Derivation of the Momentum Operator

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1 Introduction

In this paper we will derive the quantum mechanical momentum operator in the position representation for a particle in a velocity-independent potential.[1] It is often shown that $\tilde{p} = -i\hbar\nabla$ by assuming that momentum is the generator of translations, but it may not be clear why mechanical momentum (mass times velocity) is the generator of translations. In this derivation, we will show everything explicitly in hopes of making things more clear.

2 Translation Operator

Let $|\mathbf{x}\rangle$ be a position eigenstate i.e. $\hat{\mathbf{x}}\,|\mathbf{x}\rangle = \mathbf{x}\,|\mathbf{x}\rangle$. The translation operator $\hat{T}(\mathbf{a})$ is defined by

$$\hat{T}(\mathbf{a})\,|\mathbf{x}\rangle = |\mathbf{x}+\mathbf{a}\rangle$$

From this definition, we can observe the following properties

$$\hat{T}(\mathbf{0})\,|\mathbf{x}\rangle = |\mathbf{x}\rangle \quad \Rightarrow \quad \hat{T}(\mathbf{0}) = \hat{I}$$

$$\hat{T}(\mathbf{a})\hat{T}(\mathbf{b})\,|\mathbf{x}\rangle = \hat{T}(\mathbf{a})\,|\mathbf{x}+\mathbf{b}\rangle = |\mathbf{x}+(\mathbf{a}+\mathbf{b})\rangle = \hat{T}(\mathbf{a}+\mathbf{b})\,|\mathbf{x}\rangle \quad \Rightarrow \quad \hat{T}(\mathbf{a})\hat{T}(\mathbf{b}) = \hat{T}(\mathbf{a}+\mathbf{b})$$

$$\begin{aligned} \langle\psi|\,\psi\rangle &= \left\langle\psi\middle|\,\hat{T}(\mathbf{0})\,\middle|\psi\right\rangle = \left\langle\psi\middle|\,\hat{T}(-\mathbf{a})\hat{T}(\mathbf{a})\,\middle|\psi\right\rangle = \left\langle\psi\middle|\,\hat{T}(-\mathbf{a})\,\middle|\hat{T}(\mathbf{a})\psi\right\rangle = \left\langle\hat{T}^\dagger(\mathbf{a})\psi\middle|\,\hat{T}(-\mathbf{a})\,\middle|\psi\right\rangle \\ &= \left\langle\hat{T}^\dagger(\mathbf{a})\psi\middle|\,\hat{T}(-\mathbf{a})\psi\right\rangle \quad \Rightarrow \quad \hat{T}^\dagger(\mathbf{a}) = \hat{T}(-\mathbf{a}) \quad \Rightarrow \quad \hat{T}^\dagger(\mathbf{a})\hat{T}(\mathbf{a}) = 1 \end{aligned}$$

Now consider an infinitesimal transformation $\hat{T}(\boldsymbol{\epsilon})$ applied to an arbitrary state $|\psi(t)\rangle$.

$$\begin{aligned} \left\langle\mathbf{x}\middle|\,\hat{T}(\boldsymbol{\epsilon})\,\middle|\psi(t)\right\rangle &= \int d\mathbf{x}'\,\left\langle\mathbf{x}\middle|\,\hat{T}(\boldsymbol{\epsilon})\,\middle|\mathbf{x}'\right\rangle\langle\mathbf{x}'|\,\psi(t)\rangle \\ &= \int d\mathbf{x}'\,\langle\mathbf{x}|\,\mathbf{x}'+\boldsymbol{\epsilon}\rangle\,\langle\mathbf{x}'|\,\psi(t)\rangle \\ &= \int d\mathbf{x}'\,\langle\mathbf{x}|\,\mathbf{x}'\rangle\,\langle\mathbf{x}'-\boldsymbol{\epsilon}|\,\psi(t)\rangle \\ &= \int d\mathbf{x}'\delta(\mathbf{x}-\mathbf{x}')\psi(\mathbf{x}'-\boldsymbol{\epsilon},t) \\ &= \psi(\mathbf{x}-\boldsymbol{\epsilon},t) \\ &= \psi(\mathbf{x},t) - \boldsymbol{\epsilon}\cdot\nabla\psi(\mathbf{x},t) + \mathcal{O}(\epsilon^2) \\ &= (1-\boldsymbol{\epsilon}\cdot\nabla)\psi(\mathbf{x},t) \end{aligned}$$

