Exact results for spatial decay of the one-body density matrix in low-dimensional insulators

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We provide a tight-binding model of insulator, for which we derive an exact analytic form of the one-body density matrix and its large-distance asymptotics in dimensions $D = 1, 2$. The system is built out of a band of single-particle orbitals in a periodic potential. Breaking of the translational symmetry of the system results in two bands, separated by a direct gap whose width is proportional to the unique energy parameter of the model. The form of the decay is a power law times an exponential. We determine the power in the power law and the correlation length in the exponential, versus the lattice direction, the direct-gap width, and the lattice dimension. In particular, the obtained exact formulae imply that in the diagonal direction of the square lattice the inverse correlation length vanishes linearly with the vanishing gap, while in non-diagonal directions, the linear scaling is replaced by the square root one. Independently of direction, for sufficiently large gaps the inverse correlation length grows logarithmically with the gap width.

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The rapid progress in computational techniques used for calculating properties of solids enabled researchers to implement a localized real-space approach to describing such properties. It has made possible large-scale calculations based on the density functional theory \cite{1}, in particular calculating the electronic structure of solids by means of $O(N)$ methods \cite{2, 3}. In all these methods it is the one-body density matrix (DM) that is the central quantity. Its decay rate determines the degree of locality of all quantities relevant for physics and is decisive for the speed of the involved algorithms. This is why one observes a growing interest in localization properties of DM in recent years.

However, the first result concerned with the rate of decay of DM was published by W. Kohn as early as in 1959 \cite{4}. Kohn demonstrated that in a one-dimensional centrosymmetric crystal, the Wannier functions, and hence the DM, decay exponentially with sufficiently large distance. This result was extended to crystals of higher dimensionality by J. Des Cloizeaux \cite{5}.

For the reasons explained briefly above, the problem of the rate of decay of DM became the one of vital importance about forty years later. The typical questions in this respect are concerned with the dependence of the decay rate on dimensionality and energy parameters (especially the direct-gap width) of systems under study. First, Baer and Gordon \cite{6} gave general arguments that the exponential decay, discovered by Kohn, is valid irrespectively of dimensionality, and moreover, the correlation length, $\xi$, that characterizes the exponential decay, scales with the direct-gap width, $\delta$, like $\xi^{-1} \sim \sqrt{\delta}$. Then, the question of the rate of decay of DM was reconsidered by Ismail-Beigi and Arias \cite{7} in a general, model-independent context, for crystals of arbitrary dimensionality, that is in systems described by single-particle orbitals in periodic potentials. They found also the exponential decay law in insulators of arbitrary dimensionality but questioned the validity of the scaling $\xi^{-1} \sim \sqrt{\delta}$, obtained in \cite{5}. They argued that instead of the square root scaling, the linear one, $\xi^{-1} \sim \delta$, holds at least in the limit of vanishing direct-gap width. After that, He and Vanderbilt \cite{8} discovered a power-law factor, which multiplies the exponential factor in the asymptotic formula for DM in one-dimensional crystals. All these findings created a situation in which it was highly desirable to construct a $D > 1$ model of insulator whose DM could be investigated exactly in the large-distance asymptotic regime, and the dependence of power and exponential laws of decay on dimensionality and direct-gap width could be determined unambiguously.

Quite recently, an attempt at constructing such a model was made by Taraskin et al \cite{9}. They proposed a simple tight-binding model, built out of two kinds of single-particle orbitals at each lattice site, which they consider to contain the basic features of an insulator. They succeeded in demonstrating analytically the existence of a power-law factor and an exponential one in all three dimensions $D = 1, 2, 3$. However, the result was obtained only for very large values of one of the energy parameters of the model, which is in no definite relation with the direct-gap width \cite{10} (unless some additional assumptions about the energy parameters of the model are made). Moreover, the model proposed by Taraskin et al is not a kind of crystal studied in the papers cited above, since it is translation invariant.

We have succeeded in deriving analytically the exact
form of DM (in terms of special functions) and its large-distance properties for another system, which is a crystal. The system consists of one kind of single-particle orbitals at each lattice site, which are subjected to an external periodic potential. There is the unique energy parameter that determines the strength of the periodic potential. This system exhibits two bands separated by a direct gap whose width is proportional to the unique energy parameter. We have derived the power-law and exponential factors in the large distance asymptotics of DM in dimensions $D = 1, 2$, for small and large direct-gap widths, and in arbitrary direction in the $D = 2$-case.

