Propagators in Wave Mechanics

Oct. 25, 2016

$\boxed{\text{2nd Exam on Thursday, Oct. 27; Chapt. 2 materials}}$

We further discussed the SHO and obtained the second order diffential equation that the Hermite polynomials satisfy

$$\boxed{\frac{d^2 H_n}{dy^2} - 2y\frac{dH_n}{dy} + (\mathcal{E}_n - 1)H_n = 0},$$

where $y = \frac{x'}{x_0}$ (dimensionless position) and $\mathcal{E}_n = 2n+1$ (dimensionless energy).

Let's first show that one can use the Generating function of the Hermite polynomials to get the above diff. eq.

We then discuss that the generating function plays the role of Green's functions or the propagators in wave mechanics as it generates all the eigenfunctions that are the solutions of the wave equation.

So, what is the generating function of H_n ?

$$\begin{aligned} g(y,t) &\equiv e^{-t^2+2ty} \\ &= \sum_{n=0}^{\infty} \frac{1}{n!}\left(-t^2+2ty\right)^n \\ &= 1 + (-t^2+2ty) + \frac{1}{2!}(-t^2+2ty)^2 + \cdots \\ &= 1 + (2y)t + \frac{(4y^2-2)}{2!}t^2 + \cdots = H_0(y) + H_1(y)t + \frac{H_2(y)}{2!}t^2 + \cdots \end{aligned}$$

Thus,

$$\boxed{\begin{aligned} g(y,t) &= e^{-t^2+2ty} \\ &= \sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!} \end{aligned}}$$

Note that the generating function $g(y,t)$ yields all the Hermite polynomials $H_n(y)$.

From
$$\begin{aligned} \frac{\partial g(y,t)}{\partial y} &= 2t\, g(y,t) \\ &= \sum_{n=0}^{\infty} 2H_n(y)\frac{t^{n+1}}{n!} \\ &= \sum_{n=0}^{\infty} 2H_n(y)(n+1)\frac{t^{n+1}}{(n+1)!} \\ &= \sum_{n=1}^{\infty} 2n H_{n-1}(y)\frac{t^n}{n!} \\ &= \sum_{n=0}^{\infty} 2n H_{n-1}(y)\frac{t^n}{n!} \end{aligned}$$

and
$$\begin{aligned} \frac{\partial g(y,t)}{\partial y} &= \frac{\partial}{\partial y}\sum_{n=0}^{\infty} H_n(y)\frac{t^n}{n!} \\ &= \sum_{n=0}^{\infty} H_n'(y)\frac{t^n}{n!}, \end{aligned}$$

we note

$$\boxed{H_n'(y) = 2n H_{n-1}(y)}.$$

For example, $H_1'(y) = 2H_0(y)$,

$H_2'(y) = 4H_1(y)$, ... cf. $\frac{d}{dy}\big(\underbrace{4y^2-2}_{H_2(y)}\big) = 8y = 4\times\underbrace{2y}_{H_1(y)}$

Also, from $\dfrac{\partial g(y,t)}{\partial t} = (-2t+2y)\, g(y,t)$

$$= -\sum_{n=0}^{\infty} 2 H_n(y) \frac{t^{n+1}}{n!} + \sum_{n=0}^{\infty} 2y H_n(y) \frac{t^n}{n!}$$

$$= -\sum_{n=0}^{\infty} 2n\, H_{n-1}(y) \frac{t^n}{n!} + \sum_{n=0}^{\infty} 2y H_n(y) \frac{t^n}{n!}$$

and $\dfrac{\partial g(y,t)}{\partial t} = \dfrac{\partial}{\partial t}\left[\sum_{n=0}^{\infty} H_n(y) \dfrac{t^n}{n!}\right]$

$$= \sum_{n=0}^{\infty} n\, H_n(y) \frac{t^{n-1}}{n!}$$

$$\underbrace{H_1 + 2H_2 \frac{t}{2!} + 3H_3 \frac{t^2}{3!} + \cdots}$$

$$= \sum_{n=0}^{\infty} H_{n+1}(y) \frac{t^n}{n!},$$

we get the recursion relation

$$\boxed{H_{n+1}(y) = 2y H_n(y) - 2n H_{n-1}(y)}.$$

Since $H_n'(y) = 2n\, H_{n-1}(y)$,

$$H_n''(y) = 2n\, H_{n-1}'(y)$$

$H_n = 2y H_{n-1} - 2(n-1) H_{n-2}$

or $2(n-1) H_{n-2} = 2y H_{n-1} - H_n$

$$= 2n\left[2(n-1)\, H_{n-2}(y)\right]$$

$$= 2n\left[2y H_{n-1}(y) - H_n(y)\right]$$

$$= 2y (2n) H_{n-1}(y) - 2n H_n(y),$$

$H_n'(y)$

or $H_n''(y) = 2y H_n'(y) - 2n H_n(y)$

Thus, we get

$$\boxed{H_n'' - 2y H_n' + 2n H_n = 0}$$

as we obtained by solving the Schrödinger eq of SHO.

