

ON A STATISTICAL INTERRELATION BETWEEN SPECTRAL  
GAP AND TRANSITION TO SUPERCONDUCTIVITY

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**Abstract:** Recently random Schrödinger operators based on a discrete position space have drawn some attention. We illustrate the applicability of these models to a physically plausible statistical explanation of the phenomenon of superconductivity. In particular, a physically interpretable random Schrödinger operator for the description of a pair of electrons interacting with a lattice of ions is introduced. The functional dependence of the expected spectral gap of the operator on the lattice constant is studied based on a long term computer experiment. It turns out that the obtained function carries valuable statistical information about the temperature of transition to superconductivity for 24 chemical elements.

Dedicated to Professor Holger Petersson from Hagen  
on the occasion of his 70-th birthday.

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## 1. Introduction

H. Kamerlingh discovered 1911 the super-conducting state of matter in which there is no measurable electric resistance (cf. [4]). Typical for this phenomenon is the fact that the electric resistance of a substance  $X$  vanishes if an appropriate probe is cooled below a characteristic temperature  $T_{\text{sup}}(X)$  which is also called transition temperature. In context of applications one is in particular interested in substances with high transition temperatures.

The qualitative understanding of the phenomenon of superconductivity is based on the microscopic notion of the so-called Cooper pairs of electrons. The prediction of the material specific transition temperature from a microscopic model remains, however, a challenging task.

It is generally believed (cf. [4]) that superconductivity is a quantum mechanical phenomenon. On the other hand, we perceive (cf. [1] and [2] and literature cited therein) some interest in the mathematical properties of random Schrödinger operators which are relevant for the quantum mechanical description of solids. In particular, the case of discrete position space which is mathematically more easily accessible than the continuous theory and offers an attractive field for computer based studies, has recently drawn some attention.

In the present contribution we show that the concept of random Schrödinger operators based on a discrete position space can be successfully applied to the quantitative prediction of laboratory measurements in connection with the super-conducting state of matter.

The paper is organized as follows. In Section 2 a random Schrödinger operator is introduced describing a pair of electrons that are confined to a neighborhood of a finite lattice which models the sites where ions of a solid are located. The potential term of the operator is motivated by the Coulomb interaction between electrons and ions. In Section 3 we are interested in the expected width of a spectral gap of the Schrödinger operator; to our knowledge the analytical determination of the gap is a mathematically unsolved problem which we tackle by statistical evaluation of a long term computer experiment. A model function describing the dependence of the spectral gap on the (crystallographic) lattice constant is also established. In Section 4 we propose a possibility of fitting the lattice constant of a substance to its boiling point, which enables us to explore the quality of the spectral gap as a regressor for the statistical prediction of transition temperature for 24 super-conducting chemical elements.

### 2. A Schrödinger Operator for Two Electrons

Let us consider a finite lattice

$$L_a = \{na | n = 0, \dots, N\}$$

which models a discrete position space. Parameter  $a > 0$  is called lattice constant. A quantum mechanical state of an electron confined to the lattice is described by a function  $\varphi : L_a \rightarrow \mathbb{C}$  such that

$$\sum_{n=0}^N |\varphi(na)|^2 = 1.$$

In this context  $|\varphi(na)|^2$  is interpreted as the probability of location of the electron in a neighborhood of the lattice point  $na \in L_a$ . By a standard identification the set of all states can be viewed as the unit sphere in  $\mathbb{C}^{N+1}$ .

The kinetic term  $H_0 : \mathbb{C}^{N+1} \rightarrow \mathbb{C}^{N+1}$  of the discrete Schrödinger operator is defined by

$$(H_0\varphi)(na) = -\frac{\hbar^2}{2ma^2} \cdot (\varphi((n+1)a) - 2\varphi(na) + \varphi((n-1)a)) \tag{2.1}$$

for  $n = 0, \dots, N$ , where  $\hbar$  and  $m$  denote Planck constant and mass of an electron, respectively; in (2.1) the convention

$$\varphi(na) = 0 \quad \text{for } n < 0 \quad \text{and for } n > N$$

is used. (2.1) can be viewed as a discrete approximation of the kinetic term appearing in the classical 1-dimensional Schrödinger equation for the position space modelled by the real line.