Consider the model described by the following second-quantized Hamiltonian

$$H = \sum_i U_i a_i^+ a_i + t \sum_{\langle i, j \rangle} (a_i^+ a_j + h.c.).$$

(1)

In the above expression, $i, j$ represent the lattice sites of a $D$-dimensional lattice, while $\langle i, j \rangle$ stands for a pair of nearest neighbors on this lattice. The operators $\{a_i^+, a_i\}$ create, annihilate, respectively, a spinless fermion in a single-particle orbital $|k\rangle$, belonging to an orthonormal basis. The value of the external potential at site $j$ is $U_j$. Suppose that the underlying lattice is a $D$-dimensional simple cubic lattice, which consists of two inter-penetrating sublattices (the even and odd sublattices), such that the nearest neighbors of a site on one sublattice belong to the other one. Then, we set $U_j = U_1$ on the odd sublattice and $U_j = U_2$ on the even one. Under the periodic boundary conditions the Hamiltonian (1) is block-diagonalized by the plane wave orbitals $|k\rangle$ with the wave vector in the first Brillouin zone of the lattice. Specifically, shifting the energy scale to $(U_1 + U_2)/2$ and expressing all the energies in the units of the transfer in-bands of eigenenergies:

$$\Lambda_{k}^\pm = \pm 2\sqrt{(u/2)^2 + S_k^2} = \pm 2\Delta(k),$$

(2)

In (2) the wave vector $k$ is restricted to the first Brillouin zone of one of the sublattices, $u \equiv (U_2 - U_1)/2t$ is the unique energy parameter of the model, and $S_k = \frac{1}{2} \sum_{j: \langle i, j \rangle} \exp(i k (i - j))$ stands for the structure factor. Without any loss of generality, we can set $u > 0$. The two bands are mutually symmetric about zero and are separated by the gap $\delta = 2u$. For $u \neq 0$ and completely filled lower band, the system given by (1) is an insulator in the sense of the band theory, which we call the chessboard insulator. The eigenvectors corresponding to the eigenvalues $\Lambda_{k}^\pm$, $|k, \pm\rangle$, respectively, are linear combinations of the vectors $|k\rangle$ and $|k + \pi\rangle$, where $|\pi\rangle$ stands for the vector whose all components are equal to $\pi$. By means of these eigenvectors one can calculate the zero-
temperature, non-diagonal elements of DM:

$$\langle a_i^+ a_{i+r} \rangle = -\frac{1}{2} \sum_{l=1}^{D} S_l R(r), \text{ if } \sigma_r = 2m + 1,$$

$$\langle a_i^+ a_{i+r} \rangle = -\frac{u}{2} (-1)^{\sigma_r} R(r), \text{ if } \sigma_r = 2m,$$

(3)

where

$$R(r) = (2\pi)^{-D} \int_{B.Z.} dk \exp(i k r) \Delta^{-1}(k),$$

(4)

and $S_l R(r) \equiv R(r_1 + \ldots + r_l) + R(r_1 - \ldots - r_l)$, and so on for $l = 2, \ldots, D$. In (11), the D-dimensional integral is taken over the first Brillouin zone of a sublattice and $r \neq 0$. For the discussion that follows it is convenient to introduce the parameter $\sigma_r \equiv \sum_{l=1}^{D} |r_l|$, which amounts to (a noneuclidean) distance between the lattice point $r$ and the origin. Note that the matrix elements of DM depend on $R(r)$ evaluated only at the points $r$ with $\sigma_r$ even.

In the cases studied here we have found that up to a coefficient independent of $\sigma_r$,

$$R(r) \sim \sigma_r^{-\gamma} \exp(-\sigma_r/\xi),$$

(5)

for sufficiently large $\sigma_r$, with the power $\gamma$ depending only on the dimensionality of our insulator and $\xi$ depending on the direction of $r$ and the direct-gap width.

