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# Introduction to Jourdain Green's functions

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Green's functions are presented in a natural way, à la Monsieur Jourdain, spanning several fields of interest such as Ordinary Differential equations (ODE), Partial Differential Equations (PDE), Boundary Value Problems (BVP), Time dependent-Initial value problems such as driven oscillators, diffusion and wave equations, Quantum problems in wells and electronic band-structure in crystal lattices.

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## I. INTRODUCTION

"Le Bourgeois Gentillhomme" is a Molière play whose main character "Monsieur Jourdain" is unaware of the fact, his natural way of speaking is called "prose" a scholarly accurate term used by literature experts. This metaphor is a fine illustration of our work describing a most intuitive way of introducing Green's Functions with Dirac notation. A Green's function enables one to find easily solutions of inhomogeneous ordinary/partial differential/integral equations [1] encountered in various fields of physics and engineering.

Using Dirac notation we consider an operator  $\hat{L}$  acting on some unknown state  $|f\rangle$  resulting into a known state  $|h\rangle$  such that:

$$\hat{L}|f\rangle = |h\rangle \quad (1)$$

This is in fact an ordinary/partial differential/integral equation, when we express it in some representation such as  $|\mathbf{r}\rangle$  by inserting the closure relation (whose validity is granted by the fact  $|\mathbf{r}\rangle$  span a continuous Hilbert space):  $\int d\mathbf{r}' |\mathbf{r}'\rangle \langle \mathbf{r}'| = \mathbb{1}$  after multiplying both sides of eq. 1 by  $\langle \mathbf{r}|$ :

$$\int d\mathbf{r}' \langle \mathbf{r} | \hat{L} | \mathbf{r}' \rangle \langle \mathbf{r}' | f \rangle = \langle \mathbf{r} | h \rangle \quad (2)$$

This can be rewritten in ordinary functional form (see further below the mathematical conditions accompanying this formulation) without using Dirac notation as:

$$L_{\mathbf{r},\mathbf{r}'} f(\mathbf{r}') = h(\mathbf{r}) \quad (3)$$

where the functional operator  $L_{\mathbf{r},\mathbf{r}'}$  might be an integral or ordinary/partial differential.

Returning to Dirac notation, the direct solution of eq. 1 is simply:

$$|f\rangle = \hat{L}^{-1} |h\rangle \quad (4)$$

The inverse operator  $\hat{G} = \hat{L}^{-1}$  is the Green operator and the Green's functions (GF)  $G(\mathbf{r}, \mathbf{r}')$  are simply the "matrix elements" of  $\hat{G}$  in a given representation, i.e.  $G(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r} | \hat{G} | \mathbf{r}' \rangle$ .

It is possible to extract a symmetry property satisfied by GF when they are real. This means  $G(\mathbf{r}, \mathbf{r}') = \langle \mathbf{r} | \hat{G} | \mathbf{r}' \rangle = (\langle \mathbf{r}' | \hat{G} | \mathbf{r} \rangle)^* = \langle \mathbf{r}' | \hat{G}^\dagger | \mathbf{r} \rangle$  and when the Green operator is Hermitian:  $\hat{G} = \hat{G}^\dagger$  implying that the operator  $\hat{L}$  is also Hermitian (representing some physical property), we deduce the symmetry:  $G(\mathbf{r}, \mathbf{r}') = G(\mathbf{r}', \mathbf{r})$ .

The final solution of eq. 1 entails including a "hidden" (homogeneous case) contribution  $|f_0\rangle$  such that  $\hat{L}|f_0\rangle = |0\rangle$  the null state.

Thus the general solution of eq. 1 is:

$$|f\rangle = |f_0\rangle + \hat{L}^{-1}|g\rangle = |f_0\rangle + \hat{G}|h\rangle \quad (5)$$

Multiplying by  $\langle \mathbf{r} |$  and inserting the closure relation:  $\int d\mathbf{r}' |\mathbf{r}'\rangle \langle \mathbf{r}'| = \mathbb{1}$ , we get:

$$\langle \mathbf{r} | f \rangle = \langle \mathbf{r} | f_0 \rangle + \int d\mathbf{r}' \langle \mathbf{r} | \hat{G} | \mathbf{r}' \rangle \langle \mathbf{r}' | h \rangle \quad (6)$$

which can be rewritten as:

$$f(\mathbf{r}) = f_0(\mathbf{r}) + \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}') h(\mathbf{r}') \quad (7)$$

implying the use of GF when seeking solution of such equations.

The differential/integral equation satisfied by the GF  $G(\mathbf{r}, \mathbf{r}')$  is obtained from the identity  $\hat{L}\hat{G} = \mathbb{1}$ , after taking the  $\mathbf{r}, \mathbf{r}'$  matrix elements and inserting the closure relation such that:

$$\int d\mathbf{r}'' \langle \mathbf{r} | \hat{L} | \mathbf{r}'' \rangle \langle \mathbf{r}'' | \hat{G} | \mathbf{r}' \rangle = \langle \mathbf{r} | \mathbb{1} | \mathbf{r}' \rangle \quad (8)$$

Assuming the operator  $\hat{L}$  is local, his matrix elements are given by  $\langle \mathbf{r} | \hat{L} | \mathbf{r}'' \rangle = L_{\mathbf{r}, \mathbf{r}''} \delta(\mathbf{r} - \mathbf{r}'')$ , we obtain:

$$L_{\mathbf{r}, \mathbf{r}'} \langle \mathbf{r} | \hat{G} | \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') \quad \text{or} \quad L_{\mathbf{r}, \mathbf{r}'} G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (9)$$

Note that in the classical electrodynamics literature [2-6], the definition of GF might display a minus sign such that  $L_{\mathbf{r}, \mathbf{r}'} G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}')$ , however we believe that our definition is the most natural.

