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:

$$\rho(\mathbf{r},\mathbf{r}') = \int_{\mathbf{r}(0)=\mathbf{r},\mathbf{r}(\beta\hbar)=\mathbf{r}'} \mathfrak{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \left(\frac{m\dot{\mathbf{r}}^2(\tau)}{2}+V[\mathbf{r}(\tau)]\right)}, \tag{1}$$

and the end-to-end distribution is:

$$\begin{aligned}\widetilde{n}(\mathbf{x}) =& \frac{1}{Z}\int d\mathbf{r}d\mathbf{r}'\delta\left(\mathbf{r}-\mathbf{r}'-\mathbf{x}\right)\rho\left(\mathbf{r},\mathbf{r}'\right)\\ =& \frac{\int_{\mathbf{r}(0)-\mathbf{r}(\beta\hbar)=\mathbf{x}} \mathfrak{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \left(\frac{m\dot{\mathbf{r}}^2(\tau)}{2}+V[\mathbf{r}(\tau)]\right)}}{\int_{\mathbf{r}(\beta\hbar)=\mathbf{r}(0)} \mathfrak{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \left(\frac{m\dot{\mathbf{r}}^2(\tau)}{2}+V[\mathbf{r}(\tau)]\right)}}.\end{aligned} \tag{2}$$

We now perform a linear transformation in path space in the expression on the numerator:

$$\mathbf{r}(\tau) = \widetilde{\mathbf{r}}(\tau) + y(\tau)\mathbf{x}. \tag{3}$$

Here $y(\tau) = C - \frac{\tau}{\beta\hbar}$ and C is an arbitrary real number. Then the numerator is given by

$$\begin{aligned}&\int_{\mathbf{r}(0)-\mathbf{r}(\beta\hbar)=\mathbf{x}} \mathfrak{D}\mathbf{r}(\tau) e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \left(\frac{m\dot{\mathbf{r}}^2(\tau)}{2}+V[\mathbf{r}(\tau)]\right)}\\ =& e^{-\frac{m\mathbf{x}^2}{2\beta\hbar^2}}\int_{\widetilde{\mathbf{r}}(\beta\hbar)=\widetilde{\mathbf{r}}(0)} \mathfrak{D}\widetilde{\mathbf{r}}(\tau) e^{-\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\, \left(\frac{m\dot{\widetilde{\mathbf{r}}}^2(\tau)}{2}+V[\widetilde{\mathbf{r}}(\tau)+y(\tau)\mathbf{x}]\right)}.\end{aligned} \tag{4}$$

Eq. (3) transforms the open path $\mathbf{r}(\tau)$ into the closed path $\widetilde{\mathbf{r}}(\tau)$, 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

$$J(\hat{\mathbf{q}}, y) = \int n(\mathbf{p})\delta(y - \mathbf{p}\cdot\hat{\mathbf{q}})d\mathbf{p}. \tag{5}$$

The direction $\hat{\mathbf{q}}$ is defined by the experimental setup, and the momentum distribution $n(\mathbf{p})$ can be expressed in terms of the end-to-end distribution $\widetilde{n}(\mathbf{x})$ as

$$n(\mathbf{p}) = \frac{1}{(2\pi\hbar)^3}\int d\mathbf{x} e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}\widetilde{n}(\mathbf{x}). \tag{6}$$

We indicate by $x_\parallel = \mathbf{x}\cdot\hat{\mathbf{q}}$, and $\mathbf{x}_\perp$ the $\mathbf{x}$ component orthogonal to $\hat{\mathbf{q}}$. Correspondingly $p_\parallel = \mathbf{p}\cdot\hat{\mathbf{q}}$, and $\mathbf{p}_\perp$ is the $\mathbf{p}$ component orthogonal to $\hat{\mathbf{q}}$. One has

$$\begin{aligned}J(\hat{\mathbf{q}}, y) =& \frac{1}{(2\pi\hbar)^3}\int d\mathbf{x}d\mathbf{p}\ \widetilde{n}(\mathbf{x})e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}\delta(y-\mathbf{p}\cdot\hat{\mathbf{q}})\\ =& \frac{1}{(2\pi\hbar)^3}\int dx_\parallel d\mathbf{x}_\perp dp_\parallel d\mathbf{p}_\perp\ \widetilde{n}(\mathbf{x})e^{\frac{i}{\hbar}x_\parallel p_\parallel + \frac{i}{\hbar}\mathbf{p}_\perp\cdot\mathbf{x}_\perp}\delta(y-p_\parallel)\\ =& \frac{1}{2\pi\hbar}\int dx_\parallel\ \widetilde{n}(x_\parallel\hat{\mathbf{q}})e^{\frac{i}{\hbar}x_\parallel y}.\end{aligned} \tag{7}$$

Given the end to end distribution can be expressed as

$$\widetilde{n}(\mathbf{x}) = e^{-\frac{m\mathbf{x}^2}{2\beta\hbar^2}} e^{-U(\mathbf{x})}, \tag{8}$$

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

$$U(x_{\parallel}\hat{\mathbf{q}}) = -\frac{m x_{\parallel}^2}{2\beta\hbar^2} - \ln \int dy\ J(\hat{\mathbf{q}}, y) e^{-\frac{i}{\hbar} x_{\parallel} y}. \tag{9}$$

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

$$\hat{\mathbf{q}} \cdot \mathbf{F}(x_{\parallel}\hat{\mathbf{q}}) = -\frac{m x_{\parallel}}{\beta\hbar^2} + \frac{\int_0^\infty dy\ y \sin(x_{\parallel} y/\hbar) J(\hat{\mathbf{q}}, y)}{\hbar \int_0^\infty dy\ \cos(x_{\parallel} y/\hbar) J(\hat{\mathbf{q}}, y)}. \tag{10}$$

This is Eq. (6) in the text.

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