Chapter 4

The Approximate Density of States

In this chapter, the approximated density of states can be calculated by following the same procedure in Eq. (3.36). Firstly, we apply the Feynman path integral method [8] to the approximate propagator. We also calculate the preexponential factor $A(E)$ and the exponent of density of states $B(E)$. Furthermore, we determine the logarithmic derivative $n(v, z)$, which represents the characteristic of tails. Finally, tabulated results and graphs will be presented.

4.1 The Approximate Propagator

We use the variational method developed by Feynman [7] for the polaron problem and applied by Samathiyakanit [25] and Sa-yakanit [26] to calculate the density of states of a system with a screened Coulomb potential. Our trial action $S_0(\omega)$, Eq. (3.43), has the form appropriate for a nonlocal harmonic oscillator

[25,40], i.e.

$$S_0(\omega) = \int_0^t d\tau \frac{m}{2}\left[\dot{\vec{x}}^2(\tau) - \frac{1}{2t}\omega^2 \int_0^t d\sigma \left|\vec{x}(\tau) - \vec{x}(\sigma)\right|^2\right], \tag{4.1}$$

where ω is an unknown parameter to be determined. From Eq. (3.15), we can write the average propagator as

$$K(\vec{x}_2, \vec{x}_1; t) = \int D[\vec{x}(\tau)] \exp\left[\frac{i}{\hbar}(S - S_0(\omega)) + \frac{i}{\hbar}S_0(\omega)\right]. \tag{4.2}$$

Once the trial action $S_0(\omega)$ is introduced, we may find the average propagator [8,25] which, from Eq.(4.2), can be rewritten as

$$K(\vec{x}_2, \vec{x}_1; t) = K_0(\vec{x}_2, \vec{x}_1; t, \omega) \left\langle \exp[i(S - S_0(\omega))/\hbar]\right\rangle_{S_0(\omega)}, \tag{4.3}$$

where the nonlocal harmonic oscillator propagator $K_0(\vec{x}_2, \vec{x}_1; t, \omega)$ or the trial propagator can be defined as

$$K_0(\vec{x}_2, \vec{x}_1; t, \omega) = \int D[\vec{x}(\tau)] \exp\left(\frac{i}{\hbar}S_0(\omega)\right), \tag{4.4}$$

the symbol $\langle ... \rangle_{S_0(\omega)}$ means averaging with respect to the trial action $S_0(\omega)$:

$$\langle O \rangle_{S_0(\omega)} = \frac{\int D[\vec{x}(\tau)] \exp[iS_0(\omega)/\hbar] O}{\int D[\vec{x}(\tau)] \exp[iS_0(\omega)/\hbar]}. \tag{4.5}$$

The average propagator in Eq. (4.3) is an exact expression but cannot be evaluated. The cumulant expansion,

$$\langle \exp[a] \rangle = \exp\left\{ \langle a \rangle + \frac{1}{2!}[\langle a^2 \rangle - \langle a \rangle^2] - \frac{1}{3!}[\langle a^3 \rangle - 3\langle a^2 \rangle \langle a \rangle + 2\langle a \rangle^3] + ... \right\}, \tag{4.6}$$

to the first cumulant [21] allows us to obtain the approximate propagator,

$$K_1(\vec{x}_2, \vec{x}_1; t, \omega) = K_0(\vec{x}_2, \vec{x}_1; t, \omega) \exp\left[\frac{i}{\hbar} \langle S - S_0(\omega)\rangle_{S_0(\omega)}\right], \tag{4.7}$$

where the subscript 1 denotes the first order approximation. The translational invariant property is important to get the correct behavior of the prefactor which will yield density of states agreed satisfactorily with that obtained by Halperin and Lax [12]. By rewriting Eq. (4.7), we obtain

$$K_1(0, 0; t) = K_0(0, 0; t) \exp\left[\frac{i}{\hbar} \langle S - S_0(\omega)\rangle_{S_0(\omega)}\right]. \tag{4.8}$$

From Section 3.5, the diagonal part of the zeroth order propagator $K_0(0, 0; t,)$ can be calculated exactly,

$$K_0(0, 0; t) = \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} \left(\frac{\omega t}{2\sin\frac{1}{2}\omega t}\right)^3. \tag{4.9}$$

To obtain $K_1(0, 0; t)$ we have to find the average $\langle S - S_0(\omega)\rangle_{S_0(\omega)}$. Since the kinetic terms in S and $S_0(\omega)$ always cancel each other, we shall denote $\langle S\rangle_{S_0(\omega)}$ and $\langle S_0(\omega)\rangle_{S_0(\omega)}$ for convenience as the averages of the second terms respectively. The average $\langle S\rangle_{S_0(\omega)}$ can be evaluated by applying a Fourier transform of $W(\vec{x}(\tau) - \vec{x}(\sigma))$. We thus write Eq. (3.25) as

$$W(\vec{x}(\tau) - \vec{x}(\sigma)) = \int \frac{d^3q}{(2\pi)^3} W(\vec{q}) \exp\{i\vec{q}\cdot(\vec{x}(\tau) - \vec{x}(\sigma))\}, \tag{4.10}$$

where $W(\vec{q})$ denotes the Fourier transform of $W(\vec{x}(\tau) - \vec{x}(\sigma))$. For the screened Coulomb potential, $W(\vec{q})$ can be written as

$$W(\vec{q}) = \frac{2\pi\gamma^2(1 + r_e^{-2}/q^2)}{q^2\left(q^2 + r_e^{-2} + r_0^{-2}\right) r_0}. \tag{4.11}$$