Specifically, in $D = 1$-case, the function $R(r)$ at even points ($\sigma_r = r = 2m$) can be expressed by the Legendre function of the second kind, $Q_{\gamma}(x)$:

$$R(2m) = \frac{\kappa}{4\pi} \int_0^\pi \frac{\cos(2mk)dk}{\sqrt{1 - \kappa^2 \sin^2 k}} = \frac{(-1)^m}{2\pi} Q_{m-\frac{1}{2}}(1 + \frac{u^2}{2}),$$

(6)

where $\kappa^2 = (1 + (u/2)^2)^{-1}$. For sufficiently large $m$, the above expression can be cast in the form (22), where

$$\xi^{-1} = \ln\left(1 + (u/2)^2 + u/2\right), \quad \gamma = 1/2.$$ (7)

The small and large $u$ asymptotic behaviors of $\xi$ in (22) read:

$$\xi^{-1} \approx \frac{u/2 + \ldots}{u/2 + \ldots}, \quad \text{and} \quad \xi^{-1} \approx \ln u + u^{-2} + \ldots.$$ (8)

The inverse correlation length given by the formulas (22), (23), and by high-accuracy numerical calculations, plotted versus $u$, are compared in Fig. 11. The asymptotic behavior (23) has been also obtained numerically in one-dimensional crystals with periodic potentials of period greater than two (24). Naturally, in $D = 2$-case the form of $R(r)$ is more
FIG. 1: The inverse correlation length, $\xi^{-1}$, versus $u$ in $D = 1$ crystal: the data obtained from high-accuracy computation of $R(r)$ given by [10] – circles, exact analytical result [11] – thick continuous curve, the asymptotic behavior of $\xi^{-1}$, for small and large $u$, given in [12] – dotted curves.

complex [11]:

$$R(r) = \frac{1}{\pi^2} \int_0^\frac{\pi}{2} \int_0^\frac{\pi}{2} \frac{\cos(2nx) \cos(2ny)}{\sqrt{\beta^2 + \cos^2 x \cos^2 y}} \, dx \, dy$$

$$= \frac{(-1)^m}{2\pi} \frac{1}{(2\beta)^{2m+1}} \frac{\Gamma(m+n+1)\Gamma(m-n+1)}{\Gamma^2(m+1/2)}$$

$$\times F(m+1/2, m+1/2; m+n+1; -1/a)$$

$$\times F(m+1/2, m+1/2; m-n+1; -1/a),$$

where $F(a, b; c; x)$ stands for the Gauss hypergeometric function, $\Gamma(a)$ for the Euler $\Gamma$-function, and the following notation was used

$$a = 2\beta(\sqrt{1+\beta^2} + \beta), \quad \beta \equiv u/4,$$

$$r_1 + r_2 = 2m = \sigma_r, \quad r_1 - r_2 = 2n.$$  

To analyse $R(r)$ given by [10], we first consider the diagonal direction ($r_1 = r_2, n = 0$). Then, $R(r)$ can be expressed by the Legendre function of first kind [11] [12], $P^m_\nu(x)$:

$$R(r) = \frac{(-1)^m}{4\pi^3 \beta} \frac{1}{\Gamma^2(m+1/2)} \left[ P^m_\frac{1}{2} (1+2/a) \right]^2.$$  

(11)

For sufficiently large $\sigma_r = 2m$, the above $R(r)$ assumes the form [5]:

$$R(r) \underset{m \to \infty}{\approx} \frac{(-1)^m \exp(-2m/\xi)}{2\pi \beta \xi^2}$$  

(12)

with

$$\xi^{-1} = \ln(\sqrt{1+\beta^2} + \beta), \quad \gamma = 1.$$  

Note that the inverse correlation length in [13] can be obtained from that in $D = 1$-case by a change of energy scale, $u \rightarrow u/2$. Therefore, the small and large $u$ asymptotic behaviour of $\xi^{-1}$ is given by [3] with the suitable change of the energy scale. Consequently, in $D = 1$-crystal and in the diagonal direction of $D = 2$-crystal, the inverse correlation length scales linearly with the direct-gap width, $\xi^{-1} \sim \delta$, for sufficiently small $\delta$.

Second, we choose the direction along an axis, say the first axis ($r_2 = 0, \sigma_r = r_1 = 2m = 2n$). Then, the function $R(r)$ in [10] transforms into [11] [12]:

$$R(r) = \frac{(-1)^m}{\pi} Q_{m-\frac{1}{2}} (1+2a) P_{m-\frac{1}{2}} \left( \frac{a-1}{a+1} \right),$$  

(14)

with the large $m$ asymptotics:

$$R(r) \underset{m \to \infty}{\approx} \frac{(-1)^m \exp(-2m/\xi)}{\pi \sqrt{2\beta}} \frac{2m}{\cos \left( m \arccos \left( \frac{a-1}{a+1} \right) - \frac{\pi}{4} \right)},$$  

