Physics 125
Course Notes
Solving the Schrödinger Equation: Resolvents
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1 Introduction

Once a system is well-specified, the problem posed in non-relativistic quantum mechanics is to solve the Schrödinger equation. Once the solutions are known, then any question of interest can in principle be answered, by taking appropriate expectation values of operators between states made from the solutions. There are many approaches to obtaining the solutions, analytic, approximate, partial, and numerical. All have important applications. In this note, we exam the approach of obtaining analytic solutions using conventional methods of analysis. In particular, we develop a means to apply the powerful techniques of complex analysis to this problem.

2 Resolvents and Green's Functions

We have already considered the interpretation of a function of a self-adjoint operator Q, with point spectrum (eignevalues) $\Sigma(Q) = \{q_i; i = 1, 2, \dots\}$, and spectral resolution

$$Q = \sum_{k=1}^{\infty} q_k |k\rangle\langle k|, \tag{1}$$

where

$$\begin{aligned} Q|k\rangle &= q_k|k\rangle & (2)\\ \langle k|j\rangle &= \delta_{kj} & (3)\\ I &= \sum_{k=1}^{\infty} |k\rangle\langle k|. & (4) \end{aligned}$$

In particular, the eigenvectors of Q form a complete orthonormal set.

If $f(q)$ is any function defined on $\Sigma(Q)$, then we define

$$f(Q) = \sum_{k} f(q_k)|k\rangle\langle k|. \tag{5}$$

It may be observed that $[f(Q), Q] = 0$. If $f(q)$ is defined and bounded on $\Sigma(Q)$, then $f(Q)$ is a bounded operator, where the norm of an operator is defined according to:

$$\begin{aligned} \|f(Q)\|_{\text{op}} &\equiv \sup_{\|\phi\|=1} \|f(Q)\phi\| & (6) \\ &= \sup_{q\in\Sigma(Q)} |f(q)| & (7) \\ &< \infty, \quad \text{if } f(q) \text{ is bounded.} & (8) \end{aligned}$$

Now define an operator-valued function $G(z)$, called the **resolvent** of Q, of complex variable z, for all z not in $\Sigma(Q)$ by:[1]

$$G(z) = \frac{1}{Q-z}, \qquad z \notin \Sigma(Q). \tag{9}$$

For any such z the operator $G(z)$ is bounded, and we have

$$\|G(z)\|_{\text{op}} = \sup_k \frac{1}{|q_k - z|}. \tag{10}$$

The resolvent satisfies the identities

$$\begin{aligned} G(z) - G(z_0) &= \sum_k \left(\frac{1}{q_k - z} - \frac{1}{q_k - z_0} \right) |k\rangle\langle k| \\ &= \sum_k \frac{z - z_0}{(q_k - z)(q_k - z_0)} |k\rangle\langle k| \\ &= \frac{z - z_0}{(Q - z)(Q - z_0)} \\ &= (z - z_0) G(z) G(z_0), & (11) \end{aligned}$$

$$G(z) = \frac{G(z_0)}{1 + (z_0 - z)G(z_0)}, \tag{12}$$

and

$$Q = z + 1/G(z). \tag{13}$$

If the eigenvectors are written as functions of $\mathbf{x} \in R^3$ (assuming that the Hilbert space is $L_2(R^3)$), we can represent the resolvent as an integral transform on the wave functions. That is, with

$$G(z) = \frac{1}{Q-z} = \sum_k \frac{|k\rangle\langle k|}{q_k - z}, \tag{14}$$

[1]The resolvent is sometimes defined with the opposite sign. We shall see eventually that $G(z)$ also finds motivation in terms of Cauchy's integral formula.

and

$$|k\rangle = \phi_k(\mathbf{x}), \tag{15}$$

we define

$$G(\mathbf{x},\mathbf{y};z) = \sum_k \frac{\phi_k(\mathbf{x})\phi_k^*(\mathbf{y})}{q_k - z}, \tag{16}$$

so that G operates on a wave function according to

$$\left[G(z)\psi\right](\mathbf{x}) = \int_{(\infty)} d^3(\mathbf{y}) G(\mathbf{x},\mathbf{y};z)\psi(\mathbf{y}). \tag{17}$$

Thus $G(\mathbf{x},\mathbf{y};z)$ is the *kernel* of an integral transform. We may see that this correspondence is as claimed as follows: Expand

$$\psi(\mathbf{y}) = \sum_\ell \psi_\ell \phi_\ell(\mathbf{y}). \tag{18}$$

Then

$$\begin{aligned}
&\int_{(\infty)} d^3(\mathbf{y}) \sum_k \frac{\phi_k(\mathbf{x})\phi_k^*(\mathbf{y})}{q_k - z} \sum_\ell \psi_\ell \phi_\ell(\mathbf{y}) \\
&\quad = \sum_k \frac{\phi_k(\mathbf{x})}{q_k - z} \sum_\ell \psi_\ell \int_{(\infty)} d^3(\mathbf{y}) \phi_k^*(\mathbf{y}) \phi_\ell(\mathbf{y}) \\
&\quad = \sum_k \frac{\psi_l \phi_k(\mathbf{x})}{q_k - z}.
\end{aligned} \tag{19}$$

This is to be compared with

$$\begin{aligned}
\left[G(z)\psi\right](\mathbf{x}) &= \sum_k \frac{1}{q_k - z} |k\rangle\langle k| \sum_\ell \psi_\ell |\ell\rangle \\
&= \sum_k \frac{\psi_l \phi_k(\mathbf{x})}{q_k - z}.
\end{aligned} \tag{20}$$

We have thus demonstrated the representation as an integral transform. Similar results would apply on other L_2 spaces of wave functions besides $L_2(R^3)$.

Consider now the formal relation:

$$(Q - z)G(z) = (Q - z)\frac{1}{Q - z} = I. \tag{21}$$

Corresponding to this, we have operator:[2]

$$(Q_x - z)G(\mathbf{x}, \mathbf{y}; z) = \delta^{(3)}(\mathbf{x} - \mathbf{y}), \tag{22}$$

since $\delta^{(3)}(\mathbf{x}-\mathbf{y})$ is the kernel corresponding to I. This delta-function is thus symbolic of the relation:

$$(Q_x - z) \int_{(\infty)} d^{(3)}(\mathbf{y}) G(\mathbf{x}, \mathbf{y}; z)\psi(\mathbf{y}) = \psi(\mathbf{x}), \tag{23}$$

for any continuous $\psi(\mathbf{x})$ in $L_2(R^3)$ (continuous in case Q is a differential operator).

