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LETTER TO THE EDITOR

The x-ray problem revisited

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Abstract
In this letter, we revisit the x-ray problem. Assuming point interaction between the conduction electrons and the instantaneously created core-hole, the latter's Green's function can be represented as a Fredholm determinant of certain Wiener–Hopf operators acting on $L^2(0, T)$ with discontinuous symbols. Here the symbols are the local conduction electron Green's function in the frequency domain and T is the time the core-hole spends in the system before removal. In this situation, the classical theory of singular integral equations usually employed in the literature to compute the large T asymptotics of the Fredholm determinant ceased to be applicable. A rigorous theory first put forward in the context of operator theory comes into play and universal constants are found in the asymptotics.

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We consider the classical x-ray problem where the core-hole is created at the origin at $t = 0$ and removed at $t = T > 0$. The object here is to study the behaviour of the core-hole Green's function as T gets large. By first integrating out the core-hole followed by the conduction electrons [4] or using a diagrammatic approach [15] the core-hole Green's reads

$$\frac{\mathcal{G}(T)}{\mathcal{G}^{(0)}(T)} = \frac{\det(A - vB)}{\det A} \tag{1}$$

where $v > 0$, is the strength of local potential and $\mathcal{G}^{(0)}$ is the free core-hole Green's function.

The operator A has kernel,

$$\left(\mathrm{i}\frac{\partial}{\partial t} + \frac{1}{2m}\frac{\partial^2}{\partial x^2} + \varepsilon_F\right)\delta(x - x')\delta(t - t') \tag{2}$$

and B is the multiplication operator

$$\delta(x)\chi_{[0,T]}(t) \tag{3}$$

where m is the mass of the conduction electrons, ε_F is the Fermi energy, and for simplicity we have assumed that the one-dimensional electron gas has parabolic dispersion, $E_p = \frac{p^2}{2m}$.

A simple calculation shows that

$$-\ln\left(\frac{\mathcal{G}(T)}{\mathcal{G}^{(0)}(T)}\right) = \mathrm{Tr}\int_0^v (A-\lambda B)^{-1} B\,\mathrm{d}\lambda$$
$$= \int_0^v \int_0^T G_\lambda(0,t;0,t+0)\,\mathrm{d}t\,\mathrm{d}\lambda$$
$$=: \int_0^v \int_0^T g_\lambda(t,t+0)\,\mathrm{d}t\,\mathrm{d}\lambda. \tag{4}$$

Here G_λ is the time-ordered electron Green's function and satisfies

$$\left(\mathrm{i}\frac{\partial}{\partial t} + \frac{1}{2m}\frac{\partial^2}{\partial x^2} + \varepsilon_F - \lambda\delta(x)\chi_{[0,T]}(t)\right) G_\lambda(x,t;x',t') = \delta(x-x')\delta(t-t') \tag{5}$$

or equivalently the integral equation,

$$G_\lambda(x,t;x',t') = G_0(x,t;x';t') + \lambda\int_0^T G_0(x,t;0,t'')G_\lambda(0,t'';x',t')\,\mathrm{d}t''. \tag{6}$$

Putting $x = x' = 0$ in (6) gives the integral equation

$$g_\lambda(t,t') = g_0(t-t') + \lambda\int_0^T g_0(t-t'')g_\lambda(t'',t')\,\mathrm{d}t'' \tag{7}$$

where $g_\lambda(t,t') := G_\lambda(0,t;0,t')$.

We define $F(\omega)$ to be the inverse Fourier transform of $g_0(t)$ so that

$$g_0(t) = \int_{-\infty}^{\infty} \exp(-\mathrm{i}\omega t)F(\omega)\frac{\mathrm{d}\omega}{2\pi} \qquad F(\omega) = \int_{-\infty}^{\infty} \frac{\Omega(\omega)}{\omega - \frac{p^2}{2m} + \varepsilon_F + \mathrm{i}0\,\mathrm{sgn}\omega}\frac{\mathrm{d}p}{2\pi} \tag{8}$$

where Ω is a Schwartz function which regulates the artificial ultraviolet divergence due to the idealized point interaction between the core-hole and the conduction electrons. We suppose that $\Omega(0) = 1$. It will be shown later that the universal constant and exponents in T are not affected by this regularization procedure. We find, by iterating (7),

$$\frac{\mathcal{G}(T)}{\mathcal{G}^{(0)}(T)} = \det(I - v\hat{g}_{(0,T)}) \tag{9}$$

where

$$\hat{g}_{(0,T)}f(t) := \int_0^T g_0(t-t')f(t')\,\mathrm{d}t'. \tag{10}$$

This is the determinant representation of $\mathcal{G}$ mentioned earlier and is the starting point for our analysis of the large T asymptotics. In a different physical context, to be described later the function F, defined below will be appropriately modified. Computing the integral in (8) gives

$$F(\omega-\varepsilon_F) = \Omega(\omega-\varepsilon_F)\begin{cases}\mathrm{i}\,\mathrm{sgn}(\omega-\varepsilon_F)\sqrt{\frac{m}{2\omega}} & 0 \leqslant \omega < \infty \\ -\sqrt{\frac{m}{-2\omega}} & -\infty < \omega < 0.\end{cases} \tag{11}$$