### A. First-order inhomogeneous differential equations

As a direct application, we consider a first-order inhomogeneous Ordinary Differential Equation (ODE):

$$\frac{dy}{dx} - \alpha y = f(x) \quad (10)$$

Elementary Calculus states that the solution of the above linear ODE is a superposition of the general solution (without RHS)  $C \exp(\alpha x)$  ( $C$  is an arbitrary constant) and the particular solution (with RHS), that is:

$$y(x) = C \exp(\alpha x) + \exp(\alpha x) \int^x dx' \exp(-\alpha x') f(x').$$

Casting the result in the GF language, we infer that the ODE GF is  $G(x, x') = \exp(\alpha[x - x'])$  whereas the Green operator is

$$\hat{G} = (\hat{D}_x - \alpha)^{-1}, \quad \text{where} \quad \hat{D}_x = \frac{d}{dx} \quad (11)$$

with matrix elements:

$$G(x, x') = \langle x | (\hat{D}_x - \alpha)^{-1} | x' \rangle = \exp(\alpha[x - x']) \quad (12)$$

This can be shown by noting that the particular solution  $\exp(\alpha x) \int^x dx' \exp(-\alpha x') f(x')$ : can be rewritten as:

$$(\hat{D}_x - \alpha)^{-1} \langle x | f \rangle = \exp(\alpha x) \int^x dx' \exp(-\alpha x') \langle x' | f \rangle \quad (13)$$

which is equivalent to:

$$(\hat{D}_x - \alpha)^{-1} \langle x| = \exp(\alpha x) \int^x dx'' \exp(-\alpha x'') \langle x''| \quad (14)$$

Shifting the state  $\langle x|$  to the left since it commutes with the operator  $(\hat{D}_x - \alpha)^{-1}$ , we get:

$$\langle x| (\hat{D}_x - \alpha)^{-1} = \exp(\alpha x) \int^x dx'' \exp(-\alpha x'') \langle x''| \quad (15)$$

Multiplying both terms by  $|x'\rangle$ , we get:

$$\langle x| (\hat{D}_x - \alpha)^{-1} |x'\rangle = \exp(\alpha x) \int^x dx'' \exp(-\alpha x'') \langle x''|x'\rangle \quad (16)$$

recovering the Green operator matrix elements eq. 12 since  $\langle x''|x'\rangle = \delta(x'' - x')$ .

### B. 3D Poisson equation

Another example of application is the GF of the 3D Poisson partial differential equation (PDE):

$$\Delta V(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon} \quad (17)$$

The Laplacian operator  $\Delta = \nabla \cdot \nabla$  where  $\nabla = \frac{\partial}{\partial \mathbf{r}}$  plays the role of the matrix elements  $L_{\mathbf{r},\mathbf{r}}$  whereas the potential  $V(\mathbf{r})$  and  $-\frac{\rho(\mathbf{r})}{\epsilon}$  correspond to  $f(\mathbf{r})$  and  $h(\mathbf{r})$  respectively.

Hence the GF obeys the PDE:

$$\Delta G(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}') \quad (18)$$

and the full solution according to eq. 19 is:

$$V(\mathbf{r}) = V_0(\mathbf{r}) - \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}') \frac{\rho(\mathbf{r}')}{\epsilon} \quad (19)$$

with the potential  $V_0(\mathbf{r})$  solution of  $\Delta V_0(\mathbf{r}) = 0$  i.e.  $V_0(\mathbf{r})$  is a harmonic function.

The GF appearing in eq. 18 can be obtained simply by a Landau [7] argument:

Start with a point particle bearing a charge  $q$  located at the origin. The charge density is simply  $\rho(r) = q\delta(r)$ . The potential  $V(\mathbf{r})$  at any point in 3D space with dielectric constant  $\epsilon$  is the Coulomb potential  $V(\mathbf{r}) = \frac{1}{4\pi\epsilon r}$ .

Using Poisson equation we have:  $\Delta V(\mathbf{r}) = -\frac{\rho(\mathbf{r})}{\epsilon}$  meaning that  $\Delta\left(\frac{1}{4\pi\epsilon r}\right) = -\frac{\rho(\mathbf{r})}{\epsilon} = -\frac{q\delta(r)}{\epsilon}$  to obtain:

$$\Delta\left(\frac{1}{r}\right) = -4\pi\delta(r) \quad (20)$$

Thus the GF of the 3D Poisson problem eq. 18 is:

$$G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r}'|} \quad (21)$$

Let us move on from a point charge to a finite isotropic homogeneous dielectric material having a volume  $\Omega$  bounded by a surface  $\partial\Omega$ .

