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Section 1. Localization, Delocalization and Transport

EXCITON TRANSPORT AND ANDERSON LOCALIZATION IN LIOUVILLE SPACE: THE EFFECTIVE DEPHASING APPROXIMATION

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The effective dephasing approxamation (EDA) provides a self-consistent procedure for calculating the transport properties of excitons and electrons in a disordered medium. It is based on mapping the averaged Liouville space propagator into the propagator of a particle moving in an ordered lattice with an effective frequency-dependent dephasing rate, which is determined self-consistently. The Liouville equation for the averaged density matrix is isomorphic to a linearized Boltzmann equation, and the effective dephasing rate represents a generalized BGK strong-collision operator. Our results agree with the predictions of scaling theories of the Anderson transition.

We consider a quantum particle, whose motion on a lattice is described by the tight-binding Hamiltonian

$$H=\sum_{x} E_x|\boldsymbol{x}\rangle\langle \boldsymbol{x}| + \sum_{x\neq x'} \hbar J(\boldsymbol{x}-\boldsymbol{x}')|\boldsymbol{x}\rangle\langle \boldsymbol{x}'| \,, \tag{1}$$

where $|\boldsymbol{x}\rangle$ denotes the state in which the particle is localized at the lattice point $\boldsymbol{x}$, $J(\boldsymbol{x}-\boldsymbol{x}')$ is transfer matrix element between sites and E_x is the particle energy at site $\boldsymbol{x}$. In the Anderson model of diagonal disorder, $\{E_x\}$ are independent random variables with a distribution $P(E_x)$ [1,2]. The density matrix element $\rho(\boldsymbol{r},\boldsymbol{s},t)$ is defined by $\rho(\boldsymbol{r},\boldsymbol{s},t)\equiv\langle \boldsymbol{r}-\boldsymbol{s}/2|\rho|\boldsymbol{r}+\boldsymbol{s}/2\rangle$. $\rho(\boldsymbol{r},0,t)$ is a diagonal element of the density matrix, and gives the probability that the particle is located at position $\boldsymbol{r}$ at time t. For $\boldsymbol{s}\neq$ o, $\rho(\boldsymbol{r},\boldsymbol{s},t)$ is a coherence that carries information on the phase relationship between two sites separated by a displacement $\boldsymbol{s}$. Our goal is the calculation of the ensemble averaged density matrix $\langle\rho(\boldsymbol{r},\boldsymbol{s},t)\rangle$, where the angular brackets represent an average over the random site energies. The Wigner phase space distribution function $\phi(\boldsymbol{r},\boldsymbol{p},t)$ is defined by [3]

$$\phi(\boldsymbol{r},\boldsymbol{p},t)=N^{-1}\sum_{s}\exp(\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{s}/\hbar)\langle\rho(\boldsymbol{r},\boldsymbol{s},t)\rangle \,. \tag{2}$$

N is the number of lattice sites. The effective dephasing approximation is based on the following ansatz for the form of the equation of motion of $\phi(\boldsymbol{r},\boldsymbol{p},t)$ [4]:

$$\dot\phi(\boldsymbol{r},\boldsymbol{p},t)=2\sum_{a} J(\boldsymbol{a})\sin(\boldsymbol{p}\cdot\boldsymbol{a}/\hbar)\phi(\boldsymbol{r}+\boldsymbol{a}/2,\boldsymbol{p},t) + \int_0^t \mathrm{d}\tau\hat\Gamma(t-\tau)\sum_{p'}[f(\boldsymbol{p})\phi(\boldsymbol{r},\boldsymbol{p}',\tau) - f(\boldsymbol{p}')\phi(\boldsymbol{r},\boldsymbol{p},\tau)] \,. \tag{3}$$

