Spatial decay of the one-body density matrix in insulators revised

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Abstract

In the framework of the band theory, we consider two tight-binding models of insulators. The first one, proposed recently by Taraskin et al, is a translationally invariant system, built out of two independent non-overlapping bands of single-particle orbitals that are coupled by a weak inter-band hybridization. This kind of insulator exhibits unphysical properties: we show, in particular, that the one-body density matrix does not depend on the width of the gap between the bands. Consequently, there is no delocalization effect with increasing metallicity. In the second model there are also two bands. However, they are not imposed by construction but are created from a band of single-particle orbitals due to the breaking of the translational symmetry by a periodic potential. These bands are separated by a gap for all nonzero values of the unique energy parameter of the model. We demonstrate that the one-body density matrix has the same structure as in the first model. As a result, the large distance asymptotic formulae derived by Taraskin et al in dimensions $D = 1, 2, 3$, apply as well, but only for very large gap widths. In $D = 1$ and in the diagonal direction of $D = 2$ cases, we derive a stronger asymptotic formula, valid for all gap widths. The both kinds of asymptotic formulae are composed of a dimension-dependent power-law factor and a gap-dependent exponentially decaying factor. The latter asymptotics implies that the exponential decay rate vanishes linearly with the vanishing gap. In non-diagonal directions, we have found numerically that the linear scaling is replaced by the square root one. Independently of the direction, the exponential decay rate grows logarithmically with the gap width, for sufficiently large gaps.

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The rapid progress in computational techniques used for calculating properties of solids enabled researchers to use a localized real-space approach to describing such properties. It has made possible large-scale calculations based on the density functional theory \([1]\), in particular enabling researchers to use a localized real-space approach to describing such properties. It has been established that in a 1D model of an insulator the DM decays exponentially with distance. The exponential decay of DM was reconsidered by Ismail-Beigi and Arias \([5]\) a few years ago (see also the references quoted there for developments in the meantime) in a general, model-independent context, for systems described by single-particle orbitals in periodic potentials in arbitrary dimensions. Then, He and Vanderbilt \([6]\) have discovered the power-law prefactor multiplying the exponential factor in the asymptotic formula for DM. Finally, Taraskin et al \([7]\) presented their minimal model of an insulator and described, analytically and numerically, a power-law decay and an exponential decay in dimensions \(D = 1, 2, 3\).

In this communication we reconsider the model of insulator proposed in \([7]\). This is a translationally invariant system described by two kinds of single-particle orbitals between which the electrons can hop. We demonstrate that it is not a kind of insulator considered in \([5]\) or earlier papers on the subject. For instance, for those values of the energy parameters of the model for which there exist two bands separated by a gap, there is no relation between the decay rate of DM and the size of the gap. We have succeeded in deriving analytically the large distance properties of DM of another system, described by one kind of single-particle orbitals and a periodic external potential. This system exhibits two bands separated by a gap for all nonzero values of the parameter determining the strength of the potential. Specifically, in the large distance behavior of DM elements of this system we have determined the power-law factor and the exponential factor.

The model of an insulator proposed in \([7]\) (TDE insulator) is described by the following second-quantized Hamiltonian

\[
H_{tde} = \sum_{\mathbf{i}, \mu} \varepsilon_{\mu} a_{\mathbf{i}, \mu}^+ a_{\mathbf{i}, \mu} + \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \mu, \nu} t_{\mu \nu} \left( a_{\mathbf{i}, \mu}^+ a_{\mathbf{j}, \nu} + h.c. \right).
\]

In the above expression, \(\mathbf{i}, \mathbf{j}\) represent the lattice sites of a \(D\)-dimensional Bravais lattice, while \(\langle \mathbf{i}, \mathbf{j} \rangle\) stands for a pair of nearest neighbors on this lattice. The operators \(\{a_{\mathbf{i}, \mu}^+, a_{\mathbf{i}, \mu}\}\) create, annihilate, respectively, a spinless fermion in a single-particle orbital \(|\mathbf{i}, \mu\rangle\) whose bare energy is \(\varepsilon_{\mu}\), where \(\mu\) differentiates between the two kinds of involved orbitals. The orbitals \(|\mathbf{i}, \mu\rangle\) satisfy the orthonormality condition \(\langle \mathbf{j}, \nu | \mathbf{i}, \mu \rangle = \delta_{\mathbf{i}, \mathbf{j}} \delta_{\nu, \mu}\). The hopping integrals between the orbitals \(|\mathbf{i}, \mu\rangle\) and \(|\mathbf{j}, \nu\rangle\) are \(t_{\mu \nu}\), and they are nonzero only if \(\mathbf{i}, \mathbf{j}\) are nearest neighbors. If the periodic boundary conditions are imposed, then the system is diagonalized by passing to plane-wave orbitals \(|\mathbf{k}, \mu\rangle\), with the wave vector \(\mathbf{k}\) in the first Brillouin zone. In order to reduce the number of energy parameters in the model, we make the bands symmetric. Specifically, we equalize the intraband transfer integrals \(t_{11} = t_{22} = t\), introduce \(\Delta \varepsilon \equiv \varepsilon_1 - \varepsilon_2\), with \(t > 0\) and \(\Delta \varepsilon > 0\) for definitness, and shift also the zero of the energy scale to \((\varepsilon_1 + \varepsilon_2)/2\). Moreover, we express all the energies in the units of the intraband hopping \(t\). Then, the eigenenergies of the system, as functions of the wave vector \(\mathbf{k}\), form the upper, \(\lambda_+^k\), and the lower, \(\lambda_-^k\), bands \(\lambda_\pm^k\):

