CHAPTER 4

A Particle with Saddle Point Potential

In this Chapter, we consider a particle with Saddle Point Potential (SPP). This problem is related to a particle with Harmonic Potential (HP) by the complex frequency. Then the kernel of the particle with SPP relate it to the thermodynamic quantities of this system will be discussed.

4.1 The Lagrangian

We consider an electron in a two-dimensional system moving along two barriers described by SPP,

$$V(x,y) = \frac{m}{2}[\Omega_x^2 x^2 - \Omega_y^2 y^2]. \tag{4.1}$$

From Eq. (4.1), we can see that it consists of the HP and inverse HP with each frequency Ω_x and Ω_y. We consider this forms in two cases. In the first, if Ω_y is an imaginary frequency, it is still HP. In the second, Ω_y is a real frequency. It makes the system into a SPP. We show HP and SPP in Fig. (4.1) and Fig. (4.2), respectively. Now, We intend to consider the Lagrangian of a particle with SPP as

$$L = \frac{m}{2}(\dot{x}^2 + \dot{y}^2) - \frac{m}{2}(\Omega_x^2 x^2 - \Omega_y^2 y^2). \quad (4.2)$$

4.2 Kernel of The Particle with SPP

Considering Eq. (4.2), we can separate the x and y variables independently

$$L(x, \dot{x}, y, \dot{y}; t) = L_x(x, \dot{x}; t) + L_y(y, \dot{y}; t). \quad (4.3)$$

Using concepts in Eq. (3.16) we consider Eq. (4.3) . Now, we consider only x variable terms and then later consider y terms. We find the kernel from L_x as

$$L_x(x, \dot{x}; t) = \frac{m}{2}(\dot{x}^2 - \Omega_x^2 x^2). \quad (4.4)$$

From Eq. (4.4), we use variational method to obtain the equation of motion of the x trajectory

$$\ddot{x} + \Omega_x^2 x = 0. \quad (4.5)$$

Then, we use differential equation methods to find a trajectory of x path as

$$x(t) = \frac{1}{\sin \Omega_x \tau}[x_b \sin \Omega_x t + x_a \sin \Omega_x(\tau - t)]. \quad (4.6)$$

