac{\omega}{2}\tau + \mathbf{J}\sin\frac{\omega}{2}\tau. \qquad (5.6)
$$

In the second case, the argument of matrix has an off-diagnal matrix. We consider especially matrix $\mathbf{\Omega}$ and **J**. We can not change the order of $\mathbf{\Omega}$ and **J**. We can expand this exponential as

$$
e^{\mathbf{\Omega}\mathbf{J}\tau} = \mathbf{I} + \frac{1}{1!}(\mathbf{\Omega}\mathbf{J})\,\tau + \frac{1}{2!}(\mathbf{\Omega}\mathbf{J})^2\,\tau^2 + \frac{1}{3!}(\mathbf{\Omega}\mathbf{J})^3\,\tau^3 + \frac{1}{4!}(\mathbf{\Omega}\mathbf{J})^4\,\tau^4 + \ldots,
$$

we observe that $(\mathbf{\Omega}\mathbf{J})^2 = -\Omega^2\mathbf{I}$, $(\mathbf{\Omega}\mathbf{J})^3 = -\Omega^2(\mathbf{\Omega}\mathbf{J})$, $(\mathbf{\Omega}\mathbf{J})^4 = \Omega^4\mathbf{I}$, where $\Omega = (\Omega_1\Omega_2)^{1/2}$. Thus we have the easy form, that is,

$$
\begin{aligned}
e^{\mathbf{\Omega}\mathbf{J}\tau} &= \mathbf{I}(1 - \frac{\Omega^2\tau^2}{2!} + \frac{\Omega^4\tau^4}{4!} - \ldots) + \mathbf{\Omega}\mathbf{J}(\tau - \frac{\Omega^2\tau^3}{3!} + \frac{\Omega^4\tau^5}{5!} - \ldots) \\
&= \mathbf{I}\cos\Omega\tau + \mathbf{\Omega}\mathbf{J}\frac{1}{\Omega}\sin\Omega\tau.
\end{aligned}
$$

However, we can use a trick to simplify the argument of matrix in the diagonal form. We transform the coupling matrix **J**, off-diagonal matrix, to the matrix $i\mathbf{I}$.

The matrix $i\mathbf{I}$ is a diagonal matrix. Then we use the first case to obtain a proper matrix $i\mathbf{I}$ to solve this problem as

$$e^{\boldsymbol{\Omega}\mathbf{J}\tau} = e^{i\boldsymbol{\Omega}\tau} = \cos\boldsymbol{\Omega}\tau + i\sin\boldsymbol{\Omega}\tau \tag{5.7}$$

and we have just arranged to trigonometric form as

$$e^{i\boldsymbol{\Omega}\tau} - e^{-i\boldsymbol{\Omega}\tau} = 2i\sin\boldsymbol{\Omega}\tau.$$

From Eq. (5.4) we have the general solution as

$$\mathbf{r}(t) = e^{-i\omega t\mathbf{I}/2}\ [\ e^{i\boldsymbol{\Omega}t}\ A + e^{-i\boldsymbol{\Omega}t}\ B\ ]. \tag{5.8}$$

In Eq. (5.8) we can separate the exponential terms because these matrices are diagonal. Next, We must know about the boundary condition. We have the boundary condition in form

$$\mathbf{r}(0) = \begin{bmatrix} x_a \\ y_a \end{bmatrix}; \mathbf{r}(\tau) = \begin{bmatrix} x_b \\ y_b \end{bmatrix}$$

We substitute both boundary conditions into Eq. (5.8). Then we have

$$\mathbf{r}(0) \ = \ A + B, \tag{5.9}$$

$$\mathbf{r}(\tau) = e^{-i\omega\tau\mathbf{I}/2}\ [\ e^{i\boldsymbol{\Omega}\tau}\ A + e^{-i\boldsymbol{\Omega}\tau}\ B\ ]. \tag{5.10}$$

Then we solve Eq. (5.6) to find A and B by using Eqs. (5.9) and (5.10). We obtain

$$A \ = \ \frac{1}{2i}(\sin\boldsymbol{\Omega}\tau)^{-1}\ [e^{i\frac{\omega}{2}\mathbf{I}\tau}\mathbf{r}(\tau) + e^{-i\boldsymbol{\Omega}\tau}\mathbf{r}(0)], \tag{5.11}$$

$$B = \frac{1}{2i}(\sin \mathbf{\Omega}\tau)^{-1}\ [e^{i\mathbf{\Omega}\tau}\mathbf{r}(0) - e^{i\frac{\omega}{2}\mathbf{I}\tau}\mathbf{r}(\tau)]. \tag{5.12}$$

We substitute Eqs. (5.11) and (5.12) to Eq. (5.8). We obtain

$$\mathbf{r}(t) = e^{-i\frac{\omega}{2}\mathbf{I}t}(\sin \mathbf{\Omega}\tau)^{-1}[\sin \mathbf{\Omega}t e^{i\frac{\omega}{2}\mathbf{I}\tau}\ \ \mathbf{r}(\tau) + \sin \mathbf{\Omega}(\tau - t)\ \mathbf{r}(0)\ ]. \tag{5.13}$$

