Solved Problem

Green Function for Schrodinger equation

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§1 Lesson Overview

Syllabus Green function as vacuum expectation value of time ordered product of Schrodinger field.

Prerequisites Time development in quantum mechanics; Definition of Green function for a partial differential equation.

Objectives

1. To introduce the vacuum expectation value (VEV) of time ordered product of field operators. and to relate it to the Green function of the Schrodinger equation.
2. To evaluate the VEV of time ordered product using the solution of the field equations.
3. To show that the Green function is related to the propagator for Schrodinger equation in quantum mechanics.

§2 Recall and Discuss

§2.1 Solution of Time Dependent Schrodinger Equation

For time independent Hamiltonian $\widehat{H}$ the solution of the time dependent Schrodinger equation is

$$\psi(\mathbf{x},t) = \sum_n c_n e^{-iE_n(t-t_0)/\hbar} u_n(\mathbf{x}). \tag{1}$$

where E_n, u_n are the energy eigenvalues and eigenfunctions and c_n are given in terms of the wave function $\psi(\mathbf{x}, t_0$ at time t_0 by

$$c_n = \int u_n^*(\mathbf{x})\psi(\mathbf{x},t_0)\, d\mathbf{x} \tag{2}$$

§2.2 Propagator in quantum mechanics

The propagator $K(\mathbf{x},t;\mathbf{x}_0 t_0)$ for Schrodinger equation is defined as solution of the time dependent Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}K(\mathbf{x},t;\mathbf{x}_0,t_0) - \widehat{H}K(\mathbf{x},t;\mathbf{x}_0,t_0) = 0 \tag{3}$$

subject to the initial condition

$$K(\mathbf{x},t;\mathbf{x}_0,t_0)\big|_{t=t_0} = \delta^{\mathbf{x}-\mathbf{x}_0}. \tag{4}$$

The Green function $G(\mathbf{x},t;\mathbf{x}_0,t_0)$ defined by

$$G(\mathbf{x},t;\mathbf{x}_0,t_0) = \theta(t-t_0)K(\mathbf{x},t;\mathbf{x}_0,t_0) \tag{5}$$

obeys

$$i\hbar\frac{\partial}{\partial t}G(\mathbf{x},t;\mathbf{x}_0,t_0) - \widehat{H}G(\mathbf{x},t;\mathbf{x},t_0) = \delta(\mathbf{x}-\mathbf{x}_0). \qquad \text{Verify this} \tag{6}$$

§3 VEV of Time Ordered Product

(a) We will show that

$$G(\mathbf{x}-\mathbf{x}',t-t') = \langle 0|T\big(\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')\big)|0\rangle \tag{7}$$

obeys the equation for Green function of the free particle Schrodinger equation.

(b) Using the expansion of the field operator in terms of free particle wave it will be proved that function $N\exp(ik\mathbf{x} - iE_k t)$, where $E_k = \frac{\hbar^2 k^2}{2m}$. Obtain an explicit expression for this time ordered product as a function of $\mathbf{x}, t, \mathbf{x}', t'$.

(c) Have you seen this object before? Where?

Details

(a) The field operator satisfies the equation

$$i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{x},t)$$

The function $G(\mathbf{x},t;\mathbf{x}',t')$ is

$$\begin{aligned} G(\mathbf{x},t;\mathbf{x}',t') =& \langle 0|T\big(\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')\big)|0\rangle \\ =& \langle 0|\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle\theta(t-t') + \langle 0|\psi^\dagger(\mathbf{x}'t')\psi(\mathbf{x},t)|0\rangle\theta(t'-t) \end{aligned}$$

Therefore,

$$\begin{aligned} & i\hbar\frac{\partial}{\partial t}G(\mathbf{x},t;\mathbf{x}',t') \\ =& \quad \langle 0|i\hbar\frac{\partial}{\partial t}\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle\theta(t-t') + i\hbar\langle 0|\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle\delta(t-t') \\ & +i\hbar\langle 0|\psi^\dagger(\mathbf{x}',t')\frac{\partial}{\partial t}\psi(\mathbf{x},t)|0\rangle\theta(t'-t) - i\hbar\langle 0|\psi^\dagger(\mathbf{x}',t')\psi(\mathbf{x},t)|0\rangle\delta(t'-t) \end{aligned}$$

we have used $\quad \frac{d}{dt}\theta(t-t') = \delta(t-t') = -\frac{d}{dt}\theta(t'-t)$

$$\begin{aligned} =& \quad -\frac{\hbar^2}{2m}\nabla^2\langle 0|\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle\theta(t-t') - \frac{\hbar^2}{2m}\nabla^2\langle 0|\psi^\dagger(\mathbf{x}',t')\psi(\mathbf{x},t)|0\rangle\theta(t'-t) \\ & +i\hbar\langle 0|\big[\psi(\mathbf{x},t),\psi^\dagger(\mathbf{x}',t')\big]|0\rangle\delta(t-t') \end{aligned}$$