Within the body there exists a given volume density source  $\rho(\mathbf{r})$  and on the surface a charge density  $\sigma(\mathbf{r})$ , therefore the total electrostatic potential is:

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon} \int_{\Omega} \frac{\rho(\mathbf{r}')d\Omega'}{|\mathbf{r} - \mathbf{r}'|} + \frac{1}{4\pi\epsilon} \oint_{\partial\Omega} \frac{\sigma(\mathbf{r}')dS'}{|\mathbf{r} - \mathbf{r}'|} \quad (22)$$

which corresponds to eq. 19 accounting for volume and surface charges and with  $V_0(\mathbf{r}) = 0$ .

The Laplace operator possesses in fact a GF of the form  $\frac{1}{r^{d-2}}$  in  $d$  dimensions with  $r = \sqrt{\sum_{i=1}^d x_i^2}$  the Euclidian norm of  $\mathbf{r}$  and  $x_i$  its coordinates. For instance in 2D,  $G(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi} \log(|\mathbf{r} - \mathbf{r}'|)$  and in 1D,  $G(\mathbf{r}, \mathbf{r}') = \frac{1}{2}|\mathbf{r} - \mathbf{r}'|$ .

### C. 3D Boundary Value Problems (BVP)

The application of GF to a 3D BVP is to find a potential with prescribed values on a given surface (usually the material's). The boundary conditions may be of Dirichlet (specified surface potential), Neumann (specified gradient of surface) or Cauchy (mixture of both).

We apply the GF approach to deal with a 3D BVP Poisson equation.

The BVP can be solved with Green [8] second identity:

$$\int_{\Omega} [\phi(\mathbf{r})\Delta\psi(\mathbf{r}) - \psi(\mathbf{r})\Delta\phi(\mathbf{r})]d\Omega = \oint_{\partial\Omega} [\phi(\mathbf{r})\nabla\psi(\mathbf{r}) - \psi(\mathbf{r})\nabla\phi(\mathbf{r})] \cdot \mathbf{n}dS \quad (23)$$

obtained by using Laplace equation and Green divergence theorem:  $\int_{\Omega} (\nabla \cdot \mathbf{A})d\Omega = \oint_{\partial\Omega} (\mathbf{A} \cdot \mathbf{n})dS$  where  $\mathbf{n}$  is the outward normal to the finite material surface.

Taking  $\phi(\mathbf{r}) = V(\mathbf{r})$  and  $\psi(\mathbf{r}') = G(\mathbf{r}, \mathbf{r}')$ , the potential is thus expressed as:

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon} \int_{\Omega} G(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d\Omega' + \frac{1}{4\pi} \oint_{\partial\Omega} [G(\mathbf{r}, \mathbf{r}')\nabla'V_S(\mathbf{r}') - V_S(\mathbf{r}')\nabla'G(\mathbf{r}, \mathbf{r}')] \cdot \mathbf{n}'dS' \quad (24)$$

where  $\nabla' = \frac{\partial}{\partial \mathbf{r}'}$ .

If we have a Dirichlet boundary conditions,  $V_S(\mathbf{r})$  is a prescribed surface potential and we may choose a Dirichlet GF [2]  $G_D(\mathbf{r}, \mathbf{r}')$  such that  $G_D(\mathbf{r}, \mathbf{r}') = 0$  when  $\mathbf{r}' \in \partial\Omega$  to obtain finally:

$$V(\mathbf{r}) = \frac{1}{4\pi\epsilon} \int_{\Omega} G_D(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}')d\Omega' - \frac{1}{4\pi} \oint_{\partial\Omega} V_S(\mathbf{r}')\nabla'G_D(\mathbf{r}, \mathbf{r}') \cdot \mathbf{n}'dS' \quad (25)$$

Note that eq. 25 looks like eq. 22, however the GF  $G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi|\mathbf{r}-\mathbf{r}'|}$  and  $G_D(\mathbf{r}, \mathbf{r}')$  are different since  $G_D(\mathbf{r}, \mathbf{r}')$  must be harmonic over the surface  $\partial\Omega$  which is not the case of  $G(\mathbf{r}, \mathbf{r}')$ . In the case of a spherical domain  $\Omega$  of radius  $R$ , the Dirichlet GF  $G_D(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi r} + \frac{R/\rho}{4\pi r'}$  where  $\rho = Rr/r'$ .  $G_D(\mathbf{r}, \mathbf{r}')$  is zero on the surface  $\partial\Omega$  and harmonic with respect to  $r$ .

The Neumann case is treated similarly (see for instance, Jackson [2]) and the Cauchy case is more difficult since it is an ill-posed problem [9], in general.

## II. TIME EVOLUTION AND INITIAL-VALUE PROBLEMS

### A. 1D Driven harmonic oscillator

A damped oscillator is harmonic when it has a single eigen-frequency  $\omega_0$  such that its equation of motion reads:

$$\left[ \frac{d^2}{dt^2} + 2\gamma \frac{d}{dt} + \omega_0^2 \right] u(t) = F(t)/m \quad (26)$$

where  $m, F(t), \gamma$  are mass, driving force and damping of the oscillator whose displacement amplitude is  $u(t)$ . The time dependent GF  $G(t, t')$  satisfies:

$$\left[ \frac{d^2}{dt^2} + 2\gamma \frac{d}{dt} + \omega_0^2 \right] G(t, t') = \delta(t - t') \quad (27)$$

such that the displacement is  $u(t) = \int_{-\infty}^{+\infty} dt' G(t, t') F(t')/m$  implying causality (response at  $t$  should follow excitation at  $t'$ ).