Now we continue to use Eq. (5.1) to find the kernel. We set Eq. (5.1) in matrix form as

$$L = \frac{m}{2}[\ \tilde{\dot{\mathbf{r}}}\dot{\mathbf{r}} - \omega\tilde{\mathbf{r}}\mathbf{J}\dot{\mathbf{r}} - \tilde{\mathbf{r}}\mathbf{\Omega}_{\mathbf{xy}}^2\mathbf{r}\ ]. \tag{5.14}$$

We obtain the classical solutions from Eq. (5.14). Then the classical action can be obtained from the following expression

$$\begin{aligned} S_{cl} &= \frac{m}{2}\int_0^\tau \tilde{\dot{\mathbf{r}}}\dot{\mathbf{r}} - \tilde{\mathbf{r}}\ (\omega\mathbf{J}\dot{\mathbf{r}} + \mathbf{\Omega}_{\mathbf{xy}}^2\mathbf{r})\ dt \\ &= \frac{m}{2}[\tilde{\mathbf{r}}(\tau)\dot{\mathbf{r}}(\tau) - \tilde{\mathbf{r}}(0)\dot{\mathbf{r}}(0)]. \end{aligned} \tag{5.15}$$

Substituting the boundary condition into the expression in Eq. (5.15), we obtain the classical action as

$$\begin{aligned} S_{cl} = \frac{m}{2}\ \ [\ \ & \frac{\Omega_1}{\sin \Omega_1\tau}[\ (x_b^2 + x_a^2)\cos \Omega_1\tau - 2x_b x_a \cos \frac{\omega}{2}\tau + (x_a y_b - x_b y_a)\sin \frac{\omega}{2}\tau\ ] \\ + \ \ & \frac{\Omega_2}{\sin \Omega_2\tau}[\ (y_b^2 + y_a^2)\cos \Omega_2\tau - 2y_b y_a \cos \frac{\omega}{2}\tau + (x_a y_b - x_b y_a)\sin \frac{\omega}{2}\tau\ ]\ ]. \end{aligned} \tag{5.16}$$

We can easily check this classical action. If we substitute $\omega = 0$ in Eq. (5.16), we obtain $\Omega_1 = \Omega_x$ and $\Omega_2 = i\Omega_y$. The classical action of the saddle point potential in the magnetic field reduces to the classical action of the saddle point potential. If we substitute $\Omega_x = \Omega_y = 0$ to Eq. (5.16), we obtain that $\Omega_1 = \Omega_2 = \omega/2$ and the classical action reduces to the classical action of a charged particle in a constant external magnetic field.

Then the prefactor in 2 dimension can be obtained, by using Eq. (3.12), to be

$$\begin{aligned} F(\tau) &= \frac{1}{2\pi i\hbar} \begin{vmatrix} \frac{\partial^2}{\partial x_a \partial x_b} S_{cl} & \frac{\partial^2}{\partial x_a \partial y_b} S_{cl} \\ \frac{\partial^2}{\partial y_a \partial x_b} S_{cl} & \frac{\partial^2}{\partial y_a \partial y_b} S_{cl} \end{vmatrix}^{1/2} \\ &= \frac{1}{2\pi i\hbar} \begin{vmatrix} -m\frac{\Omega_1}{\sin\Omega_1\tau}\cos\frac{\omega\tau}{2} & \frac{m}{2}[\frac{\Omega_1}{\sin\Omega_1\tau} + \frac{\Omega_2}{\sin\Omega_2\tau}]\sin\frac{\omega\tau}{2} \\ -\frac{m}{2}[\frac{\Omega_1}{\sin\Omega_1\tau} + \frac{\Omega_2}{\sin\Omega_2\tau}]\sin\frac{\omega\tau}{2} & -m\frac{\Omega_2}{\sin\Omega_2\tau}\cos\frac{\omega\tau}{2} \end{vmatrix}^{1/2} \\ &= (\frac{m}{2\pi i\hbar}) \\ &\times \; [\frac{\Omega_1}{\sin\Omega_1\tau}\frac{\Omega_2}{\sin\Omega_2\tau}\cos^2\frac{\omega\tau}{2} + \frac{1}{4}[\frac{\Omega_1}{\sin\Omega_1\tau} + \frac{\Omega_2}{\sin\Omega_2\tau}]^2 \sin^2\frac{\omega\tau}{2}\;]^{1/2}. \end{aligned} \tag{5.17}$$

Thus the exact propagator for the particle with SPP in magnetic field by using Eqs. (5.16) and (5.17) are given as

$$K(\mathbf{r_b}, \mathbf{r_a}; \tau) = F(\tau)\exp\{\frac{i}{\hbar}S_{cl}(\mathbf{r_b}, \mathbf{r_a}; \tau)\}. \tag{5.18}$$

5.3 The Partition Function and Free Energy of The Particle with SPP in Magnetic Field

We can find the density matrix from the kernel Eq. (5.18), that is, $\rho(\mathbf{r_b},\mathbf{r_a},\beta)\equiv K(\mathbf{r_b},\mathbf{r_a},-i\hbar\beta)$. To find the partition function, we consider a trace of the density matrix. Then, we have

$$Z \equiv Tr\ \rho(\mathbf{r_b},\mathbf{r_a},\tau) = F(\tau)\ Tr\ e^{(i/\hbar)S_{cl}}. \tag{5.19}$$

