CHAPTER 1

SOME QUANTUM BACKGROUND

We assume basic quantum mechanics as in e.g. [**603**] (cf. also [**170, 177, 175**]).

1. deBROGLIE-BOHM MECHANICS

This is covered e.g. in [**170, 440**] but we sketch matters here following [**170**]. There are many ways to derive or develop the dBB theory but for simplicity first look at a 1-D SE of the form (**1A**) $-(\hbar^2/2m)\partial_x^2\psi+V(x)\psi=i\hbar\partial_t\psi$. Then putting $\psi=Rexp(iS/\hbar)$ yields

$$\partial_t S+\frac{S_x^2}{2m}+V-\frac{\hbar^2 R_{xx}}{2mR}=0;\ \partial_t(R^2)+\frac{1}{m}\partial_x(R^2S_x)=0 \tag{1.1}$$

which in e.g. three space dimensions can be written (with $P=R^2=|\psi|^2$, and (**1B**) $Q=-(\hbar^2/2m)(\Delta R/R)$) is the quantum potential (QP)

$$\partial_t S+\frac{1}{2m}|\nabla S|^2+V+Q=0;\ \partial_t P+\frac{1}{m}\nabla\cdot(P\nabla S)=0 \tag{1.2}$$

Writing $\rho=mP$ one has formulas

$$\frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}=\frac{1}{4}\left[\frac{2\Delta\rho}{\rho}-\left(\frac{\nabla\rho}{\rho}\right)^2\right] \tag{1.3}$$

and for $\mathbf{v}=\dot{\mathbf{q}}$ with $p=mv=\partial_x S$ (cf. however p. 8.3 and [**177, 187, 310, 843**])

$$\partial_t\rho+\partial_x(\rho\dot{q})=0;\ \partial_t S+\frac{p^2}{2m}+V-\frac{\hbar^2}{3m}\frac{\partial_x^2\sqrt{\rho}}{\sqrt{\rho}}=0 \tag{1.4}$$

Now we observe that ($P=0$ for large x)

$$\int P\frac{\partial_x^2\sqrt{P}}{\sqrt{P}}dx=\frac{1}{4}\int\left(2P''-\frac{(P')^2}{P}\right)dx=-\frac{1}{4}\int\frac{(P')^2}{P}dx=-\frac{1}{4}FI \tag{1.5}$$

FI is Fisher information or better Fisher channel capacity (cf. [**318, 321**]). Hence, writing Q via P,

$$\int PQdx=\frac{\hbar^2}{8m}\int\frac{(P')^2}{P}dx=\frac{\hbar^2}{8m}FI \tag{1.6}$$

For the differential entropy (**1C**) $\mathfrak{S}=-\int\rho log(\rho)dx$ one has

$$\partial_t\mathfrak{S}=-m\int[P_t log(P)+P_t]dx=-m\int P_t(log(P)+1)dx \tag{1.7}$$

From (1.1) we have $P_t = -(1/m)(PS')'$ ($P' \sim \partial_x P$ etc.) so

$$(1.8)\qquad \partial_t \mathfrak{S} = \int (PS')'[log(P)+1]dx = -\int (PS')\frac{P'}{P}dx = -\int S'P'dx$$

At this point one often refers to diffusion or hydrodynamical processes and thinks of $S' = p = m\dot{q}$ (omitting boldface for vectors in 1-D) where $v = \dot{q}$ represents some collective velocity field related to a free for example with say $v = -(\hbar/2m)(\nabla P/P)$ involving an $v = -u$ (cf. [**170, 332, 333**]). Note that the typical Bohmian hypothesis $p \sim S'$ or $p \sim \nabla S$ is not valid for particle models and does not lead to correct quantum trajectories (cf. [**187, 297, 310, 311, 312, 589, 590**]) but we will continue to use this notation for hydrodynamical and diffusion processes essentially for historical purposes (cf. also [**843**] in this connection). Then (1.1) gives (**1D**) $P_t + (Pv)' = 0$ and it is interesting to note that this form of velocity involving $\nabla P/P$ or $\nabla\rho/\rho$ comes up in the form of momentum fluctuations or perturbations in work of Hall-Reginatto [**400, 401, 402, 736**] on the exact uncertainty principle and in Crowell [**246**] in a fluctuation context. Indeed in [**246**] one takes (**1E**) $\delta\rho = (\hbar/2i)(\nabla\rho/\rho)$ (think of $m=1$ for convenience) with

$$(1.9)\quad <\delta\rho> = \int \rho\delta\rho dx = \frac{\hbar}{2i}\int \nabla\rho dx = 0;\ <(\delta\rho)^2> = c\int\left[\frac{(\nabla\rho)^2}{\rho}\right]dx \sim FI$$

Thus from (1.3) and (**1B**) Q can be written as

$$(1.10)\qquad Q = -\frac{\hbar^2}{4m}\left[\frac{1}{2}(\delta p)^2 - \frac{\Delta\rho}{\rho}\right] = \frac{\hbar^2}{4m}\left[\nabla(\delta p) + \frac{1}{2}(\delta p)^2\right]$$

The exact uncertainty principle involves the characterization of quantum fluctuations as being generated by momentum fluctuations $\nabla P/P$ under certain quite general assumptions. This principle can be applied in many interesting circumstances (cf. [**170, 171, 400, 401, 402, 736**]).