Thus we can write Eq. (3.16) as

$$\langle S \rangle_{S_0(\omega)} = \frac{i}{2\hbar} \int_0^t \int_0^t d\tau d\sigma \int \frac{d^3q}{(2\pi)^3} W(\vec{q}) \langle \exp[i\vec{q} \cdot (\vec{x}(\tau) - \vec{x}(\sigma))] \rangle_{S_0(\omega)}. \tag{4.12}$$

The average of the right-hand side of Eq. (4.12) can be expanded in terms of cumulants. Since S_0 is quadratic, one can easily keep only the second order cumulant approximation [25]. Therefore, Eq. (4.12) becomes

$$\langle S \rangle_{S_0(\omega)} = \frac{i}{2\hbar} \int_0^t \int_0^t d\tau d\sigma \int \frac{d^3q}{(2\pi)^3} W(\vec{q}) \exp(\kappa_1 + \kappa_2), \tag{4.13}$$

where

$$\kappa_1 = i\vec{q} \cdot \langle (\vec{x}(\tau) - \vec{x}(\sigma)) \rangle_{S_0(\omega)}, \tag{4.14}$$

and

$$\kappa_2 = -\frac{1}{2}\vec{q}^2 \left[\frac{1}{3} \left\langle (\vec{x}(\tau) - \vec{x}(\sigma))^2 \right\rangle_{S_0(\omega)} - \langle x(\tau) - x(\sigma) \rangle^2_{S_0(\omega)} \right]. \tag{4.15}$$

Then Eq.(4.13) can be rewritten as

$$\langle S \rangle_{S_0(\omega)} = \frac{i}{2\hbar} \int_0^t \int_0^t d\tau d\sigma \int \frac{d^3q}{(2\pi)^3} W(\vec{q}) \exp\left[i\vec{q} \cdot \vec{A} - q^2 B \right], \tag{4.16}$$

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where

$$\vec{A} = \langle \vec{x}\,(\tau) - \vec{x}\,(\sigma) \rangle_{S_0(\omega)}\,, \tag{4.17}$$

and

$$B = \frac{1}{2}\left[\frac{1}{3}\left\langle (\vec{x}\,(\tau) - \vec{x}\,(\sigma))^2 \right\rangle_{S_0(\omega)} - \langle x\,(\tau) - x\,(\sigma) \rangle^2_{S_0(\omega)}\right]. \tag{4.18}$$

Now, consider the average of the trial action in Eq. (4.1),

$$\langle S_0\,(\omega) \rangle_{S_0(\omega)} = -\frac{m\omega^2}{4t}\int\limits_0^t\int\limits_0^t d\tau d\sigma \left\langle (\vec{x}\,(\tau) - \vec{x}\,(\sigma))^2 \right\rangle_{S_0(\omega)}. \tag{4.19}$$

We can calculate the approximate propagator by substituting Eqs. (4.16) and (4.19) into Eq. (4.8). We will present this calculation in the next section.

4.2 Calculations of $\vec{A}$, B and $\left\langle (\vec{x}\,(\tau) - \vec{x}\,(\sigma))^2 \right\rangle_{S_0(\omega)}$

We are interested in the average $\langle S - S_0\,(\omega) \rangle_{S_0(\omega)}$. From Eqs. (4.16) and (4.19) we can express the quantity $\langle S - S_0\,(\omega) \rangle_{S_0(\omega)}$ in terms of the averages $\langle \vec{x}\,(\tau) \rangle_{S_0(\omega)}$, $\langle \vec{x}\,(\tau) \cdot \vec{x}\,(\sigma) \rangle_{S_0(\omega)}$ and $\langle (\vec{x}\,(\tau) - \vec{x}\,(\sigma))^2 \rangle_{S_0(\omega)}$. The transition element of the functional [8] can be written as

$$\left\langle \exp\left[\frac{i}{\hbar}\int \vec{f}(\tau)\cdot\vec{x}\,(\tau)\,d\tau\right]\right\rangle_{s_0(\omega)} = \int\limits_a^b \exp\left[\frac{i}{\hbar}\left(S_0\,(\omega) + \int \vec{f}(\tau)\cdot\vec{x}\,(\tau)\,d\tau\right)\right] D[\vec{x}\,(\tau)], \tag{4.20}$$

where $\vec{f}\,(\tau)$ is any arbitrary function of time. If the original action S is Gaussian, the action $S^f_{0,cl}$ will be equal to $S_0\,(\omega) + \int\limits_0^t \vec{f}(\tau)\cdot\vec{x}\,(\tau)\,d\tau$. This means that the path integral on the right-hand side of Eq. (4.20) can be reduced to an exponential function multiplied by the transition element. The result is

$$\left\langle \exp\left[\frac{i}{\hbar}\int \vec{f}(\tau)\cdot\vec{x}(\tau)\,d\tau\right]\right\rangle_{s_0(\omega)} = \left\{\exp\left[\frac{i}{\hbar}\left(S^f_{0,cl} - S_{0,cl}\right)\right]\right\}. \tag{4.21}$$

Functional derivative [8] of Eq. (4.21) with respect to $\vec{f}(\tau)$ gives

$$\left\langle \vec{x}(\tau)\exp\left[\frac{i}{\hbar}\int \vec{f}(\tau)\cdot\vec{x}(\tau)\,d\tau\right]\right\rangle_{s_0(\omega)} = \frac{\delta S^f_{0,cl}}{\delta\vec{f}(\tau)}\left\{\exp\left[\frac{i}{\hbar}\left(S^f_{0,cl} - S_{0,cl}\right)\right]\right\}. \tag{4.22}$$

Therefore, evaluating both sides by using $\vec{f}(\tau) = 0$ [8], we obtain

$$\langle\vec{x}(\tau)\rangle_{s_0(\omega)} = \left.\frac{\delta S^f_{0,cl}}{\delta\vec{f}(\tau)}\right|_{\vec{f}(\tau)=0}. \tag{4.23}$$