Now we just consider only a trace term which separates into two similar integrals

$$\begin{aligned} Tr\ e^{(i/\hbar)S_{cl}} &= \int_{-\infty}^{\infty} dx_a\ \exp\{\frac{i}{\hbar}\frac{m}{2}\frac{\Omega_1}{\sin\Omega_1\tau}2(\cos\Omega_1\tau-\cos\frac{\omega\tau}{2})x_a^2\} \\ &\times \int_{-\infty}^{\infty} dy_a\ \exp\{\frac{i}{\hbar}\frac{m}{2}\frac{\Omega_2}{\sin\Omega_2\tau}2(\cos\Omega_2\tau-\cos\frac{\omega\tau}{2})y_a^2\}. \end{aligned} \tag{5.20}$$

We use a gaussian integration to evaluate each integral as

$$\begin{aligned} \int_{-\infty}^{\infty} dx_a \exp\{\frac{i}{\hbar}\frac{m\Omega_1}{\sin\Omega_1\tau}(\cos\Omega_1\tau-\cos\omega\tau/2)\ x_a^2\} &= (\frac{\pi i\hbar\ \sin\Omega_1\tau}{m\Omega_1[\cos\Omega_1\tau-\cos\omega\tau/2]})^{1/2}, \\ \int_{-\infty}^{\infty} dy_a \exp\{\frac{i}{\hbar}\frac{m\Omega_2}{\sin\Omega_2\tau}(\cos\Omega_2\tau-\cos\omega\tau/2)\ y_a^2\} &= (\frac{\pi i\hbar\ \sin\Omega_2\tau}{m\Omega_2[\cos\Omega_2\tau-\cos\omega\tau/2]})^{1/2}. \end{aligned} \tag{5.21}$$

Thus, the total result, we get as

$$\begin{aligned} Z &\equiv \frac{1}{2}[\frac{\Omega_1}{\sin\Omega_1\tau}\frac{\Omega_2}{\sin\Omega_2\tau}\cos^2\frac{\omega\tau}{2}+\frac{1}{4}(\frac{\Omega_1}{\sin\Omega_1\tau}+\frac{\Omega_2}{\sin\Omega_2\tau})^2\sin^2\frac{\omega\tau}{2}]^{1/2} \\ &\times (\frac{\sin\Omega_1\tau}{\Omega_1}\frac{\sin\Omega_2\tau}{\Omega_2})^{1/2} \\ &\times [\frac{1}{4}\frac{1}{\sin(\frac{\Omega_1+\omega/2}{2})\tau\ \sin(\frac{\Omega_1-\omega/2}{2})\tau\ \sin(\frac{\Omega_2+\omega/2}{2})\tau\ \sin(\frac{\Omega_2-\omega/2}{2})\tau}]^{1/2} \end{aligned} \tag{5.22}$$

From this Partition function Eq. (5.22), we change τ to $-i\beta\hbar$ for the thermodynamic form. Then, we have

$$\begin{aligned} Z &= \frac{1}{2}[-\frac{\Omega_1}{\sinh\Omega_1\beta\hbar}\frac{\Omega_2}{\sinh\Omega_2\beta\hbar}\cosh^2\frac{\omega\beta\hbar}{2}+\frac{1}{4}(\frac{\Omega_1}{\sinh\Omega_1\beta\hbar}+\frac{\Omega_2}{\sinh\Omega_2\beta\hbar})^2\sinh^2\frac{\omega\beta\hbar}{2}]^{1/2} \\ &\times (-\frac{\sinh\Omega_1\beta\hbar}{\Omega_1}\frac{\sinh\Omega_2\beta\hbar}{\Omega_2})^{1/2} \\ &\times [\frac{1}{4}\frac{1}{\sinh(\frac{\Omega_1+\omega/2}{2})\beta\hbar\ \sinh(\frac{\Omega_1-\omega/2}{2})\beta\hbar\ \sinh(\frac{\Omega_2+\omega/2}{2})\beta\hbar\ \sinh(\frac{\Omega_2-\omega/2}{2})\beta\hbar}]^{1/2}. \end{aligned} \quad (5.23)$$

Eq. (5.23) shows that this is the partition function of the particle with SPP in magnetic field in closed form. Now we can find F from Eq. (2.4), we obtain

$$\begin{aligned} F &= \frac{\hbar}{2}(\Omega_1+\Omega_2)+\frac{1}{2\beta}\{\ \ln[1-e^{-\beta\hbar(\Omega_1-\omega/2)}] \\ &+ \ln[1-e^{-\beta\hbar(\Omega_1+\omega/2)}]+\ln[1-e^{-\beta\hbar(\Omega_2-\omega/2)}]+\ln[1-e^{-\beta\hbar(\Omega_2+\omega/2)}] \\ &- \ln[\ \cosh^2\frac{\omega\beta\hbar}{2}-\frac{1}{4}[\frac{\Omega_1}{\sinh\Omega_1\beta\hbar}+\frac{\Omega_2}{\sinh\Omega_2\beta\hbar}]^2\frac{\sinh\Omega_1\beta\hbar}{\Omega_1}\frac{\sinh\Omega_2\beta\hbar}{\Omega_2}\sinh^2\frac{\omega\beta\hbar}{2}\ ]\}. \end{aligned} \quad (5.24)$$

