Anderson transition of three dimensional phonon modes

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Anderson transition of the phonon modes is studied numerically. The critical exponent for the divergence of the localization length is estimated using the transfer matrix method, and the statistics of the modes is analyzed. The latter is shown to be in excellent agreement with the energy level statistics of the disordered electron system belonging to the orthogonal universality class.

Anderson localization, which was originally proposed for disordered electron system, is now widely discussed in many random systems of classical waves, such as photons and phonons. Especially interesting is the Anderson transition in three dimensional (3D) systems, where the wave form changes from extended to exponentially localized one. In disordered electron systems, this can be well described by the scaling theory and universal behaviors of localization length, conductance distribution as well as level statistics have been demonstrated. The important point is that the Anderson transition is classified into a few universality classes.

Recently, Song and Kim have shown that the 3D phonon modes in disordered lattice undergo Anderson transition. However, whether this Anderson transition is classified into the same universality classes as electron systems remains to be studied. In this short note, we demonstrate the Anderson transition of 3D phonon modes and discuss its critical behavior, and show that it is classified into the orthogonal universality class of disordered electron system.

We begin with the following equation of motion for the lattice displacement $u(r,t)$,

$$
M \frac{d^2}{dt^2} u(r,t) = \sum_{i=x,y,z} [K_i(r-e_i)(u(r-e_i,t) - u(r,t)) + K_i(r)(u(r+e_i,t) - u(r,t))]
$$

where $r$ is the lattice position, and $e_i$ the unit vector in the $i$-th direction ($i=x,y,z$). Here we have assumed the simple cubic structure, and the displacement is represented by a scalar quantity for simplicity. $K_i(r)$ is the spring constant connecting the site at $r$ and that at $r+e_i$. Only the nearest neighbor interaction is taken into account.

Putting $u(r,t) = e^{-i\omega t}u(r)$ and setting $\Omega = \omega^2$, we reduce the problem to the matrix eigenvalue problem which is similar to the tight binding model where the transfer energy as well as the potential energy is random. The difference is that off diagonal elements $H_{ij}$'s are correlated in the phonon system such that

$$
\sum_j H_{ij} = 0. \quad (2)
$$

The correlation of the matrix element is very important especially in the one dimensional systems. Without the correlation, i.e., when $H_{ij}$'s are independent random variables, all the states are localized. When only the off-diagonal elements are random, the states delocalize at the band center ($E = 0$) with the localization length $\xi \sim |\log E|$ [14]. With the above correlation, the localization length diverges according to the power law of the mode frequency.

In the actual simulation, the random spring constant $K_i$'s are independently and uniformly distributed between $0.1K_0$ and $1.9K_0$. We scale the frequency $\omega$ by $\sqrt{K_0/M}$ and the length by the lattice constant. The density of modes $D(\Omega)$ obtained by diagonalizing $14 \times 14 \times 14$ systems for 935 configurations is shown in Fig. 1.

We then discuss the critical behavior of the mode $u$. We apply the transfer matrix method to calculate the decay length $\lambda_N$ for $N \times N \times L$ system along $z$-direction, setting $L$ much larger than $N$ and $\lambda_N$. In actual calculations, $N$ is varied from 8 to 12, and the simulation is stopped when the relative error of $\lambda_N$ becomes smaller than 2%.

In Fig.2, we plot $\Lambda_N = \lambda_N/N$ as the function of $\Omega$. For extended modes, $\Lambda_N$ is an increasing function with respect to $N$, while it is a decreasing function for localized modes. At the critical point $\Omega_c$ becomes $N$ independent. The common crossing point in Fig. 2, therefore, gives the critical point $\Omega_c$, which is estimated to be

$$
\Omega_c = 13.0 \pm 0.2. \quad (3)
$$

The critical exponent $\nu$ for the localization length (or the correlation length) $\xi$ which characterizes the divergence of $\xi$

$$
\xi \sim |\Omega - \Omega_c|^{-\nu} \quad (4)
$$
can be estimated by expanding $\Lambda_N$ as

$$
\Lambda_N = \Lambda_c + A_1 N^{1/\nu}(|\Omega - \Omega_c| + \cdots) \quad (5)
$$

In the present simulation, $\nu$ is estimated to be

$$
\nu = 1.2 \pm 0.2. \quad (6)
$$

Recent precise estimate of $\nu_{\text{And}}$ in the Anderson model gives

$$
\nu_{\text{And}} = 1.59 \pm 0.03 \quad (7)
$$
for 3D orthogonal universality class, i.e., systems without magnetic fields. Present estimate of $\nu$ for phonon mode localization length is considerably smaller than $\nu_{\text{And}}$. This, however, should not be taken seriously, since when the transition occurs near the band edge, we tend to underestimate $\nu$. \[16\]

In fact, if we study the level statistics regarding $\Omega$ close to the critical point, we obtain the same critical level statistics for the Anderson model belonging to the orthogonal universality class. The distribution function $P(s)$ for the nearest neighbor spacing of the two successive modes $s$ near the critical points ($12.5 < \Omega < 13.5$) is plotted in Fig.3, together with the critical level statistics for the orthogonal universality class in electron systems. \[8\] The coincidence between the two is excellent, and we conclude that the Anderson transition of phonon modes is classified into the orthogonal universality class in the disordered electron systems. The critical behavior in 3D is not altered by the correlation of the matrix elements (Eq.(2)).

In the present model, we have assumed the simple cubic lattice where the general vector displacement problem can be reduced to the scalar displacement problem (isotropic Born model). \[7\] In real lattices, all the components of the displacement vectors should be taken into account. \[17\] Such a model is very difficult to analyze by the transfer matrix calculation. The present method of level statistics might be a powerful tool to investigate the phonon Anderson transition in such realistic lattices, which is a problem left for the future.

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Figure captions

Fig. 1: The density $D(\Omega)$ of the square frequency $\Omega$.

Fig. 2: Normalized decay length $\Lambda_N$ vs. $\Omega$ for $N=8$ ($\triangle$), 9($\bullet$), 10 ($\circ$) and 12 ($\triangleleft$). The dashed lines are the 3rd order polynomial fit to the data. Common crossing point indicates the critical point $\Omega_c$, and the $N$-dependence of the slope at $\Omega_c$ gives the localization length exponent $\nu$.

Fig. 3: Distribution function $P(s)$ for the nearest neighboring $\Omega$’s close to $\Omega_c$ ($\bullet$). That for the disordered electron systems ($\circ$) as well as the Poisson (broken line) and the Winger (solid line) distributions is also shown for comparison.