The possible quantum mechanical states of a pair of electrons are elements of the tensor product  $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$  with the orthonormal basis  $(e_i \otimes e_j)_{i,j=0}^N$ , where  $e_i$  denotes the  $i$ -th canonical unit column vector in  $\mathbb{C}^{N+1}$ . By the linear isomorphism  $\Psi : \mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1} \rightarrow \mathbb{C}^{(N+1)^2}$  which is defined by

$$\Psi(e_i \otimes e_j) = e_i e_j' \quad (i, j = 0, \dots, N),$$

where  $e_j'$  denotes the transpose of column vector  $e_j$ , we can identify tensor product  $\mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$  with  $\mathbb{C}^{(N+1)^2}$ .

The kinetic term

$$H_0^2 : \mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1} \rightarrow \mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$$

of the Schrödinger operator for a pair of electrons is given by

$$H_0^2 := H_0 \otimes I_{N+1} + I_{N+1} \otimes H_0,$$

where  $I_{N+1} : \mathbb{C}^{N+1} \rightarrow \mathbb{C}^{N+1}$  denotes the identity map.

Let  $X_0, \dots, X_N, Y_0, \dots, Y_N$  be stochastically independent random vectors that are distributed uniformly over the cube

$$C := [-a/2, a/2]^3 \subset \mathbb{R}^3.$$

If two electrons are located in neighborhoods of two lattice points  $ma, na \in L_a$ , then their positions are modelled by

$$X_m + ma \cdot e_1 \quad \text{and} \quad Y_n + na \cdot e_1;$$

this smearing out of the positions will turn out to be necessary in view of the singularity in the Coulomb potential. The Coulomb repulsion between these electrons is given by

$$V_r(m, n) = \frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{d(X_m + ma \cdot e_1, Y_n + na \cdot e_1)}$$

for  $m, n = 0, \dots, N$ , where  $e_1, e, \varepsilon_0$  and  $d$  denote the first canonical unit vector in  $\mathbb{R}^3$ , the charge of an electron, the permittivity of vacuum and the Euclidean distance, respectively. Analogously, the Coulomb attraction between the electrons and the ions (the latter being located exactly at the lattice points of  $L_a$ ) can be expressed by

$$V_a^{(1)}(m) = -\frac{e^2}{4\pi\varepsilon_0} \cdot \sum_{k=0}^N \frac{1}{d(X_m + ma \cdot e_1, ka \cdot e_1)}$$

and

$$V_a^{(2)}(n) = -\frac{e^2}{4\pi\varepsilon_0} \cdot \sum_{k=0}^N \frac{1}{d(Y_n + na \cdot e_1, ka \cdot e_1)}$$

for  $m, n = 0, \dots, N$ . The (random) potential term  $V : \mathbb{C}^{(N+1)^2} \rightarrow \mathbb{C}^{(N+1)^2}$  of the Schrödinger operator is defined by

$$(V\psi)(m, n) := (V_r(m, n) + V_a^{(1)}(m) + V_a^{(2)}(n))\psi(m, n).$$

for  $m, n = 0, \dots, N$ .

Finally, the announced random Schrödinger operator

$$H : \mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1} \rightarrow \mathbb{C}^{N+1} \otimes \mathbb{C}^{N+1}$$

describing two electrons located in a neighborhood of lattice  $L_a$  is defined by