This shows that the generating function has in principle all the information of the solution for the Schrödinger eq.

Let's now recall the Schrödinger picture:

$$|\alpha, t\rangle = \mathcal{U}(t, t_0) |\alpha, t_0\rangle$$

$$= e^{\frac{-iH(t-t_0)}{\hbar}} |\alpha, t_0\rangle$$

$$= \sum_a |a\rangle\langle a| \, e^{\frac{-iH(t-t_0)}{\hbar}} |\alpha, t_0\rangle$$

$$= \sum_a |a\rangle \, e^{\frac{-iE_a(t-t_0)}{\hbar}} \langle a|\alpha, t_0\rangle$$

Projecting this in 3-dim. position space, we get

$$\langle \vec{x}'' |\alpha, t\rangle = \sum_a \langle \vec{x}'' | a\rangle \, e^{\frac{-iE_a(t-t_0)}{\hbar}} \langle a| \int d^3\vec{x}' \, |\vec{x}'\rangle\langle \vec{x}'|\alpha, t_0\rangle$$

$$= \int d^3\vec{x}' \underbrace{\boxed{\sum_a \langle \vec{x}'' | a\rangle\langle a|\vec{x}'\rangle \, e^{\frac{-iE_a(t-t_0)}{\hbar}}}}_{K(\vec{x}'', t; \vec{x}', t_0)} \langle \vec{x}'|\alpha, t_0\rangle$$

$K(\vec{x}'', t; \vec{x}', t_0)$ Green's function or propagator

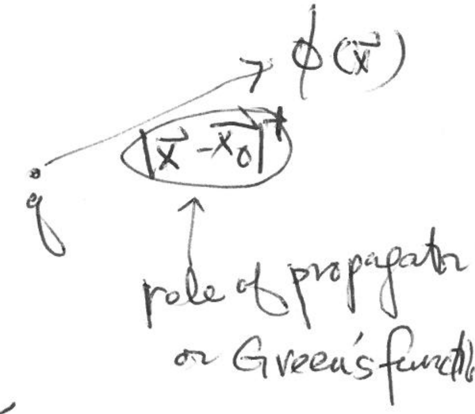
$$\boxed{\psi(\vec{x}'',t) = \int d^3\vec{x}'\, \underbrace{K(\vec{x}'',t;\vec{x}',t_0)}_{\text{called as Green's function, propagator, kernel, etc.}}\, \psi(\vec{x}',t_0)}$$

<u>Green's function method is based on Causality.</u>

For example, electrostatic potential from a point charge is given by

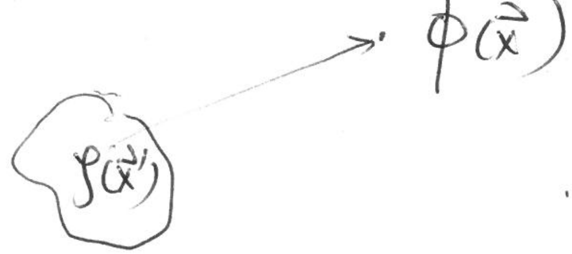
$$\phi(\vec{x}) = \frac{q \leftarrow \text{source}}{|\vec{x}-\vec{x}_0|}$$

resulted potential



Once the Green's function is known, then one can get the resulted potential from any given charge distribution. Causality!

$$\phi(\vec{x}) = \int \frac{\rho(\vec{x}')}{|\vec{x}-\vec{x}'|} d^3\vec{x}'$$



$$= \int G(\vec{x}-\vec{x}')\rho(\vec{x}')\,d^3\vec{x}'$$

Green's function. Boundary conditions are already implemented in the Green's function.