5.4 Calculated Results

In this section we present the calculated results for the case of the particle with SPP in magnetic field. The magnetic field, as well known, forces the particle into circular motion with translation motion in one dimension. From Eq. (5.24), we can calculate the free energy of the particle with SPP to compare with Eq.(4.19). We obtain the particles with HP and with SPP in Figs. (5.1) and (5.2), respectively, which are exactly the same as in Figs. (4.3) and (4.4). In Fig. (5.3), we show the case of the particle in magnetic field when saddle point potential is zero. For weak magnetic field, the circular motion is weak, the magnetic field has a small effect on the particle. Therefore the free energy of the particle with SPP in magnetic field does not change appreciably as can be seen in Fig (5.4), comparing to Fig. (5.3). When we increase the magnetic field, the particle is bounded by the magnetic field and the behavior of the free energy tends to smooth out as can be seen in Fig. (5.5). The further increase of magnetic field makes all singular behavior smooth as can be seen in Figs. (5.6)-(5.8).

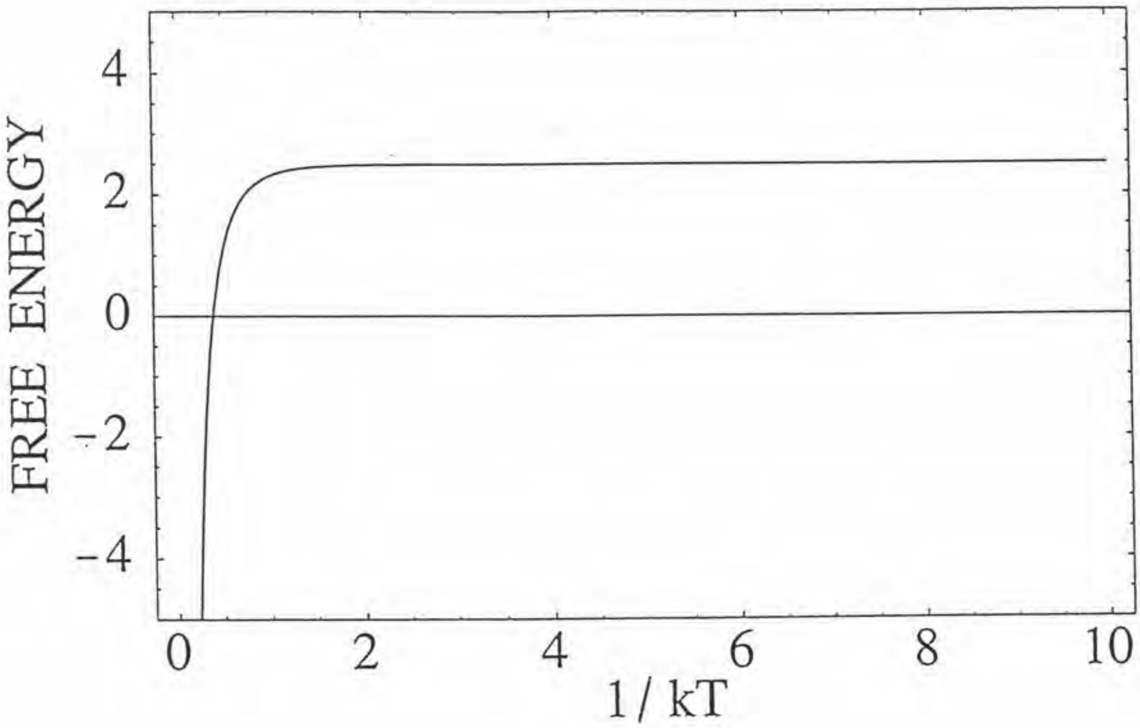

Figure 5.1: The free energy of the particle with HP when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3i$ and $\omega = 0$