\[
\lambda_\pm^k = 2S_k \pm 2 \left[ (\Delta \varepsilon/4)^2 + \tau^2 S_k^2 \right]^{1/2},
\]

where \(S_k\) is the spin quantum number.
Figure 1: Curves of constant gap $\delta$ for $D = 2$. The thick curve corresponds to $\delta = 0$; it splits the $\tau \geq 0$, $\Delta \varepsilon \geq 0$ quadrant into two disjoint regions of $\delta \geq 0$ and $\delta < 0$.

where $\tau \equiv t_{12}/t$ is the interband transfer integral in the units of $t$, $\tau > 0$ for definitness, and $S_k = \frac{1}{2} \sum_{j \in \{i,j\}} \exp(i k (\vec{r}_i - \vec{r}_j))$ stands for the structure factor. Clearly, $\lambda^+_{\vec{k}}$ and $\lambda^-_{\vec{k}}$ are mutually symmetric about zero and there are two independent energy parameters: $\tau$ and $\Delta \varepsilon$. Let $\delta = \min_k \lambda^+_{\vec{k}} - \max_k \lambda^-_{\vec{k}}$ be the width of the gap (if $\delta \geq 0$) or the overlap of the two bands (if $\delta < 0$). In Fig. 1 we display the curves of constant $\delta$, in the plane $(\tau, \Delta \varepsilon)$, for $D = 2$. It is seen that if the bare energies of the two kinds of single-particle orbitals are such that $\Delta \varepsilon > 8$, then for any hybridization $\tau > 0$ the width of the gap $\delta > 0$. Otherwise, the hybridization has to be large enough. Generally, we need $\Delta \varepsilon > 4D$ to have a gap for arbitrarily small $\tau$. Now, consider the TDE insulator, i.e. we set $\delta > 0$ and fill up completely with spinless electrons the lower band. Moreover, the underlying Bravais lattice is assumed to be a $D$-dimensional simple cubic lattice, with lattice vectors expressed in the units of the lattice constant (i.e. the components $j_l, l = 1, \ldots, D, \vec{j}$ are integer). Then, the zero-temperature matrix elements of DM are given by the zero-temperature averages $\langle a^+_{i,\mu} a_{i+r,\nu} \rangle$, which in the thermodynamic limit assume the form

$$
\langle a^+_{i,\mu} a_{i+r,\nu} \rangle = (2(2\pi)^D)^{-1} \int_{-\pi}^\pi \cdots \int_{-\pi}^\pi d\vec{k} \exp(i \vec{k} \vec{r}) \left[ 1 \mp A \Delta^{-1}(\vec{k}) \right],
$$

$$
\langle a^+_{i,\mu} a_{i+r,\nu} \rangle = -(2(2\pi)^D)^{-1} \int_{-\pi}^\pi \cdots \int_{-\pi}^\pi d\vec{k} \exp(i \vec{k} \vec{r}) S_k \Delta^{-1}(\vec{k}),
$$