In the classical theory of integral operators the function F is called the symbol of the finite convolution operator, or finite Wiener–Hopf operator. The often stated theorem which yields the asymptotics of determinants of such operators is the classical result of Kac–Akhiezer–Hirschman [10–13]. However since the symbol has singularities at $\omega = \varepsilon_F$ and $\omega = 0$, this theorem no longer applies, and alternative methods are required to deal with such singularities. We note here that the theorem is already violated with one singularity. It is clear that the kernel which is the Fourier transform of $F(\omega-\varepsilon_F)$ has identical Fredholm determinant with that of $\det(I - v\hat{g}_{(0,T)})$.

There have been previous attempts in the physics literature to deal with such symbols, although much of the attempts are formal in nature. In the original paper [15], where a flat band approximation is used, $F(\omega)$ is replaced by the following:

$$F(\omega) = D_0(\alpha + \mathrm{i}\pi\,\mathrm{sgn}\omega) \qquad \omega \in \mathbb{R} \tag{12}$$

where D_0 is the density of states at the Fermi level and in this context ε_F is set to 0. The inverse Fourier transform of (12) gives rise to a linear combination of $\delta(t)$ and $P\frac{1}{t}$, where P is the principal value operator. Using this, (7) becomes a singular integral equation of the form,

$$a\phi(t) + \frac{b}{\mathrm{i}\pi} P \int_0^T \frac{\phi(t')}{t - t'}\,\mathrm{d}t' = \varrho(t) \qquad t \in [0, T] \tag{13}$$

where a and b are constants and $a^2 - b^2 \neq 0$. Now the 'driving term' ϱ, which is again a linear combination of a principal value operator and a Dirac delta, and which is neither in $L^2[0, T]$ nor belongs to the Hölder class, invalidates a straightforward application of the standard solution theory of singular integral equations described, for example, in [14]. In [15], a formal computation, which claims to give an exact expression for $\mathcal{G}(T)/\mathcal{G}^{(0)}(T)$, shows that it is asymptotic to

$$\exp\{a_1 T + a_2 \log T + a_3 + \mathrm{o}(1)\} \tag{14}$$

as $T \to \infty$, where a_j, $j = 1, 2, 3$, are constants independent of T. Indeed, a_1, contains a divergent term, which is, however, harmless, since it can be renormalized by a redefinition of the core-level. This is due to the choice of $F(\omega)$ in (12). There is also controversy [9] as to the precise value of a_2. Finally a_3 has so far not been computed, heuristically or otherwise, although attempts have been made [16].

On the other hand, in the mathematics literature singular symbols have been studied for some time. Older results from this literature as well as some recent progress in evaluating such asymptotics rigorously confirm the above form of the asymptotics. The reader is referred to [2, 3, 5, 6, 8]. We present those results here so that at least the value of the constants a_1 and a_2 can be conjectured with a high degree of certainty.

We begin by considering a class of symbols called the pure Fisher–Hartwig singular symbols. These are defined by

$$\psi_{\alpha,\beta}(\omega) = \left(\frac{\omega - 0\mathrm{i}}{\omega - \mathrm{i}}\right)^{\alpha} \left(\frac{\omega + 0\mathrm{i}}{\omega + \mathrm{i}}\right)^{\beta}.$$

(We specify the arguments of $\omega \pm 0\mathrm{i}$ and $\omega \pm \mathrm{i}$ to be zero or close to it when ω is large and positive.) This has the behaviour

$$\psi_{\alpha,\beta}(\omega) \sim |\omega|^{\alpha+\beta}\,\mathrm{e}^{\frac{1}{2}\mathrm{i}\pi(\alpha-\beta)\mathrm{sgn}\omega} \qquad \text{as} \quad \omega \to 0.$$

We associate a convolution operator with this symbol on $L^2[0, T]$ by convolving with the Fourier transform of $\psi - 1$. Let us call this operator plus the identity $W_T(\psi)$. Note that this symbol has the behaviour of our previous F defined in (11).