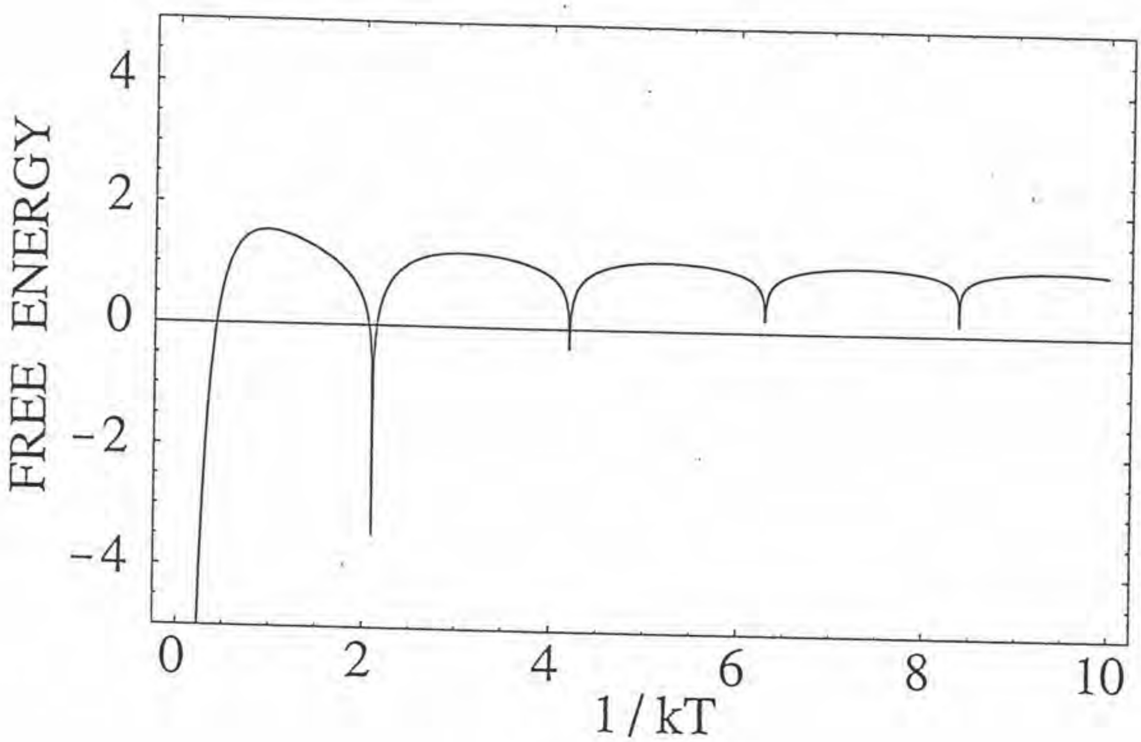

Figure 5.2: The free energy of the particle with SPP when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3$ and $\omega = 0$

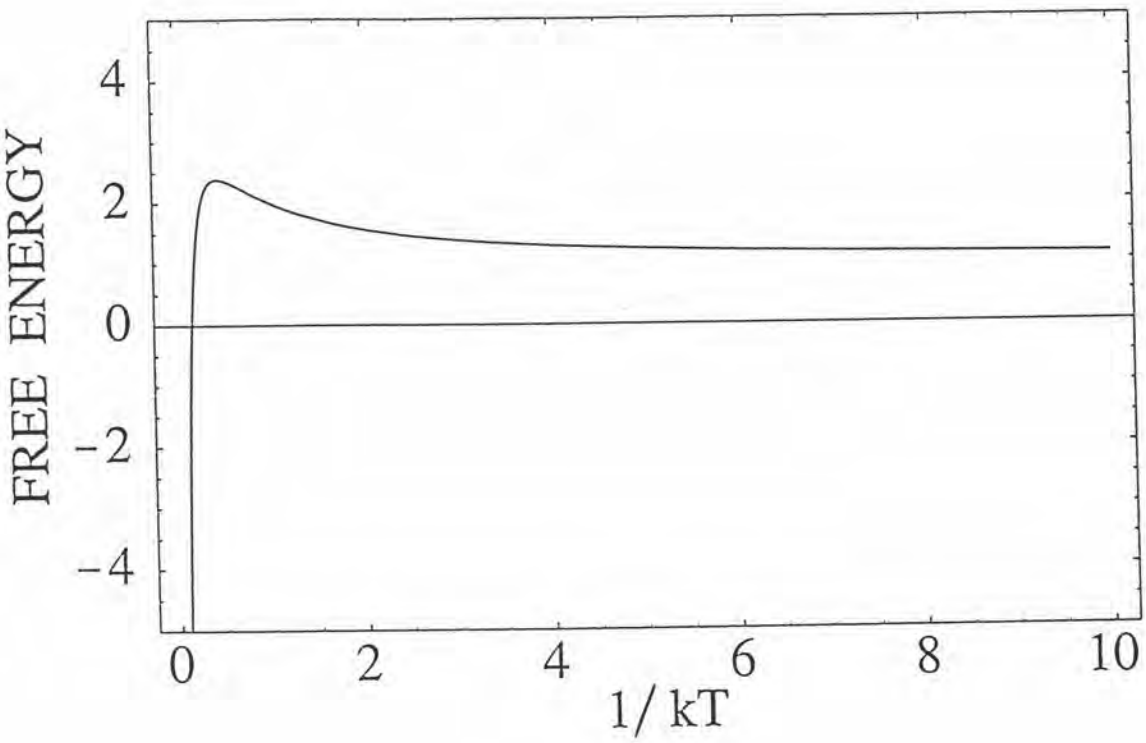

Figure 5.3: The free energy of the particle in magnetic field when $m = 1$, $\hbar = 1$, $\Omega_x = 0$, $\Omega_y = 0$ and $\omega = 2$