Therefore, according to the definition of the corresponding position representation operator $\tilde{A}\psi(\mathbf{x},t) = \left\langle\mathbf{x}\middle|\,\hat{A}\,\middle|\psi(t)\right\rangle$, we have

$$\tilde{T}(\boldsymbol{\epsilon}) = 1 - \boldsymbol{\epsilon}\cdot\nabla$$

[1] Goldstein mentions on page 405 that the canonical momentum is not equivalent to the mechanical momentum when you have velocity dependent potentials. Indeed, this assumption is needed for the derivation shown here.

3 Momentum Operator

Suppose $|\psi\rangle$ represents a particle in a time-independent potential. Let's perform an infinitesimal Galilei boost by applying a time-dependent translation.

$$|\psi(t)\rangle \rightarrow \hat{T}(d\mathbf{v}_0 t)\,|\psi(t)\rangle$$

This will change the velocity of the particle by an infinitesimal amount $d\mathbf{v}_0$.[2] This will allow us to identify the momentum operator after requiring that the kinetic energy changes by the appropriate amount after this boost. Plugging the boosted wave function into the Schrödinger equation,

$$\begin{aligned}
\hat{H}\left(\hat{T}(d\mathbf{v}_0 t)\,|\psi(t)\rangle\right) &= i\hbar\frac{\partial}{\partial t}\left(\hat{T}(d\mathbf{v}_0 t)\,|\psi(t)\rangle\right)\\
&= i\hbar\frac{\partial}{\partial t}\left(\hat{T}(d\mathbf{v}_0 t)\right)|\psi(t)\rangle + i\hbar\hat{T}(d\mathbf{v}_0 t)\frac{\partial}{\partial t}\,|\psi(t)\rangle\\
&= i\hbar\frac{\partial}{\partial t}\left(\hat{T}(d\mathbf{v}_0 t)\right)|\psi(t)\rangle + \hat{T}(d\mathbf{v}_0 t)\hat{H}\,|\psi(t)\rangle
\end{aligned}$$

Applying $\langle\psi(t)|\,\hat{T}^\dagger(d\mathbf{v}_0 t)$ to both ends of the chain of equations,

$$\left\langle\psi(t)\middle|\,\hat{T}^\dagger(d\mathbf{v}_0 t)\hat{H}\hat{T}(d\mathbf{v}_0 t)\,\middle|\psi(t)\right\rangle = i\hbar\left\langle\psi(t)\middle|\,\hat{T}^\dagger(d\mathbf{v}_0 t)\frac{\partial}{\partial t}\left(\hat{T}(d\mathbf{v}_0 t)\right)\middle|\psi(t)\right\rangle + \left\langle\psi(t)\middle|\,\hat{H}\,\middle|\psi(t)\right\rangle$$