We can continue this process to get the second derivative as

$$\langle\vec{x}(\tau)\cdot\vec{x}(\sigma)\rangle_{s_0(\omega)} = \left.\left[\frac{\hbar}{i}\frac{\delta^2 S^f_{0,cl}}{\delta\vec{f}(\tau)\delta\vec{f}(\sigma)} + \frac{\delta S^f_{0,cl}}{\delta\vec{f}(\tau)}\frac{\delta S^f_{0,cl}}{\delta\vec{f}(\sigma)}\right]\right|_{\vec{f}(\tau)=0}. \tag{4.24}$$

First, we find a variation of $S^f_{0,cl}$ with respect to $\vec{f}(\tau)$, we have

$$\begin{aligned}
\frac{\delta S^f_{0,cl}}{\delta\vec{f}(\tau)} &= \frac{1}{\sin\omega\tau}\Big[\vec{x}_2(\sin\omega\tau - 2\sin\frac{1}{2}\omega t\sin\frac{1}{2}\omega\tau\sin\frac{1}{2}\omega\tau\,(t-\tau)) \\
&\quad +\vec{x}_1(\sin\omega\,(t-\tau) - 2\sin\frac{1}{2}\omega t\sin\frac{1}{2}\omega\tau\sin\frac{1}{2}\omega\,(t-\tau))\Big] \\
&\quad -\frac{1}{m\omega\sin\omega t}\left[\int_0^\tau d\sigma\vec{f}(\sigma)\sin\omega\,(t-\tau)\sin\omega\sigma + \int_\tau^t \vec{f}(\sigma)\sin\omega\,(t-\sigma)\sin\omega\tau\right] \\
&\quad +\frac{4}{m\omega\sin\omega\tau}\Big[\int_0^t d\sigma\vec{f}(\sigma)\sin\frac{1}{2}\omega\,(t-\sigma)\sin\frac{1}{2}\omega\tau \\
&\quad \times\sin\frac{1}{2}\omega\,(t-\sigma)\sin\frac{1}{2}\omega\sigma\Big].
\end{aligned} \tag{4.25}$$

Finally substituting Eq. (4.25) into Eq. (4.23), we get for $\vec{f}(\tau)=0$

$$\begin{aligned}\langle\vec{x}(\tau)\rangle_{S_0(\omega)} &= \frac{1}{\sin\omega t}[\vec{x}_2(\sin\omega\tau - 2\sin\frac{1}{2}\omega t\sin\frac{1}{2}\omega\tau\sin\frac{1}{2}\omega\tau(t-\tau) \\ &+\vec{x}_1(\sin\omega(t-\tau) - 2\sin\frac{1}{2}\omega t\sin\frac{1}{2}\omega\tau\sin\frac{1}{2}\omega(t-\tau))]. \quad (4.26)\end{aligned}$$

Now, evaluating $\dfrac{\delta^2 S^f_{0,cl}}{\delta\vec{f}(\tau)\delta\vec{f}(\sigma)}$ by making a variation of $\dfrac{\delta S^f_{0,cl}}{\delta\vec{f}(\tau)}$ with respect to $\vec{f}(\sigma)$, we have

$$\begin{aligned}\frac{\delta^2 S^f_{0,cl}}{\delta\vec{f}(\tau)\delta\vec{f}(\sigma)} &= -\frac{1}{m\omega\sin\omega t}\Big[\sin\omega(t-\tau)\sin\omega\sigma H(\tau-\sigma) \\ &+\sin\omega(\tau-\sigma)\sin\omega\tau H(\sigma-\tau)] \\ &+\frac{4}{m\omega\sin\omega t}[\sin\frac{1}{2}\omega(t-\tau)\sin\frac{1}{2}\omega\tau \\ &\times\sin\frac{1}{2}\omega(t-\sigma)\sin\frac{1}{2}\omega\sigma\Big]. \quad (4.27)\end{aligned}$$

From Eq. (4.24) and using Eqs. (4.25), and (4.27), we get

$$\begin{aligned}\langle\vec{x}(\tau)\cdot\vec{x}(\sigma)\rangle_{S_0(\omega)} &= \frac{3i\hbar}{m\omega\sin\omega t}\Big[\sin\omega(t-\tau)\sin\omega\sigma H(\tau-\sigma) \\ &+\sin\omega(\tau-\sigma)\sin\omega\tau H(\sigma-\tau)\Big] \\ &-\frac{12i\hbar}{m\omega\sin\omega t}\Big[\sin\frac{1}{2}\omega(t-\tau)\sin\frac{1}{2}\omega\tau\sin\frac{1}{2}\omega(t-\sigma)\sin\frac{1}{2}\omega\sigma\Big] \\ &+(\langle\vec{x}(\tau)\rangle_{S_0(\omega)}\cdot\langle\vec{x}(\sigma)\rangle_{S_0(\omega)}), \quad (4.28)\end{aligned}$$

where $H(t)$ is the Heaviside step function. Substituting the average of $\vec{x}$, Eq.