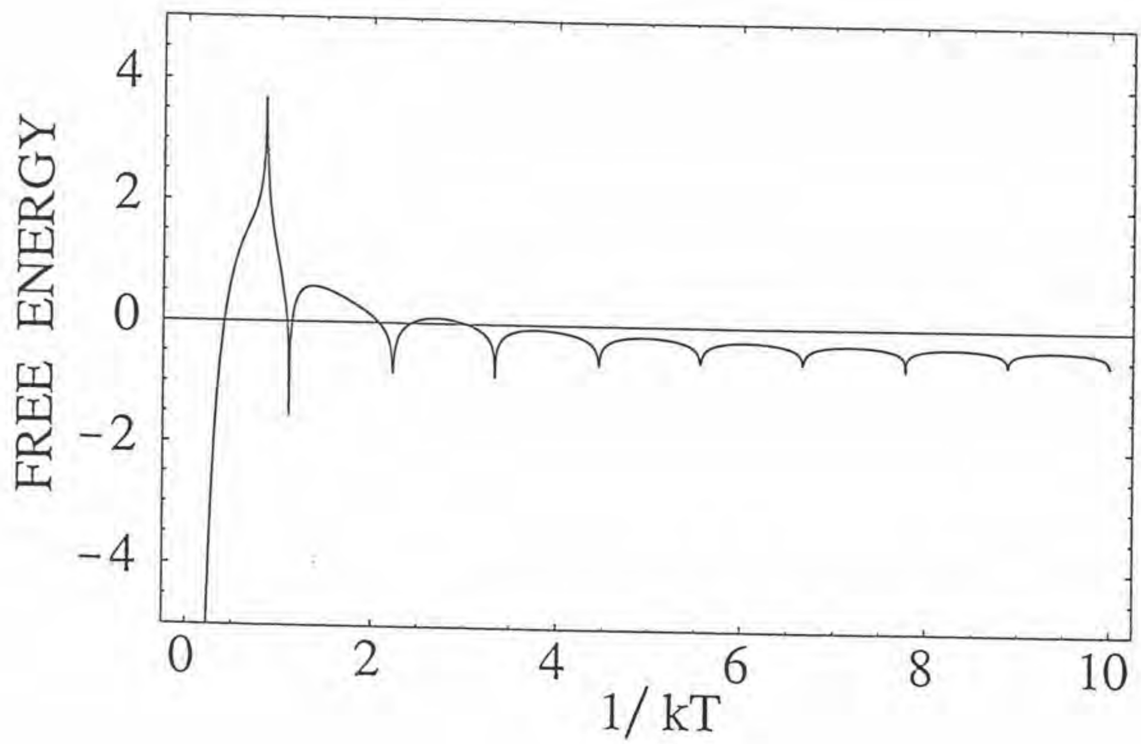

Figure 5.4: The free energy of the particle with SPP in the magnetic field when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3$, and $\omega = 2$

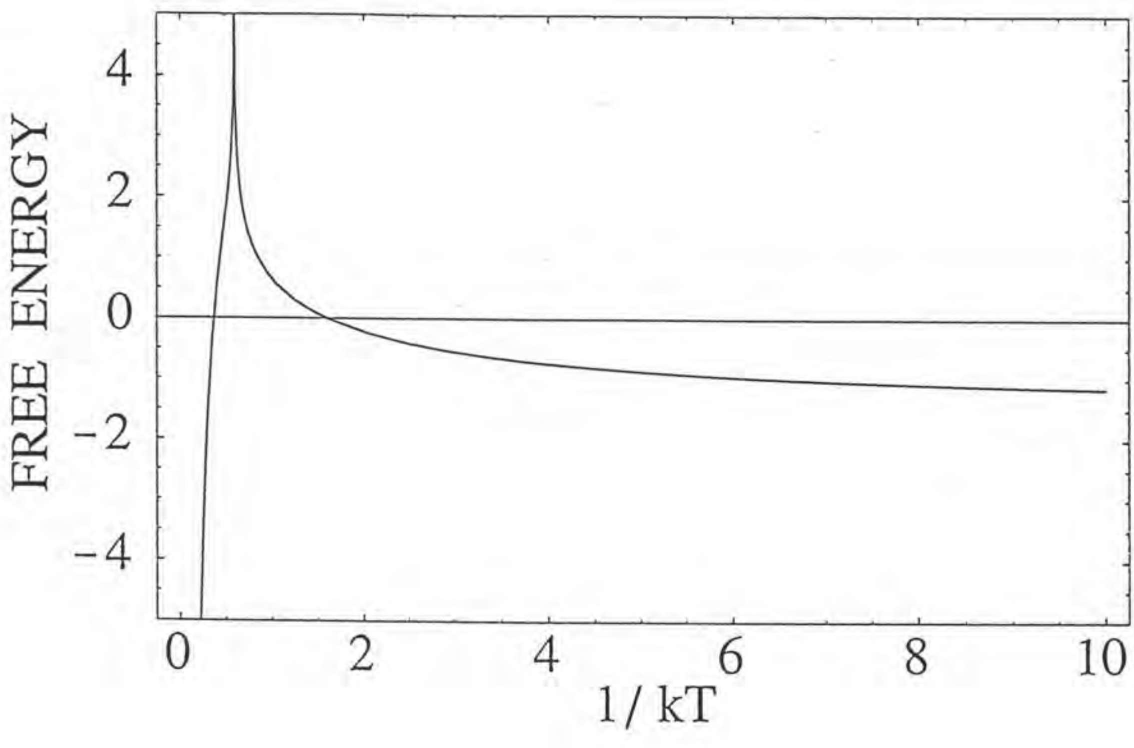

Figure 5.5: The free energy of the particle with SPP in the magnetic field when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3$, and $\omega = 6$