If we define $|\psi'(t)\rangle = \hat{T}(d\mathbf{v}_0 t)\,|\psi(t)\rangle$,

$$\begin{aligned}
\left\langle\psi'(t)\middle|\,\hat{H}\,\middle|\psi'(t)\right\rangle - \left\langle\psi(t)\middle|\,\hat{H}\,\middle|\psi(t)\right\rangle &= i\hbar\left\langle\psi(t)\middle|\,\hat{T}^\dagger(d\mathbf{v}_0 t)\frac{\partial}{\partial t}\left(\hat{T}(d\mathbf{v}_0 t)\right)\middle|\psi(t)\right\rangle\\
&= i\hbar\int d\mathbf{x}'\int d\mathbf{x}''\int d\mathbf{x}'''\,\langle\psi(t)|\,\mathbf{x}'\rangle\left\langle\mathbf{x}'\middle|\,\hat{T}^\dagger(d\mathbf{v}_0 t)\,\middle|\mathbf{x}''\right\rangle\frac{\partial}{\partial t}\left\langle\mathbf{x}''\middle|\,\hat{T}(d\mathbf{v}_0 t)\,\middle|\mathbf{x}'''\right\rangle\langle\mathbf{x}'''|\,\psi(t)\rangle\\
&= i\hbar\int d\mathbf{x}'\int d\mathbf{x}''\int d\mathbf{x}'''\,\langle\psi(t)|\,\mathbf{x}'\rangle\,(1 - t d\mathbf{v}_0\cdot\nabla)\,\langle\mathbf{x}'|\,\mathbf{x}''\rangle\frac{\partial}{\partial t}\left((1 - t d\mathbf{v}_0\cdot\nabla)\,\langle\mathbf{x}''|\,\mathbf{x}'''\rangle\right)\langle\mathbf{x}'''|\,\psi(t)\rangle\\
&= i\hbar\int d\mathbf{x}'\,\langle\psi(t)|\,\mathbf{x}'\rangle\,(1 - t d\mathbf{v}_0\cdot\nabla)(-d\mathbf{v}_0\cdot\nabla)\,\langle\mathbf{x}'|\,\psi(t)\rangle\\
&= -i\hbar\int d\mathbf{x}'\,\langle\psi(t)|\,\mathbf{x}'\rangle\,(d\mathbf{v}_0\cdot\nabla)\,\langle\mathbf{x}'|\,\psi(t)\rangle
\end{aligned}$$

to first order in $d\mathbf{v}_0$. Removing the connecting equations and writing the matrix elements in integral form we have

$$\int d\mathbf{x}'\psi'^*(\mathbf{x}',t)\tilde{H}\psi'(\mathbf{x}',t) = \int d\mathbf{x}'\psi^*(\mathbf{x}',t)\left(\tilde{H} - i\hbar d\mathbf{v}_0\cdot\nabla\right)\psi(\mathbf{x}',t)$$

The only issue now is that the integral on the left contains the boosted wave function and the integral on the right does not. However, we know what effect a boost should have on the expectation value of the Hamiltonian, so we can modify the Hamiltonian to account for the boost and use the unboosted wave function.

$$\tilde{H} = \frac{\tilde{p}^2}{2m} + V(\mathbf{x}) \quad\rightarrow\quad \tilde{H}' = \frac{(\tilde{p} + m d\mathbf{v}_0)\cdot(\tilde{p} + m d\mathbf{v}_0)}{2m} + V(\mathbf{x})$$

Our assumption that the potential is velocity independent was used here. So equating the integrands,

$$\frac{(\tilde{p} + m d\mathbf{v}_0)\cdot(\tilde{p} + m d\mathbf{v}_0)}{2m} + V(\mathbf{x}') = \frac{\tilde{p}^2}{2m} + V(\mathbf{x}') - i\hbar d\mathbf{v}_0\cdot\nabla$$

To first order in $d\mathbf{v}_0$ we have

$$d\mathbf{v}_0\cdot\tilde{p} = d\mathbf{v}_0\cdot(-i\hbar\nabla) \quad\Rightarrow\quad \tilde{p} = -i\hbar\nabla$$

[2] Note that we do not want the velocity to be finite because the translation operator expression we obtained is only valid for infinitesimal translations. It is possible to iteratively apply the infinitesimal translation operator to construct finite translations, but it is difficult due to the fact that the wave function is evolving while the sequence of infinitesimal translations is being applied.

4 References

- Jordan, T.: Why $-i\nabla$ is the momentum. Am. J. Phys. 43, 10891093 (1975)
- Reese, R.: A Derivation of the Quantum Mechanical Momentum Operator in the Position Representation. http://www.hep.upenn.edu/~rreece/docs/notes/derivation_of_quantum_mechanical_momentum_operator_in_position_representation.pdf