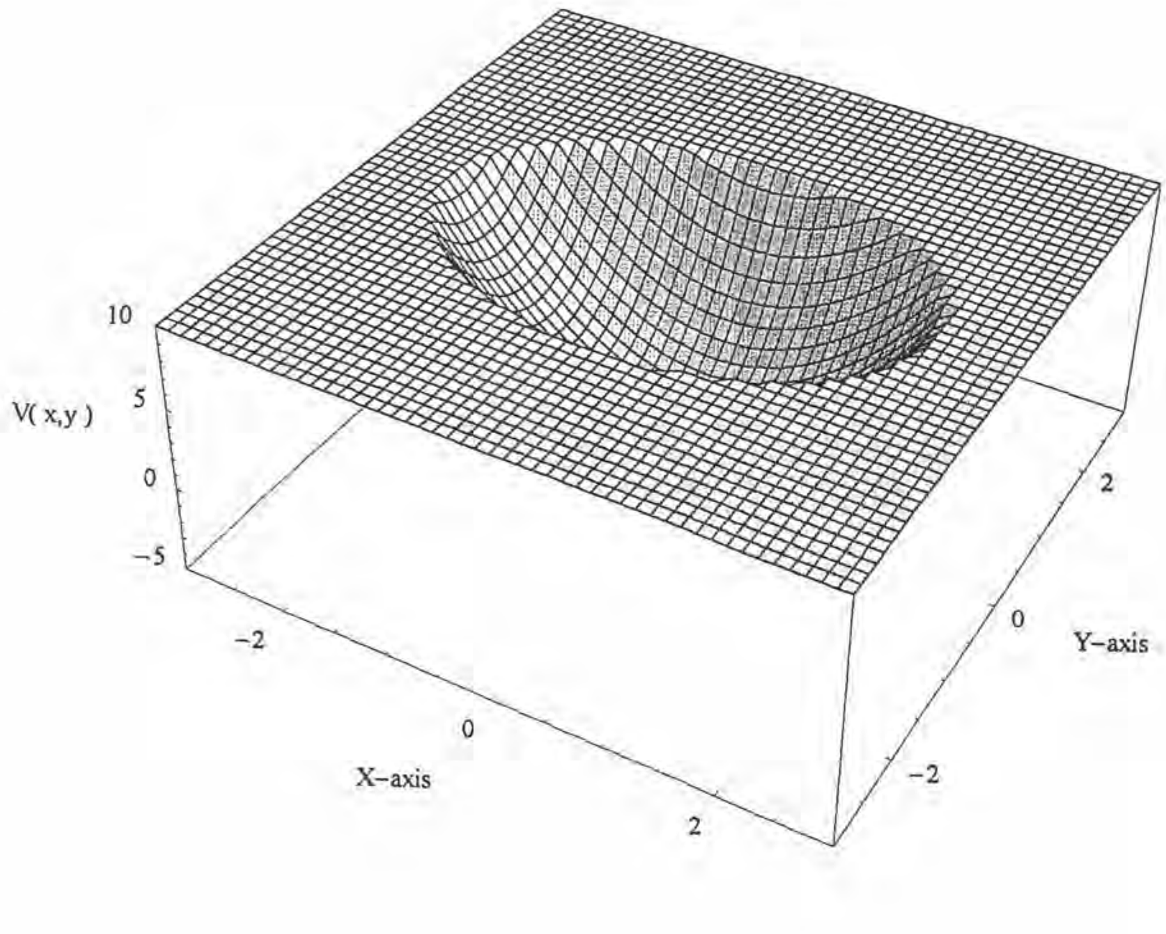

Figure 4.1: The HP when $m = 1, \Omega_x = 2$ and $\Omega_y = 3i$

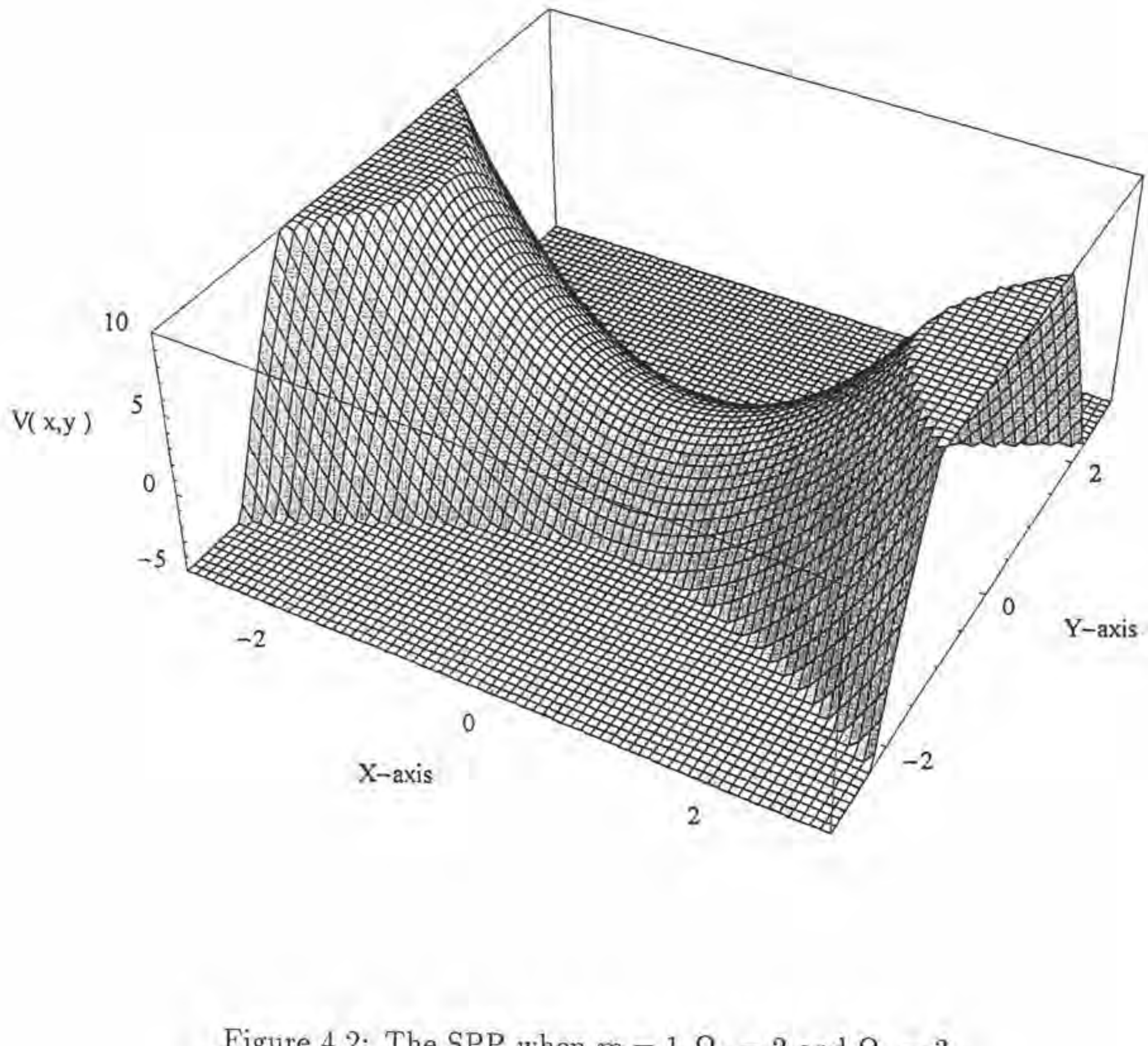

Figure 4.2: The SPP when $m = 1, \Omega_x = 2$ and $\Omega_y = 3$

Now, we find a classical action of x, S^x_{cl} as

$$\begin{aligned} S^x_{cl} &= \int_0^\tau L_x(x,\dot{x};t)dt \\ &= \frac{m}{2}\int_0^\tau(\dot{x}^2-\Omega_x^2x^2)dt \\ &= \frac{m}{2}\int_0^\tau(\dot{x}^2+\ddot{x}x)dt \\ &= \frac{m}{2}\dot{x}x|_0^\tau \\ &= \frac{m}{2}[x_b\dot{x}(\tau)-x_a\dot{x}(0)]. \end{aligned} \quad (4.7)$$

Using Eq. (4.6) we get S^x_{cl} as

$$S^x_{cl} = \frac{m}{2}\frac{\Omega_x}{\sin\Omega_x\tau}[(x_b^2+x_a^2)\cos\Omega_x\tau - 2x_bx_a] \quad (4.8)$$

and the prefactor can be found from formula of Eq. (3.12). We have

$$F_x(\tau) = [\frac{m}{2\pi i\hbar}\frac{\Omega_x}{\sin\Omega_x\tau}]^{1/2}. \quad (4.9)$$

Then, we have a kernel, $K_x(x_b,x_a;\tau)$, for a trajectory of x as