The GF is readily obtained with Fourier Transform (FT) methods [10] by introducing the frequency dependent GF  $G(\omega, t') = \int_{-\infty}^{+\infty} dt e^{i\omega t} G(t, t')$ .

Taking the FT of eq. 27, we get:

$$[-\omega^2 - 2i\gamma\omega + \omega_0^2]G(\omega, t') = \int_{-\infty}^{+\infty} dt e^{i\omega t} \delta(t - t') = e^{i\omega t'} \quad (28)$$

obtaining:  $G(\omega, t') = -\frac{e^{i\omega t'}}{\omega^2 + 2i\gamma\omega - \omega_0^2}$

The GF  $G(t, t')$  can be obtained with an inverse FT such that:

$$G(t, t') = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} G(\omega, t') \quad (29)$$

The denominator being a quadratic can be factored such that  $G(t, t')$  can be written as:

$$G(t, t') = - \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-t')}}{(\omega - \omega_1)(\omega - \omega_2)} \quad (30)$$

where the poles  $\omega_{1,2} = -i\gamma \pm \sqrt{\omega_0^2 - \gamma^2}$ .

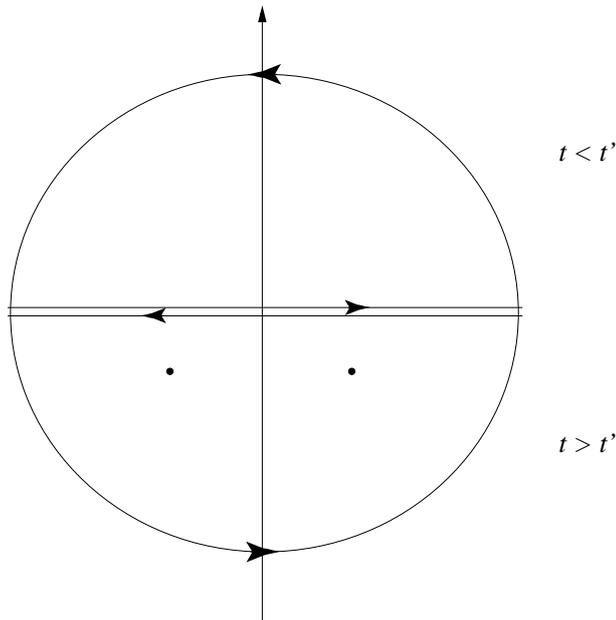


FIG. 1: The contour is closed in the upper half-plane when  $t < t'$  yielding zero result. When  $t > t'$ , it is closed in the lower half-plane containing both poles (black dots) yielding a non-zero result and expressing causality.

The integral can be evaluated with complex contour integration such that for  $t < t'$  the contour is closed in the upper half-plane with zero result whereas in the opposite case  $t > t'$  it is closed in the lower half-plane with both poles inside (see fig. 1) so that  $G(t, t')$  reads:  $G(t, t') = i\Theta(t - t') \left[ \frac{e^{-i\omega_1(t-t')}}{(\omega_1 - \omega_2)} + \frac{e^{-i\omega_2(t-t')}}{(\omega_2 - \omega_1)} \right]$  where  $\Theta(t - t')$  is the Heaviside step function expressing causality (since it is zero when  $t < t'$  and 1 when  $t > t'$ ).

Finally we can write  $G(t, t')$  as:

$$\begin{aligned}
G(t, t') &= \Theta(t - t') e^{-\gamma(t-t')} \frac{\sin(\sqrt{\omega_0^2 - \gamma^2} (t - t'))}{\sqrt{\omega_0^2 - \gamma^2}}, & \gamma < \omega_0 & \text{ under-damped} \\
&= \Theta(t - t') e^{-\gamma(t-t')} \frac{\sinh(\sqrt{\gamma^2 - \omega_0^2} (t - t'))}{\sqrt{\gamma^2 - \omega_0^2}}, & \gamma > \omega_0 & \text{ over-damped} \\
&= \Theta(t - t') e^{-\gamma(t-t')} (t - t'), & \gamma = \omega_0 & \text{ critically-damped}
\end{aligned} \tag{31}$$

The displacement is obtained from the GF as  $u(t) = \frac{1}{m} \int_{-\infty}^{+\infty} dt' G(t, t') F(t')$  for an arbitrary driving term  $F(t)$  without using other means such as the Fourier or Laplace transforms for instance.

In addition, note that most of the literature concerned with driven oscillators in mathematics, physics or engineering uses a limited set of driving term  $F(t)$  such as impulse, step, ramp, exponential, trigonometric that are mathematically straightforward to solve with Fourier or Laplace methods whereas with the GF method, the driving term is completely arbitrary.

## B. 1D Diffusion equation

Consider the 1D diffusion (heat) equation:  $(\frac{\partial}{\partial t} - D \frac{\partial^2}{\partial x^2})u(x, t) = 0$  with initial condition for the temperature profile :  $u(x, 0) = f(x)$  in the case of an infinite rod:  $-\infty < x < \infty$  possessing diffusion constant  $D$ . We impose the asymptotic condition at all times:  $u(x, t) \rightarrow 0$  for  $|x| \rightarrow \infty$ .

