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Department of Physics

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Quantum Field Theory — Problem Sheet 2

Problem 3: Propagators of Schrödinger Theory

Consider a non-relativistic particle of mass m, which moves in one dimension under the influence of a potential $V(x)$. Then the corresponding wave function $\psi(x,t)$ evolves from an initial wave function

$$\psi(x_0,t_0) = \psi_0(x_0,t_0) \tag{1}$$

given at time t_0 according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right\}\psi(x,t) \tag{2}$$

In the following you solve this initial value problem (1), (2) with the help of the fundamental solutions

$$u_n(x,t) = \varphi_n(x)\,\exp\left\{-\frac{i}{\hbar}E_n t\right\} \tag{3}$$

where $\varphi_n(x)$ represent the eigenfunctions and E_n the eigenvalues of the Hamilton operator:

$$\left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right\}\varphi_n(x) = E_n\varphi_n(x)\,. \tag{4}$$

Note that the quantum numbers n can be both discrete and continuous. The orthonormality and completeness relation of the fundamental solutions are then given by

$$\left(u_n(x,t), u_{n'}(x,t)\right) = \delta(n-n')\,, \tag{5}$$

$$\sum\!\!\!\!\!\!\!\int_n u_n(x,t)u_n^*(x_0,t) = \delta(x-x_0)\,, \tag{6}$$

Here $\delta(n-n')$ in the orthonormality relation (5) represents the Kronecker symbol for discrete and the Dirac delta function for continuous quantum numbers, respectively. Correspondingly one has to use in the completeness relation (6) the sum (integral) for discrete (continuous) quantum numbers. Furthermore, the scalar product of the Schrödinger theory is defined via

$$\left(\psi_1(x,t), \psi_2(x,t)\right) = \int_{-\infty}^{\infty} dx\,\psi_1^*(x,t)\psi_2(x,t)\,. \tag{7}$$

a) Using the completeness relation (6) the solution $\psi(x,t)$ of the Schrödinger equation (2) can be decomposed in the fundamental solutions $u_n(x,t)$:

$$\psi(x,t) = \sum\!\!\!\!\!\!\!\int_n c_n u_n(x,t)\,. \tag{8}$$

Determine the expansion coefficients c_n from the initial condition (1). Show that the time evolution of the wave function $\psi(x,t)$ is related to the initially given wave function (1) according to

$$\psi(x,t) = (G_{\mathrm{I}}^*(x,t;x_0,t_0), \psi_0(x_0,t_0)) \; . \tag{9}$$

Show that the propagator $G_{\mathrm{I}}(x,t;x_0,t_0)$ depends on the fundamental solutions $u_n(x,t)$ via

$$G_{\mathrm{I}}(x,t;x_0,t_0) = \sum\!\!\!\!\!\!\int_n \; u_n(x,t)u_n^*(x_0,t_0) \tag{10}$$

(2 points)

b) Prove the following properties of the propagator $G_{\mathrm{I}}(x,t;x_0,t_0)$:

- It solves the initial value problem

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}G_{\mathrm{I}}(x,t;x_0,t_0) &= \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right\} G_{\mathrm{I}}(x,t;x_0,t_0)\,, && (11)\\ G_{\mathrm{I}}(x,t_0;x_0,t_0) &= \delta(x-x_0)\,. && (12)\end{aligned}$$

- It obeys the group property $G_{\mathrm{I}}(x_3,t_3;x_1,t_1) = (G_{\mathrm{I}}^*(x_3,t_3;x_2,t_2), G_{\mathrm{I}}(x_2,t_2;x_1,t_1))$.
- It fulfills the symmetry relation $G_{\mathrm{I}}(x,t;x_0,t_0) = G_{\mathrm{I}}^*(x_0,t_0;x,t)$. (3 points)

c) Consider now the special case of a freely moving non-relativistic particle. The fundamental solutions of the Schrödinger equation for $V(x) = 0$ are given by plane waves:

$$u_p(x,t) = N_p \exp\left\{\frac{i}{\hbar}(px - E_p t)\right\} \; . \tag{13}$$

Which dispersion E_p do you get? Find the normalization constants N_p from the orthonormality relation (5) and verify the completeness relation (6). Perform the integration in (10) explicitly and determine the propagator $G_{\mathrm{I}}^{\mathrm{FP}}(x,t;x_0,t_0)$ of the free particle. Show that the propagator $G_{\mathrm{I}}^{\mathrm{FP}}(x,t;x_0,t_0)$ of the free particle fulfills, indeed, the properties of **3b)**.
Note: Prove the Fresnel integral

$$\int_{-\infty}^{\infty} dx\, e^{-ix^2} = \sqrt{\frac{\pi}{i}} \; . \tag{14}$$

To this end use the complex integral $I = \oint_{\mathcal{C}_R} dz\, e^{-z^2}$ along the closed curve

$$\mathcal{C}_R = \begin{cases} z(t) = t & ; t \in [0,R]\,, \\ z(t) = Re^{it} & ; t \in [0,\pi/4]\,, \\ z(t) = te^{i\pi/4} & ; t \in [R,0] \end{cases} \tag{15}$$

and reduce the Fresnel integral (14) in the limit $R \to \infty$ to the Gaussian integral $\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}$. (6 points)

d) Within the realm of perturbation theory investigate now the impact of an external potential upon the non-relativistic particle, where one has to solve the Schrödinger equation with respect to an additional inhomogeneity:

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right\} \psi(x,t) + \xi(x,t)\,. \tag{16}$$

To this end perform a decomposition of the inhomogeneity $\xi(x,t)$ with respect to the eigenfunctions $\varphi_n(x)$ and a Fourier transformation with respect to the time:

$$\xi(x,t) = \sum\!\!\!\!\!\!\int_n \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar}\, \varphi_n(x) \exp\left\{ -\frac{i}{\hbar} E t \right\} \xi(n,E)\,. \tag{17}$$

With a corresponding decomposition of the particular solution $\psi(x,t)$ of the inhomogeneous Schrödinger equation (16) you obtain a connection between the respective expansion coefficients $\xi(n,E)$ and $\psi(n,E)$. Prove the integral

$$\lim_{\eta\downarrow 0} \int_{-\infty}^{\infty} \frac{dE}{2\pi\hbar} \frac{1}{E - E_n + i\eta} \exp\left\{ -\frac{i}{\hbar} E(t-t_0) \right\} = -\frac{i}{\hbar}\,\Theta(t-t_0) \exp\left\{ -\frac{i}{\hbar} E_n (t-t_0) \right\} \tag{18}$$

with the help of the residue theorem, where $\Theta(t-t_0)$ denotes the Heaviside function:

$$\Theta(t-t_0) = \begin{cases} 1 & ; t > t_0\,, \\ 0 & ; t < t_0\,. \end{cases} \tag{19}$$

Prove with this that the particular solution $\psi(x,t)$ has the following form:

$$\psi(x,t) = \int_{-\infty}^{\infty} dx_0 \int_{-\infty}^{\infty} dt_0\, G_{\mathrm{II}}(x,t;x_0,t_0)\, \xi(x_0,t_0)\,. \tag{20}$$

What is the relation between the propagators $G_{\mathrm{I}}(x,t;x_0,t_0)$ and $G_{\mathrm{II}}(x,t;x_0,t_0)$? Prove that the propagator $G_{\mathrm{II}}(x,t;x_0,t_0)$ is a particular solution of the following inhomogeneous Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} G_{\mathrm{II}}(x,t;x_0,t_0) = \left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \right\} G_{\mathrm{II}}(x,t;x_0,t_0) + \delta(x-x_0)\delta(t-t_0)\,. \tag{21}$$