where $A \equiv \Delta \varepsilon/4\tau$ and $\Delta(\vec{k}) \equiv (A^2 + S_k^2)^{1/2}$. Clearly, the matrix elements of DM depend on the two energy parameters of TDE insulator only through their ratio $\Delta \varepsilon/\tau$, hence in that part of $(\tau, \Delta \varepsilon)$-plane where $\delta \geq 0$, they are constant along the rays with the slope $4A$, emerging from the origin $(0, 0)$. Consequently, the DM does not depend on the width of the gap between the upper band and the lower one. In other words, by following a suitable curve in the region $\delta \geq 0$, we can impose any relation between the parameter $A$ and the gap width $\delta$. For instance, along the lines of constant $\tau$ the parameter $A$ is an increasing function of $\delta$, whose minimum is $A_{\tau}$, and the limit $A \to A_{\tau}^+$ is equivalent to the limit $\delta \to 0^+$. Only for a sufficiently strong hybridization, $\tau \geq 1$, the minimum $A_{\tau}$ attains zero and then $A \to 0^+$ is equivalent to $\delta \to 0^+$.
are no density-density correlations between the electrons, that is, the correlations \( \langle \hat{a}_{j, \mu}^+ \hat{a}_{j, \mu'} \rangle \) vanish identically in some lattice directions.

Now, consider the model, where only one sort (\( \mu \) fixed) of single-particle orbitals \( | \vec{j}, \mu \rangle \equiv | \vec{j} \rangle \) is present, whose Hamiltonian is

\[
H_{cb} = \sum_{i} U_i a_i^+ a_i + t \sum_{\langle i, j \rangle} \left( a_i^+ a_j + h.c. \right),
\]

where we used the same notation as in (1) but with the fixed index \( \mu \) suppressed, and \( U_j \) denotes a periodic external potential. Suppose that the underlying Bravais lattice consists of two interpenetrating sublattices that differ by a primitive translation, i.e. the nearest neighbors of a site on one sublattice belong the other one. Then, we set \( U_j = U_1 \) on one sublattice and \( U_j = U_2 \) on the other one. Under periodic boundary conditions the Hamiltonian (5) is diagonalized by plane wave orbitals \( | \vec{k} \rangle \) with the wave vector in the first Brillouin zone of a sublattice. Specifically, shifting the energy scale to \((U_1 + U_2)/2\) and expressing all the energies in the units of the transfer integral \( t \), we obtain the upper \( \Lambda_+^k \) and the lower \( \Lambda_-^k \) bands of eigenenergies labeled by \( \vec{k} \):

\[
\Lambda_+^k = \pm 2 \sqrt{(u/2)^2 + S_k^2} \equiv \pm 2 \Delta_{cb}(\vec{k}),
\]

where \( u \equiv (U_2 - U_1)/2t \) is the unique energy parameter of the model. Without any loss of generality we can set \( u > 0 \). As in the TDE insulator, the two bands are mutually symmetric about zero and are separated by a nonzero gap \( \delta_{cb} = 2u \), for any nonzero \( u \). For \( u \neq 0 \) and completely filled lower band, the system given by (5) is an insulator in the sense of the band theory, which we call the chessboard insulator. In contrast to TDE insulator, the chessboard insulator belongs to the class of insulators, for which a definite scaling of the exponential decay rate versus the vanishing gap is expected [3]. Let the underlying lattice be a D-dimensional simple cubic lattice. For definiteness, we set \( U_j = U_2 \) at the sites of the even sublattice. The zero temperature, non-diagonal elements of DM are given by

\[
\langle a_i^+ a_{i+r} \rangle = (2\pi)^{-D} \int_{B.Z.} d\vec{k} \exp(i\vec{k}\vec{r}) \gamma_k^{-2} \left\{ u^2 + (-1)^{\sigma_r} \beta_k^2 - (-1)^{\sigma_l} \right\} \left[ 1 + (-1)^{\sigma_r} u \beta_k \right], \quad r \neq 0,
\]

where the D-dimensional integral is taken over the first Brillouin zone of a sublattice, \( \vec{r} \neq 0 \), and the following abbreviations have been used

\[
\sigma_r \equiv \sum_{l=1}^{D} r_l, \quad \beta_k \equiv 2S_k + 2\Delta_{cb}(\vec{k}), \quad \gamma_k^2 \equiv 4\beta_k \Delta_{cb}(\vec{k}).
\]

Without any loss of generality, we can assume that for all \( l = 1, \ldots, D \), \( r_l > 0 \). Then, \( \sigma_r \) is a (noneuclidean) distance between the lattice point \( \vec{r} \) and the origin. To reveal the structure of DM given by (7), it is convenient to rewrite it separately for \( \sigma_r \) even and odd:

\[
\langle a_i^+ a_{i+r} \rangle = -(2\pi)^{-D} \int_{B.Z.} d\vec{k} \exp(i\vec{k}\vec{r}) S_k \Delta_{cb}^{-1}(\vec{k}), \quad \text{if} \quad \sigma_r = 2m + 1,
\]

\[
\langle a_i^+ a_{i+r} \rangle = -(-1)^{\sigma_l} (2(2\pi)^D)^{-1} u \int_{B.Z.} d\vec{k} \exp(i\vec{k}\vec{r}) \Delta_{cb}^{-1}(\vec{k}), \quad \text{if} \quad \sigma_r = 2m.
\]
It appears that the large distance behavior of DM elements for the chessboard insulator is determined by the function $R_{cb}(\mathbf{r})$,

$$R_{cb}(\mathbf{r}) = (2\pi)^{-D} \int_{B.Z.} \, d\mathbf{k} \exp(i\mathbf{k}\mathbf{r}) \Delta_{cb}^1(\mathbf{k}),$$