The kernel $G(\mathbf{x}, \mathbf{y}; z)$ is called the **Green's function** for the (differential) operator Q. This Green's function is the "kernel for a resolvent"(as with the resolvent, the sign convention is not universal). It is the solution of the homogeneous differential equation (Eqn. 22), which satisfies "the" boundary conditions since it may be expressed in an expansion of basis vectors satisfying the boundary conditions:

$$G(\mathbf{x}, \mathbf{y}; z) = \sum_{k=1}^{\infty} \frac{\phi_k(\mathbf{x})\phi_k^*(\mathbf{y})}{q_k - z}. \tag{24}$$

From this relation, we also see the symmetry property:

$$G(\mathbf{x}, \mathbf{y}; z)^* = G(\mathbf{y}, \mathbf{x}; z^*). \tag{25}$$

Our definition of $G(z) \equiv \frac{1}{Q-z}$ suggests that the resolvent is an analytic (operator-valued) function of z in the complement of the spectrum of Q. For any point $z_0 \notin \Sigma(Q)$, we have the power series:

$$G(z) = G(z_0) \sum_{n=0}^{\infty} \left[(z - z_0)G(z_0)\right]^n. \tag{26}$$

This series converges in norm inside any disk $|z - z_0| < \rho$ which does not intersect $\Sigma(Q)$. Further, for the n^{th} term in the series, we have

$$\|G(z_0) \left[(z - z_0)G(z_0)\right]^n \|_{\text{op}} \leq \left(\frac{\rho}{\rho_0}\right)^n \frac{1}{\rho_0}, \tag{27}$$

[2] We use a subscript x on Q to denote that, if, for example, Q is a differential operator, the differentiation is on variable $\mathbf{x}$.

where

$$\frac{1}{\rho_0} = \|G(z_0)\|_{\rm op} = \text{distance}\,[z_0, \Sigma(Q)]\,. \tag{28}$$

Since the resolvent is "analytic" we may use contour integration. For example, in Fig. 1 we suppose that contour C_4 encircles a single, non-degenerate, eigenvalue q_4. Then

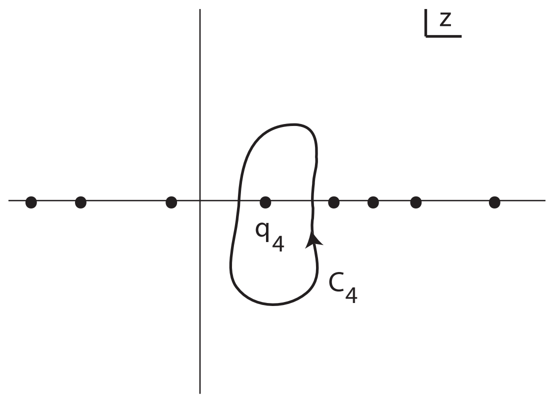

Figure 1: The complex z plane, with eigenvalues of Q indicated on the real axis. A contour is shown encircling one of the eigenvalues.

$$\begin{aligned}
\frac{1}{2\pi i}\int_{C_4} G(z)\,dz &= \frac{1}{2\pi i}\int_{C_4}\sum_{k=1}^{\infty}\frac{|k\rangle\langle k|}{q_k - z}\,dz && (29)\\
&= \frac{1}{2\pi i}\int_{C_4}\frac{|\phi_4\rangle\langle\phi_4|}{q_4 - z}\,dz && (30)\\
&= |\phi_4\rangle\langle\phi_4|\lim_{z\to q_4}\left(\frac{z-q_4}{q_4-z}\right) && (31)\\
&= -|\phi_4\rangle\langle\phi_4|. && (32)
\end{aligned}$$

That is,

$$|\phi_4\rangle\langle\phi_4| = -\frac{1}{2\pi i}\int_{C_4} G(z)\,dz. \tag{33}$$

The contour integral of G around an eigenvalue of Q gives the projection onto the one-dimensional subspace of the corresponding eigenvector of Q.

Now suppose that the spectrum of Q is bounded below, *i.e.*, there exists an $\alpha > -\infty$ such that $q_k > \alpha, \forall k$. Of particular interest is the Hamiltonian, which has this property. In this case, we may consider a contour which encircles all eigenvalues, as in Fig. 2: Then we have

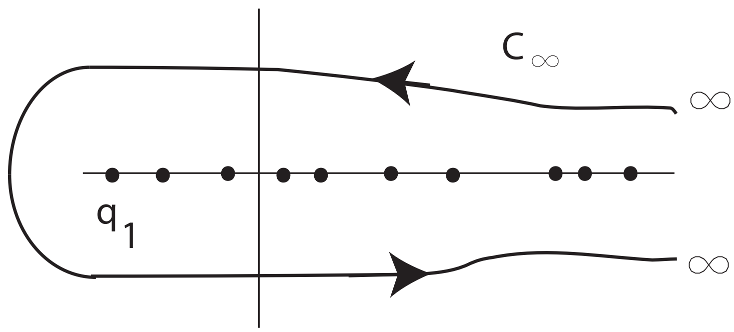

Figure 2: A contour which encircles the entire spectrum of Q.

$$I = -\frac{1}{2\pi i}\int_{C_\infty} G(z)\, dz, \tag{34}$$

as may be proven by a limiting process, and noting that convergence is all right.

According to Cauchy's integral formula, we can express analytic functions of Q in terms of contour integrals: Let $f(z)$ be a function which is analytic in a region which contains C_∞. Then

$$f(Q) = \frac{1}{2\pi i}\int_{C_\infty} \frac{f(z)\, dz}{z - Q} = -\frac{1}{2\pi i}\int_{C_\infty} dz f(z)G(z), \tag{35}$$

assuming the integral converges. In particular consider the function $f(z) = e^{-izt}$:

$$U(t) = e^{-itQ} = -\frac{1}{2\pi i}\int_{C_\infty} G(z)e^{-izt}\, dz = \sum_{k=1}^{\infty} |k\rangle\langle k| e^{-itq_k}, \tag{36}$$

with the restriction that $\mathrm{Im}(t) \leq 0$.