$$\boxed{\vec{\nabla}^2\left(\frac{1}{|\vec{x}-\vec{x}'|}\right) = -4\pi\delta(\vec{x}-\vec{x}')}$$

$$\boxed{\vec{\nabla}^2 G(\vec{x}-\vec{x}') = -4\pi\delta(\vec{x}-\vec{x}')}$$

$$\boxed{\vec{\nabla}^2\phi(\vec{x}) = -4\pi\rho(\vec{x})}$$

$$K(\vec{x}'', t; \vec{x}', t_0) = \sum_a \langle \vec{x}'' | a \rangle \langle a | \vec{x}' \rangle e^{\frac{-iE_a(t-t_0)}{\hbar}}$$

$$= \sum_a \langle \vec{x}'' | e^{\frac{-iHt}{\hbar}} | a \rangle \langle a | e^{\frac{iHt_0}{\hbar}} | \vec{x}' \rangle$$

$$= \langle \vec{x}'' | e^{\frac{-iH(t-t_0)}{\hbar}} | \vec{x}' \rangle$$

$$= \langle \vec{x}'', t | \vec{x}', t_0 \rangle \sim e^{\frac{iS_{cl}}{\hbar}} \text{ (path integral)}$$

__Ex.__ SHO in 1-dim.

$$K(x'', t; x', t_0) = \sum_n u_n(x'') u_n^*(x') e^{\frac{-iE_n(t-t_0)}{\hbar}}$$

$$= \sum_n \underbrace{\left[u_n(x'') e^{\frac{-iE_n t}{\hbar}} \right]}_{\psi_n(x'', t)} \underbrace{\left[u_n^*(x') e^{\frac{iE_n t_0}{\hbar}} \right]}_{\psi_n^*(x', t_0)}$$

$$= \sum_n \frac{1}{\pi^{1/4} 2^{n/2} \sqrt{n!} \sqrt{x_0}} e^{-\frac{1}{2}\left(\frac{x''}{x_0}\right)^2} H_n\left(\frac{x''}{x_0}\right) e^{-i\omega(n+\frac{1}{2})t}$$

$$\times \frac{1}{\pi^{1/4} 2^{n/2} \sqrt{n!} \sqrt{x_0}} e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2} H_n\left(\frac{x'}{x_0}\right) e^{i\omega(n+\frac{1}{2})t_0}$$

$$= \sum_n \frac{1}{\pi^{1/2} 2^n n! x_0} e^{-\frac{1}{2}\frac{x''^2 + x'^2}{x_0^2}} H_n\left(\frac{x''}{x_0}\right) H_n\left(\frac{x'}{x_0}\right) e^{-i\omega(n+\frac{1}{2})(t-t_0)}$$

$$= \frac{1}{\sqrt{\pi} x_0} e^{-\left\{\frac{x''^2 + x'^2}{2x_0^2} + i\frac{\omega}{2}(t-t_0)\right\}} \sum_n \frac{\left[e^{-i\omega(t-t_0)}\right]^n}{2^n n!} H_n\left(\frac{x''}{x_0}\right) H_n\left(\frac{x'}{x_0}\right)$$

⑦

$$\boxed{e^{-(x^2+y^2)} \sum_{n=0}^{\infty} \left(\frac{t^n}{2^n n!}\right) H_n(x) H_n(y) = \frac{1}{\sqrt{1-t^2}} e^{-\frac{x^2+y^2-2xyt}{1-t^2}} \quad (\text{e.g. } t=0 \text{ case})}$$

$$e^{-\frac{x''^2+x'^2}{x_0^2}} \sum_n \frac{\left[e^{-i\omega(t-t_0)}\right]^n}{2^n n!} H_n\left(\frac{x''}{x_0}\right) H_n\left(\frac{x'}{x_0}\right)$$

$$= \frac{1}{\left[1-e^{-2i\omega(t-t_0)}\right]^{\frac{1}{2}}} e^{-\frac{\left(\frac{x''}{x_0}\right)^2+\left(\frac{x'}{x_0}\right)^2-2\left(\frac{x''}{x_0}\right)\left(\frac{x'}{x_0}\right)e^{-i\omega(t-t_0)}}{1-e^{-2i\omega(t-t_0)}}}$$

$$= \frac{e^{i\frac{\omega}{2}(t-t_0)}}{\left[e^{i\omega(t-t_0)}-e^{-i\omega(t-t_0)}\right]^{\frac{1}{2}}} e^{-\frac{(x''^2+x'^2)\overbrace{e^{i\omega(t-t_0)}}^{\cos\omega(t-t_0)+i\sin\omega(t-t_0)}-2x''x'}{x_0^2\left[e^{i\omega(t-t_0)}-e^{-i\omega(t-t_0)}\right]}}$$

