Kachelriess Problems 2.1 and 2.2

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Revision 2

Goals

- Set up problem 2.1 (free particle only)
- Explain notation and some basic facts about QM that are required for this problem
- Solve problem 2.1 (free particle only)
- Show the solution of problem 2.2 using the resolution of the identity

Problem 2.1 – Free particle

Problem statement: Find the propagator for the free particle, in terms of the action for the free particle.

Review of classical mechanics

$$S_{free}(q) = \int_{t_1}^{t_2} dt \, \frac{m\dot{q}^2}{2}$$

Notice that $\boldsymbol{q' \equiv q(t_2);\ q \equiv q(t_1)}$

The Lagrangian is $L(q) = \frac{m\dot{q}^2}{2}$. The momentum is $p = m\dot{q}$

We also need the Hamiltonian, $H(q,p) = p\dot{q} - L(q,\dot{q}) = \frac{p^2}{m} - \frac{p^2}{2m} = \frac{p^2}{2m}$

The Propagator

Comment: See solution to 2.2 for difference between propagator and Green's function.

Definition $K(q',t';q,t) = \langle q'|\exp[-i(t'-t)H|q\rangle$

What do the symbols on the right mean?

- In math, we start with a Hilbert space with vectors *v,w* etc. In physics we use Dirac notation where those vectors become $|q\rangle$, etc. and we refer to these as states.
- In math, we speak of a linear operator $\hat{O}$ transforming a vector through the action $\hat{O}v$. In Dirac notation we write $\hat{O}|q\rangle$.
- The notation $|q\rangle$ identifies a particular vector (state), as the **unique** vector with the property $\hat{Q}|q\rangle = q|q\rangle$. We say that "state $|q\rangle$ is the eigenstate, with eigenvalue *q* of the operator $\hat{Q}$."
  - More generally, there are several states with the same eigenvalue. We distinguish them by $|q,\alpha\rangle$.
  - Caveat: mathematical care is required for dealing with continuous-valued eigenvectors and eigenstates.
  - The state label (e.g. "q") is purely a convention that is context-dependent.
- Hilbert spaces have inner products. We write (*v,w*). In Dirac notation, we write $\langle v|w\rangle$ or with the previous states $\langle q'|q\rangle$. The inner product of the state $|v\rangle$ with the state $\hat{O}|w\rangle$ is written as $\langle v|\hat{O}|w\rangle$.
  - So far, we haven't explicitly talked about the meaning of $\langle v|$. Mathematically it is the dual of $|v\rangle$.
  - $\langle v|w\rangle = \langle w|v\rangle^*$
- What is $\exp[-i(t'-t)H]$? $I + [-i\delta t\ H] + \frac{[-i\delta t]^2}{2!}H^2 + \ldots$ where "I" is the identity operator. (cf. equation 2.8).

Very important manipulation in Quantum Mechanics – basis expansion!

(Resolution of the Identity)

- A Hilbert space has an orthonormal basis, $\hat{e}^i$
  - $(\hat{e}^i, \hat{e}^j) = \delta^{i,j}$
  - Any vector *v* can be written in the form $v = \sum a_n \, \hat{e}^n$ where $a_n = (\hat{e}^n, v)$. So $v = \sum (\hat{e}^n, v) \, \hat{e}^n$. In Dirac notation, this is $|v\rangle = \sum \langle \hat{e}^n | v \rangle | \hat{e}^n \rangle$ or $|v\rangle = \sum (|\hat{e}^n\rangle \langle \hat{e}^n|) v\rangle$. **NOTICE THAT THIS EXPRESSION HAS THE FORM $|v\rangle = \hat{O}|v\rangle$ so $\hat{O}$ is the identity operator where $\hat{O} = \sum |\hat{e}^n\rangle\langle\hat{e}^n|$.** $\sum |\hat{e}^n\rangle\langle\hat{e}^n| = I$
- There are an infinite number of possible bases. Switch from basis $\hat{e}^i$ to basis $\hat{f}^i$ by inserting the resolution of the identity. $|\hat{f}^j\rangle = \sum |\hat{e}^n\rangle\langle\hat{e}^n| \hat{f}^j\rangle$
  - If the basis is continuous, replace the sum by an integral
- Example bases: $|q\rangle$ are normalized eigenvectors of $\hat{Q}$, $|p\rangle$ are normalized eigenvectors of $\hat{P}$ and $|q\rangle = \int \frac{dp}{2\pi} \, |p\rangle\langle p|q\rangle$