We note also, going back to (1.8) with $P' \sim \nabla P$, when (as in the Brownian motion situation) $S' = -(\hbar/2m)(P'/P)$, then (**1F**) $\partial_t\mathfrak{S} = (\hbar/2m)\int[(P')^2/P]dx \sim \hat{c}FI$ showing that $\partial_t\mathfrak{S} \geq 0$ and exactly how it varies. This feature also arises in studying Ricci flow and information on this is provided in [**172, 506, 507, 621, 693, 836**]. Let $P(x)$ be a probability distribution on $\mathbf{R}$ or $\mathbf{R}^3$; we work in $\mathbf{R}$ for simplicity. Consider a differential entropy $\mathfrak{S} = -\int P\,log(P)dx$ and assume one wants to specify some value $\bar{A} = \int A(x)P(x)dx$. Then consider extremizing

$$(1.11)\qquad \tilde{\mathfrak{S}} = -\int Plog(P)dx + \lambda(1 - \int Pdx) + \alpha(\bar{A} - \int APdx)$$

Recall $log(1+x) \sim x$ for x small and write

$$(1.12)\quad \delta\tilde{\mathfrak{S}} = -\int[(P+\delta P)log(P+\delta P) - Plog(P)]\,dx - \lambda\int\delta Pdx - \alpha\int A\delta Pdx$$

$$= -\int\left\{(P+\delta P)log\left[P\left(1+\frac{\delta P}{P}\right)\right] - Plog(P)\right\}dx - \int(\lambda+\alpha A)\delta Pdx$$

$$\approx -\int\delta P(x)\,[log(P)+1+\lambda+\alpha A]\,dx$$

Since δP is arbitrary one obtains (**1G**) $log(P) + 1 + \lambda + \alpha A = 0$ or $P = exp[-1 - \lambda - \alpha A] = (1/Z)exp(-\alpha A)$ where $Z = exp(1 + \lambda)$ and $\int P dx = 1 \Rightarrow Z = \int exp[-\alpha A(x)]dx$. Here a suitable candidate for A would be the total energy of a system and if S is determined by P alone with $P \sim p = (1/m)S'$ as above then A would have to be the fluctuation energy determined by the quantum potential.

1.1. SUBQUANTUM THERMODYNAMICS. We go here to [**392**] for a derivation of the SE from vacuum fluctuations and diffusion waves in subquantum thermodynamics (cf. also [**93, 123, 329, 332, 333, 335, 334, 532, 878**] for background). Grössing's work in [**392**] specifies the energy in quantum mechanics arising from sub-quantum fluctuations via nonequilibrium thermodynamics. The ideas are motivated and discussed at great length in e.g. papers 1, 2, and 4 in [**392**] and we only summarize here following [**392**]-6. To each particle of nature is attributed an energy $E = \hbar\omega$ for some kind of angular frequency ω and one can generally assume that "particles" are actually dissipative systems maintained in a nonequilibrium steady-state by a permanent source of kinetic energy, or heat flow, which is not identical with the kinetic energy of the particle, but an additional contribution. Thus it is assumed here that (**1H**) $E_{tot} = \hbar\omega + [(\delta p)^2/2m]$ where δp is the additional fluctuating momentum component of the particle of mass m. Similarly the particle's environment is considered to provide detection probability distributions which can be modeled by wave-like intensity distributions $I(x,t) = R^2(x,t)$ with R being the wave's real valued amplitude; thus one assumes (**1I**) $P(x,t) = R^2(x,t)$ with $\int P d^n x = 1$ (note $x \sim \mathbf{x}$). In [**392**]-1 it was proposed to merge some results of nonequilibrium thermodynamics with classical wave mechanics in such a manner that the many microscopic degrees of freedom associated with the hypothesized sub-quantum medium can be recast into the more "macroscopic" properties that characterize the wave-like behavior on the quantum level. Thus one considers a particle as being surrounded by a large "heat bath" so that the momentum distribution in this region is given by the usual Maxwell-Boltzmann distribution. This corresponds to a "thermostatic" regulation" of the reservoir's temperature which is equivalent to saying that the energy lost to the thermostat can be regarded as heat. This leads to emergence at the equilibrium-type probability density ratio (**1J**) $[P(x,t)/P(x,0)] = exp[-(\Delta\mathcal{Q})/kT)]$ where T is the reservoir temperature and $\Delta\mathcal{Q}$ the exchanged heat between the particle and its environment. The conditions (**1H**)-(**1J**) are sufficient to derive the SE. Thus first, via Boltzmann, the relation between heat and action is given via an action function $S = \int (E_{kin} - V)dt$ with $\delta S = \delta \int E_{kin} dt$ via

$$\Delta\mathcal{Q} = 2\omega\delta S = 2\omega[\delta(S)(t) - \delta S(0)] \tag{1.13}$$