The first term in eq. (3) represents the free motion of the particle on an ordered lattice. The index $\boldsymbol{a}$ runs over all displacements in the lattice. If we take $\hat\Gamma(t)=\gamma\delta(t)$, then the second term has the form of the BGK strong-collision operator in the Boltzmann equation, in which γ is the collision rate and $f(\boldsymbol{p})$ is the distribution of momenta after a collision. We take $f(\boldsymbol{p})=1/N$ if $\boldsymbol{p}$ is in the first Brillouin zone and is 0 otherwise. The frequency-dependent collision rate $\Gamma(\epsilon)$ is the Laplace transform of $\hat\Gamma(t)$,

$$\Gamma(\epsilon)=\int_0^\infty \mathrm{d}t\,\exp(-\epsilon t)\hat\Gamma(t) \,. \tag{4}$$

The transport properties of the quantum particle can be determined from $P(\boldsymbol{r},t)$, the probability that the particle undergoes a displacement $\boldsymbol{r}$ in time t. $\hat P(\boldsymbol{k},\epsilon)$, is the Fourier-Laplace transform of $P(\boldsymbol{r},t)$. The generalized wavevector and frequency dependent diffusion coefficient $D(\boldsymbol{k},\epsilon)$ is defined by

$$\hat P(\boldsymbol{k},\epsilon)=[\epsilon+k^2D(\boldsymbol{k},\epsilon)]^{-1} \,, \tag{5}$$

and is related to $\Gamma(\epsilon)$ by

$$k^2D(\boldsymbol{k},\epsilon)=Q^{-1}(\boldsymbol{k},\epsilon)-\Gamma(\epsilon)-\epsilon \,, \tag{6}$$

where $Q(\boldsymbol{k},\epsilon)$ is given by eq. (7b). The EDA is a self-consistent equation for $\Gamma(\epsilon)$ [4]:

$$\Gamma(\epsilon)=\Gamma_0+2\Delta^2\Omega^{-1}\int \mathrm{d}\boldsymbol{k}[Q(\boldsymbol{k},\epsilon)^{-1}-\Gamma(\epsilon)]^{-1} \,, \tag{7a}$$

$$Q(\boldsymbol{k},\epsilon)=\pi^{-d}\int_0^\pi \mathrm{d}q_1\ldots\int_0^\pi \mathrm{d}q_d[\epsilon+\Gamma(\epsilon) + 4iJ\sum_{j=1}^{d}\sin(q_j)\sin(k_j/2)]^{-1} \,, \tag{7b}$$

where d is the dimensionality, $k_j=\boldsymbol{k}\cdot\boldsymbol{x}_j$, $\boldsymbol{x}_j$ is the lattice vector in the jth direction, Γ_0 is a noncritical contribution to $\Gamma(\epsilon)$, and we assume nearest neighbor coupling J, Ω is the volume of the first Brillouin zone, and Δ is the variance of the site energy distribution $P(E_x)$. The dimensionless parameter $\chi=\Delta^2/J^2$ is crucial in determining the transport properties of the model. Eqs. (7) predict a metal–insulator transition at $\chi=\chi^*\cong 3.957$. In the vicinity of the critical point in three dimensions, eqs. (7) assume the form

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$$[\Gamma(\epsilon)/\Gamma_0]\{1-\chi/\chi^* + (\chi/2\pi)[\epsilon\Gamma(\epsilon)/8J^2]^{1/2}\}=1\,. \tag{8}$$

For $\chi>\chi^*$, $\Gamma(\epsilon)$ diverges as ϵ^{-1} as $\epsilon\to 0$. For $\chi<\chi^*$, $\Gamma(\epsilon)$ approaches a finite limit as $\epsilon\to 0$. At $\chi=\chi^*$, $\Gamma(\epsilon)$ diverges as $\epsilon^{-1/3}$. χ^* has been estimated by a variety of numerical methods for the original Anderson model, in which the site energies are uniformly distributed between $-W/2$ and $W/2$. Our value of $\chi^*=3.957$ corresponds to $(W/J)^*=6.9$. The EDA approach yields a prediction for χ^* that is within a factor of two of the current numerical predictions (~ 15). The solution of the EDA yields [4]