APPLY THIS

Recall $K(q',t';q,t) = \langle q'|e^{-i\delta t\hat{H}}|q\rangle = \langle q'|e^{-i\delta t\frac{\hat{p}^2}{2m}}|q\rangle = \int \frac{dp}{2\pi}\langle q'|e^{-i\delta t\frac{\hat{p}^2}{2m}}|p\rangle\langle p|q\rangle$

The reason for using the resolution of the identity is to convert to a basis of $\hat{P}$ eigenvectors so that we can use the property $e^{-i\delta t\frac{\hat{p}^2}{2m}}|p\rangle = e^{-i\delta t\frac{p^2}{2m}}|p\rangle$. Then the integral in red becomes $\int \frac{dp}{2\pi} e^{-i\delta t\frac{p^2}{2m}}\langle q'|p\rangle\langle p|q\rangle$.

ONE OTHER IMPORTANT PROPERTY $\langle p|q\rangle = e^{-ipq}$ and (complex conjugation) $\langle q'|p\rangle = e^{ipq'}$

Finally $K(q',t';q,t) = \int \frac{dp}{2\pi}(e^{-i\delta t\frac{p^2}{2m}})(e^{-ip(q-q')}) = \int \frac{dp}{2\pi} e^{-i[\delta t\frac{p^2}{2m}+p(q-q')]}$

AN IMPORTANT IDENTITY (see Example 2.1) $\int \frac{dp}{2\pi} e^{-i(ap^2+bp)} = e^{i\frac{b^2}{4a}}[\frac{1}{\sqrt{a}}\int\frac{dp}{2\pi}e^{-ip^2}]$

This is an example of a common kind of integral where an exponential appears with a quadratic argument. Ignore issues having to do with convergence of the integral (sometimes resolved by adding –iε to "a").

$K(q',t';q,t) = e^{i\frac{m(q-q')^2}{2\delta t}}N$ where N is independent of q and q' $(N = [\sqrt{\frac{2m}{\delta t}}\int\frac{dp}{2\pi}e^{-ip^2}])$

Suppose δt is very small (required for Problem 2.1 even if Kachelriess doesn't say so).

Then $\int_t^{t+\delta t} dt'\,\dot{q}^2 \simeq \int_t^{t+\delta t} dt'\,\frac{[q(t+\delta t)-q(t)]^2}{\delta t^2} = \frac{[q(t+\delta t)-q(t)]^2}{\delta t^2}\int_t^{t+\delta t} dt' = \frac{[q'-q]^2}{\delta t}$

And $e^{i\frac{m(q-q')^2}{2\delta t}} \simeq e^{i\int_t^{t+\delta t}dt'\frac{m\dot{q}^2}{2}} = e^{iS_{free}}$. Finally $K(q',t';q,t) \simeq N\,e^{iS_{free}}$.

Problem 2.2: Properties of propagator K

First show $\left(i\frac{d}{dt'} + \frac{1}{2m}\frac{d^2}{dx'^2} - V(x')\right)K(x',t';x,t) = 0$ *(not what Kachelriess asks for!)*