The last term becomes equal time commutator due to $\delta(t-t')$ function. Therefore, we get

$$i\hbar\frac{\partial}{\partial t}G(\mathbf{x},t;\mathbf{x}',t') + \frac{\hbar^2}{2m}\nabla^2 G(\mathbf{x},t,\mathbf{x}',t') = i\hbar\delta(t-t')\delta(\mathbf{x}-\mathbf{x}')$$

(b) The field $\psi(\mathbf{x},t)$ obeys free particle equation therefore we write it as a superposition

$$\psi(\mathbf{x},t) = \iiint_{-\infty}^{\infty} \frac{d^3k}{(2\pi)^{3/2}}\exp(i\mathbf{k}\cdot\vec{\mathbf{x}} - iE_k t/\hbar)\, a(\mathbf{k})$$

of free particle solutions $\dfrac{1}{(2\pi)^{3/2}}\exp(i\mathbf{k}\cdot\mathbf{x} - iE_k t/\hbar)$. Now

$$\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t') \quad = \quad \iiint_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^{3/2}}e^{i\mathbf{k}\cdot\mathbf{x}-iE_kt/\hbar}a(\mathbf{k}) \times \iiint_{-\infty}^{\infty}\frac{d^3q}{(2\pi)^{3/2}}e^{-i\mathbf{q}\cdot\mathbf{x}'+iE_qt'/\hbar}a^\dagger(\mathbf{q})$$

Therefore, the vacuum expectation value of the time ordered product becomes

$$\begin{aligned} & \langle 0|T\big[\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')\big]|0\rangle \\ & = \iiint_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^{3/2}}\iiint_{-\infty}^{\infty}\frac{d^3q}{(2\pi)^{3/2}}e^{i(\mathbf{k}\cdot\vec{\mathbf{x}}-E_kt/\hbar)}e^{-i(\mathbf{q}\cdot\mathbf{x}'-E_qt/\hbar)} \\ & \times \big\{\langle 0|a(\mathbf{k})a^\dagger(\mathbf{q})|0\rangle\theta(t-t') + \langle 0|a^\dagger(\mathbf{q})a(\mathbf{k})|0\rangle\theta(t'-t)\big\} \end{aligned}$$

The last term vanishes because $a|0\rangle = 0$. Also

$$\begin{aligned} \langle 0|a(\mathbf{k})a^\dagger(\mathbf{q})|0\rangle\theta(t-t') &= \langle 0|\big[a(\mathbf{k}),a^\dagger(\mathbf{q})\big]|0\rangle\theta(t-t') + \langle 0|a^\dagger(\mathbf{q})a(\mathbf{k})|0\rangle\theta(t-t') \\ &= \delta(\mathbf{k}-\mathbf{q})\theta(t-t') \qquad (8) \end{aligned}$$

Substituting in Eq.(1) and using $\delta(\mathbf{k}-\mathbf{q})$ to do the $\mathbf{q}$ integrals gives

$$\langle 0|T\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle = \theta(t-t')\iiint_{-\infty}^{\infty}\frac{d^3k}{(2\pi)^3}\exp\left[\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}') - \frac{i\hbar^2}{2m}\frac{(t-t')\mathbf{k}^2}{\hbar}\right]$$

The integrals over $\mathbf{k}$ are now Gaussian and can be done by completing the sequences. This gives the answer for the vacuum expectation value of the time ordered product as

$$\langle 0|T\psi(\mathbf{x},t)\psi^\dagger(\mathbf{x}',t')|0\rangle = \theta(t-t')\left[\frac{m}{2\pi i\hbar(t-t')}\right]^{3/2}\exp\left(\frac{im(\mathbf{x}-\mathbf{x}')^2}{2\hbar(t-t')}\right)$$

(c) This expression is just the Green function for free particle wave function in Schrodinger quantum mechanics.

$$\psi(\mathbf{x},t) = \iiint d\mathbf{x}' G(\mathbf{x},t;\mathbf{x}',t')\psi(\mathbf{x}',t')d\mathbf{x}'$$

§4 EndNotes

§4.1 Green function

The Green function for a partial differential equation

$$LG(\mathbf{x},t;\mathbf{x}_0,t_0) = \delta(\mathbf{x}-\mathbf{x}_0) \tag{9}$$

will depend on $t-t_0$ if the operator L does not depend on time explicitly. In this case the solution can be obtained in terms of eigenfunctions of L, as you have seen in quantum mechanics. The Green function can be written as

$$G(\mathbf{x},t;\mathbf{x},t_0) = \theta(t-t_0))K(\mathbf{x},t;\mathbf{x}_0,t_0) \tag{10}$$

and $K(\mathbf{x},t;\mathbf{x}_0,t_0)$ obeys the equation

$$LK(\mathbf{x},t;\mathbf{x},t_0) = 0, \qquad \text{where } K(\mathbf{x},t;\mathbf{x}_0,t_0)\big|_{t=t_0} = \delta(\mathbf{x}-\mathbf{x}_0) \tag{11}$$

As you would realize that the corresponding objects in quantum mechanics and field theory discussed in this lesson are just special cases for $L = H$.