Since $\psi - 1$ is only known to be in L^2 a determinant for $W_T(\psi)$ is not defined necessarily. We must use the regularized determinant $\det_2 W_T(\psi)$. In the case where both determinants are defined for an operator A we have

$$\det{}_2 A = \det A\,\mathrm{e}^{-\mathrm{Tr}(A-I)}.$$

Now it follows from the results in [3] that if $|\mathcal{R}\rceil(\alpha \pm \beta)| < 1$ then

$$\frac{\det_2 W_T(\psi_{\alpha,\beta})}{G_2(\psi_{\alpha,\beta})^T} \sim \left(\frac{T}{2}\right)^{\alpha\beta} E(\alpha, \beta)$$

where

$$G_2(\psi) = \exp\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}(\log\psi(\omega) - \psi(\omega) + 1)\,\mathrm{d}\omega\right) \qquad E(\alpha,\beta) = \frac{G(1+\alpha)G(1+\beta)}{G(1+\alpha+\beta)}$$

and where G is the Barnes G-function, an entire function satisfying $G(z+1) = \Gamma(z)G(z)$ with the initial condition $G(1) = 1$.

The results of [3] can be modified so that a product of such functions times a smooth function can be considered. This has already been done when $\alpha = -\beta$ and in a few other special cases. However, the more general case follows now from the Toeplitz localization techniques of [7] which can be modified to apply to the Wiener–Hopf case as well. If we consider a product of two such functions, one with a singularity at zero and the other with a singularity at ε_F, and then multiplying the product by a 'nice' function b, the asymptotic formula obtained is as follows: let

$$\psi(\omega) = b(\omega)\psi_{\alpha_1,\beta_1}(\omega)\psi_{\alpha_2,\beta_2}(\omega - \varepsilon_F).$$

Then

$$\det{}_2 W_T(\psi) \sim G_2(\psi)^T \left(\frac{T}{2}\right)^{\alpha_1\beta_1+\alpha_2\beta_2} E \tag{15}$$

where the constant E is a product of three terms, that is $E = E_1E_2E_3$ where

$$E_1 = \frac{G(1+\alpha_1)G(1+\beta_1)}{G(1+\alpha_1+\beta_1)}\frac{G(1+\alpha_2)G(1+\beta_2)}{G(1+\alpha_2+\beta_2)}$$

and

$$E_2 = \exp\left(\frac{1}{2\pi}\int_0^{\infty} tS(t)S(-t)\,\mathrm{d}t\right)$$

where $S(t)$ is the Fourier transform of $\log b(\omega)$. The last factor is given by

$$E_3 = \frac{(1-\mathrm{i}\varepsilon_F)^{2\alpha_1\beta_2}(1+\mathrm{i}\varepsilon_F)^{2\alpha_2\beta_1}}{(2\mathrm{i}-\varepsilon_F)^{\alpha_2\beta_1}(-2\mathrm{i}-\varepsilon_F)^{\alpha_1\beta_2}\varepsilon_F^{\alpha_2\beta_1+\alpha_1\beta_2}}\frac{b_-(-\mathrm{i})^{\alpha_1}b_-(\varepsilon_F-\mathrm{i})^{\alpha_2}b_+(\mathrm{i})^{\beta_1}b_+(\varepsilon_F+\mathrm{i})^{\beta_2}}{b_-(0)^{\alpha_1}b_-(\varepsilon_F)^{\alpha_2}b_+(0)^{\beta_1}b_+(\varepsilon_F)^{\beta_2}}.$$

In this last factor all arguments are taken between $-\pi$ and π and the functions $b_\pm$ are the normalized Wiener–Hopf factors of b. For definitions of these factors and similar results, the reader is referred to [5] where the constant was first conjectured, although in the above form it appears here for the first time as far as the authors are aware. Also, it should be noted that while this is the formula for the regularized determinant, in the case that the ordinary determinant exists, for instance when $\alpha = \beta$ or if the function Ω is sufficiently small, then the asymptotic formula given above in (15) only changes by the factor G_2. It is replaced with

$$G_1(\psi) = \exp\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\log\psi(\omega)\,\mathrm{d}\omega\right).$$

This follows immediately from the definition of the regularized determinant.

It is interesting to note that in the above the first factor is the product of the constants that arise for a single singularity, the second term is the constant for nice symbols and the third factor is what arises from the interaction of all three.