(4.26) , into Eq. (4.17) , we arrive

$$\begin{aligned}\vec{A} &= \langle \vec{x}\,(\tau)\rangle_{S_0(\omega)} - \langle \vec{x}\,(\sigma)\rangle_{S_0(\omega)} \\ &= \left[\frac{\sin\frac{1}{2}\omega\,(\tau-\sigma)\cos\frac{1}{2}\omega[t-(\tau+\sigma)]}{\sin\frac{1}{2}\omega t}\right](\vec{x}_2-\vec{x}_1).\end{aligned} \tag{4.29}$$

From Eq. (4.18), we can write B [25] as

$$B = \frac{1}{6}\left[\left\langle (\vec{x}\,(\tau)-\vec{x}\,(\sigma))^2\right\rangle_{S_0(\omega)} - \langle \vec{x}\,(\tau)-\vec{x}\,(\sigma)\rangle^2_{S_0(\omega)}\right]. \tag{4.30}$$

Note that, in Eq. (4.30), we have set

$$\langle (x\,(\tau)-x\,(\sigma))\rangle^2_{S_0(\omega)} = \frac{1}{3}\langle \vec{x}\,(\tau)-\vec{x}\,(\sigma)\rangle^2_{S_0(\omega)}. \tag{4.31}$$

Eq. (4.30) can be written as

$$\begin{aligned}B &= \frac{1}{6}\Big[\left\langle \vec{x}^2\,(\tau)\right\rangle_{S_0(\omega)} - 2\langle \vec{x}\,(\tau)\cdot\vec{x}\,(\sigma)\rangle_{S_0(\omega)} + \left\langle \vec{x}^2\,(\sigma)\right\rangle_{S_0(\omega)} - \langle \vec{x}\,(\tau)\rangle^2_{S_0(\omega)} \\ &\quad +2\langle \vec{x}\,(\tau)\rangle_{S_0(\omega)}\cdot\langle \vec{x}\,(\sigma)\rangle_{S_0(\omega)} - \langle \vec{x}\,(\sigma)\rangle^2_{S_0(\omega)}\Big].\end{aligned} \tag{4.32}$$

Another way to calculate B is to consider the average of $(\vec{x}\,(\tau)-\vec{x}\,(\sigma))^2$ in Eq. (4.30) which is equal to

$$\begin{aligned}\left\langle (\vec{x}\,(\tau)-\vec{x}\,(\sigma))^2\right\rangle_{S_0(\omega)} &= \frac{6i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right] \\ &\quad +\langle \vec{x}\,(\tau)-\vec{x}\,(\sigma)\rangle^2_{S_0(\omega)}.\end{aligned} \tag{4.33}$$

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The last term of the above equation is the square of Eq. (4.29). Putting Eq. (4.33) into Eq. (4.30), we can rewrite B as follows

$$B = \frac{i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right]. \tag{4.34}$$

It is worth to note that B has the following property

$$B\left(|\tau-\sigma|\right) = B(t-|\tau-\sigma|). \tag{4.35}$$

4.3 Evaluating the Approximate Density of States

The average of $\langle S - S_0(\omega)\rangle_{S_0(\omega)}$ has been considered in previous section and we know that

$$\langle S - S_0(\omega)\rangle_{S_0(\omega)} = \langle S\rangle_{S_0(\omega)} - \langle S_0(\omega)\rangle_{S_0(\omega)}. \tag{4.36}$$

We can use Eq. (4.16) to write the average action which is the first term of the right-hand side of Eq. (4.36) by using Eqs. (4.17), (4.18), (4.29), and (4.34)

$$\begin{aligned}\langle S\rangle_{S_0(\omega)} &= \frac{i}{2\hbar}\int_0^t\int_0^t d\tau d\sigma\int\frac{d^3q}{(2\pi)^3}W(\vec{q})\exp\Bigg\{i\vec{q} \\ &\times\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\cos\frac{1}{2}\omega[t-(\tau+\sigma)]}{\sin\frac{1}{2}\omega t}\right]\cdot(\vec{x}_2-\vec{x}_1) \\ &-q^2\frac{i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right]\Bigg\}.\end{aligned} \tag{4.37}$$

In the above equation, we can calculate the exponential term by setting $(\vec{x}_2-\vec{x}_1) = 0$ [25], so that

$$\exp\left\{i\vec{q}\left[\frac{\sin\frac{1}{2}\omega\left(\tau-\sigma\right)\cos\frac{1}{2}\omega[t-(\tau+\sigma)]}{\sin\frac{1}{2}\omega t}\right](\vec{x}_2-\vec{x}_1)-q^2\frac{i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right]\right\}$$
$$= \exp\left\{-q^2\frac{i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right]\right\}. \tag{4.38}$$

If we define

$$g\left(\tau,\sigma\right) = \frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}, \tag{4.39}$$

with the property similar to B in Eq. (4.35), we can then write the exponential term on the right-hand side of Eq. (4.38) as

$$\exp\left\{-q^2\frac{i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right]\right\} = \exp\left\{-q^2\frac{i\hbar}{m\omega}g\left(\tau,\sigma\right)\right\}. \tag{4.40}$$

Now, Eq. (4.37) becomes

$$\langle S\rangle_{S_0(\omega)} = \frac{i}{2\hbar}\int_0^t\int_0^t d\tau d\sigma\int\frac{d^3q}{\left(2\pi\right)^3}W\left(\vec{q}\right)\exp\left\{-q^2\frac{i\hbar}{m\omega}g\left(\tau,\sigma\right)\right\}. \tag{4.41}$$

Substituting Eq. (4.11) into Eq. (4.41) , we get

$$\begin{aligned}\langle S\rangle_{S_0(\omega)} &= \frac{i\pi\gamma^2}{\hbar r_0}\int_0^t\int_0^t d\tau d\sigma\int\frac{d^3q}{(2\pi)^3}\frac{(1+\frac{r_e^{-2}}{q^2})}{q^2\left(q^2+r_e^{-2}+r_0^{-2}\right)}\\ &\quad\times\exp\left\{-q^2\frac{i\hbar}{m\omega}g\left(\tau,\sigma\right)\right\}.\end{aligned} \tag{4.42}$$