$$\Gamma(\epsilon)=\begin{cases}\Gamma_0(1-\chi/\chi^*)^{-1}-\epsilon^{1/2}(\chi/2\pi)\Gamma_0^{3/2} \\ \quad\times(8J^2)^{-1/2}[1-\chi/\chi^*]^{-5/2}\,, & \chi<\chi^*\,, \\ 8J^2[(2\pi/\chi)(\chi/\chi^*-1)]^2\epsilon^{-1} \\ \quad+2\Gamma_0(\chi/\chi^*-1)^{-1}\,, & \chi>\chi^*\,, \\ [4(2)^{1/2}\pi\Gamma_0 J/\chi^*]^{2/3}\epsilon^{-1/3}\,, & \chi=\chi^*\,.\end{cases} \tag{9}$$

$$P(0,t)=\begin{cases}t^{-3/2}(2\Delta^2)^{-1}(\chi/2\pi)\Gamma_0^{3/2}(8J^2)^{-1/2} \\ \quad\times(1-\chi/\chi^*)^{-5/2}\,, & \chi<\chi^*\,, \\ 8J^2(2\Delta^2)^{-1}[(2\pi/\chi)(\chi/\chi^*-1)]^2\,, & \chi>\chi^*\,, \\ t^{-2/3}(2\Delta^2)^{-1}[2^{5/2}\pi\Gamma_0 J/\chi^*]^{2/3}\,, & \chi=\chi^*\,.\end{cases} \tag{10}$$

The second moment of $P(\boldsymbol{r},t)$ is

$$\langle r^2(t)\rangle=\begin{cases}t[2J^2l^2(1-\chi/\chi^*)/\Gamma_0]\,, & \chi<\chi^*\,, \\ l^2[(4\pi/\chi)(\chi/\chi^*-1)]^{-2}\,, & \chi>\chi^*\,, \\ t^{2/3}l^2\{J^2\chi^*/(2^{3/2}\pi\Gamma_0)\}^{2/3}\,, & \chi=\chi^*\,.\end{cases} \tag{11}$$

In the delocalized regime ($\chi<\chi^*$), the transport is diffusive at long times: $\langle r^2(t)\rangle$ increases linearly with time, and $P(0,t)$ decays as $t^{-3/2}$. In the localized regime ($\chi>\chi^*$), $\langle r^2(t)\rangle$ is bounded, and $P(0,t)$ decays to a nonzero value, indicating that there is a finite probability at all times that the particle is to be found at its original site. At the critical point ($\chi=\chi^*$), the particle is weakly localized, $\langle r^2(t)\rangle$ increases as $t^{2/3}$, and $P(0,t)$ decays as $t^{-2/3}$.

We conclude by summarizing the implications of this work. The EDA is based on the physical intuition that the ensemble-averaged density matrix of a particle moving in a random potential satisfies an effective Liouville equation which contains a generalized frequency-dependent dephasing rate $\Gamma(\epsilon)$. $\Gamma(\epsilon)$ describes the loss of phase coherence between different points in space and can be viewed as a generalized scattering rate in a Boltzmann equation with a BGK collision kernel. The effective Liouville equation (eq. (3)) is capable of describing coherent motion ($\Gamma=0$) and incoherent motion (when $\Gamma(0)$ is finite and large compared with the intersite coupling J). The signature of localization is an infrared divergence in $\Gamma(\epsilon)$: $\Gamma(\epsilon)\sim\epsilon^{-\alpha}$. The correspondence between the EDA and the Boltzmann equation indicates that the applicability of the EDA method extends beyond the treatment of lattice models such as the Anderson problem to the general problem of the localization of a classical or quantum particle and the propagation of light in disordered media [5]. This is one of the major advantages of the EDA. While the Anderson model is extremely valuable in providing an insight into the problem of transport in disordered systems, it is clearly oversimplified. Electronic motion in solids and glasses at finite temperatures is coupled to other degrees of freedom (e.g. phonons or coupling to internal molecular degrees of freedom). In addition, electron–electron interactions affect the transport as well. The Anderson model does not address the many-body aspects and the dynamic nature of the disorder in these systems. The present mapping of the ensemble-averaged equation of motion onto an effective Liouville (Boltzmann) equation is ideally suited for treating these more general types of disorder [6], and for developing a semiclassical theory of localization.

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