We define a time dependent GF  $G(x, t)$  and drawing from our experience with time independent GF, we infer that space-time dependent  $G(x, t)$  should be solution of:

$$\left( \frac{\partial}{\partial t} - D \frac{\partial^2}{\partial x^2} \right) G(x, x', t, t') = \delta(x - x') \delta(t - t') \tag{32}$$

The temperature profile  $u(x, t)$  should be written as:

$$u(x, t) = \int_{-\infty}^{-\infty} d\xi f(\xi) G(x - \xi, t) \tag{33}$$

Taking the spatial FT of eq. 32 gives  $G(k, t)$  after defining:

$$G(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \exp(-ikx) G(x, t) \tag{34}$$

$$U(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \exp(-ikx) u(x, t) \tag{35}$$

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \exp(-ikx) f(x) \tag{36}$$

we get the GF after taking the inverse spatial FT of  $G(k, t)$ :

$$G(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk \exp(ikx) G(k, t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \tag{37}$$

### Note on the 1D Schrödinger equation:

Time-dependent Schrödinger equation may be considered as a diffusion equation in imaginary time [11]. Considering a free particle of mass  $m$ , 1D Schrödinger equation writes:  $(i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}) G(x, x', t, t') = \delta(x - x') \delta(t - t')$ . Comparing with eq. 32 and making the replacements  $t \rightarrow \frac{t}{i\hbar}$ ,  $D \rightarrow -\frac{\hbar^2}{2m}$ ,  $G(x, t) \rightarrow \frac{1}{i\hbar} G(x, t)$ , we get the 1D free particle Green's function as:  $G(x, t) = \frac{1}{i\hbar} \sqrt{\frac{m}{2i\pi\hbar t}} \exp\left(\frac{imx^2}{2\hbar t}\right)$ .

### C. 1D wave equation

Consider the 1D wave equation:  $(\frac{\partial^2}{\partial t^2} - v^2 \frac{\partial^2}{\partial x^2})u(x, t) = 0$  with  $u(x, t)$  the wave amplitude.

In order to derive the GF:  $\frac{1}{2v}\Theta(vt - |x|)$  where  $\Theta(t)$  is the Heaviside function, we consider the solution with initial conditions  $u(x, 0) = f(x)$  and  $(\frac{\partial u(x, t)}{\partial t})_{t=0} = g(x)$  as given by d'Alembert [12] method:

$$u(x, t) = \frac{1}{2}[f(x + vt) + f(x - vt)] + \frac{1}{2v} \int_{x-vt}^{x+vt} g(x') dx' \quad (38)$$

If we suppose that  $Q(x, x', t)$  is the solution with initial value  $Q(x, x', 0) = \delta(x - x')$  and  $(\frac{\partial Q(x, x', t)}{\partial t})_{t=0} = 0$ , whereas  $P(x, x', t)$  is the solution with initial value  $P(x, x', 0) = 0$  and  $(\frac{\partial P(x, x', t)}{\partial t})_{t=0} = \delta(x - x')$ , the solution can be recast into:

$$u(x, t) = \int_{-\infty}^{\infty} f(x') Q(x, x', t) dx' + \int_{-\infty}^{\infty} g(x') P(x, x', t) dx' \quad (39)$$

with  $P$  and  $Q$  defined by:

$$P(x, x', t) = \frac{1}{2v} \Theta(vt - |x - x'|) \quad (40)$$

$$Q(x, x', t) = \frac{\partial P(x, x', t)}{\partial t} = \frac{1}{2} [\delta(x - x' - vt) + \delta(x - x' + vt)] \quad (41)$$

$$(42)$$

Relation 39 can be viewed as a double GF solution with one ( $Q(x, x', t)$ ) involving the initial condition on the amplitude  $u(x, 0) = f(x)$  and the other ( $P(x, x', t)$ ) pertaining to the initial time derivative of the amplitude  $(\frac{\partial u(x, t)}{\partial t})_{t=0} = g(x)$ .

### III. 1D STATIONARY QUANTUM MECHANICS

The stationary Schrödinger equation reads:

$$\hat{H} |\psi\rangle = E |\psi\rangle \quad \text{or} \quad (E - \hat{H}) |\psi\rangle = 0 \quad (43)$$

This eigenvalue equation is a special case of the previous relation  $\hat{L} |f\rangle = |h\rangle$  since  $|h\rangle$  is proportional to  $|f\rangle$ . Thus the corresponding Green operator is  $\hat{G} = (E - \hat{H})^{-1}$ .

Since  $\hat{H}$  is a physical operator, it is Hermitian and possesses a set of eigenstates labeled by an integer  $n$  such that  $\hat{H} |n\rangle = E_n |n\rangle$ . The closure relation (whose validity is granted by the fact the set  $|n\rangle$  spans a discrete Hilbert space) is  $\sum |n\rangle \langle n| = \mathbb{1}$ .