Using the relation

$$\frac{1}{q^2\left(q^2+r_e^{-2}+r_0^{-2}\right)} = \frac{1}{\left(r_e^{-2}+r_0^{-2}\right)q^2} - \frac{1}{\left(r_e^{-2}+r_0^{-2}\right)\left[\left(r_e^{-2}+r_0^{-2}\right)+q^2\right]} \tag{4.43}$$

and

$$\frac{r_e^{-2}}{q^4\left(q^2+r_e^{-2}+r_0^{-2}\right)} = \frac{1}{\left(r_e^{-2}+r_0^{-2}\right)r_e^2q^4} - \frac{1}{\left(r_e^{-2}+r_0^{-2}\right)r_e^2}\left\{\frac{1}{\left(r_e^{-2}+r_0^{-2}\right)q^2} - \frac{1}{\left(r_e^{-2}+r_0^{-2}\right)\left[\left(r_e^{-2}+r_0^{-2}\right)+q^2\right]}\right\}. \tag{4.44}$$

Let $Q^2 = \left(r_e^{-2}+r_0^{-2}\right)$, where Q is an inverse screening length. Therefore the average action is

$$\begin{aligned}\langle S\rangle_{S_0(\omega)} &= \frac{i\pi\gamma^2}{\hbar r_0}\left(1-\frac{1}{r_e^2Q^2}\right)\int_0^t\int_0^t d\tau d\sigma\int\frac{d^3q}{(2\pi)^3}\left[\frac{1}{Q^2q^2}-\frac{1}{Q^2\left(Q^2+q^2\right)}\right] \\ &\times\exp\left\{-q^2\frac{i\hbar}{m\omega}g(\tau,\sigma)\right\} \\ &+\frac{i\pi\gamma^2}{\hbar r_0}\int_0^t\int_0^t d\tau d\sigma\int\frac{d^3q}{(2\pi)^3}\frac{1}{r_e^2q^4Q^2}\exp\left\{-q^2\frac{i\hbar}{m\omega}g(\tau,\sigma)\right\}\end{aligned} \tag{4.45}$$

Here we assume Eq. (4.45) is hold as t is large [28]. Then it is easy to show that

$$\int_0^t\int_0^t f\left(|\tau-\sigma|\right)d\tau d\sigma = 2\int_0^t dx\,(t-x)\,f(x), \tag{4.46}$$

where $x = |\tau-\sigma|$. Using $x = x't$ we may write Eq. (4.46) as

$$\int_0^t\int_0^t f\left(|\tau-\sigma|\right)d\tau d\sigma = 2t^2\int_0^1 dx'\,(1-x')\,f(x'). \tag{4.47}$$

Considering the double integral of the equation (4.42), we obtain

$$\int_0^t\int_0^t d\tau d\sigma\exp\left\{-q^2\frac{i\hbar}{m\omega}g(\tau,\sigma)\right\} = 2t^2\int_0^1 dx'\,(1-x')\exp\left\{-q^2\frac{i\hbar}{m\omega}g(x')\right\}. \tag{4.48}$$

In the same way, by putting Eq. (4.48) into Eq. (4.45), we have

$$\langle S\rangle_{S_0(\omega)} = \frac{2i\pi\gamma^2 t^2}{\hbar r_0}\left(1-\frac{1}{r_e^2Q^2}\right)\int_0^1 dx'\,(1-x')\int\frac{d^3q}{(2\pi)^3}\left[\frac{1}{Q^2q^2}-\frac{1}{Q^2\left(Q^2+q^2\right)}\right] \times\exp\left\{-q^2\frac{i\hbar}{m\omega}g\left(x'\right)\right\} +\frac{2i\pi\gamma^2 t^2}{\hbar r_0}\int_0^1 dx'\,(1-x')\int\frac{d^3q}{(2\pi)^3}\frac{1}{r_e^2q^4Q^2}\exp\left\{-q^2\frac{i\hbar}{m\omega}g\left(x'\right)\right\}. \quad (4.49)$$

Using the formula

$$\int\frac{d^3q}{(2\pi)^3} = \frac{1}{2\pi^2}\int_0^\infty q^2dq, \quad (4.50)$$

$$\int_0^\infty dq q^2\exp\left(-q^2y\right) = \frac{1}{4}\sqrt{\frac{\pi}{y^3}}, \quad (4.51)$$

and the identity

$$\left(q^2+Q^2\right)^{-1} = \int_0^\infty dy\exp\left[-\left(q^2+Q^2\right)y\right], \quad (4.52)$$

$$\left(q^2\right)^{-1} = \int_0^\infty dy\exp\left[-\left(q^2\right)y\right], \quad (4.53)$$

and inserting the Eqs. (4.50), (4.51), (4.52) and (4.53) into (4.49) and performing the $\vec{q}$ integration, we obtain

$$\langle S\rangle_{S_0(\omega)} = \frac{i\gamma^2t^2}{4\sqrt{\pi}\hbar r_0Q^2}\left(1-\frac{1}{r_e^2Q^2}\right)\int_0^1 dx'\,(1-x')\left\{\int_0^\infty dy\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2} -\int_0^\infty dy\exp\left(-Q^2y\right)\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2}\right\} +\frac{i\gamma^2t^2}{4\sqrt{\pi}\hbar r_0r_e^2Q^2}\int_0^1 dx'\,(1-x')\int_0^\infty dy\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-1/2} \quad (4.54)$$

When the Debye screening length is sufficiently large such as in HDCS, Eq. (4.54) can be rewritten as

$$\begin{aligned}\langle S\rangle_{S_0(\omega)} &= \frac{i\gamma^2 t^2}{4\sqrt{\pi}\hbar r_0 Q^2}\int_0^1 dx'\left(1-x'\right)\left\{\int_0^\infty dy\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2}\right. \\ &\left. -\int_0^\infty dy\exp\left(-Q^2 y\right)\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2}\right\} \qquad (4.55)\end{aligned}$$