(11)

since,

$$\langle a^+_i a_{i+r} \rangle = -\frac{1}{2} \sum_{l=1}^D S_l R_{cb}(\mathbf{r}), \quad \text{if} \quad \sigma_r = 2m + 1,$$

(12)

$$\langle a^+_i a_{i+r} \rangle = -\frac{u}{2} (-1)^{\sigma_i} R_{cb}(\mathbf{r}), \quad \text{if} \quad \sigma_r = 2m,$$

(13)

where $S_l R_{cb}(\mathbf{r}) \equiv R_{cb}(r_1 + 1, \ldots, r_D) + R_{cb}(r_1 - 1, \ldots, r_D)$, etc. Note that the matrix elements of DM depend on $R_{cb}(\mathbf{r})$ evaluated only at the points $\mathbf{r}$ with $\sigma_r$ even. Similar relations hold in the case of TDE insulator. On introducing

$$\mathcal{R}(\mathbf{r}) \equiv (2(2\pi)^D)^{-1} \int_{-\pi}^\pi \cdots \int_{-\pi}^\pi \, d\mathbf{k} \exp(i\mathbf{k}\mathbf{r}) \Delta^{-1}(\mathbf{k}),$$

(14)

we obtain

$$\langle a^+_i a_{i+r,2} \rangle = -\frac{1}{2} \sum_{l=1}^D S_l \mathcal{R}(\mathbf{r}),$$

(15)

$$\langle a^+_i a_{i+r,2} \rangle = \mp A \mathcal{R}(\mathbf{r}).$$

(16)

In what follows, we limit our analysis to the $D = 1, 2$ cases. Then, one finds easily that

$$\mathcal{R}(\mathbf{r}) = \begin{cases} 0, & \text{if} \quad \sigma_r \text{ is odd}, \\ R_{cb}(\mathbf{r})|_{u=A}, & \text{if} \quad \sigma_r \text{ is even}. \end{cases}$$

(17)

Therefore, as in the case of the chessboard insulator, the DM elements depend only on $\mathcal{R}(\mathbf{r})$ evaluated at the points with $\sigma_r$ even. Consequently, the matrix elements $\langle a^+_i a_{i+r,2} \rangle$ vanish at the lattice directions with $\sigma_r$ even, while $\langle a^+_i a_{i+r,\mu} \rangle$ vanish at the lattice directions with $\sigma_r$ odd. Moreover, the large distance behavior of the DM elements of both insulators under considerations, is given by the function $R_{cb}(\mathbf{r})$ restricted to the points with $\sigma_r$ even. In all the cases studied here we have found that up to a coefficient independent of $\sigma_r$

$$R_{cb}(\mathbf{r}) \sim \sigma_r^{-\gamma} \exp(-\sigma_r/\xi(\epsilon)),$$

(18)

for sufficiently large $\sigma_r$, where $\epsilon$ stands for an energy parameter and $\xi(\epsilon)$ is the correlation length.

Apparently, a straightforward way to obtain a large $\sigma_r$ asymptotics of $R_{cb}(\mathbf{r})$ is to expand $\Delta_{cb}(\mathbf{k})$ in powers of $u^{-2}$, for large $u$, carry out the integrals of products of cosine functions and to approximate the Euler $\Gamma$-functions, that arise, by the leading term of the Stirling’s asymptotic expansion. Then, in $D = 1$ case we obtain the inverse correlation length

$$\xi_{tde}^{-1}(u) = \ln u + u^{-2},$$

(19)

while in directions of finite nonzero slope $\chi \equiv r_1/r_2$ of the $D = 2$ case,

$$\xi_{tde}^{-1}(u) = \ln u + u^{-2}(2 + \chi + \chi^{-1}) - \sum_{\alpha=-1,1} (1 + \chi^{\alpha})^{-1} \ln(1 + \chi^{\alpha}),$$

(20)
Figure 2: The calculated numerically exactly function $R_{cb}(r)$, denoted $\rho_{\text{numer}}$, divided by its TDE asymptotics, denoted $\rho_{\text{asympt}}$, which up to a constant is given by (20), versus distance $\sigma_r$, for $D = 2, \chi = 1, 2, 4$, and two values of $u$.

and the exponent $\gamma = D/2$. A similar procedure gives asymptotic formulae along the axes. The asymptotics (18) with (19) or (20) – the TDE asymptotics, on setting $u = 2A$ amounts to the corresponding asymptotics derived in [7].