The principal application of all this occurs when $Q = H$ is the Hamiltonian. For real t in this case, $U(t)$ is the **time development transformation**, or **evolution operator**. Note that it satisfies (assuming H carries no explicit time dependence):

$$i\frac{d}{dt}U(t) = i\frac{d}{dt}e^{-itH} = HU(t) \tag{37}$$

$$U(0) = I. \tag{38}$$

We shall consider this case ($Q = H$) henceforth. The kernel of the integral transform representing $U(t)$ is:

$$U(\mathbf{x},\mathbf{y};t) = -\frac{1}{2\pi i}\int_{C_\infty} dz e^{-itz} G(\mathbf{x},\mathbf{y};z) \tag{39}$$

$$= \sum_{k=1}^{\infty} \phi_k(\mathbf{x})\phi_k^*(\mathbf{y})e^{-iq_k t}. \tag{40}$$

If we know $U(\mathbf{x},\mathbf{y};t)$ then we can solve the time-dependent Schrödinger equation given any initial wave function. Corresponding to the above differential equation (Eqn. 37), we have for $U(\mathbf{x},\mathbf{y};t)$:

$$\begin{aligned} i\partial_t U(\mathbf{x},\mathbf{y};t) &= \sum_{k=1}^{\infty} \phi_k(\mathbf{x})\phi_k^*(\mathbf{y})q_k e^{-iq_k t} \\ &= \sum_{k=1}^{\infty} H_x\phi_k(\mathbf{x})\phi_k^*(\mathbf{y})e^{-iq_k t} \\ &= H_x U(\mathbf{x},\mathbf{y};t), \end{aligned} \tag{41}$$

and initial condition

$$U(\mathbf{x},\mathbf{y};0) = \delta^{(3)}(\mathbf{x}-\mathbf{y}). \tag{42}$$

Hence, if $\psi(\mathbf{x})$ is any wave function, then $\psi(\mathbf{x};t)$ defined by:

$$\psi(\mathbf{x};t) \equiv \int_{(\infty)} d^3(\mathbf{y}) U(\mathbf{x},\mathbf{y};t)\psi(\mathbf{y}) \tag{43}$$

satisfies the Schrödinger equation,

$$i\partial_t\psi(\mathbf{x};t) = H_x\psi(\mathbf{x};t), \tag{44}$$

and initial condition

$$\psi(\mathbf{x};0) = \psi(\mathbf{x}). \tag{45}$$

We remark that the resolvent and Green's function, and $U(t)$, actually exist for a larger class of operators, not just those with a pure point spectrum. For example, the resolvent exists for any self-adjoint operator which is bounded below. In particular, we have existence for the Hamiltonian of a free particle, with $H = p^2/2m$. However, we cannot in general express $G(z)$ and $U(t)$ as sums over states, and the Green's function cannot be expressed as a sum over products of eigenfunctions. The contour integral relation:

$$U(\mathbf{x}, \mathbf{y}; t) = -\frac{1}{2\pi i} \int_{C_\infty} dz e^{-itz} G(\mathbf{x}, \mathbf{y}; z) \tag{46}$$

remains valid. We have resorted to the case with a pure point spectrum, with sums over states, in order to develop the feeling for how things work without getting bogged down in mathematical issues.

3 Connection between Schrödinger Equation and Diffusion Equation

Suppose

$$H = -\frac{1}{2m}\nabla^2 + V(\mathbf{x}), \tag{47}$$

and recall

$$U(t) = e^{-itH} = \sum_{k=1}^{\infty} |k\rangle\langle k| e^{iq_k t}. \tag{48}$$

These relations still make sense mathematically if we consider imaginary times $t = -i\tau$ where $\tau \geq 0$:

$$U(-i\tau) = e^{-\tau H}, \tag{49}$$

and then

$$\frac{d}{d\tau} U(-i\tau) = -HU(-i\tau). \tag{50}$$

The corresponding equation for the kernel is thus:

$$\begin{aligned} \partial_\tau U(\mathbf{x}, \mathbf{y}; -i\tau) &= -H_x U(\mathbf{x}, \mathbf{y}; -i\tau) \\ &= \frac{1}{2m}\nabla_x^2 U(\mathbf{x}, \mathbf{y}; -i\tau) - V(x) U(\mathbf{x}, \mathbf{y}; -i\tau). \end{aligned} \tag{51}$$

This is in the form of a **diffusion equation**. Thus, the Schrödinger equation is closely related to a diffusion equation, corresponding to the Schrödinger equation with imaginary time.

However, there is a difference. The Schrödinger equation can be solved in both time directions – "backward prediction" is all right. But the diffusion equation can, for general initial conditions, only be solved in the forward time direction. This is because the operator $U(-i\tau) = e^{-\tau H}$ has the entire Hilbert space as its domain for $\tau > 0$, but not for $\tau < 0$ (since $e^{-\tau H} = \sum_k e^{-\tau\omega_k}|k\rangle\langle k|$, and the $e^{-\tau\omega_k}$ "weight" has unbounded contributions for $\tau < 0$. On the other hand $U(t) = e^{-itH}$ is a unitary operator for all real t, and hence the entire Hilbert space is its domain for all real t.

4 A Brief Revisit to Statistical Mechanics

In the note on density matrices we gave the density matrix for the canonical thermodynamic distribution. With $U(t) = e^{itH}$, we may also write it in terms of U:

$$\rho(T) = \frac{e^{-H/T}}{Z(T)} = \frac{1}{Z(T)} U(-i/T), \tag{52}$$

where we have made the substitution $t = -i/T$. As long as $T \geq 0$, this substitution is mathematically acceptable. The inverse temperature corresponds to an imaginary time coordinate. With this substitution, we also have the partition function:

$$\begin{aligned} Z(T) &= \mathrm{Tr}\left(e^{-H/T}\right) \\ &= \mathrm{Tr}\left[U(-i/T)\right] \qquad (53) \\ &= \int_{(\infty)} d^3(\mathbf{x}) U(\mathbf{x}, \mathbf{y}; -i/T). \qquad (54) \end{aligned}$$

5 Practical Matters

We see that the objects $G(z)$, $U(z)$, *etc.*, are potentially very useful tools towards solving the Schrödinger equation, calculating the partition function, and perhaps other applications. We'll also make the connection of $G(z)$ with perturbation theory later. Let us here address the question of how one goes about constructing these tools in practice in an explicit problem. "Closed form" solutions for the Green's function exist for special cases (with special symmetries of H), and useful forms can be constructed for one-dimensional problems (hence also for spherically symmetric problems in three-dimensions). Otherwise, we can attempt to apply perturbation theory methods towards obtaining useful approximations.

5.1 General Procedure to Construct the Green's Function for a One-dimensional Schrödinger Equation

Let

$$H = -\frac{1}{2m}\frac{d^2}{dx^2} + V(x), \tag{55}$$

where $x \in (a,b)$ (and $a \to -\infty$, $b \to \infty$ is permissible). The Hilbert space is $L_2(a,b)$. Assume $V(x)$ is such that H is bounded below.