$$= \frac{e^{i\frac{\omega}{2}(t-t_0)}}{\left[2i\sin\omega(t-t_0)\right]^{1/2}} e^{-\frac{(x''^2+x'^2)\cos\omega(t-t_0)-2x''x'}{2x_0^2 i\sin\omega(t-t_0)}} \times e^{-\frac{x''^2+x'^2}{2x_0^2}}$$

$$\therefore K(x'',t;x',t_0) = \frac{1}{\sqrt{\pi}\,x_0} e^{\frac{x''^2+x'^2}{2x_0^2}} e^{-i\frac{\omega}{2}(t-t_0)} e^{-\frac{x''^2+x'^2}{2x_0^2}} e^{i\frac{\omega}{2}(t-t_0)}$$

$$\times \frac{1}{\left[2i\sin\omega(t-t_0)\right]^{1/2}} e^{\frac{i\{(x''^2+x'^2)\cos\omega(t-t_0)-2x''x'\}}{2x_0^2\sin\omega(t-t_0)}}$$

$$= \frac{1}{x_0\sqrt{2\pi i\sin\omega(t-t_0)}} \exp\left[\frac{i\{(x''^2+x'^2)\cos\omega(t-t_0)-2x''x'\}}{2x_0^2\sin\omega(t-t_0)}\right]$$

Eq. (2.6.18) p.119

(8)

Note that in some sense, we found that the generating function as the Green's function since Green's function generates all the eigenfunctions $\psi_n(x'',t)\,\psi_n^*(x',t_0)$.

Properties of $K(\vec{x}'',t\,;\vec{x}',t_0)$

i) $t<t_0$; $K(\vec{x}'',t\,;\vec{x}',t_0)=0$

ii) $t>t_0$; $i\hbar\frac{\partial}{\partial t}\underbrace{\psi(\vec{x}'',t)}_{\int d^3\vec{x}'\,K\,\psi(\vec{x}',t_0)}=\left\{-\frac{\hbar^2}{2m}\vec{\nabla}''^2+V(\vec{x}'')\right\}\underbrace{\psi(\vec{x}'',t)}_{\int d^3\vec{x}'\,K\,\psi(\vec{x}',t_0)}$ for any $\psi(\vec{x}',t_0)$

or $$i\hbar\frac{\partial}{\partial t}K(\vec{x}'',t\,;\vec{x}',t_0)=\left\{-\frac{\hbar^2}{2m}\vec{\nabla}''^2+V(\vec{x}'')\right\}K(\vec{x}'',t\,;\vec{x}',t_0)$$

or $$\left[-\frac{\hbar^2}{2m}\vec{\nabla}''^2+V(\vec{x}'')-i\hbar\frac{\partial}{\partial t}\right]K(\vec{x}'',t\,;\vec{x}',t_0)=0.$$

iii) $t\to t_0$;

$$\lim_{t\to t_0}K(\vec{x}'',t\,;\vec{x}',t_0)=\lim_{t\to t_0}\sum_a\langle\vec{x}''|a\rangle\langle a|\vec{x}'\rangle e^{\frac{-iE_a(t-t_0)}{\hbar}}$$
$$=\sum_a\langle\vec{x}''|a\rangle\langle a|\vec{x}'\rangle=\langle\vec{x}''|\vec{x}'\rangle=\delta^3(\vec{x}''-\vec{x}')$$

Since the Kernel is nontrivial in the region $t\to t_0$, let's integrate over $t_0-\epsilon<t<t_0+\epsilon$ as $\epsilon\to 0$;

mean value in the interval

$$\lim_{\epsilon\to 0}\int_{t_0-\epsilon}^{t_0+\epsilon}dt\left\{-\frac{\hbar^2}{2m}\vec{\nabla}''^2+V(\vec{x}'')-i\hbar\frac{\partial}{\partial t}\right\}K(\vec{x}'',t\,;\vec{x}',t_0)=\lim_{\epsilon\to 0}\Big[2\epsilon\left\{-\frac{\hbar^2}{2m}\vec{\nabla}''^2+V(\vec{x}'')\right\}K(\vec{x}'',\bar{t}\,;\vec{x}',t_0)$$
$$-i\hbar K(\vec{x}'',t_0+\epsilon\,;\vec{x}',t_0)+i\hbar\underbrace{K(\vec{x}'',t_0-\epsilon\,;\vec{x}',t_0)}_{0\text{ due to causality}}\Big]=-i\hbar K(\vec{x}'',t_0\,;\vec{x}',t_0)=-i\hbar\delta^3(\vec{x}''-\vec{x}')$$

