What Is a Single - Particle Model?

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Although transport phenomena involve many particles, the entire description can be framed in terms of single-particle eigenstates, which are thus crucial. This chapter is motivated by this central idea. Skills such as probing charge density, predicting current flow through a device, and estimating noise are typical outcomes expected from a robust transport theory. Despite 'charge density' and 'current' being many-particle quantities, it is beneficial to consider them when solving the single-particle Schrödinger equation. Ultimately, macroscopic charge and current densities are statistical sums of microscopic densities carried by single-particle states or arising from transitions between them. Therefore, it makes sense to examine single-particle eigenstates from this perspective. Associating a charge density with a single-particle wave function is relatively straightforward. Generally, if $\Phi(\mathbf{r}, t)$ is the wave function of a single-particle state $|\Phi(t)\rangle$, then $|\Phi(\mathbf{r}, t)|^2$ represents the probability density of finding the particle at position $\mathbf{r}$ when it is in the time-dependent state $|\Phi(t)\rangle$. Intuitively, the charge density of the corresponding state $|\Phi(t)\rangle$ for a particle with charge q is given by:

$$\rho(\mathbf{r}, t) = q|\Phi(\mathbf{r}, t)|^2 \tag{1}$$

for a particle with charge. Moreover, it is possible to define a current density $\mathbf{J}(\mathbf{r}, t)$ for the state $|\Phi(t)\rangle$ to satisfy the continuity equation:

$$\nabla \cdot \mathbf{J}(\mathbf{r}, t) + \frac{\partial \rho(\mathbf{r}, t)}{\partial t} = 0 \tag{2}$$

Starting from the time-dependent Schrödinger equation in the position representation, it can be shown that:

$$\mathbf{J}(\mathbf{r}, t) = -\frac{iq\hbar}{2m}[\Phi^*(\mathbf{r}, t)\nabla\Phi(\mathbf{r}, t) - (\nabla\Phi^*(\mathbf{r}, t))\Phi(\mathbf{r}, t)] = -\frac{q\hbar}{m}\Im\{(\nabla\Phi^*(\mathbf{r}, t))\Phi(\mathbf{r}, t) \tag{3}$$

is the appropriate expression for the current density. From this equation, we deduce that single states can carry current only if their wave functions have a non-zero imaginary component. If $|\Phi\rangle$ is an energy eigenstate, meaning it is an eigenvector of the one-particle Hamiltonian, the time variable t can be omitted. In this case, the continuity equation simplifies to:

$$\nabla \cdot \mathbf{J}(\mathbf{r}) = 0 \tag{4}$$

implying that the current is incompressible. The solution of the Schrödinger equation for a particle in a constant potential is notable for several reasons. Firstly, it requires minimal mathematical effort. If we denote the constant potential energy by U_0, Schrödinger's equation can be rewritten as:

$$\nabla^2 \phi(\mathbf{r}) + \alpha \phi(\mathbf{r}) = 0 \tag{5}$$

where α is independent of the position vector $\mathbf{r}$:

$$\alpha = \frac{2m}{\hbar^2}(E - U_0). \tag{6}$$

If the domain Ω has a simple geometry (such as rectangular boxes, cylinders, spheres, etc.) where the coordinate surfaces align with the domain boundaries, can be solved by separation of variables. For more detailed treatments and examples of this technique, we refer to standard textbooks on mathematical physics and quantum mechanics, such as those by Morse and Feshbach, and Flügge. Additionally, the constant potential is an idealization of the periodic crystal potential that governs perfect metals and semiconductors, at least when considered infinite in all directions.