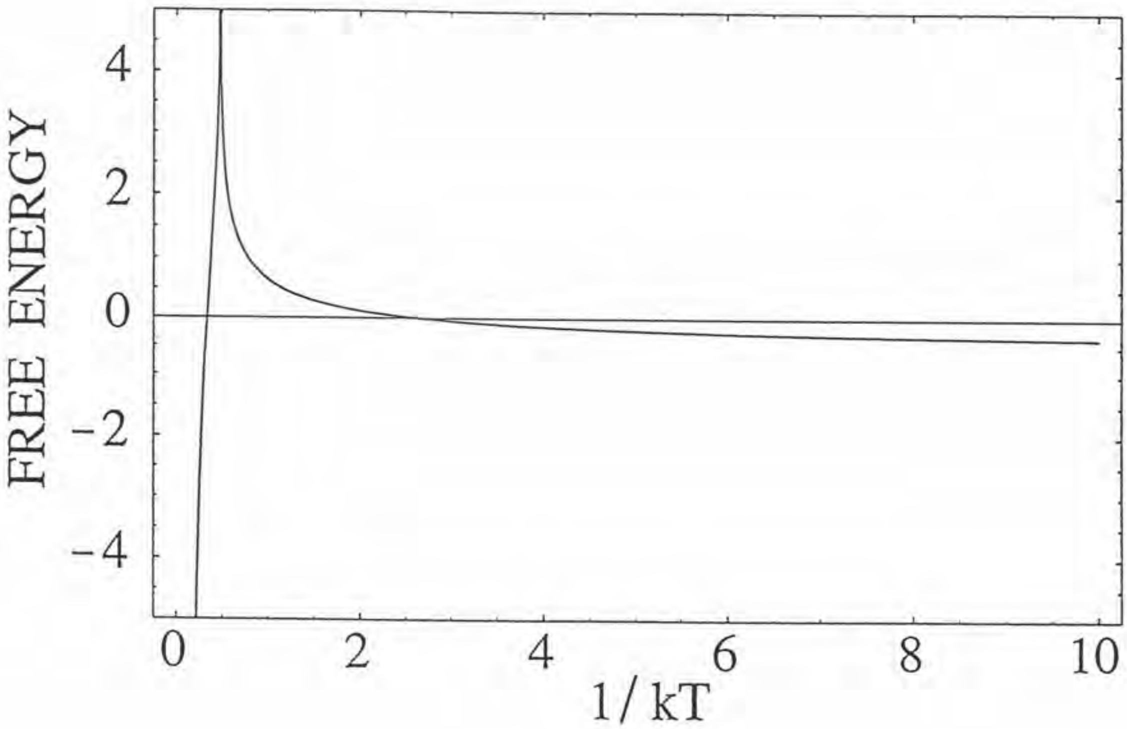

Figure 5.6: The free energy of the particle with SPP in the magnetic field when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3$, and $\omega = 10$

