



# A Note on the Exact Green Function for a Quantum System Decorated by Two or More Impurities

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The exact Green function is constructed for a quantum system, with known Green function, which is decorated by two delta function impurities. It is shown that when two such impurities coincide they behave as a single singular potential with combined amplitude. The results are extended to N impurities and higher dimensions.

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## 1. INTRODUCTION

The one dimensional harmonic oscillator or square well, for example, for which the energy -dependent Green function  $G_0(x, x'; E)$  is known, have been taken for many years as solvable models for semi-conductor quantum wells [1]. Frequently delta function potentials are placed at various points to simulate defects or impurities. In the case of a single impurity potential,  $V(x) = \lambda\delta(x - a)$ , the Green function for the composite system is known to be [2]

$$G(x, x'; E) = G_0(x, x') + \lambda \frac{G_0(x, a; E)G_0(a, x')}{1 - \lambda G_0(a, a; E)} \quad (1)$$

In this note a corresponding formula is derived for the case  $V(x) = \lambda\delta(x - a) + \mu\delta(x - b)$  On the basis of the analogy of the algebraic structure the result is extended to N-impurities and for a standard interpretation of the Dirac delta function, to higher dimension.

## 2. CALCULATION

We first note that the same argument can be used for the time dependent-, as well as the energy-dependent Green functions, so we shall omit the third argument and write simply  $G(x, x')$ .

Beginning with the Dyson equation, noting that  $G_0(x, y) = G_0(y, x)$

$$G(x, x') = G_0(x, x') + \int G_0(x, y)V(y)G(y, x')dy, \quad (2)$$

where the integration extends over the system domain, one has the set of equations

$$G(x, x') = G_0(x, x') + \lambda G_0(x, a)G(a, x') + \mu G_0(x, b)G(b, x') \quad (3)$$

$$G(a, x') = G_0(a, x') + \lambda G_0(a, a)G(a, x') + \mu G_0(a, b)G(b, x'), \quad (4)$$

$$G(b, x') = G_0(b, x') + \lambda G_0(a, b)G(a, x') + \mu G_0(b, b)G(b, x'). \quad (5)$$

The linear Equations (4) and (5) are easily solved for  $G(a, x')$  and  $G(b, x')$ :

$$G(a, x') = \frac{G_0(a, x') + \mu[G_0(b, x')G_0(a, b) - G_0(a, x')G_0(b, b)]}{D} \tag{6}$$

$$G(b, x') = \frac{G_0(b, x') + \lambda[G_0(a, x')G_0(a, b) - G_0(b, x')G_0(a, a)]}{D} \tag{7}$$

with

$$D = [1 - \lambda G_0(a, a)][1 - \mu G_0(b, b)] - \lambda \mu [G_0(a, b)]^2. \tag{8}$$

By inserting (6) and (7) into (3) we obtain the desired expression

$$\begin{aligned} G(x, x') &= G_0(x, x') \\ &+ \frac{1}{D} \{ \lambda G_0(x, a) G_0(a, x') + \mu G_0(x, b) G_0(b, x') \\ &+ \lambda \mu [G_0(x, a) (G_0(a, b) G_0(a, x') - G_0(b, b) G_0(b, x')) \\ &+ G_0(x, b) (G_0(a, b) G_0(a, x') - G_0(a, a) G_0(a, x'))] \}. \tag{9} \end{aligned}$$

### 3. DISCUSSION

By setting  $\mu$  to 0 (9) reduces to (1), proving this expression as well. The most salient feature of (9) is the denominator  $D$  whose zeros form the exact spectrum of the composite system. For example, when  $a$  and  $b$  coincide,  $D$  reduces to  $1 - (\lambda + \mu)G_0(a, a)$  and (9) reduces to (1) with  $\lambda$  replaced by the amplitude  $\lambda + \mu$ . I.e., the two impurities combine to form one with combined amplitude. This generalizes the result of Fassari and Rinaldi [3], for two identical defects symmetrically placed with respect to the center of a harmonic oscillator. An expression similar to (9) has been derived recently by Horing (private communication) for the case of a quantum dot in a magnetic field.

Two further points can be made. Nothing in the derivation of (9) restricts it to the line. If we accept the standard definition  $\delta(\vec{x}) = \prod_{j=1}^d \delta(x_j)$ , then (9), and its consequences, are valid for  $d$ -dimensional quantum systems. This has been proven function-theoretically for the three dimensional quantum dot with two symmetrically placed identical impurities by Albeverio et al. [4].

A second observation is that  $D$  is simply the Cramer determinant for the pair of simultaneous linear Equations (4) and (5). In the case of impurity potential

$$V(x) = \sum_{j=1}^N \lambda_j \delta(x - a_j) \tag{10}$$

there will be  $N$  such equations and the determinant is easily evaluated. The general result is

If a quantum system having Green function  $G_0(x, y)$  is decorated with  $N$  delta function impurities  $\lambda_j \delta(x - a_j)$ ,  $j = 1, 2, \dots, N$ , then the new energy levels are the roots of

$$D_N = \prod_{j=1}^N A_{jj} - \sum_{j=2}^N (-1)^j \sum_{1 \leq k_1 < \dots < k_j \leq N} A_{k_1 k_2} A_{k_2 k_3} \dots A_{k_j k_1} = 0 \tag{11}$$

where  $A_{lm} = \delta_{lm} - \lambda_l G_0(a_l, a_m)$ .

Thus,

$$\begin{aligned} D_3 &= \prod_{j=1}^3 [1 - \lambda_j G_0(a_j, a_j)] - \sum_{i < j} \lambda_i \lambda_j G_0(a_i, a_j) G_0(a_j, a_i) \\ &+ \lambda_1 \lambda_2 \lambda_3 G_0(a_1, a_2) G_0(a_2, a_3) G_0(a_3, a_1), \tag{12} \end{aligned}$$

which reduces to the  $N = 1$  and  $N = 2$  cases appropriately and shows that any two coinciding impurities coalesce as indicated above.

Note that if all the  $\lambda$ s and  $a$ 's coincide then

$$D_N = (1 - \lambda G_0(a, a))^N - \sum_{j=2}^N \binom{N}{j} \lambda^j G_0(a, a)^j = (1 - N\lambda G_0(a, a)). \tag{13}$$

Equation (11) might offer a new approach to Kronig-Penney-type systems for periodic or random unit cells.

Finally, it should be pointed out that the work in this note is paralleled in the theory of quantum graphs introduced by Linus Pauling about 1930 to describe electrons in molecules which has developed into a sophisticated and important branch of quantum physics [5]. For relations of this discipline to the present work see the papers by Andrade et al. [6] and Andrade and Severini [7].

### AUTHOR CONTRIBUTIONS

The author confirms being the sole contributor of this work and has approved it for publication.

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