Thus, we find

$$\left[-\frac{\hbar^2}{2m}\vec{\nabla}''^2+V(\vec{x}'')-i\hbar\frac{\partial}{\partial t}\right]K(\vec{x}'',t;\vec{x}',t_0)=-i\hbar\,\delta^3(\vec{x}''-\vec{x}')\,\delta(t-t_0)$$

Check for S.H.O in 1+1 dim

$$K(x'',t_0;x',t_0)=\lim_{\epsilon\to 0}\frac{1}{x_0\sqrt{2\pi i\epsilon}}\,e^{i\frac{(x''-x')^2}{2x_0^2\epsilon}}=\delta(x''-x')$$

as expected.

where

$$\epsilon=\omega(t-t_0)$$

$$\sin\epsilon\approx\epsilon\,,\quad\cos\epsilon\approx 1$$

$$\int_{-\infty}^{\infty}e^{\frac{i(x''-x')^2}{2x_0^2\epsilon}}dx''=\sqrt{2\pi i\epsilon}\;x_0\,,\quad\text{i.e.}\int_{-\infty}^{\infty}dx''\,\delta(x''-x')=1.$$

$$\int_{-\infty}^{\infty}e^{-r^2x^2}dx=\frac{\sqrt{\pi}}{r}\,,\quad\text{where } r^2=\frac{1}{2i\epsilon x_0^2}$$

$$\frac{1}{r}=\sqrt{2i\epsilon}\;x_0$$

Formulae Reminder

Dispersion of Operator: $<(\Delta A)^2> = <A^2> - <A>^2$

Algebra of Spin ½ Operators: $[S_i\,, S_j] = i\hbar\varepsilon_{ijk}S_k$, $\{S_i\,, S_j\} = \dfrac{\hbar^2}{2}\delta_{ij}I$

Trigonometry: $\cos\theta = 2\cos^2\dfrac{\theta}{2} - 1$, $\sin\theta = 2\sin\dfrac{\theta}{2}\cos\dfrac{\theta}{2}$

Matrix Representation of spin ½ eigenstates:

$$|1/2,1/2> \doteq \begin{bmatrix}1\\0\end{bmatrix}, \quad |1/2,-1/2> \doteq \begin{bmatrix}0\\1\end{bmatrix}$$

$$<1/2,1/2| \doteq \begin{bmatrix}1 & 0\end{bmatrix}, \quad <1/2,-1/2| \doteq \begin{bmatrix}0 & 1\end{bmatrix}$$

Unitary Operator: $UU^+ = U^+U = I$

Position Wavefunction: $\psi_\alpha(x') = <x'|\alpha>$

Normalization of Wavefunction: $\int_{-\infty}^{\infty} dx'\, |\psi_\alpha(x')|^2 = 1$

Completeness of Position Space: $\int_{-\infty}^{\infty} dx'\, |x'><x'| = I$

Commutation Relation between Position and Momenetum Operators:

$$[x,p] = i\hbar$$

Simple Harmonic Oscillator:

$$[a, a^+] = 1,$$

$$a^+ | n> = \sqrt{n+1} \, | n+1>,$$

$$a | n> = \sqrt{n} \, | n-1>,$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^+),$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(-a + a^+).$$

Time Evolution Operator:

$$U(t, t_0 = 0) \equiv U(t) = \exp\left(\frac{-iHt}{\hbar}\right).$$

Heisenberg Picture Observable:

$$A^{(H)}(t) = U^+(t) A^{(S)} U(t),$$

$$\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}\left[A^{(H)}, H\right].$$

Baker-Hausdorff Lemma:

$$\exp(iG\lambda) A \exp(-iG\lambda) = A + i\lambda[G, A] + \left(\frac{i^2\lambda^2}{2!}\right)[G,[G, A]] + \cdots + \left(\frac{i^n\lambda^n}{n!}\right)[G,[G,[G, \cdots [G, A]]] \cdots] + \cdots$$

Propagator for a free particle in one dimension:

$$K(x'', t\,;\, x', t_0) = \sqrt{\frac{m}{2\pi i\hbar(t-t_0)}}\exp\left[\frac{im(x''-x')^2}{2\hbar(t-t_0)}\right]$$

Gaussian Integrations:

$$\int_0^\infty dx\, e^{-r^2x^2} = \frac{\sqrt{\pi}}{2r} \quad ; \quad \int_0^\infty dx\, x\, e^{-r^2x^2} = \frac{1}{2r^2} \quad ; \quad \int_0^\infty dx\, x^2 e^{-r^2x^2} = \frac{\sqrt{\pi}}{4r^3}$$