Let z be a complex number with $\mathrm{Im}(z) \neq 0$, and consider solutions $u(x;z)$ of the following differential equation:

$$Hu(x;z) = zu(x;z), \tag{56}$$

with boundary condition that the solutions must vanish at the endpoints of the interval. Let $u_L(x;z)$ be a solution satisfying the boundary conditions at the left endpoint, and let $u_R(x;z)$ be a solution satisfying the boundary conditions at the right endpoint. Consider the quantity, called the **Wronskian**:

$$W(z) \equiv u_L'(x;z)u_R(x;z) - u_L(x;z)u_R'(x;z). \tag{57}$$

We only give the Wronskian a z argument, because it has the remarkable property that is is independent of x:

$$\begin{aligned} \frac{dW}{dx} &= u_L'' u_R - u_L u_R'' \\ &= -2m(z-V)u_L u_R - u_L\left[-2m(z-V)\right]u_R \\ &= 0. \end{aligned} \tag{58}$$

Thus, the Wronskian may be evaluated at any convenient value of x.

Now define

$$G(x,y;z) \equiv \frac{2m}{W(z)}\left[u_L(x;z)u_R(y;z)\theta(y-x) + u_L(y;z)u_R(x;z)\theta(x-y)\right], \tag{59}$$

where the step function $\theta(x)$ is defined by:

$$\theta(x) \equiv \begin{cases} 0 & \text{if } x<0, \\ 1/2 & \text{if } x=0 \\ 1 & \text{if } x>0. \end{cases} \tag{60}$$

Since u_L and u_R are continuous functions on (a, b), with continuous first derivatives (in order to be in the domain of H), it follows that

1. $G(x, y; z)$ is a continuous function of x, for $x \in (a, b)$.

2. $G(x, y; z)$ is a differentiable function of x, and the first derivative is continuous at all points $x \in (a, b)$, except for $x = y$, where there is a discontinuity of magnitude:

$$\lim_{\epsilon \to 0^+} \left[(\partial_1 G)(x + \epsilon, x; z) - (\partial_1 G)(x - \epsilon, x; z) \right] = -2m, \tag{61}$$

   where the notation ∂_1 is used to mean "differentiation with respect to the first argument".

3. For $x \neq y$, G satisfies the differential equation

$$H_x G(x, y; z) = zG(x, y; z), \qquad (x \neq y). \tag{62}$$

   We may include the point $x = y$ by writing

$$(H_x - z)G(x, y; z) = \delta(x - y). \tag{63}$$

   This corresponds to the right magnitude for the discontinuity in the first derivative.

4. If H is self-adjoint, then $G(x, y; z)$ is, in fact, our earlier discussed Green's function. It is given by Eqn. 59 for all z (including real z), not in the specturm of H. The discrete eigenvalues of H correspond to poles of G as a function of z. Thus, the bound states can be found by searching for the poles of G, in a suitably cut complex plane (if H has a continuous spectrum, we have a branch cut).

5.2 Example: Force-free Motion

Let us evaluate the Green's function for force-free motion, $V(x) = 0$, in $x \in (-\infty, \infty)$ configuration space:

$$Hu(x; z) = -\frac{1}{2m} \frac{d^2}{dx^2} u(x; z) = zu(x; z). \tag{64}$$

We must have $u_L \to 0$ as $x \to -\infty$, and $u_R \to 0$ as $x \to \infty$. Then we have solutions of the form:

$$u_L(x;z) = e^{-i\rho x}, \qquad u_R(x;z) = e^{i\rho x}, \tag{65}$$

where

$$\rho = \sqrt{2mz}. \tag{66}$$

We select the branch of the square route so that the imaginary part of ρ is positive, as long as z is not along the non-negative real axis. We know that the spectrum of H is the non-negative real axis. Thus, we cut the z-plane along the positive real axis.

To obtain the Wronskian, note that $u_L' = -i\rho u_L$ and $u_R' = i\rho u_R$. Evaluate at $x = 0$ for convenience: $u_L(0) = u_R(0) = 1$. Hence,

$$W(z) = (-i\rho) - (i\rho) = -2i\rho = -2i\sqrt{2mz}. \tag{67}$$

Thus, we obtain the Green's function:

$$\begin{aligned} G(x,y;z) &= \frac{2m}{-2i\sqrt{2mz}}\left[e^{-i\rho x}e^{i\rho y}\theta(y-x) + e^{-i\rho y}e^{i\rho x}\theta(x-y)\right] \\ &= i\sqrt{\frac{m}{2z}}e^{i\rho|x-y|}. \end{aligned} \tag{68}$$

We could have noticed from the start that G had to be a function of $(x-y)$ only, by the translational invariance of the problem.

Let us continue, and obtain the time development transformation $U(x,y;t)$:

$$U(x,y;t) = -\frac{1}{2\pi i}\int_{C_\infty} dz e^{itz} G(x,y;z), \tag{69}$$

where C_∞ is the contour in Fig. 3 With $\rho^2 = 2mz$, we may make the substitution $z = \rho^2/2m$ and $dz = \rho d\rho/m$, to obtain the integral in the ρ plane:

$$U(x,y;t) = -\frac{im}{2\pi i}\int_{\infty+i\epsilon}^{-\infty+i\epsilon} \frac{d\rho}{m} e^{it\rho^2/2m} e^{i\rho|x-y|}. \tag{70}$$

We may take the $\epsilon \to 0$ limit, and guarantee convergence by evaluating the integral at complex time $t \to t - i\tau$, where $\tau > 0$:

$$U(x,y;t-i\tau) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\rho \exp\left\{-\left[\rho^2\left(\frac{1}{2m}(\tau+it)\right) - \rho i|x-y|\right]\right\}. \tag{71}$$

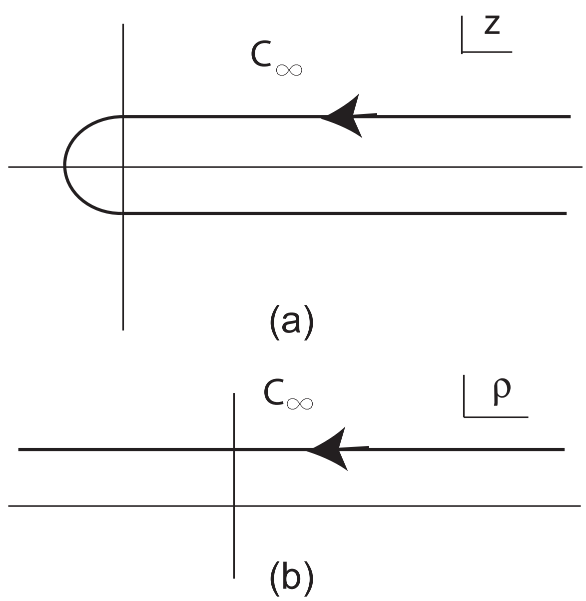

Figure 3: The contour C_∞: (a) in the z plane; (b) in the ρ plane.