Considering the "matrix elements" of the Green operator in the 1D space  $x$  representation, we have:

$$G(x, x') = \langle x | \hat{G} | x' \rangle = \langle x | (E - \hat{H})^{-1} | x' \rangle \quad (44)$$

we insert twice the closure relation before and after  $(E - \hat{H})^{-1}$  to get:

$$G(x, x') = \sum_{n, n'} \langle x | n' \rangle \langle n' | (E - \hat{H})^{-1} | n \rangle \langle n | x' \rangle = \sum_{n, n'} \langle x | n' \rangle \langle n' | (E - \hat{H})^{-1} | n \rangle \langle n | x' \rangle \quad (45)$$

Since  $|n\rangle$  are orthogonal eigenstates of  $\hat{H}$  the matrix elements are:  $\langle n' | (E - \hat{H})^{-1} | n \rangle = (E - E_n)^{-1} \delta_{n, n'}$ . Thus we write using  $\psi_n(x) = \langle x | n \rangle$ :

$$G(x, x') = \sum_n \frac{\psi_n(x) \psi_n^*(x')}{(E - E_n)} \quad (46)$$

### A. Application to the 1D infinite potential well

The eigenvalues of the 1D infinite potential well with width  $a$  are:  $E_n = \frac{\hbar^2}{2m} (\frac{n\pi}{a})^2$  and the eigenstates are:  $\psi_n(x) = \sqrt{\frac{2}{a}} \sin(\frac{n\pi x}{a})$ .

Thus the corresponding GF is:

$$G(x, x') = \frac{2}{a} \sum_n \frac{\sin(\frac{n\pi x}{a}) \sin(\frac{n\pi x'}{a})}{(E - E_n)} \quad (47)$$

### B. Application to Density of States evaluation

In a system with discrete energy eigenvalues  $E_n$ , the density of states is given by:

$$D(E) = \sum_n \delta(E - E_n) \quad (48)$$

Consider the retarded/advanced Green operator  $G^\pm(E)$ :

$$G^\pm(E) = (E - \hat{H} \pm i\epsilon)^{-1} \quad (49)$$

The Sokhotski-Plemelj [13] theorem states that:

$$\frac{1}{x \pm i\epsilon} = P\left(\frac{1}{x}\right) \mp i\pi\delta(x) \quad (50)$$

It can be shown by simply writing:  $\frac{1}{x \pm i\epsilon} = \frac{x - (\pm i\epsilon)}{x^2 + \epsilon^2}$  and expanding:  $\frac{1}{x \pm i\epsilon} = \frac{x}{x^2 + \epsilon^2} \mp i \frac{\epsilon}{x^2 + \epsilon^2}$ .

where the principal value is defined as:  $P\left(\frac{1}{x}\right) = \lim_{\epsilon \rightarrow 0} \frac{x}{x^2 + \epsilon^2}$ .

Similarly  $\delta(x) = \pi \lim_{\epsilon \rightarrow 0} \frac{\epsilon}{x^2 + \epsilon^2}$ .

Performing an "analytic continuation" from function to operator allows us to write:

$$G^\pm(E) = (E - \hat{H} \pm i\epsilon)^{-1} = P\left(\frac{1}{E - \hat{H}}\right) \mp i\pi\delta(E - \hat{H}) \quad (51)$$

Thus:  $G^+(E) - G^-(E) = -2i\pi\delta(E - \hat{H})$  and taking the trace:

$Tr[G^+(E) - G^-(E)] = \sum_n \langle n | G^+(E) - G^-(E) | n \rangle = -2i\pi\delta(E - E_n)$ , we get the density of states:

$$D(E) = -\frac{1}{2i\pi} Tr[G^+(E) - G^-(E)] \quad (52)$$

## IV. LATTICE GREEN'S FUNCTIONS

In a perfect crystal the electrons are subjected to a periodic potential  $\hat{V}_P$  and their physics is described by a single electron Schrödinger equation with Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m} \Delta + \hat{V}_P(\mathbf{r}) \quad (53)$$

The eigenstates of such Hamiltonian are Bloch functions  $|n, \mathbf{k}\rangle$  with  $n$  the band index and  $\mathbf{k}$  the wavevector.

In the case of tight-binding (TB) electronic states in a lattice of parameter  $a$ , the Hamiltonian writes in the site representation:

$$\hat{H} = \sum_{\mathbf{l}} \epsilon_{\mathbf{l}} |\mathbf{l}\rangle \langle \mathbf{l}| + \sum_{\mathbf{k}, \mathbf{l}} V_{\mathbf{k}, \mathbf{l}} |\mathbf{k}\rangle \langle \mathbf{l}| \quad (54)$$

with  $\epsilon_{\mathbf{l}}$  local energy at site  $\mathbf{l}$  (that reduces to a single value  $\epsilon_0$  by translational symmetry) and  $V_{\mathbf{k}, \mathbf{l}}$  overlap integral between neighboring sites  $\mathbf{k}$  and  $\mathbf{l}$  (that reduces to a single value  $V_0$  between nearest neighbor sites). Note that a spatial FT links the site (direct lattice) representation to the wavevector (reciprocal lattice) representation:

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} \exp(i\mathbf{k} \cdot \mathbf{l}) |\mathbf{l}\rangle \quad (55)$$

with  $N$  the number of unit cells.

**Note:** We introduce a slight notation change to indicate eigenstates in the reciprocal space by  $|\mathbf{k}\rangle$  in order not to confuse them with eigenstates in the site representation  $|\mathbf{k}\rangle$  corresponding to site  $\mathbf{k}$ .