While the TDE asymptotics obtained for the chessboard insulator and the corresponding one for the TDE insulator have the same structure, their physical content is very different. The energy parameter $u$ is in one to one correspondence with the gap width of the chessboard insulator. In contrast, $A$ is in no definite relation with the gap width of the TDE insulator.

To test the quality of the asymptotic formula (18) with (20), one can compare it with a calculated numerically exactly function $R_{cb}(r)$. The log-log plot of both functions is too rough for such a test. We have plotted, in Fig. 2 $R_{cb}(r)$ calculated numerically exactly, divided by its TDE asymptotics. It is seen that, in the case of $D=2$ chessboard insulator, the TDE asymptotics is reasonably good only for as large values of $u$ as 16 or higher.

To obtain an asymptotics stronger than the TDE asymptotics, valid for small and large values of $u$, we have applied to the integrals in (11) the Laplace asymptotic expansion. Unfortunately, we have succeeded to carry out the calculations only in the $D = 1$ case (more results on the correlation function in this case can be found in [8]) and for the diagonal direction in the $D = 2$ case. The result is of the form (18), with the inverse correlation length

$$\xi^{-1}(\epsilon) = \ln(\epsilon + \sqrt{\epsilon^2 + 1}), \quad \epsilon = (2D)^{-1}u,$$

and the exponent $\gamma = D/2$. Making a similar comparison as that displayed in Fig. 2 we find a satisfactory agreement, see Fig. 3. Apparently, in the limit of the vanishing gap the inverse correlation length (21) vanishes proportionally to the gap width. In the one-dimensional case, the same result has been obtained numerically for periodic potentials of period higher than 2 [8].

Assuming that the asymptotic behavior of $R_{cb}(r)$ is of the form (18) with the exponent $\gamma$ independent of $u$, we have found numerically, see Fig. 4, that in non-diagonal directions the inverse correlation length vanishes as $\sqrt{u}$ as $u \to 0$. For sufficiently large $u$, depending on the direction, the correlation length behaves as in the diagonal case, i.e. obeys (21). Our data show also that the decay rate of DM elements is the slowest in the diagonal direction.
Figure 3: The calculated numerically exactly function $R_{cb}(r)$, denoted $\rho_{\text{numer}}$, divided by its asymptotics $\rho_{\text{asympt}}$ that up to a constant is given by (21), versus distance $\sigma_r$, for $D = 2$, $\chi = 1$ and three values of $u$.

Figure 4: The inverse correlation length, $\xi^{-1}$, obtained from the calculated numerically exactly function $R_{cb}(r)$, versus $u$, for $D = 2$ and three non-diagonal directions. Thin continuous curves are the fits by the function $\text{const} \sqrt{u}$. The thick curve represents $\xi^{-1}$ in the diagonal direction, according to (21).
In summary, this work has been inspired by the recent paper of Taraskin et al. on spatial decay of DM in a translationally invariant model of insulator – the TDE insulator. Having found that the TDE model shows unphysical features, we have carried out similar studies of another model of insulator – the chessboard insulator, whose translational symmetry is broken. In contrast to TDE insulator, in the chessboard insulator there is a unique energy parameter which determines both, the gap between the bands and the DM elements. We have succeeded in deriving analytically a dimension-dependent power-law factor, predicted in [6], with the exponent $\gamma = D/2$, and a gap-dependent exponential decay rate, discussed extensively in [5]. Specifically, in $D = 1, 2, 3$ cases, the DM elements of the chessboard insulator obey the asymptotics derived for TDE insulator by Taraskin et al, which we have found to hold only for very large gap widths. In $D = 1$ case and along the diagonal in $D = 2$ case, we have derived a stronger asymptotic formula, valid for arbitrary gap widths. The latter asymptotics implies that the inverse correlation length of the chessboard insulator vanishes linearly with the vanishing gap width. Concerning non-diagonal directions, on assuming that the exponent $\gamma$ is independent of the gap width, we have found numerically that the inverse correlation length vanishes as the square root of the gap width. Independently of the direction, the inverse correlation length grows logarithmically with the gap width, for sufficiently large gaps. A more comprehensive discussion will be given in a separate article [9].

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