(15)

where the inverse correlation length depends on $u$ as follows:

$$\xi^{-1} \approx \ln \left( \sqrt{\beta+\sqrt{1+\beta^2}} \right),$$  

and $\gamma = 1$. Along an axis, the first terms of the small and large $u$ asymptotic expansions of $\xi^{-1}$ read:

$$\xi^{-1} \approx \left( 1 + \frac{1}{12} \frac{u}{2} - \ldots \right),$$

and $\xi^{-1} \approx \frac{3}{u^2} - \ldots.$

(16)

Finally, we consider a general non-axial direction. Let, for definitness, $0 < n < m$. In this case we have not been able to obtain a large $m$ asymptotics of the function $R(r)$ in [10] for arbitrary values of $u$. However, we succeeded in deriving the asymptotic form [15] for sufficiently small and sufficiently large values of $u$. For sufficiently small values of $u$, we have found $\gamma = 1$ and the inverse correlation length

$$\xi^{-1} \approx -\frac{1}{2} \left( 1 + \eta \ln(\sqrt{1+\beta^2}+\beta) + \ln \left( \frac{2}{b+2} \left( 1 - \frac{2a}{b} \right)^\eta \right) \right),$$  

(18)

where the following notation has been used:

$$b \equiv (1+\eta)a + \sqrt{(1+\eta)^2a^2 + 4\eta},$$

$$\eta \equiv n/m = (\chi - 1)/(\chi + 1), \quad \chi \equiv r_1/r_2.$$  

(19)

Around zero, the asymptotic expansion of the above $\xi^{-1}$ has the form

$$\xi^{-1} \approx \frac{u}{2} \left( 1 + \frac{1}{24} \frac{1+\eta^2}{\eta} \frac{u}{2} - \ldots \right).$$  

(20)

Apparently, a straightforward way to obtain a large $\sigma_r$ asymptotics of $R(r)$ is to expand $\Delta(k)$ in powers of $u^{-2}$, for large $u$, carry out the integrals of products of cosine
In Fig. 2, we have displayed the analytic results for the inverse correlation length, $\xi^{-1}$, versus $u$, for different directions $\chi$ in $D = 2$ crystal: the data obtained from high-accuracy computation of $\mathcal{R}(r) - $ symbols, exact analytical result along the diagonal (13) and along an axis (10) – thick continuous curve, exact analytical result along a direction given by slope $\chi$ (18) – thin continuous curves, exact analytical results for large $u$, given by (17) and (21) – dots. In the insert we show the log-log plot of $\xi^{-1}$ versus $u$, and the dotted curve represents the first term of small $u$ asymptotics (20).

functions and to approximate the Euler $\Gamma$-functions, that arise, by the leading term of the Stirling’s asymptotic expansion. Such a procedure leads to the large-distance asymptotics of $\mathcal{R}(r)$ (analogous to the one derived in [9]), which consists of the power-law factor with $\gamma = 1$ and the exponential factor with the inverse correlation length of the form

$$
\xi^{-1} = \ln u + (2 + \chi + \chi^{-1})u^{-2} - \sum_{\alpha=-1,1} (1 + \chi^\alpha)^{-1} \ln(1 + \chi^\alpha). \tag{21}
$$

In Fig. 2 we have displayed the analytic results for $\xi^{-1}$ versus $u$, obtained for $D = 2$-crystal, and the same function determined by means of high-accuracy numerical calculations.

To summarize, our work has been inspired by the recent results of Taraskin et al [8], concerning the spatial decay of DM in a translation invariant model of insulator, where the relation between the decay and the direct-gap width has not been established. To the best of our knowledge, we provide in this letter the first example of insulator being a crystal (with broken translational symmetry) of dimension greater than one, where the relation between decay properties of DM and the direct-gap width can be established exactly, in the whole range of this parameter. Specifically, for arbitrary direct-gap width the large-distance asymptotics of DM consists of the power law factor with the power $\gamma = D/2$ and an exponential factor with the correlation length depending on direction and the direct-gap width.

There is an excellent agreement between our analytic results and high-accuracy numerical results presented in the figures. It is worth to emphasize that, by the general arguments given in [2], these results should not depend on the underlying lattice.

As particularly interesting, we consider the results concerning the scaling of the correlation length $\xi$ with the vanishing direct-gap width $\delta$, which is physically the most interesting regime, in the $D = 2$-crystal: $\xi^{-1} \sim \delta$ in the diagonal direction while $\xi^{-1} \sim \sqrt{\delta}$ in non-diagonal directions. They resolve the controversy that has arisen in the literature in this respect [10, 11, 12]: of which these two scalings holds in insulators? Apparently, the answer is more subtle than the question asked: both, depending on lattice direction.

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