We compute by completing the square in the exponent:

$$U(x,y;t-i\tau) = \frac{1}{2\pi} e^{a^2} \int_{-\infty}^{\infty} d\rho \exp\left\{ -\frac{\left[\rho - a/\sqrt{\frac{1}{2m}(\tau+it)}\right]^2}{2\sigma^2} \right\}, \tag{72}$$

where

$$a = \frac{i}{2} \frac{|x-y|}{\sqrt{\frac{1}{2m}(\tau+it)}} \tag{73}$$

$$\sigma = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{\frac{1}{2m}(\tau+it)}}. \tag{74}$$

The integral is now in the form of the integral of a Gaussian, and has the value $\sqrt{2\pi}\sigma$. Therefore,

$$\begin{aligned} U(x,y;t-i\tau) &= \frac{1}{2\pi}\sqrt{2\pi}\frac{1}{\sqrt{\frac{1}{2m}(\tau+it)}} e^{a^2} \\ &= \sqrt{\frac{m}{2\pi(\tau+it)}} \exp\left[-\frac{m(x-y)^2}{2(\tau+it)} \right], \end{aligned} \tag{75}$$

with $\text{Re}\sqrt{\tau + it} > 0$.

It is interesting to look at this result for $t = 0$:

$$U(x, y, -i\tau) = \sqrt{\frac{m}{2m\tau}} \exp\left[-\frac{m(x-y)^2}{2\tau}\right]. \tag{76}$$

Referring back to our earlier discussion, we see that this gives the solution to the diffusion equation, or, for example, to the heat conduction problem (for a homogeneous medium) with an initial heat distribution proportional to $\delta(x-y)$. As time τ increases, the heat propagates out from $x = y$, spreading according to a broadening Gaussian.

In quantum mechanics, we are more interested in the limit $\tau \to 0^+$. The only subtle issue is the phase in $\sqrt{\tau + it}$. Let

$$\sqrt{\tau + it} = \sqrt{Re^{i\theta}} = \sqrt{R}e^{i\theta/2}, \tag{77}$$

where $R = \sqrt{\tau^2 + t^2} \underset{\tau \to 0^+}{\to} |t|$. Referring to Fig. 4, for $t > 0$ we have $0 < \theta < \pi/2$, approaching $\theta = \pi/2$ as $\tau \to 0^+$. Similarly, for $t < 0$ we have $-\pi/2 < \theta < 0$, approaching $\theta = -\pi/2$ as $\tau \to 0^+$. Hence,

$$\sqrt{\tau + it} \to_{\tau \to 0^+} \sqrt{|t|} \begin{cases} e^{i\pi/4} = \frac{1}{\sqrt{2}}(1+i), & t > 0, \\ e^{-i\pi/4} = \frac{1}{\sqrt{2}}(1-i), & t < 0. \end{cases} \tag{78}$$

Thus,

$$U(x, y; t) = \frac{1}{2}\left(1 - i\frac{t}{|t|}\right)\sqrt{\frac{m}{2\pi|t|}} \exp\left[\frac{im(x-y)^2}{2t}\right]. \tag{79}$$

This is the time development transformation for the free particle Schrödinger equation in one dimension, where we have kept proper track of the phase for all times.

We may check that the behavior of this transformation is as expected when we transform by time t, followed by transforming by time $-t$. The result ought to be what we started with, *i.e.*, this product should be the identity. Thus, we consider the product

$$U(y_2, x; -t)U(x, y_1; t) = \frac{m}{2\pi|t|} \exp\left\{\frac{im}{2t}\left[(x-y_1)^2 - (x-y_2)^2\right]\right\}. \tag{80}$$

Integrating over the intermediate variable x:

$$\int_{-\infty}^{\infty} dx U(y_2, x; -t)U(x, y_1; t) \quad = \quad \frac{m}{|t|} \exp\left[\frac{im}{2t}(y_1^2 - y_2^2)\right] \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \exp\left[\frac{im}{t}(y_2 - y_1)x\right]$$

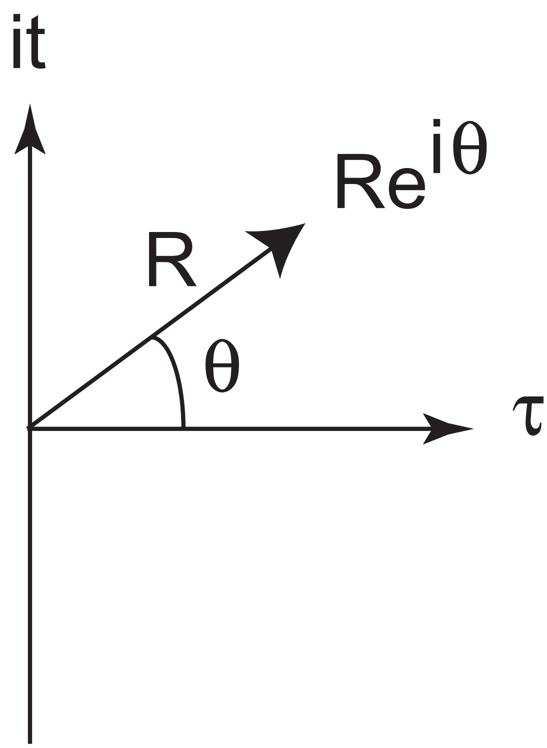

Figure 4: Illustration to help in the evaluation of the phase of the free particle time development transformation.

$$
\begin{aligned}
&= \frac{m}{|t|} \exp\left[\frac{im}{2t}(y_1^2 - y_2^2)\right] \delta\left[\frac{m}{t}(y_2 - y_1)\right] \\
&= \delta(y_2 - y_1). \qquad (81)
\end{aligned}
$$

This has the hoped-for behavior.