Considering the average of the second term in Eq. (4.36), which equals to Eq. (4.19), and using Eq. (4.33), we get

$$\begin{aligned}\langle S_0\rangle_{S_0(\omega)} &= -\frac{m\omega^2}{4t}\int_0^t\int_0^t d\tau d\sigma\left\{\frac{6i\hbar}{m\omega}\left[\frac{\sin\frac{1}{2}\omega(\tau-\sigma)\sin\frac{1}{2}\omega[t-(\tau-\sigma)]}{\sin\frac{1}{2}\omega t}\right]\right. \\ &\left. +\left\langle\vec{x}\left(\tau\right)-\vec{x}\left(\sigma\right)\right\rangle^2_{S_0(\omega)}\right\}. \qquad (4.56)\end{aligned}$$

Here $\left\langle\vec{x}\left(\tau\right)-\vec{x}\left(\sigma\right)\right\rangle^2_{S_0(\omega)}$ is the average of $\vec{A}$ in Eq. (4.29) squared. To overcome this, Eq. (4.56) can be carried out to be

$$\begin{aligned}\left\langle S_0\left(\omega\right)\right\rangle_{S_0(\omega)} &= \frac{3}{2}i\hbar\left(\frac{1}{2}\omega t\cot\frac{1}{2}\omega t-1\right) \\ &+\frac{1}{2}m\left[\frac{1}{2}\omega t\cot\frac{1}{2}\omega t-\left(\frac{1}{2}\omega t\csc\frac{1}{2}\omega t\right)^2\right]\frac{\left|\vec{x}_2-\vec{x}_1\right|^2}{2t}, \qquad (4.57)\end{aligned}$$

we neglect the second term of the average trial action because $(\vec{x}_2-\vec{x}_1)=0$ [25]. Thus

$$\left\langle S_0\left(\omega\right)\right\rangle_{S_0(\omega)}=\frac{3}{2}i\hbar\left(\frac{1}{2}\omega t\cot\frac{1}{2}\omega t-1\right). \qquad (4.58)$$

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Collecting terms from Eqs. (4.55) and (4.58), we can write

$$\begin{aligned}\frac{i}{\hbar}\left\langle S-S_0\left(\omega\right)\right\rangle_{S_0(\omega)} &= -\frac{\gamma^2t^2}{4\sqrt{\pi}\hbar^2r_0Q^2}\int\limits_0^1 dx'\left(1-x'\right)\\ &\quad\times\int\limits_0^\infty dy\left[1-\exp\left(-Q^2y\right)\right]\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2}\\ &\quad+\frac{3}{2}\left(\frac{1}{2}\omega t\cot\frac{1}{2}\omega t-1\right).\end{aligned}\tag{4.59}$$

We can write the density of states Eq. (3.36) as

$$\rho\left(E\right)=\frac{1}{2\pi\hbar}\int\limits_{-\infty}^{+\infty}dtK_0(0,0;t)\exp\left[\frac{i}{\hbar}Et+\frac{i}{\hbar}\left\langle S-S_0\left(\omega\right)\right\rangle_{S_0(\omega)}\right].\tag{4.60}$$

Substituting Eqs. (4.9) , and (4.59) into Eq. (4.60) , we have

$$\begin{aligned}\rho\left(E\right) &= \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{+\infty}dt\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\left(\frac{\omega t}{2\sin\frac{1}{2}\omega t}\right)^3\exp\left\{\frac{i}{\hbar}Et\right.\\ &\quad-\frac{\gamma^2t^2}{4\sqrt{\pi}\hbar^2r_0Q^2}\int\limits_0^1 dx'\left(1-x'\right)\int\limits_0^\infty dy\left[1-\exp\left(-Q^2y\right)\right]\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2}\\ &\quad\left.+\frac{3}{2}\left(\frac{1}{2}\omega t\cot\frac{1}{2}\omega t-1\right)\right\}.\end{aligned}\tag{4.61}$$

Eq. (4.61) is rewritten as

$$\begin{aligned}\rho\left(E\right) &= \frac{1}{2\pi\hbar}\int\limits_{-\infty}^{+\infty}dt\left(\frac{m}{2\pi i\hbar t}\right)^{3/2}\left(\frac{\omega t}{2\sin\frac{1}{2}\omega t}\right)^3\exp\left\{\frac{i}{\hbar}Et-\frac{\gamma^2t^2}{8\sqrt{\pi}\hbar^2r_0Q^2}\right.\\ &\quad\times\int\limits_0^\infty dy\left[1-\exp\left(-Q^2y\right)\right]\left[y+\frac{i\hbar}{m\omega}g\left(x'\right)\right]^{-3/2}\\ &\quad\left.+\frac{3}{2}\left(\frac{1}{2}\omega t\cot\frac{1}{2}\omega t-1\right)\right\}.\end{aligned}\tag{4.62}$$

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The obtained density of states is still too complicated and cannot be calculated exactly. We consider it in the asymptotic approximation that we suppose ω is very large

$$
\begin{aligned}
g(x') &= \frac{\sin\frac{1}{2}\omega x' \sin\frac{1}{2}\omega(t-x')}{\sin\frac{1}{2}\omega t} \\
&\cong \frac{1}{2i},
\end{aligned}
\tag{4.63}
$$

$$
\left(\sin\frac{1}{2}\omega t\right)^{-3} \cong -8i\exp\left(-\frac{3}{2}i\omega t\right), \tag{4.64}
$$

$$
\frac{1}{2}\omega t\cot\frac{1}{2}\omega t - 1 \cong \frac{i}{2}\omega t. \tag{4.65}
$$