$$H := H_0^2 + \Psi^{-1}V\Psi.$$

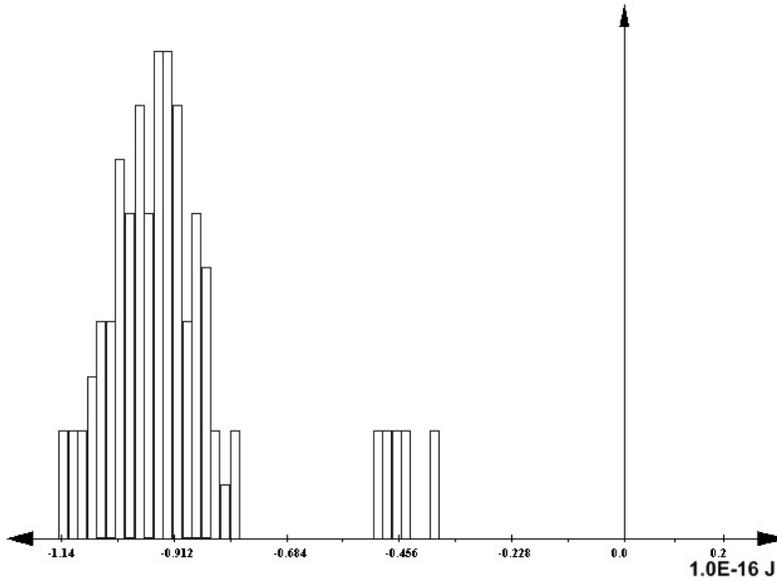


Figure 1: Histogram estimate of the spectral density

### 3. The Expected Spectral Gap

Since the introduced Schrödinger operator  $H$  is self-adjoint and acts on a finite dimensional Hilbert space, it can be represented by a Hermitian matrix. The spectral decomposition of this matrix can be performed numerically by the Jakobi algorithm (cf. [5]). From the obtained spectrum the spectral density can be estimated by the histogram method (for the notions of the thermodynamic limit and of the spectral density cf. [2]). Figure 1 shows a typical histogram estimate of the spectral density obtained in a computer experiment for Schrödinger operators  $H$  based on realizations of the random vectors  $X_0, \dots, X_N, Y_0, \dots, Y_N$  introduced in Section 2. In particular the spectral gap revealed by the histogram can be extracted from the spectrum.

To estimate the expected width of the spectral gap 1600 independent replicas of the random Schrödinger operator have been generated and the corresponding average width has been computed for the number  $N + 1 = 10$  of points in lattice  $L_a$ .

This experiment has been repeated 200 times, where lattice constant  $a$  has

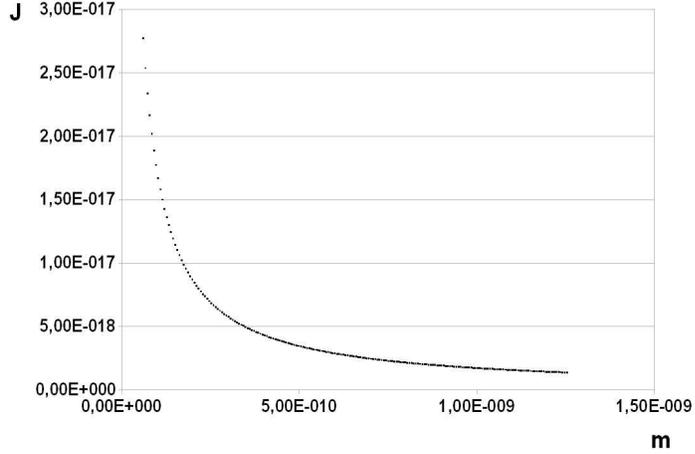


Figure 2: Lattice constant vs. average spectral gap

been varied within the relevant interval  $[0.6 \cdot 10^{-10}\text{m}, 1.25 \cdot 10^{-9}\text{m}]$  containing typical values of the crystallographic lattice constant. Figure 2 shows the obtained estimates of the expected spectral gap  $G$  as function of lattice constant  $a$ . To describe the dependence between  $a$  and  $G$  analytically, we consider the ansatz

$$G(a) = \gamma \cdot a^{-1}, \quad (3.1)$$

where constant  $\gamma$  can be fitted to the computer experimental data by the least squares method yielding  $\hat{\gamma} = 1.7037 \cdot 10^{-27} \text{Jm}$ . The average relative error in the prediction  $\hat{G}(a) = \hat{\gamma} \cdot a^{-1}$  of the 200 spectral gap values attains 1.53% which underlines the quality of fit  $\hat{G}$ .