(cf. [**392**] for more details). Next the kinetic energy of the thermostat is $kT/2$ per degree of freedom and the average kinetic energy of an oscillator is $(1/2)\hbar\omega$ so equality of average kinetic energies demands (**1K**) $kT/2 = \hbar\omega/2$ or $\hbar\omega = kT = 1/\beta$. Combining (**1H**), (1.13), and (**1K**) yields then

$$P(x,t) = P(x,0)e^{-\frac{2}{\hbar}[\delta S(x,t) - \delta S(x,0)]} \tag{1.14}$$

leading to a momentum fluctuation

$$\delta p(x,t) = \nabla(\delta S(x,t)) = -\frac{\hbar}{2}\frac{\nabla P(x,t)}{P(x,t)} \tag{1.15}$$

and an additional kinetic energy term

$$\delta E_{kin} = \frac{1}{2m}\nabla(\delta S)\cdot\nabla(\delta S) = \frac{1}{2m}\left(\frac{\hbar}{2}\frac{\nabla P}{P}\right)^2 \tag{1.16}$$

The action integral then becomes

$$A = \int L d^n x dt = \int P(x,t)\left[\partial_t S + \frac{1}{2m}\nabla S\cdot\nabla S + \frac{1}{2m}\left(\frac{\hbar}{2}\frac{\nabla P}{P}\right)^2 + V\right] \tag{1.17}$$

We emphasize here that

$$(\bigstar\bigstar)\int P(\nabla S\cdot\delta p)d^n x = \int P(\nabla S\cdot\nabla(\delta S))d^n x = 0$$

(i.e. the fluctuations terms δp are uncorrelated with the momentum $p \sim \nabla S$). Now one uses the Madelung form (**1L**) $\psi = Rexp[(i/\hbar)S]$ where $R = \sqrt{P}$ to obtain (**1M**) $[\nabla\psi/\psi]^2 = [\nabla P/2P]^2 + [\nabla S/\hbar]^2$ leading to (1.17) in the form

$$A = \int L dt = \int d^n x dt\left[|\psi|^2(\partial_t S + V) + \frac{\hbar^2}{2m}|\nabla\psi|^2\right] \tag{1.18}$$

(cf. [**848**] for $|\psi|^2 \sim P$). Then via $|\psi|^2\partial_t S = -(i\hbar/2)(\psi^*\dot{\psi} - \dot{\psi}^*\psi)$ one has (**1N**) $L = -(i\hbar/2)(\psi^*\dot{\psi} - \dot{\psi}^*\psi) + (\hbar^2/2m)\nabla\psi\cdot\nabla\psi^* + V\psi\psi^*$ leading to the SE (**1O**) $i\hbar\partial_t\psi = [-(\hbar^2/2m)\nabla^2 + V]\psi$ along with the "modified" Hamilton-Jacobi equation (cf. [**843**] for another version of the Madelung theory).

$$\partial_t S + \frac{1}{2m}(\nabla S)^2 + V + Q = 0;\ Q = -\frac{\hbar^2}{4m}\left[\frac{1}{2}\left(\frac{\nabla P}{P}\right)^2 - \frac{\Delta P}{P}\right] = -\frac{\hbar^2}{2m}\frac{\Delta R}{R} \tag{1.19}$$

Then define (**1P**) $\mathbf{u} = (\delta\mathbf{p}/m) = -(\hbar/2m)(\nabla P/P)$ and $k_{\mathbf{u}} = -(1/2)(\nabla P/P) = -(\nabla R/R)$ so that Q can be rewritten as

$$Q = \frac{m\mathbf{u}\cdot\mathbf{u}}{2} - \frac{\hbar}{2}(\nabla\cdot\mathbf{u}) = \frac{\hbar^2}{2m}(k_{\mathbf{u}}\cdot k_{\mathbf{u}} - \nabla\cdot k_{\mathbf{u}}) \tag{1.20}$$

Using (1.13) and (1.14) one can also write (**1Q**) $\mathbf{u} = (1/2\omega m)\nabla\mathcal{Q}$.