Next, we approximate the density of states using Eqs. (4.63), (4.64) and (4.65). Considering the ground state contribution to the density of states, and letting $t \to \infty$, we can write

$$
\begin{aligned}
\rho(E) &= \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dt \left(\frac{m}{2\pi i\hbar t}\right)^{3/2} (i\omega t)^3 \exp\left\{\frac{i}{\hbar}Et - \frac{\gamma^2 t^2}{8\sqrt{\pi}\hbar^2 r_0 Q^2}\right. \\
&\quad \left.\times\int_0^{\infty} dy\left[1-\exp\left(-Q^2 y\right)\right]\left[y+\frac{\hbar}{2m\omega}\right]^{-3/2} - \frac{3}{4}i\omega t\right\}.
\end{aligned}
\tag{4.66}
$$

Using the formula [26]

$$
\int_{-\infty}^{+\infty} dt\,(it)^p \exp\left(-\beta^2 t^2 - ict\right) = 2^{-p/2}\sqrt[2]{\pi}\beta^{-p-1}\exp\left(\frac{-c^2}{8\beta^2}\right) D_p\left(\frac{c}{\beta\sqrt[2]{2}}\right), \tag{4.67}
$$

p is constant, and $D_p(z)$ denotes the parabolic cylinder function. Thus Eq. (4.66) becomes

$$
\rho(E) = \frac{1}{4\hbar}\left(\frac{2^{1/2}}{\pi}\right)^{1/2}\omega^3\left(\frac{m}{2\pi\hbar}\right)^{3/2}\beta^{-5/2}\exp\left(\frac{-c^2}{8\beta^2}\right) D_{3/2}\left(\frac{c}{\beta\sqrt[2]{2}}\right), \tag{4.68}
$$

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where

$$c = \frac{\left(\frac{3}{4}\hbar\omega - E\right)}{\hbar}, \tag{4.69}$$

$$E_\omega = \hbar\omega, \tag{4.70}$$

$$\beta^2 = \frac{\xi_Q}{8\hbar^2\sqrt{\pi}Q}\int_0^\infty dy\left[1-\exp\left(-Q^2y\right)\right]\left[y+\frac{\hbar}{2m\omega}\right]^{-3/2}. \tag{4.71}$$

From Eq. (4.71), we calculate the variable β as follows:

$$\beta^2 = \frac{\xi_Q}{4\hbar^2}\exp\left(\frac{E_Q}{E_\omega}\right)\left\{1 - D_{-3}\left(\left(\frac{E_Q}{E_\omega}\right)^{1/2}\right)\right\}, \tag{4.72}$$

where

$$E_Q = \frac{\hbar^2 Q^2}{2m}, \tag{4.73}$$

and the typical fluctuation which has the dimension of energy squared can be written as

$$\xi_Q = \gamma^2. \tag{4.74}$$

Next, we will find that the two-parameter model can be used to obtain the density of states proposed by Halperin and Lax [12] written in the form:

$$\rho(E) = \left[A(E)/\xi_Q^2\right]\exp\left[-B(E)/2\xi_Q\right]. \tag{4.75}$$

The density of states is expressed in the analytic form with the dimensionless functions of the preexponential $a(v,z)$ and the exponent $b(v,z)$ [26], respectively.

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Moreover, numerical results $a(\upsilon, z)$ and $b(\upsilon, z)$ are very important to finding the density of states of HDCS. For a screened Coulomb potential [12], we get

$$A(E) = (E_Q Q)^3 \, a(\upsilon, z), \tag{4.76}$$

and

$$B(E) = E_Q^2 b(\upsilon, z), \tag{4.77}$$

where

$$\upsilon = -\frac{E}{E_Q}. \tag{4.78}$$

We thus show the density of states for the system with a screened Coulomb potential [12,26] to be

$$\rho(E) = \left[(E_Q Q)^3 \, a(\upsilon, z) / \xi_Q^2\right] \exp\left[-E_Q^2 b(\upsilon, z) / 2\xi_Q\right], \tag{4.79}$$

where

$$z = \left(\frac{2E_Q}{E_\omega}\right)^{1/2}. \tag{4.80}$$

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Comparing Eq. (4.68) with Eq. (4.79), we can calculate $a(\upsilon, z)$ and $b(\upsilon, z)$ by using the variables in Eqs. (4.69), (4.70), (4.72), (4.73), (4.74), (4.78) and (4.80),

$$a(\upsilon, z) = \frac{\left(\frac{3}{2}z^{-2} + \upsilon\right)^{3/2}}{4\sqrt{2}\pi^2 z^6 \exp(z^2)\left[1 - D_{-3}(z')\right]^2}, \tag{4.81}$$

and

$$b(\upsilon, z) = \frac{\left(\frac{3}{2}z^{-2} + \upsilon\right)^2}{2\exp\left(\frac{1}{2}z^2\right)\left[1 - D_{-3}(z')\right]}, \tag{4.82}$$

where $z' = z/\sqrt{2}$, υ is the dimensionless energy. We can express analytically $a(\upsilon, z)$ and $b(\upsilon, z)$ in terms of parabolic cylinder functions. We can get the density of states by substituting Eqs. (4.81) and (4.82) into Eq. (4.79) . The critical exponent interested is the the logarithmic derivative of the exponent $b(\upsilon, z)$ [12,26], we have

$$n(\upsilon, z) = \frac{d\ln b(\upsilon, z)}{d\ln \upsilon} \tag{4.83}$$

or,

$$n(\upsilon, z) = \frac{\upsilon}{b(\upsilon, z)}\frac{db(\upsilon, z)}{d\upsilon} \tag{4.84}$$

By using Eq. (4.82) , we can see that

$$n(\upsilon, z) = \frac{2\upsilon}{\left(\frac{3}{2}z^{-2} + \upsilon\right)}. \tag{4.85}$$

For this reason, the kinetic energy of localization $T(\upsilon, z)$ [12] can also be written as

$$T(\upsilon, z) = \frac{3}{2}z^{-2}, \tag{4.86}$$

where z is a function of υ.