For a numerical illustration of estimate  $\hat{\gamma}$  we point out that

$$\hat{\gamma} \approx \frac{\hbar \cdot c}{20},$$

where  $c$  denotes the velocity of light.

#### 4. The Statistical Evaluation

To explore the predictive power of the expected spectral gap (whose approximation is obtained in Section 3) w.r.t. the material specific transition temperature  $T_{sup}(X)$ , we utilize the laboratory data for 24 super-conducting chemical ele-

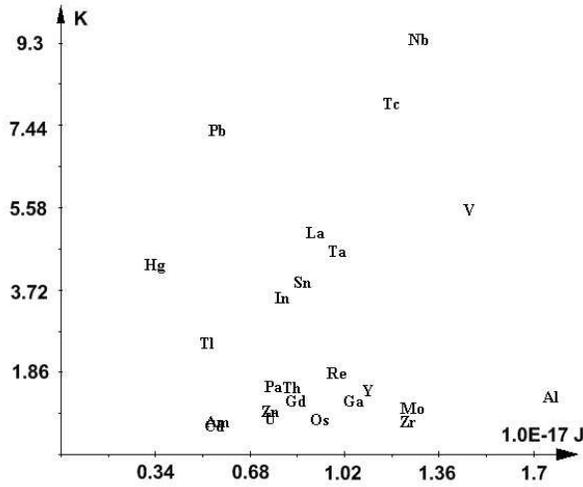


Figure 3: Spectral gap versus transition temperature

ments.

The interaction between molecules of a substance  $X$  can be modelled by the Lennard-Jones potential  $\Phi_X$  which is given by

$$\Phi_X(r) = 4U_X \cdot \left( \left( \frac{r_X}{r} \right)^{12} - \left( \frac{r_X}{r} \right)^6 \right).$$

$\Phi_X(r)$  represents the potential energy of a configuration of two molecules of substance  $X$  at distance  $r$ . In [3] a possibility of fitting parameters  $U_X$  and  $r_X$  of  $\Phi_X$  to the boiling point of substance  $X$  is presented.

We utilize this possibility and put

$$a_X := 2^{1/6} \cdot r_X \tag{4.1}$$

for the element specific lattice constant  $a_X$ . Note that Lennard-Jones potential  $\Phi_X$  attains its minimum at  $r = a_X$ .

In Figure 3 the values of  $\widehat{G}(a_X)$  are graphed on the horizontal axis versus the temperatures  $T_{sup}(X)$  of transition to superconductivity on the vertical axis for 24 chemical elements  $X$ . After removal of the outliers Al, Hg, Mo, Pb, Zr the empirical correlation coefficient attains the value 0.65258 which indicates a moderate correlation between the considered quantities. The linear ansatz

$$k_B T_{sup}(X) = \gamma_0 + \gamma_1 \cdot \widehat{G}(a_X), \tag{4.2}$$

where  $k_B$  denotes Boltzmann constant, entails the least-squares estimates

$$\hat{\gamma}_0 = -4.2971 \cdot 10^{-23} \text{J} \quad \text{and} \quad \hat{\gamma}_1 = 9.25178 \cdot 10^{-6}$$

of parameters  $\gamma_0$  and  $\gamma_1$ .

We interpret the region below the expected spectral gap of the random Schrödinger operator introduced in Section 2 as the range of energy corresponding to the association of electrons in Cooper pairs. The wider the spectral gap the higher the required temperature at which there is a tendency for thermal decay of Cooper pairs entailing a destruction of the super-conducting phase; in this sense ansatz (4.2) is microscopically justified and physically plausible. (4.2) and (3.1) suggest, moreover, an increase of  $T_{sup}(X)$  for decreasing values of lattice constant  $a_X$ , which statistically explains the observation of increased transition temperature under high pressure reported for some substances.

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