The tight-binding (TB) single-band electronic dispersion for the square lattice of parameter  $a$  is:

$$\epsilon(\mathbf{k}) = \epsilon_0 + 2V_0[\cos(k_x a) + \cos(k_y a)] \quad (56)$$

where  $\epsilon_0$  is a mean energy,  $V_0$  the neighboring sites overlap integral and  $k_x, k_y$  wavevectors that belong to the Brillouin zone  $[-\pi/a, \pi/a] \times [-\pi/a, \pi/a]$ .

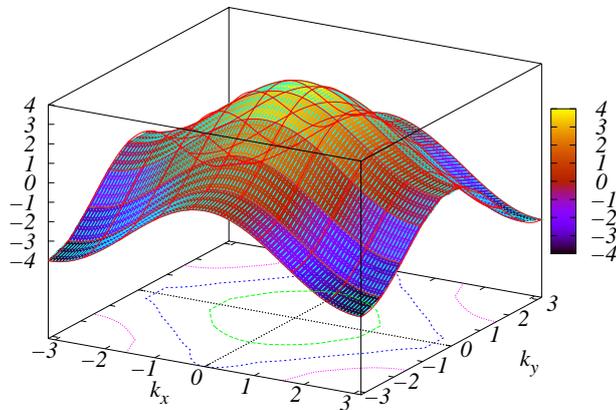


FIG. 2: (Color on-line) Dispersion relation  $\epsilon(\mathbf{k}) = \epsilon(k_x, k_y) = \epsilon_0 + 2V_0[\cos(k_x a) + \cos(k_y a)]$  in the Brillouin zone  $[-\pi, \pi] \times [-\pi, \pi]$  with  $a = 1, \epsilon_0 = 0, |V_0| = 1$  displaying saddle or extremal points at values  $(k_x, k_y)$  such as  $(0, 0), (0, \pm\pi), (\pm\pi, 0), (\pm\pi, \pm\pi) \dots$  at which  $|\nabla_{\mathbf{k}} \epsilon(\mathbf{k})| = 2V_0 a \sqrt{\sin^2(k_x a) + \sin^2(k_y a)} = 0$ , Van Hove singularities in the DOS are expected at the corresponding energy values such as  $E = \pm 4, E = 0$ .

### A. Electronic density of states

The density of states (DOS) is obtained from  $\epsilon(\mathbf{k})$  with formula [14]:

$$D(E) = \frac{\Omega}{(2\pi)^d} \oint_{\epsilon(\mathbf{k})=E} \frac{dS_E}{|\nabla_{\mathbf{k}} \epsilon(\mathbf{k})|} \quad (57)$$

with  $\nabla_{\mathbf{k}} = \frac{\partial}{\partial \mathbf{k}}$  and  $\Omega$  is a normalization volume as in the plane wave case:  $\frac{1}{\sqrt{\Omega}} \exp(i\mathbf{k} \cdot \mathbf{r})$ . The integration element  $dS_E$  indicate the quadrature is performed over constant energy surfaces  $\epsilon(\mathbf{k}) = E$ .

We may derive the DOS with lattice GF starting from the lattice Green operator defined as usual by:

$$\hat{G}(E) = (E - \hat{H})^{-1} \quad (58)$$

The GF is obtained from matrix elements of  $\hat{G}(E)$  with respect to Bloch  $|n, \mathbf{k}\rangle$  states as:

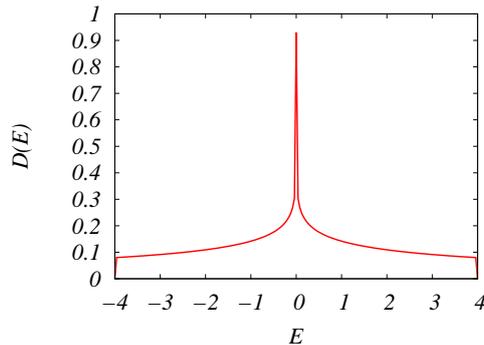


FIG. 3:  $D(E)$  of the tight-binding square lattice with  $\epsilon_0 = 0$  and  $|V_0| = 1$  yielding discontinuities at the band edges  $E = \pm 4$  and a sharp singularity at midband  $E = 0$ .

$$G(n, \mathbf{k}, n', \mathbf{k}', E) = \langle n, \mathbf{k} | \left( \frac{1}{E - \hat{H}} \right) | n', \mathbf{k}' \rangle = \langle n, \mathbf{k} | \left( \frac{1}{E - \epsilon(\mathbf{k}')} \right) | n', \mathbf{k}' \rangle \quad (59)$$

Orthogonality of eigenstates being given by:  $\langle n, \mathbf{k} | n', \mathbf{k}' \rangle = \delta_{nn'} \delta_{\mathbf{k}\mathbf{k}'}$  yields:

$$G(n, \mathbf{k}, n', \mathbf{k}', E) = \delta_{nn'} \delta_{\mathbf{k}\mathbf{k}'} \left( \frac{1}{E - \epsilon(\mathbf{k})} \right) \quad (60)$$

In the single band case ( $n = 1$ ) we express the Green operator in wavevector (reciprocal space) representation using the closure relation (whose validity is granted by the fact  $|\mathbf{k}\rangle$  span a discrete Hilbert space)  $\sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}| = \mathbf{1}$  and orthogonality of wavevector eigenstates  $\langle \mathbf{k} | \mathbf{k}' \rangle = \delta_{\mathbf{k}, \mathbf{k}'}$ :

$$\hat{G}(E) = \sum_{\mathbf{k}} |\mathbf{k}\rangle \langle \mathbf{k}| (E - \hat{H})^{-1} \sum_{\mathbf{k}'} |\mathbf{k}'\rangle \langle \mathbf{k}'| = \sum_{\mathbf{k}'} \frac{|\mathbf{k}'\rangle \langle \mathbf{k}'|}{E - \epsilon(\mathbf{k}')} \quad (61)$$