4.4 Results

We begin with the minimization of the parameter $b\left(v, z\right)$ by considering its derivative with respect to z [12,22]. We can see that

$$-12z^{-3}\exp\left(\frac{1}{2}z^2\right)\left(\frac{3}{2}z^{-2}+v\right)\left(1-D_{-3}\left(z'\right)\right)-\left(\frac{1}{2}zD_{-3}\left(z'\right)+3\sqrt{2}D_{-4}\left(z'\right)\right)$$
$$\times\exp\left(\frac{1}{2}z^2\right)\left(\frac{3}{2}z^{-2}+v\right)^2+2z\exp\left(\frac{1}{2}z^2\right)\left(\frac{3}{2}z^{-2}+v\right)^2\left(1-D_{-3}\left(z'\right)\right)=0, \tag{4.87}$$

by using the formula

$$\frac{d}{dz}D_p\left(z\right)+\frac{1}{2}zD_p\left(z\right)-pD_{p-1}\left(z\right)=0. \tag{4.88}$$

Before considering the numerical evaluation of $a\left(v, z\right)$ and $b\left(v, z\right)$ in Eqs. (4.81) and (4.82), we can also evaluate the quantities analytically by introducing an approximation. For a strong screening $v << 1$ ($Q \to \infty$ or $z \to \infty$), Eq. (4.87) can be evaluated easily,

$$z = \left(2v/3\right)^{-1/2}, \tag{4.89}$$

by using the asymptotic properties of the parabolic cylinder function

$$D_p\left(z\right)_{z\to\infty} \approx \exp\left(-\frac{1}{4}z^2\right)z^p. \tag{4.90}$$

The numerical values of z and v in Eq. (4.89) are shown in Table 4.1.

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υ	z
10^{-1}	3.87
10^{-2}	12.25
10^{-3}	38.73
10^{-4}	122.47

Table 4.1: Numerical results of υ and z for a strong screening [$\upsilon << 1$ and $z \to \infty$].

Putting Eq. (4.89) into Eq. (4.81), we get

$$a(\upsilon) \approx 10^{-2}\upsilon^{9/2}e^{-3/2\upsilon} \quad , \tag{4.91}$$

and in the same way, we find from Eq. (4.82) that

$$b(\upsilon) \approx \upsilon^2 e^{-3/4\upsilon}. \tag{4.92}$$

Of course, when we substitute Eq. (4.89) into Eqs. (4.85) and (4.86), we have $n(\upsilon) \approx 1$ and $T(\upsilon)/\upsilon \approx 1$. For a weak screening, $\upsilon >> 1$ ($Q \to 0$ or $z \to 0$), Eq. (4.87) can also be evaluated easily and get

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$$z = \left[\upsilon/3(2\sqrt{2} - \sqrt{\pi})\right]^{-1/3} , \tag{4.93}$$

by using the formula

$$D_{p+1}(z) - zD_p(z) + pD_{p-1}(z) = 0. \tag{4.94}$$

The numerical values of z and υ in Eq. (4.93) are shown in Table 4.2.

v	z
10^1	0.68
10^2	0.32
10^3	0.15
10^4	0.07

Table 4.2: Numerical results of v and z for a weak screening [$v >> 1$ and $z \to 0$].

Substituting Eq. (4.93) into Eqs. (4.81) and (4.82), we can write

$$a(v) = 10^{-2}v^{7/2}, \tag{4.95}$$

and

$$b(v) = v^2. \tag{4.96}$$

Similarly, the resulting Eqs. (4.85) and (4.86) are $n(v) \approx 2$ and $T(v)/v \approx 0$. The asymptotic values of $a(v)$, $b(v)$, $n(v)$ and $T(v)$ are given in Table 4.3 and other values are tabulated in Table 4.4.

$v << 1$	$v >> 1$
$z \approx (2v/3)^{-1/2}$	$z \approx [v/3(2\sqrt{2} - \sqrt{\pi})]^{-1/3}$
$a(v) \approx 10^{-2}v^{9/2}e^{-3/2v}$	$a(v) \approx 10^{-2}v^{7/2}$
$b(v) \approx v^2 e^{-3/4v}$	$b(v) \approx v^2$
$n(v) \approx 1$	$n(v) \approx 2$
$T(v)/v \approx 1$	$T(v)/v \approx 0$

Table 4.3: The limiting values of $a(v)$, $b(v)$, $n(v)$ and $T(v)/v$ calculated from the present method for the case of a screened Coulomb potential.

v	z	$a(v)$	$b(v)$	$n(v)$	$T(v)$
10^4	0.07	6.56×10^{11}	1.25×10^8	1.94	2.85×10^2
10^3	0.17	1.09×10^8	1.15×10^6	1.90	5.48×10^1
10^2	0.38	1.33×10^4	9.61×10^3	1.81	1.02×10^1
10^1	0.85	1.41	6.80×10^1	1.66	2.08
10^0	1.81	3.51×10^{-5}	2.21×10^{-1}	1.37	4.60×10^{-1}
10^{-1}	4.28	2.62×10^{-15}	1.78×10^{-6}	1.10	8.20×10^{-2}
10^{-2}	12.41	0	0	1.01	9.75×10^{-3}
10^{-3}	38.78	0	0	1.00	9.97×10^{-4}
10^{-4}	122.49	0	0	1.00	1.00×10^{-4}

Table 4.4: Numerical results of the function $a(v)$, $b(v)$, $n(v)$ and $T(v)/v$ for a screened Coulomb potential.