Now we need to identify only the α and β. This computation yields that $\alpha_1 = 0$, $\beta_1 = -1/2$, $\alpha_2 = -\beta_2 = -\theta/\pi$, where $\tan\theta = v\Omega(0)\sqrt{\frac{m}{2\varepsilon_F}}$. This yields the following answer:

$$\det{}_2 W_T(\psi) \sim G_2(1 - vF)^T \left(\frac{T}{2}\right)^{-\frac{\theta^2}{\pi^2}} E_1E_2E_3 \tag{16}$$

where

$$E_1 = G\left(1 + \frac{\theta}{\pi}\right) G\left(1 - \frac{\theta}{\pi}\right)$$

and

$$E_2 = \exp\left(\frac{1}{2\pi}\int_0^\infty t S(t) S(-t)\, \mathrm{d}t\right)$$

where $S(t)$ is the Fourier transform of

$$\ln\left(\frac{1 - vF(\omega)}{\psi_{0,-1/2}(\omega)\psi_{-\theta/\pi,\theta/\pi}(\omega - \varepsilon_F)}\right).$$

The last factor is given by

$$E_3 = \frac{(1 + \mathrm{i}\varepsilon_F)^{\frac{\theta}{2\pi}}}{(2\mathrm{i} - \varepsilon_F)^{\frac{\theta}{\pi}} \varepsilon_F^{\frac{\theta}{2\pi}}} \frac{b_-(\varepsilon_F - \mathrm{i})^{\frac{-\theta}{\pi}} b_+(\mathrm{i})^{-1/2} b_+(\varepsilon_F + \mathrm{i})^{\frac{\theta}{\pi}}}{b_-(\varepsilon_F)^{-\frac{\theta}{\pi}} b_+(0)^{-1/2} b_+(\varepsilon_F)^{\frac{\theta}{\pi}}}.$$

An allied problem which arises from the study of the x-ray photo emission of a two-dimensional electron gas under the influence of a constant magnetic field [17], where

$$F(\omega - \varepsilon_F) = \Omega(\omega - \varepsilon_F) \sum_{n=0}^{\infty} \frac{\exp(-\alpha n)}{\omega - n\omega_\mathrm{c} + \mathrm{i}\delta \operatorname{sgn}(\omega - \varepsilon_F)} \tag{17}$$

where $\alpha > 0$ provides a high energy cut-off and ω_c, a fixed positive parameter, is the cyclotron frequency and we think of δ as a small positive constant which we later let tend to zero.

This symbol is again discontinuous and in this case since $\alpha = -\beta$ the previously mentioned analysis also applies. For this purpose, we first compute the jump of $1 - vF$. We consider the quantity

$$\alpha - \beta = \frac{1}{\mathrm{i}\pi} \ln \frac{(1 - vF)_{\omega=\varepsilon_F^+}}{(1 - vF)_{\omega=\varepsilon_F^-}}. \tag{18}$$

This is seen to be

$$\frac{1}{\mathrm{i}\pi} \ln\left(\frac{1 - c + \mathrm{i}d}{1 - c - \mathrm{i}d}\right) \tag{19}$$

where

$$c = -v\Omega(0) \sum_{n=0}^{\infty} \frac{\exp(-\alpha n)(\varepsilon_F - n\omega_\mathrm{c})}{(\varepsilon_F - n\omega_\mathrm{c})^2 + \delta^2} \tag{20}$$

and

$$d = -v\Omega(0)\delta \sum_{n=0}^{\infty} \frac{\exp(-\alpha n)}{(\varepsilon_F - n\omega_\mathrm{c})^2 + \delta^2}. \tag{21}$$

This yields asymptotics again of the form found in equation (15) except that there is just one singularity. The form these take is

$$\det{}_2 W_T(\psi) \sim G_2(1 - vF)^T \left(\frac{T}{2}\right)^{-\theta^2/\pi^2} E \tag{22}$$

where θ is the arctangent of $\frac{d}{1-c}$.

Let us now consider these asymptotics as δ tends to zero. If Ω is nice enough, say bounded, continuous and integrable, then the G_2 term tends to a limit. This is also true of the

β term. In fact, a straightforward calculation shows that if $\varepsilon_F \neq p\omega_c$ for any positive integer p then θ tends to zero as δ tends to zero.

If $\varepsilon_F = p\omega_c$ for some p then to compute the limit, we note that $d = a/\delta + O(\delta)$ with a constant and negative and that $1 - c = 1 + O(\delta)$. Thus as δ tends to zero, θ approaches $-\pi/2$ and the exponent in formula (22) approaches $-1/4$.

However, it should be pointed out that from the extensive work in the past that as far as the asymptotics go, these limits are sometimes correct at least in the first two terms, but that the constant terms do not always yield a correct answer when limit processes are interchanged. In any case, if the x-ray case bears resemblance to the classical work done in the Ising model, then the appearance of the '1/4' is no surprise.

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