$$\begin{aligned} K_x(x_b,x_a;\tau) = [\frac{m}{2\pi i\hbar}\frac{\Omega_x}{\sin\Omega_x\tau}]^{1/2} \\ \times\exp\{\frac{i}{\hbar}\frac{m}{2}\frac{\Omega_x}{\sin\Omega_x\tau}[(x_b^2+x_a^2)\cos\Omega_x\tau - 2x_bx_a]\}. \end{aligned} \quad (4.10)$$

For y-direction, we also find a trajectory of y path $y(t)$, the classical action S^y_{cl}, the prefactor $F_y(\tau)$ and the kernel $K_y(y_b,y_a;\tau)$. It is similar but only different in trigonometric terms which are in hyperbolic forms. We have a prefactor $F_y(\tau)$ as

$$F_y(\tau) = [\frac{m}{2\pi i\hbar}\frac{\Omega_y}{\sin\Omega_y\tau}]^{1/2}. \quad (4.11)$$

and have a kernel, $K_y(y_b, y_a; \tau)$, for trajectory of y as

$$K_y(y_b, y_a; \tau) = [\frac{m}{2\pi i\hbar}\frac{\Omega_y}{\sinh\Omega_y\tau}]^{1/2}$$
$$\times\exp\{\frac{i}{\hbar}\frac{m}{2}\frac{\Omega_y}{\sinh\Omega_y\tau}[(y_b^2+y_a^2)\cosh\Omega_y\tau - 2y_by_a]\}. \tag{4.12}$$