5.3 Example: Reflecting Wall

The translation invariance of the example above will be lost if the configuration space is changed to a half-line $x \in [0, \infty)$. This may be interpreted as a free-particle problem, except with a reflecting wall at $x = 0$. Again,

$$H = -\frac{1}{2m}\frac{d^2}{dx^2}. \qquad (82)$$

We still have $u_R(x;z) = e^{i\rho x}$, but now the left boundary condition is $u_L(0;z) = 0$. Hence, a left solution is

$$u_L(x;z) = \sin(\rho x). \tag{83}$$

We obtain $W = \rho$, by evaluating at $x = 0$. Thus,

$$\begin{aligned} G(x,y;z) &= \frac{2m}{\rho}\left[\sin(\rho x)e^{i\rho y}\theta(y-x) + \sin(\rho y)e^{i\rho x}\theta(x-y)\right] \\ &= \frac{m}{i\rho}\left[\left(e^{i\rho(x+y)} - e^{i\rho(y-x)}\right)\theta(y-x) + \left(e^{i\rho(x+y)} - e^{i\rho(x-y)}\right)\theta(x-y)\right] \\ &= i\sqrt{\frac{m}{2z}}\left[e^{i\rho|x-y|} - e^{i\rho(x+y)}\right]. \end{aligned} \tag{84}$$

This Green's function is not translation invariant. However, if $x \to \infty$, $y \to \infty$ such that $x - y$ is finite, then this Green's function tends toward our first example ($\mathrm{Im}\rho > 0$ is still our branch). This is compatible with the intuition that the local physics far from the wall at $x = 0$ should be nearly independent of the existence of the wall.

5.4 Example: Force-free Motion in Three Dimensions

Consider the Green's function problem for force-free motion in three dimensions:

$$H = -\frac{1}{2m}\nabla^2, \tag{85}$$

where $x \in R^3$. The resolvent is most easily found in momentum space, since $H = -p^2/2m$ is just multiplication by a factor there. Hence, the resolvent in momentum space is:

$$G(z) = \frac{1}{\frac{\mathbf{p}^2}{2m} - z}. \tag{86}$$

The Green's function in momentum space is, formally:

$$G(\mathbf{x},\mathbf{y};z) = \sum_k \frac{\phi_k(\mathbf{x})\phi_k^*(\mathbf{y})}{\omega_k - z}, \tag{87}$$

where

$$\begin{aligned} \omega_k &= \frac{\mathbf{p}^2}{2m}, & (88) \\ \phi_k(\mathbf{x}) &= \frac{1}{(2\pi)^{3/2}}e^{i\mathbf{p}\cdot\mathbf{x}}. & (89) \end{aligned}$$

That is,

$$G(\mathbf{x},\mathbf{y};z) = \frac{1}{(2\pi)^3}\int_{(\infty)} d^3(\mathbf{p})\frac{1}{\frac{\mathbf{p}^2}{2m}-z}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}. \tag{90}$$

To evaluate this integral, let us first evaluate another handy integral, the Fourier transform of the "Yukawa potential":

$$\begin{aligned} Y &= \int_{(\infty)} d^3(\mathbf{x})e^{-i\mathbf{x}\cdot\mathbf{p}}\frac{e^{-\mu r}}{4\pi r}, \quad \text{where } r\equiv|\mathbf{x}| && (91)\\ &= \int_0^\infty\int_{-1}^1\int_0^{2\pi} d\phi d\cos\theta dr r^2\frac{1}{4\pi r}\exp(-\mu r - irp\cos\theta), \quad \text{where } \mathbf{x}\cdot\mathbf{p} = rp\cos\theta \\ &= \frac{1}{2}\int_0^\infty\int_{-1}^1 d\cos\theta dr r e^{-\mu r}e^{-irp\cos\theta} \\ &= \frac{i}{2p}\int_0^\infty dr\int_0^\infty \left(e^{-irp}-e^{irp}\right) \\ &= \frac{i}{2p}\left(\frac{1}{\mu+ip}-\frac{1}{\mu-ip}\right) \\ &= \frac{1}{\mathbf{p}^2+\mu^2}. && (92)\end{aligned}$$

We notice in passing that the Coulomb potential corresponds to $\mu\to 0$, with

$$\int_{(\infty)} d^3(\mathbf{x})e^{-i\mathbf{x}\cdot\mathbf{p}}\frac{1}{4\pi|\mathbf{x}|} = \frac{1}{\mathbf{p}^2}. \tag{93}$$

The inverse Fourier transform theorem tells us that then:

$$\frac{1}{(2\pi)^{3/2}}\int_{(\infty)} d^s(\mathbf{p})\frac{1}{\mathbf{p}^2+\mu^2}e^{i\mathbf{x}\cdot\mathbf{p}} = (2\pi)^{3/2}\frac{e^{-\mu|\mathbf{x}|}}{4\pi|\mathbf{x}|}. \tag{94}$$

Hence,

$$\begin{aligned} G(\mathbf{x},\mathbf{y};z) &= \frac{1}{(2\pi)^3}\int_{(\infty)} d^3(\mathbf{p})\frac{1}{\frac{\mathbf{p}^2}{2m}-z}e^{i(\mathbf{x}-\mathbf{y})\cdot\mathbf{p}} \\ &= 2m\frac{e^{-i\rho|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}. && (95)\end{aligned}$$

We have selected the branch of the square root function so that $\mathrm{Im}\rho < 0$. We could just as well have selected the branch with $\mathrm{Im}\rho > 0$, in which case the Green's function is:

$$G(\mathbf{x},\mathbf{y};z) = 2m\frac{e^{i\rho|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}; \quad \rho = \sqrt{2mz}. \tag{96}$$

6 Perturbation Theory with Resolvents

Let H and $\bar{H} = H + V$ be self-adjoint operators. The choice of symbol is motivated by the fact that we are especially interested in the case in which H is a Hamiltonian, and $\bar{H}$ is another Hamiltonian related to the first by the addition of a potential term. We form the resolvents (with $z \notin \Sigma(H), \Sigma(\bar{H})$):

$$\begin{aligned} G(z) &= \frac{1}{H - z} && (97) \\ \bar{G}(z) &= \frac{1}{\bar{H} - z} = \frac{1}{H + V - z}. && (98) \end{aligned}$$

Then, noting that

$$V = \frac{1}{\bar{G}(z)} - \frac{1}{G(z)}, \tag{99}$$

it may readily be verified that

$$\bar{G}(z) = G(z) - G(z)V\bar{G}(z) = G(z) - \bar{G}(z)VG(z) \tag{100}$$

and

$$\bar{G}(z) = G(z) - G(z)VG(z) + G(z)V\bar{G}(z)VG(z). \tag{101}$$

These identities are very important in perturbation theory – if $G(z)$ is known for Hamiltonian H, then we may learn something about a perturbed Hamiltonian $H + V$.