(4 points)

e) Summarize the previous results by deriving the Lippmann-Schwinger integral equation for the propagator $G_{\mathrm{I}}(x,t;x_0,t_0)$:

$$\begin{aligned} G_{\mathrm{I}}(x,t;x_0,t_0) &= G_{\mathrm{I}}^{\mathrm{FP}}(x,t;x_0,t_0) \\ &\quad - \frac{i}{\hbar} \int_{-\infty}^{\infty} dx_0' \int_{t_0}^{t} dt_0'\, G_{\mathrm{I}}^{\mathrm{FP}}(x,t;x_0',t_0')\, V(x_0')\, G_{\mathrm{I}}(x_0',t_0';x_0,t_0)\,. \end{aligned} \tag{22}$$

In case that the potential $V(x)$ is small, the propagator $G_{\mathrm{I}}(x_0', t_0'; x_0, t_0)$ on the right-hand side of the Lippmann-Schwinger integral equation can be approximated by the free-particle propagator $G_{\mathrm{I}}^{\mathrm{FP}}(x_0', t_0'; x_0, t_0)$. Determine the propagator $G_{\mathrm{I}}(x, t; x_0, t_0)$ in this order by assuming a harmonic oscillator for the potential $V(x)$. To this end prove the integral

$$\int_{-\infty}^{\infty} dx\, x^2\, e^{ix^2} = \frac{i}{2}\sqrt{i\pi} \tag{23}$$

with the help of the Fresnel integral (14). (5 points)

f) Within a second quantization of the Schrödinger theory both fields $\psi(x,t)$ and $\psi^*(x,t)$ go over into the field operators $\hat{\psi}(x,t)$ and $\hat{\psi}^\dagger(x,t)$. In case of a bosonic field quantization one has to postulate equal-time canonical commutator relations between the field operators $\hat{\psi}(x,t)$ and $\hat{\psi}^\dagger(x,t)$:

$$\left[\hat{\psi}(x,t), \hat{\psi}(x_0,t)\right]_- = \left[\hat{\psi}^\dagger(x,t), \hat{\psi}^\dagger(x_0,t)\right]_- = 0\,, \quad \left[\hat{\psi}(x,t), \hat{\psi}^\dagger(x_0,t)\right]_- = \delta(x - x_0)\,. \tag{24}$$

Expand both field operators with respect to the fundamental solutions $u_n(x,t)$:

$$\hat{\psi}(x,t) = \sum_n\!\!\!\!\!\!\int \hat{c}_n\, u_n(x,t)\,, \qquad \hat{\psi}^\dagger(x,t) = \sum_n\!\!\!\!\!\!\int \hat{c}_n^\dagger\, u_n^*(x,t)\,. \tag{25}$$

Determine the commutator relations between the operators $\hat{c}_n$ and $\hat{c}_n^\dagger$. Determine with this

- the commutator of the field operators at different times

$$\left[\hat{\psi}(x,t), \hat{\psi}^\dagger(x_0,t_0)\right]_- = ?\,, \tag{26}$$

- the vacuum expectation value of the time-ordered product of the field operators

$$-\frac{i}{\hbar}\,\langle 0|\hat{T}\left(\hat{\psi}(x,t)\hat{\psi}^\dagger(x_0,t_0)\right)|0\rangle = ?\,. \tag{27}$$

Here the action of the time-ordering operator $\hat{T}$ upon two field operators $\hat{A}(x,t)$ and $\hat{B}(x,t)$ is defined according to

$$\hat{T}\left(\hat{A}(x,t)\hat{B}(x_0,t_0)\right) = \Theta(t - t_0)\,\hat{A}(x,t)\hat{B}(x_0,t_0) + \Theta(t_0 - t)\,\hat{B}(x_0,t_0)\hat{A}(x,t) \tag{28}$$

and the vacuum state $|0\rangle$ is given by $\hat{c}_n|0\rangle = 0$ for all n. With which propagators can you identify (26) and (27), respectively? (3 points)

Drop the solutions in the post box on the 5th floor of building 46 or send them via email to radonjic@physik.uni-kl.de until November 12, 2020 at 12.00!