Then, we obtain the total kernel for the particle with SPP as

$$K(\mathbf{r_b}, \mathbf{r_a}; \tau) = K_x(x_b, x_a; \tau)K_y(y_b, y_a; \tau). \tag{4.13}$$

4.3 The Partition Function and Free Energy of a particle with SPP

We change the result in the form of a density matrix and relate it to the partition function by $Z = Tr[\rho] \equiv Tr[K]$. When we can find the partition function, we can find the free energy. Now we can show the density matrix from the kernel Eq. (4.13), that is

$$\rho(\mathbf{r_b}, \mathbf{r_a}; \beta) \equiv K(\mathbf{r_b}, \mathbf{r_a}; -i\hbar\beta) \tag{4.14}$$

where $\tau = -i\hbar\beta$. To find the partition function, we consider a trace of Eq. (4.14). Then, we have

$$\begin{aligned} Z &\equiv Tr\ \rho(\mathbf{r_b}, \mathbf{r_a}, \tau) \\ &= F_x(\tau)F_y(\tau)\ Tr\ e^{(i/\hbar)[S_{cl}^x + S_{cl}^y]} \end{aligned} \tag{4.15}$$

where $F_x(\tau)$ and $F_y(\tau)$ are prefactors previously defined in Eqs. (4.9) and (4.11).

Now we just consider only a trace term that can separate into two similar integrals

$$\begin{aligned} Tr\ e^{(i/\hbar)[S^x_{cl}+S^y_{cl}]} &= \int_{-\infty}^{\infty} dx_a\ \exp\{\frac{i}{\hbar}\frac{m}{2}\frac{\Omega_x}{\sin\Omega_x\tau}2[\cos\Omega_x\tau-1]x_a^2\} \\ &\times \int_{-\infty}^{\infty} dy_a\ \exp\{\frac{i}{\hbar}\frac{m}{2}\frac{\Omega_y}{\sinh\Omega_y\tau}2[\cosh\Omega_y\tau-1]y_a^2\}. \quad (4.16) \end{aligned}$$

We use a Gaussian integration to evaluate each integral as

$$\begin{aligned} \int_{-\infty}^{\infty} dx_a\ \exp\{\frac{i}{\hbar}\frac{m\Omega_x}{\sinh\Omega_x\tau}[\cosh\Omega_x\tau-1]x_a^2\} &= (\frac{\pi i\hbar\sinh\Omega_x\tau}{m\Omega_x[\cosh\Omega_x\tau-1]})^{1/2}, \\ \int_{-\infty}^{\infty} dy_a\ \exp\{\frac{i}{\hbar}\frac{m\Omega_y}{\sinh\Omega_y\tau}[\cosh\Omega_y\tau-1]y_a^2\} &= (\frac{\pi i\hbar\sinh\Omega_y\tau}{m\Omega_y[\cosh\Omega_y\tau-1]})^{1/2}. \quad (4.17) \end{aligned}$$

Thus, the total result becomes

$$\begin{aligned} Z &\equiv (\frac{m}{2\pi i\hbar})(\frac{\Omega_x}{\sin\Omega_x\tau})^{1/2}(\frac{\Omega_y}{\sinh\Omega_y\tau})^{1/2} \\ &\times (\frac{\pi i\hbar}{m})(\frac{\sin\Omega_x\tau}{\Omega_x[\cos\Omega_x\tau-1]})^{1/2}(\frac{\sinh\Omega_y\tau}{\Omega_y[\cosh\Omega_y\tau-1]})^{1/2} \\ &= \frac{1}{2}[\frac{1}{\cos\Omega_x\tau-1}]^{1/2}[\frac{1}{\cosh\Omega_y\tau-1}]^{1/2}. \quad (4.18) \end{aligned}$$

