Supplemental material for displaced path integral formulation for the momentum distribution of quantum particles

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Derivation of Eq. (3) in the text:
Within Feynman’s path integral representation the density operator is given by:
\[ \rho(\mathbf{r}, \mathbf{r}') = \int_{\mathbf{r}(0)=\mathbf{r}, \mathbf{r}(\beta\hbar)=\mathbf{r}'} \mathcal{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left( \frac{m\dot{\mathbf{r}}^2(\tau)}{2} + V[\mathbf{r}(\tau)] \right)} \],
and the end-to-end distribution is:
\[ \bar{n}(\mathbf{x}) = \frac{1}{Z} \int d\mathbf{r} d\mathbf{r}' \delta(\mathbf{r} - \mathbf{r}') \rho(\mathbf{r}, \mathbf{r}') = \frac{1}{Z} \int_{\mathbf{r}(0)-\mathbf{r}(\beta\hbar)=\mathbf{x}} \mathcal{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left( \frac{m\dot{\mathbf{r}}^2(\tau)}{2} + V[\mathbf{r}(\tau)] \right)} \]

\[ = e^{-\frac{m\dot{\mathbf{r}}^2}{2\beta\hbar}} \int_{\mathbf{r}(\beta\hbar)=\mathbf{r}(0)} \mathcal{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left( \frac{m\dot{\mathbf{r}}^2(\tau)}{2} + V[\mathbf{r}(\tau)] \right)} \].

Eq. (3) transforms the open path \( \mathbf{r}(\tau) \) into the closed path \( \mathbf{r}(\tau) \), and the free particle contribution comes naturally from the derivative of \( y(\tau) \). The choice of the constant \( C \) influences the variance of free energy perturbation and thermodynamic integration estimators in the text. It is found that the lowest variance is achieved when \( C = 1/2 \), since this choice has the smallest displacement from the closed path configuration. This is Eq. (3) in the text.

Next we present the derivation of Eq. (6) in the text:
The Compton profile is given by
\[ J(\mathbf{q}, y) = \int n(\mathbf{p}) \delta(\mathbf{y} - \mathbf{p} \cdot \mathbf{q}) d\mathbf{p} \].

The direction \( \mathbf{q} \) is defined by the experimental setup, and the momentum distribution \( n(\mathbf{p}) \) can be expressed in terms of the end-to-end distribution \( \bar{n}(\mathbf{x}) \) as
\[ n(\mathbf{p}) = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{x} e^{i\mathbf{p} \cdot \mathbf{x}} \bar{n}(\mathbf{x}). \]

We indicate by \( x_|| = \mathbf{x} \cdot \mathbf{q} \), and \( x_\perp \) the \( \mathbf{x} \) component orthogonal to \( \mathbf{q} \). Correspondingly \( p_|| = \mathbf{p} \cdot \mathbf{q} \), and \( p_\perp \) is the \( \mathbf{p} \) component orthogonal to \( \mathbf{q} \). One has
\[ J(\mathbf{q}, y) = \frac{1}{(2\pi\hbar)^3} \int d\mathbf{x} dp_\perp \bar{n}(\mathbf{x}) e^{i\mathbf{p}_\perp \cdot \mathbf{x}_\perp} \delta(\mathbf{y} - \mathbf{p}_\perp) \]
\[ = \frac{1}{(2\pi\hbar)^3} \int dx_\perp dp_\perp \bar{n}(\mathbf{x}) e^{i\mathbf{p}_\perp \cdot \mathbf{x}_\perp} \delta(y - p_\perp) \]
\[ = \frac{1}{2\pi\hbar} \int dx_\perp \bar{n}(x_\perp \mathbf{q}) e^{i\mathbf{x}_\perp \mathbf{p}_\perp}. \]
Given the end to end distribution can be expressed as

\[ \tilde{n}(x) = e^{-\frac{mx^2}{2\hbar^2}} e^{-U(x)}, \]  
(8)

the potential of mean force \( U(x) \) can be obtained from the Compton profile as

\[ U(x\parallel \hat{q}) = -\frac{mx^2}{2\beta\hbar^2} \ln \int dy J(\hat{q}, y)e^{-\frac{x\parallel y}{\hbar}}. \]  
(9)

The mean force \( \mathbf{F}(x) \) is the gradient of \( U(x) \). Taking into account that \( J(\hat{q}, y) \) is an even function of \( y \) one obtains

\[ \hat{q} \cdot \mathbf{F}(x\parallel \hat{q}) = -\frac{mx^2}{\beta\hbar^2} + \frac{1}{\hbar} \int_0^\infty dy \cos(x\parallel y/\hbar)J(\hat{q}, y). \]  
(10)

This is Eq. (6) in the text.

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