We could try to iterate these identities still further:

$$\begin{aligned} \bar{G}(z) &= G(z) - \bar{G}(z)VG(z) \\ &= G(z) - G(z)VG(z) + \bar{G}(z)VG(z)VG(z) \\ &= \sum_{n=0}^{N} \left[-G(z)V\right]^n G(z) + (-)^{N+1}\bar{G}(z) \left[VG(z)\right]^{N+1}. \end{aligned} \tag{102}$$

If V is such that the "remainder" term above approaches 0 as $N \to \infty$, then we have the **Liouville-Neumann Series**:

$$\bar{G}(z) = G(z) \sum_{n=0}^{\infty} \left[-VG(z)\right]^n. \tag{103}$$

We may state a convergence theorem:

Theorem: Let H and V be self-adjoint operators. Let $G(z)$ be the resolvent for H, and let $D_H \subset D_V$. If

$$\|V\phi\| < \alpha_1\|\phi\| + \alpha_2\|H\phi\|, \quad \forall\phi \in D_H, \tag{104}$$

where $\alpha_1 > 0$ and $0 < \alpha_2 < 1$, then the Liouville-Neumann series converges in operator norm for some open region of the complex plane.

Proof: Let $\psi \in \mathcal{H}$ and $z \notin \Sigma(H)$. Then

$$\phi = G(z)\psi = \frac{1}{H-z}\psi \in D_H, \tag{105}$$

since $\frac{H}{H-z}$ is a bounded operator. By assumption we have

$$\|V\phi\| = \|VG(z)\psi\| < \alpha_1\|G(z)\psi\| + \alpha_2\|\frac{H}{H-z}\psi\|. \tag{106}$$

Since ψ is arbitrary, this implies:

$$\|VG(z)\|_{\text{op}} < \alpha_1\|G(z)\|_{\text{op}} + \alpha_2\|\frac{H}{H-z}\|_{\text{op}}. \tag{107}$$

Let $z = x + iy$ (x, y real). Use

$$\|f(H)\|_{\text{op}} = \sup_{\omega\in\Sigma(H)} |f(\omega)|, \tag{108}$$

to obtain

$$\|G(z)\|_{\text{op}} = \|\frac{1}{H-z}\|_{\text{op}} \leq \left|\frac{1}{x-z}\right| = \frac{1}{|y|}, \tag{109}$$

and

$$\|\frac{H}{H-z}\|_{\text{op}} = \sup_{\omega\in\Sigma(H)} \left|\frac{\omega}{\omega-z}\right| < 1. \tag{110}$$

The last part expresses the fact that $\lim_{\omega\to\infty}\left|\frac{\omega}{\omega-z}\right| = 1$.

We thus have

$$\|VG(z)\|_{\text{op}} < \frac{\alpha_1}{|y|} + \alpha_2. \tag{111}$$

Since $\alpha_2 < 1$, for large enough $y = y_0$, say, we have the result

$$\|VG(z)\|_{\text{op}} < 1 \quad \text{whenever } |y| > y_0. \tag{112}$$

Hence, the series converges in operator norm whenever $|y| > y_0$.[3]

[3] If the spectrum of H is bounded below, it will also converge for $x < x_0$, for small enough x_0.

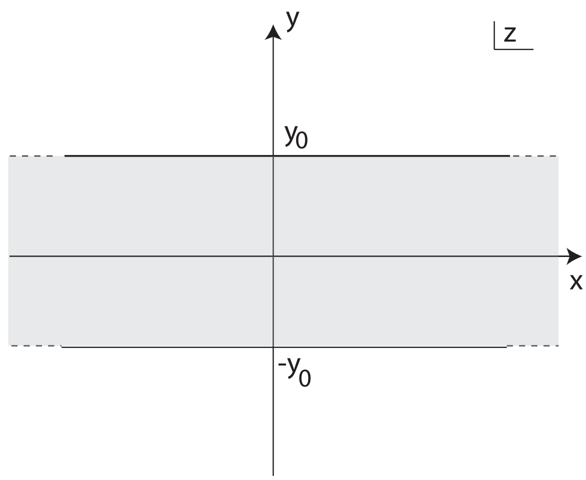

Figure 5: The region of convergence of the perturbation series is the unshaded area.

This series is the basis for the Born expansion in scattering theory, as will be discussed in another note.

Consider now the case where H is the Hamiltonian for force-free motion:

$$H = -\frac{1}{2m}\nabla^2, \qquad \mathbf{x} \in R^3, \tag{113}$$

$V = V(\mathbf{x})$ is a potential function, and $\bar{H} = H + V$. Then the identity

$$\bar{G}(z) = G(z) - G(z)V\bar{G}(z) \tag{114}$$

corresponds to the integral equation:

$$\bar{G}(\mathbf{x}, \mathbf{y}; z) = G(\mathbf{x}, \mathbf{y}; z) - \int_{(\infty)} d^3(\mathbf{x}')G(\mathbf{x}, \mathbf{x}'; z)V(\mathbf{x}')\bar{G}(\mathbf{x}', \mathbf{y}; z), \tag{115}$$

and

$$\bar{G}(z) = G(z) - G(z)VG(z) + G(z)V\bar{G}(z)VG(z) \tag{116}$$

corresponds to:

$$\begin{aligned} \bar{G}(\mathbf{x}, \mathbf{y}; z) &= G(\mathbf{x}, \mathbf{y}; z) - \int_{(\infty)} d^3(\mathbf{x}')G(\mathbf{x}, \mathbf{x}'; z)V(\mathbf{x}')G(\mathbf{x}', \mathbf{y}; z) \qquad (117) \\ &+ \int\int_{(\infty)} d^3(\mathbf{x}')d^3(\mathbf{y}')G(\mathbf{x}, \mathbf{x}'; z)V(\mathbf{x}')\bar{G}(\mathbf{x}', \mathbf{y}'; z)V(\mathbf{y}')G(\mathbf{y}', \mathbf{y}; z), \end{aligned}$$

where $z \notin \Sigma(H)$, $z \notin \Sigma(\bar{H})$.