From this partition function, we change $\tau = t_b - t_a$ to $-i\beta\hbar$ for the thermodynamic form. Then, we have

$$\begin{aligned} Z &= \frac{1}{2}[\cosh(\beta\hbar\Omega_x)-1]^{-1/2}[\cos(\beta\hbar\Omega_y)-1]^{-1/2} \\ &= \frac{1}{2}[2\sinh^2(\beta\hbar\frac{\Omega_x}{2})]^{-1/2}[-2\sin^2(\beta\hbar\frac{\Omega_y}{2})]^{-1/2} \\ &= \frac{1}{4}\frac{1}{\sinh(\beta\hbar\Omega_x/2)}\frac{1}{\sinh(i\beta\hbar\Omega_y/2)}. \quad (4.19) \end{aligned}$$

Eq. (4.19) shows the partition function of the saddle point terms in closed form. Now we can find F from Eq. (2.4) $F = -\beta^{-1}\ln Z$. We obtain

$$
\begin{aligned}
F &= \beta^{-1}\ln\left[4\sinh\left(\beta\hbar\Omega_x/2\right)\sinh\left(i\beta\hbar\Omega_y/2\right)\right] \\
&= \frac{\hbar}{2}(\Omega_x + i\Omega_y) + \beta^{-1}\ln\left[1 - e^{-\beta\hbar\Omega_x}\right] + \beta^{-1}\ln\left[1 - e^{-i\beta\hbar\Omega_y}\right]. \qquad (4.20)
\end{aligned}
$$

We can plot F against $1/kT$. The particles with HP and with SPP have been shown in Figs. (4.3) and (4.4), respectively.

4.4 Calculated Results

In this section we calculate the free energy of the particle with SPP. In order to give a comparision with the particle with HP, we present the case of the particle with HP which can be obtained from the case of the particle with SPP by setting Ω_y in complex frequency. This will bring the system to the particle with HP in two dimensions. The result is shown in Fig. (4.3) . For the case of the particle with SPP, the result is given in Fig. (4.4). As can be seen the free energy shows discontinuous behaviors. This is due to the decay of the particle in the y-direction. In the particle with HP case, the particle is completely bounded in the harmonic well. For the particle with SPP, the particle can be moved out of the potential in the y-direction. In the next section when we apply the magnetic field to the system, the particle again is bounded to the harmonic potential for strong magnetic field.