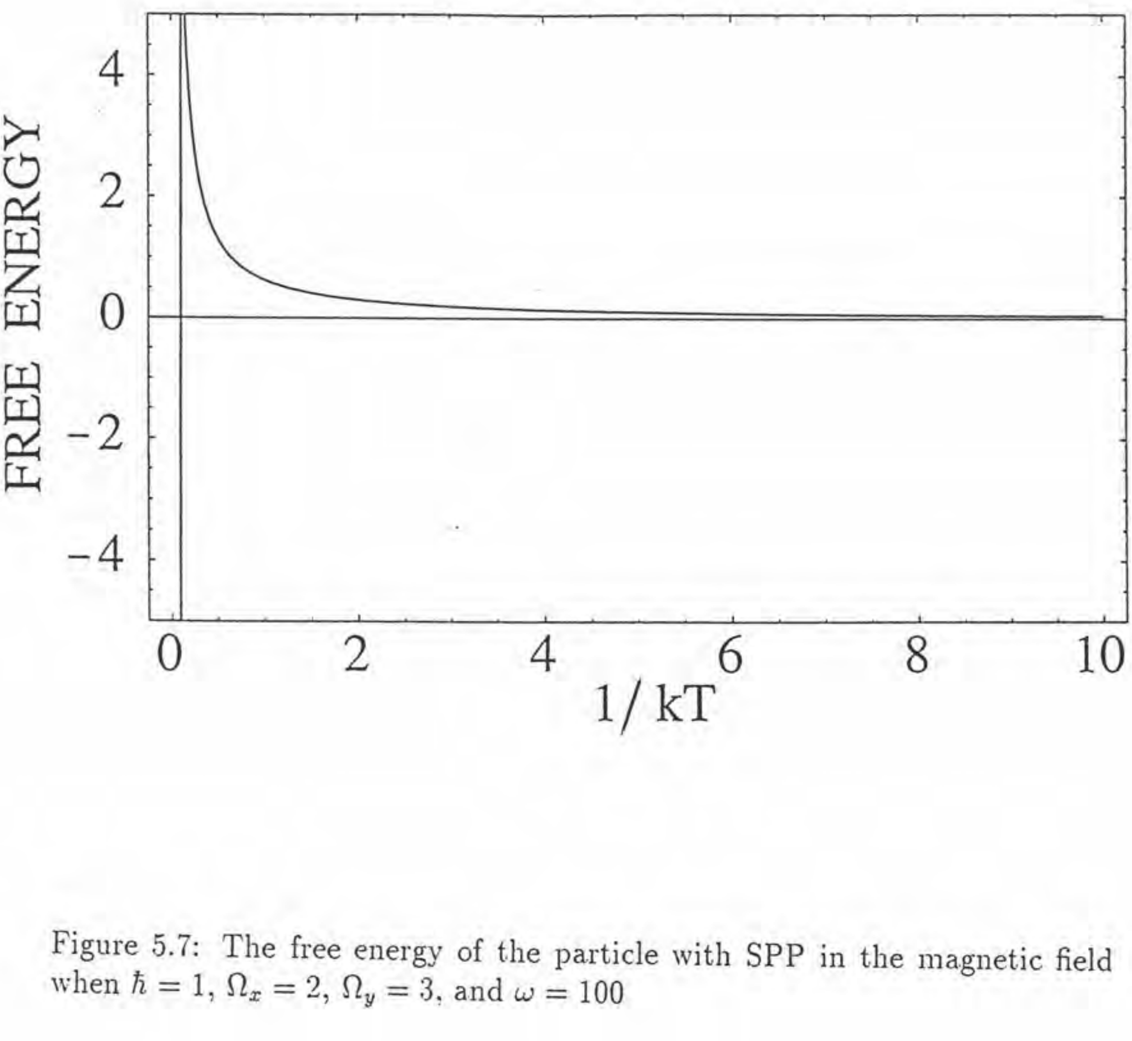

Figure 5.7: The free energy of the particle with SPP in the magnetic field when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3$, and $\omega = 100$

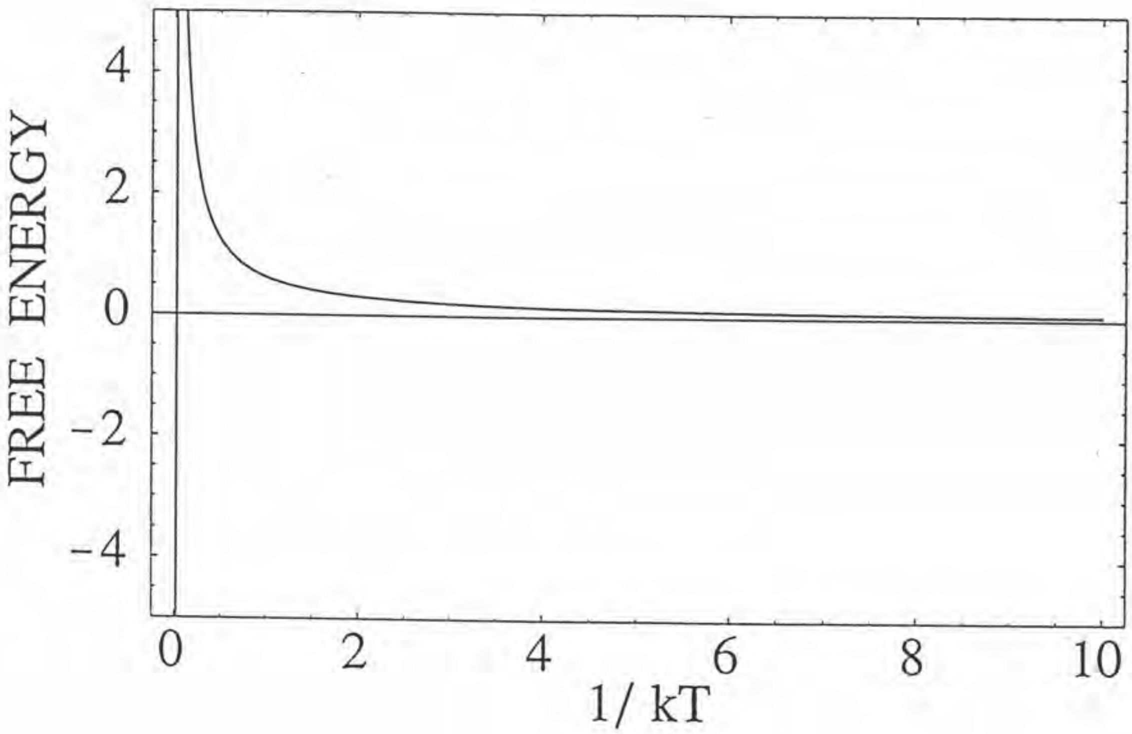

Figure 5.8: The free energy of the particle with SPP in the magnetic field when $\hbar = 1$, $\Omega_x = 2$, $\Omega_y = 3$, and $\omega = 1000$