Therefore the TB single-band DOS becomes using  $D(E) = -\frac{1}{2i\pi} \text{Tr}[G^+(E) - G^-(E)]$  the trace being a sum over wavevector states transformed into an integration over the Brillouin zone such that:

$$\sum_{\mathbf{k}} \xrightarrow{\Omega \rightarrow \infty} \left[ \frac{\Omega}{N(2\pi)^d} \right] \int d^d \mathbf{k} \quad (62)$$

The 2D DOS requires the calculation of lattice integrals [15] appearing when taking matrix elements of the Green operator:  $I(E) = \langle \mathbf{k} | \sum_{\mathbf{k}'} \frac{|\mathbf{k}'\rangle \langle \mathbf{k}'|}{E - \epsilon(\mathbf{k}')} | \mathbf{k} \rangle = \sum_{\mathbf{k}} \frac{1}{E - \epsilon(\mathbf{k})}$ , thus:

$$\begin{aligned} I(E) &= \frac{a^2}{(2\pi)^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \frac{dk_x dk_y}{E - \epsilon(\mathbf{k})} \\ &= \frac{a^2}{(2\pi)^2} \int_{-\pi/a}^{\pi/a} \int_{-\pi/a}^{\pi/a} \frac{dk_x dk_y}{E - \epsilon_0 - 2V_0 \cos(k_x a) - 2V_0 \cos(k_y a)}. \end{aligned} \quad (63)$$

since  $\Omega = Na^2$  and  $d^2 \mathbf{k} = dk_x dk_y$ .

The DOS was obtained analytically with a mathematical "Tour de Force" by Morita and Horiguchi in a series of papers [16]:

$$D(E) = \frac{2}{\pi^2 B} \Theta(B - |E - \epsilon_0|) K \left( \sqrt{1 - \frac{(E - \epsilon_0)^2}{B^2}} \right). \quad (64)$$

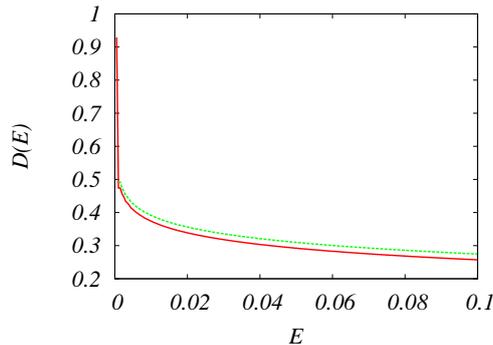


FIG. 4: (Color on-line) Comparison of the exact DOS expression 64 (in red) and the approximate logarithmic behavior (in green) around  $E = 0$  originating from  $K(z \sim 1) \sim \log(4) - \frac{1}{2} \log(1 - z) \dots$  where  $z = \sqrt{1 - \frac{(E - \epsilon_0)^2}{B^2}}$ .

$B = 4|V_0|$  and  $K(z)$  with  $z = \sqrt{1 - \frac{(E - \epsilon_0)^2}{B^2}}$  is the complete elliptic integral of the first kind defined from  $F(\phi, z)$  the Legendre elliptic integral of the first kind [17, 18]:

$$K(z) \equiv F(\pi/2, z), \quad F(\phi, z) = \int_0^\phi \frac{d\theta}{\sqrt{1 - z^2 \sin^2 \theta}} \quad (65)$$

$D(E)$  is displayed in Fig. 3 showing discontinuities (due to logarithmic behavior of the GF) at the band edges  $\pm \frac{(E - \epsilon_0)}{B}$  and a sharp behavior at the middle of the band ( $E = 0$ ).

DOS singularities (also called Van Hove [11]) originate from saddle or extremal points in the dispersion relation  $\epsilon(\mathbf{k})$  as observed in Fig. 2.

At a saddle point we have  $\nabla_{\mathbf{k}}\epsilon(\mathbf{k}) = 0$  and since  $D(E)$  is inversely proportional to  $|\nabla_{\mathbf{k}}\epsilon(\mathbf{k})|$  (see eq. 57) the singularity arises.

The sharp logarithmic behavior around  $E = 0$  can be explained from the properties of the complete elliptic integral of the first kind  $K(z)$ . Generally, logarithmic behavior is characteristic of 2D systems [11].

For  $\epsilon_0$  and  $E = 0$  we get  $z = 1$  around which  $K(z)$  behaves as [19]:

$$K(z \sim 1) \sim \log(4) - \frac{1}{2} \log(1 - z) \dots \quad (66)$$

Behavior of the dispersion relation around  $E = 0$  and the approximate analytic expression of  $K(z)$  are compared in Fig. 4.

Discontinuities around the the band edges  $\frac{(E - \epsilon_0)}{B} = \pm 4$  are due to the Heaviside factor  $\Theta(B - |E - \epsilon_0|)$  preventing occurrence of singularities originating from saddle points at  $E = \pm 4$  (see Fig. 2).

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