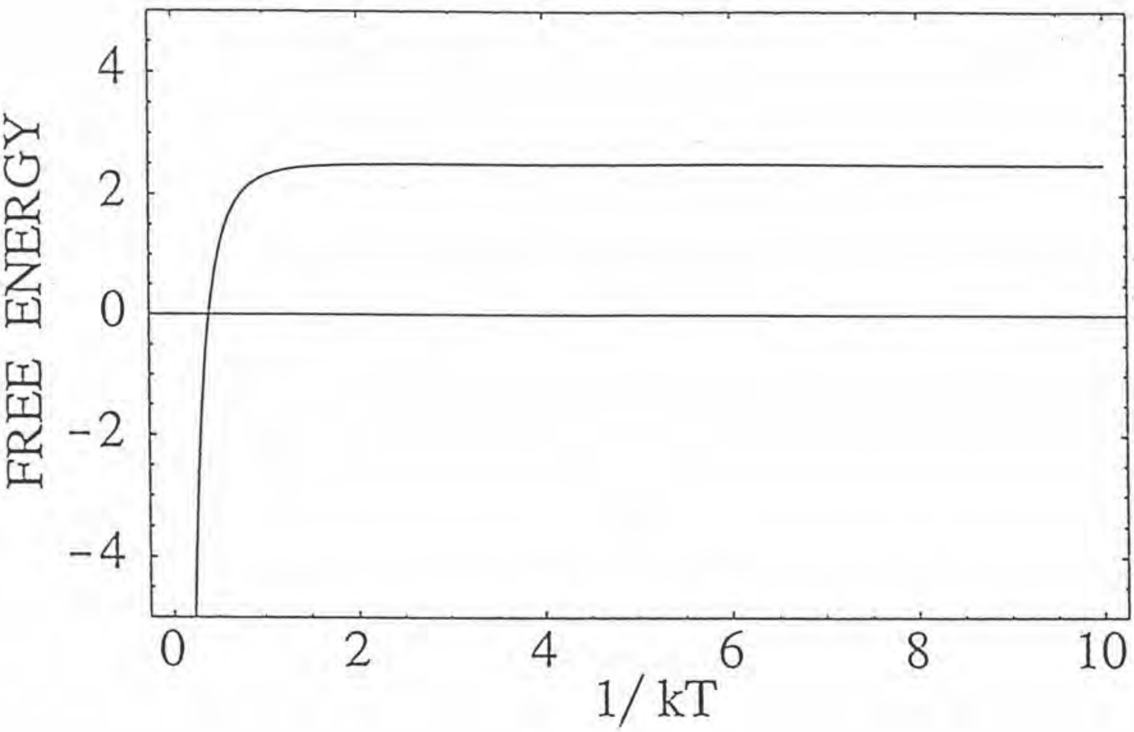

Figure 4.3: The free energy of the particle with HP when $\hbar = 1$, $\Omega_x = 2$ and $\Omega_y = 3i$

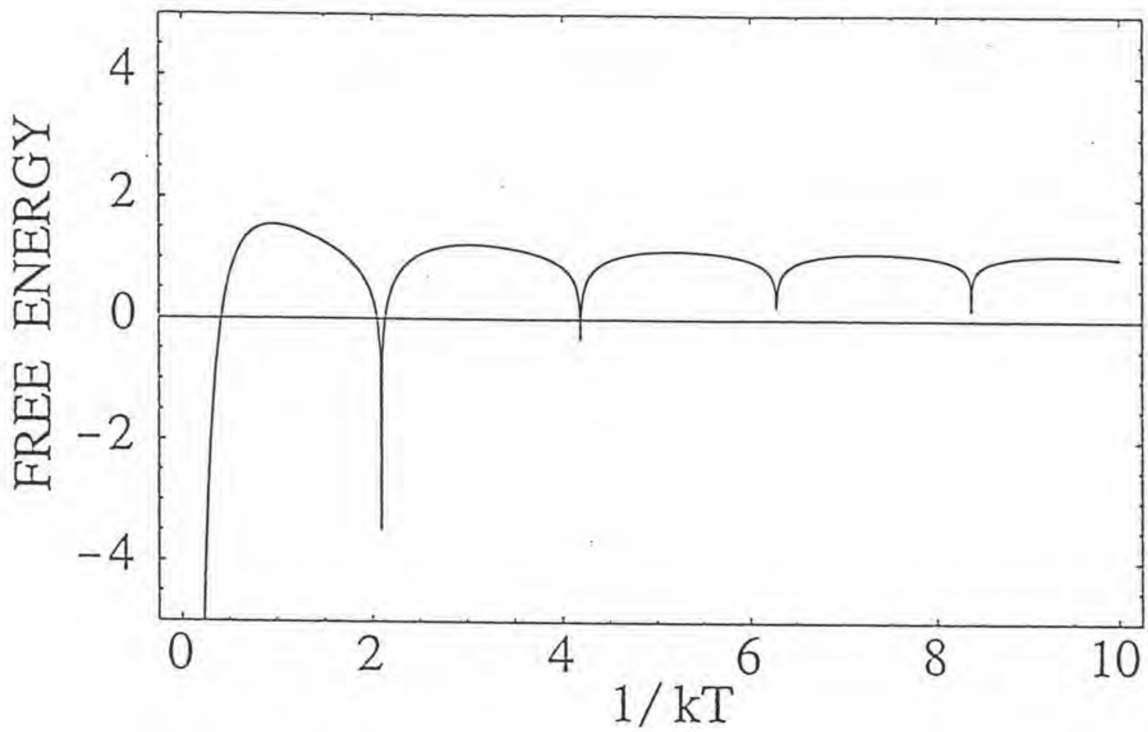

Figure 4.4: The free energy of the particle with SPP when $\hbar = 1$, $\Omega_x = 2$ and $\Omega_y = 3$