We can also express the Schrödinger Equation for eigenstates of the perturbed Hamiltonian in the form of an integral equation. Let $\bar{\phi}_k$ be an eigenstate of $\bar{H}$, corresponding to eigenvalue $\bar{\omega}_k$. Use the identity $\bar{G}(z) = G(z) - G(z)V\bar{G}(z)$, and operate on $\bar{\phi}_k$, noting that $(\bar{\omega}_k - z)\bar{G}(z)\bar{\phi}_k = \bar{\phi}_k$:

$$\bar{\phi}_k = (\bar{\omega}_k - z)G(z)\bar{\phi}_k - G(z)V\bar{\phi}_k. \tag{118}$$

If $\bar{\omega}_k \notin \Sigma(H)$, we may now substitute $z = \bar{\omega}_k$ to obtain:

$$\bar{\phi}_k = -G(\bar{\omega}_k)V\bar{\phi}_k. \tag{119}$$

Using our free particle Green's function, Eqn. 96, this corresponds to the integral equation:

$$\bar{\phi}_k(\mathbf{x}) = -\frac{2m}{4\pi}\int_{(\infty)} d^3(\mathbf{y})\frac{\exp\left(i\sqrt{2m\bar{\omega}_k}|\mathbf{x}-\mathbf{y}|\right)}{|\mathbf{x}-\mathbf{y}|}V(\mathbf{y})\bar{\phi}_k(\mathbf{y}). \tag{120}$$

In the case of a discrete bound state spectrum ($\bar{\omega}_k < 0$),

$$i\sqrt{2m\bar{\omega}_k} = -\sqrt{2m|\bar{\omega}_k|} < 0, \tag{121}$$

and this portion of the integrand falls off rapidly as $|\mathbf{y}|$ becomes large. This equation can be more convenient for studying the properties of $\bar{\phi}_k$ than using the Schrödinger equation itself.

7 Exercises

1. Prove identities 12 and 13.

2. Prove the power series expansion for resolvent $G(z)$ (Eqn. 26):

$$G(z) = G(z_0)\sum_{n=0}^{\infty}\left[(z-z_0)G(z_0)\right]^n.$$

   You may wish to attempt to do this either "directly", or via iteration on the identity of Eqn. 11.

3. Prove the result in Eqn. 34.

4. Let's consider once again the Hamiltonian

$$H = -\frac{1}{2m}\frac{d^2}{dx^2}, \tag{122}$$

but now in configuration space $x \in [a, b]$ ("infinite square well").

   (a) Construct the Green's function, $G(x, y; z)$ for this problem.

   (b) From your answer to part (a), determine the spectrum of H.

   (c) Notice that, using

   $$G(x, y; z) = \sum_{k=1}^{\infty} \frac{\phi_k(x)\phi_k^*(x)}{\omega_k - z}, \tag{123}$$

   the normalized eigenstate, $\phi_k(x)$, can be obtained by evaluating the residue of G at the pole $z = \omega_k$. Do this calculation, and check that your result is properly normalized.

   (d) Consider the limit $a \to -\infty$, $b \to \infty$. Show, in this limit that $G(x, y; z)$ tends to the Green's function we obtain in this note for this Hamiltonian on $x \in (-\infty, \infty)$:

   $$G(x, y; z) = i\sqrt{\frac{m}{2z}}e^{i\rho|x-y|}. \tag{124}$$

5. Let us investigate the Green's function for a slightly more complicated situation. Consider th potential:

$$V(x) = \begin{cases} V & |x| \leq \Delta \\ 0 & |x| > \Delta \end{cases} \tag{125}$$

   (a) Determine the Green's function for a particle of mass m in this potential.

   Remarks: You will need to construct your "left" and "right" solutions by considering the three different regions of the potential, matching the functions and their first derivatives at the boundaries. Note that the "right" solution may be very simply obtained from the "left" solution by the symmetry of the problem. In your solution, let

   $$\rho = \sqrt{2m(z - V)} \tag{126}$$

   $$\rho_0 = \sqrt{2mz}. \tag{127}$$

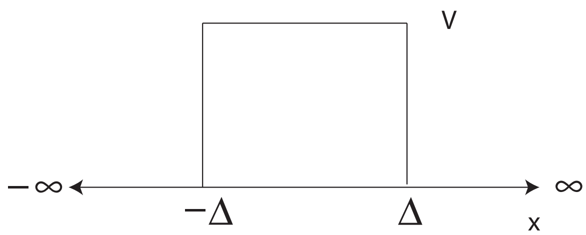

Figure 6: The "finite square potential".

Make sure that you describe any cuts in the complex plane, and your selected branch. You may find it convenient to express your answer to some extent in terms of the force-free Green's function:

$$G_0(x, y; z) = \frac{im}{\rho} e^{i\rho_0|x-y|}. \tag{128}$$

(b) Assume $V > 0$. Show that your Green's function $G(x, y; z)$ is analytic in your cut plane, with a branch point at $z = 0$.

(c) Assume $V < 0$. Show that $G(x, y; z)$ is analytic in your cut plane, except for a finite number of simple poles at the bound states of the Hamiltonian.

6. Find the time development transformation $U(x, y; t)$ for the one-dimensional harmonic oscillator:

$$H = \frac{p^2}{2m} + \frac{k}{2}x^2, \qquad \omega \equiv \sqrt{k/m}. \tag{129}$$

Be sure to clearly specify any choice of branch.

Note that you can approach this problem in different ways, *e.g.*, by directly integrating the differential equation U must satisfy, or by considering its expansion in terms of eigenfunctions of H (and perhaps using the creation and annihilation operators).

7. Let us investigate the application of the time development transformation for the harmonic oscillator that we computed in the previous exercise. Explicitly, let us consider the problem of finding the wave function at time t corresponding to an initial ($t = 0$) wave function:

$$\phi(x; 0) = \left(\frac{\alpha m\omega}{2\pi}\right)^{1/4} \exp\left[-\frac{\alpha m\omega}{4}(x-a)^2\right], \tag{130}$$

where $\alpha > 0$. Our initial wave function thus corresponds to a Gaussian probability in position, with $\langle x \rangle = a$, and $\langle (x-a)^2 \rangle = 1/\alpha m\omega$. Using $U(x, y; t)$ we can solve for $\phi(x; t)$ in closed form with this initial wave function.

(a) Solve for $\phi(x; t)$. Do not go to great effort to simplify your result in this part – we'll consider a case with simple cancellations in part (b).

(b) From your answer to part (a), show that, for $\alpha = 2$:

$$\phi(x;t) = (\frac{m\omega}{\pi})^{\frac{1}{4}} \exp\left\{-\frac{m\omega}{2}(x - a\cos\omega t)^2 - \frac{i\omega}{2}\left[t + 2max\sin\omega t - m\frac{a^2}{2}\sin 2\omega t\right]\right\}. \tag{131}$$

You should give some thought to how you might have attacked this problem using "elementary methods", without knowing $U(x, y; t)$.

(c) Notice that the choice $\alpha = 2$ corresponds to an initial state wave function something like a "displaced" ground state wave function. Solve for the probability distribution to find the particle at x as a function of time (for $\alpha = 2$). Your result should have a simple form and should have an obvious classical correspondence.