Recall $K(x',t';x,t) = \langle x'|\exp[-i(t'-t)H]|x\rangle$

- $i\frac{d}{dt'}K(x',t';x,t) = \langle x'|H\exp[-i(t'-t)H]|x\rangle = \left\langle x'\middle|\left[\frac{\hat{P}^2}{2m} + V(\hat{Q})\right]\exp[-i(t'-t)H]\middle|x\right\rangle$
  - $\langle x'|[V(\hat{Q})]\exp[-i(t'-t)H]|x\rangle = \boldsymbol{V(x')\langle x'|\exp[-i(t'-t)H]|x\rangle}$
  - $\frac{1}{2m}\langle x'|[\hat{P}^2]\exp[-i(t'-t)H]|x\rangle = \frac{1}{2m}\int\frac{dp}{2\pi}\langle x'|p\rangle\langle p|[\hat{P}^2]\exp[-i(t'-t)H]|x\rangle$ (resolution of identity)

$$= \boldsymbol{\frac{1}{2m}\int\frac{dp}{2\pi}\langle p|\exp[-i(t'-t)H]|x\rangle\, p^2 e^{ipx'}}$$

- $\frac{1}{2m}\frac{d^2}{dx'^2}K(x',t';x,t) = \frac{1}{2m}\frac{d^2}{dx'^2}\langle x'|\exp[-i(t'-t)H]|x\rangle = \frac{1}{2m}\frac{d^2}{dx'^2}\int\frac{dp}{2\pi}\langle x'|p\rangle\langle p|\exp[-i(t'-t)H]|x\rangle$

$= \frac{1}{2m}\frac{d^2}{dx'^2}\int\frac{dp}{2\pi}\langle x'|\exp[-i(t'-t)H]|p\rangle e^{ipx'} = \boldsymbol{\frac{-1}{2m}\int\frac{dp}{2\pi}\langle x'|\exp[-i(t'-t)H]|p\rangle\, p^2 e^{ipx'}}$

- **-V(x')** $\boldsymbol{K(x',t';x,t)}$

Bold colored terms add up to 0!

Problem 2.2 cont'd: Properties of Green's function G

Reference – Wikipedia article on "Propagator" (doesn't seem explained by Kachelriess)

$$\boldsymbol{G(x',t',x,t) \equiv \theta(t'-t)K(x',t',x,t)}$$

$$[i\partial_{t'} - H(x',t')]G(x',t',x,t) =$$

$$\{i\frac{d}{dt'} + \frac{1}{2m}\frac{d^2}{dx'^2} - V(x')\}G(x',t',x,t)$$

$$= \left[\frac{d}{dt'}\theta(t'-t)\right]K(x',t',x,t) - i\theta(t'-t)\{i\frac{d}{dt'} + \frac{1}{2m}\frac{d^2}{dx'^2} - V(x')\}K(x',t',x,t)$$

The term in red is 0 from the first part of this problem. Only the first term is new.

But $\frac{d}{dt'}\theta(t'-t)$ = δ(t'-t), and K(x',t,x,t) = δ(x'-x), so

$$\boldsymbol{[i\partial_{t'} - H(x',t')]G(x',t',x,t) = \delta(t'-t)\,\delta(x'-x)}$$

which is why G is called a Green's function.

Some random stuff

Adjoint operators

We have expressions like $\langle a|\hat{O}|b\rangle$ and we know what $\hat{O}|b\rangle$ is. Does $\langle a|\hat{O}$ mean anything? It should for notational consistency.

$\langle a|\hat{O} \;\equiv\; \langle a'|$ where $|a'\rangle = \hat{O}\,|a\rangle$. We also employ the definition of adjoint as follows:

$[\langle a|\hat{O}]\,||b\rangle = \langle a|[\hat{O}^{\dagger}|b\rangle]$ and $\hat{O}^{\dagger}$ is called the **adjoint** of $\hat{O}$. Observables are always **self-adjoint** (the operator equivalent of *real*), meaning $\hat{O}^{\dagger}$ = $\hat{O}$.

An application of this idea is the expression $\langle p|\hat{P}|q\rangle$. It isn't practical to operate with $\hat{P}$ on the vector $|q\rangle$. However, using the above information, we find that $\langle p|\hat{P}$ = p $\langle p|$, so $\langle p|\hat{P}|q\rangle$ = p $\langle \mathrm{p}|\mathrm{q}\rangle$.