Generally a steady state oscillator in nonequilibrium thermodynamics corresponds to a kinetic energy at the sub-quantum level providing the necessary energy to maintain a constant oscillation frequency ω and some excess kinetic energy resulting in a fluctuating momentum contribution δp to the momentum p of the particle (note $p \sim \mathbf{p}$). Similarly a steady state resonator representing a "particle" in a thermodynamic environment will not only receive kinetic energy from it but in order to balance the stochastic influence of the buffeting momentum fluctuations it will also dissipate heat into the environment. There is a vacuum fluctuation theorem (VFT) from [**392**]-1 which proposes that larger energy fluctuations of the oscillating system correspond to higher probability of heat dissipated into the environment (rather that absorbed). The corresponding balancing velocity is called (after Einstein) the "osmotic" velocity. Thus recalling the stochastic "forward" movement $\mathbf{u} \sim (\delta\mathbf{p}/m)$, the current $\mathbf{J} = P\mathbf{u}$ has to be balanced by $-\mathbf{u}$, i.e. $\mathbf{J} = -P\mathbf{u}$. Putting (**1P**) into the definition of the "forward" diffusive current $\mathbf{J}$ and recalling the diffusivity $D = \hbar/2m$ one has (**1R**) $\mathbf{J} = P\mathbf{u} = -D\nabla P$ and when combined with the continuity equation $\dot{P} = -\nabla\cdot\mathbf{J}$ this gives (**1S**) $\partial_t P = D\nabla^2 P$. Here (**1R**) and (**1S**) are the first and second of the Fick laws of diffusion and $\mathbf{J}$ is called the diffusion current.

Returning now to (**1Q**) one defines $\Delta\mathcal{Q} = \mathcal{Q}(t) - \mathcal{Q}(0) < 0$ and maintaining heat flow as positive one writes $-\Delta\mathcal{Q}$ for heat dissipation and puts this in (**1Q**) to get the osmotic velocity (**1T**) $\bar{\mathbf{u}} = -\mathbf{u} = D(\nabla P/P) = -(1/2\omega m)\nabla\mathcal{Q}$ with osmotic current (**1U**) $\bar{\mathbf{J}} = P\bar{\mathbf{u}} = D\nabla P = -(P/2\omega m)\nabla\mathcal{Q}$. As a corollary to Fick's second law one has then

$$\partial_t P = -\nabla\cdot\bar{\mathbf{J}} = -D\nabla^2 P = \frac{1}{2\omega m}[\nabla P\cdot\nabla\mathcal{Q} + P\nabla^2\mathcal{Q}] \tag{1.21}$$

Next one looks for a thermodynamic meaning for the quantum potential Q. Take first $Q = 0$ and look at the osmotic velocity (**1T**) that represents the heat dissipation from the particle into its environment. From (1.20) one has (**1V**) $(\hbar/2)(\nabla\cdot\mathbf{u}) = (1/2)(m\mathbf{u}\cdot\mathbf{u})$. Inserting now (**1T**) instead of (**1Q**) yields the thermodynamic corollary of a vanishing QP as (**1W**) $\nabla^2\mathcal{Q} = (1/2\hbar\omega)(\nabla\mathcal{Q})^2$. Returning to (1.21) put first (**1K**) into (**1S**) to get (**1X**) $P = P_0 exp[-(\Delta\mathcal{Q}/\hbar\omega)]$ and one obtains then from (1.21)

$$\partial_t P = \frac{P}{2\omega m}\left[\nabla^2\mathcal{Q} - \frac{(\nabla\mathcal{Q})^2}{\hbar\omega}\right] \Rightarrow \partial_t P = -\frac{P}{2\omega m}\nabla^2\mathcal{Q} \tag{1.22}$$

(via (**1W**)). Now from (**1X**) one has also (**1Y**) $\partial_t P = -(P/\hbar\omega)\partial_t\mathcal{Q}$ so comparison of (1.22) and (**1X**) yields (**1Z**) $\nabla^2\mathcal{Q} - (1/D)\partial_t\mathcal{Q} = 0$ ($\tilde{\mathcal{Q}} = (1/\hbar\omega)\mathcal{Q}$ is inserted here in a second version of the last paper in [**392**]). This is nothing but a classical heat equation obtained by the requirement that the quantum potential $Q = 0$; it shows that even for free particles both in the quantum and classical case one can identify a heat dissipation process emanating from the particle. A non-vanishing quantum potential then is a means of describing the spatial and temporal dependencies of the corresponding thermal flow in the case that the particle is not free.

Various particular solutions to (**1Z**) are indicated for the case $Q = 0$ as well as when $Q \neq 0$. Examples are discussed with a view toward resolving a certain "particle in a box" problem of Einstein. In [**392**]-1 one concentrated on the momentum fluctuations δp generated from the environment to the particle while in [**392**]-3 one develops the idea of excess energy developed as heat from the particle to its environment (which is described via the quantum potential). In fact one can rewrite (1.19) as

$$\partial_t S + \frac{1}{2m}(\nabla S)^2 + V + \frac{\hbar^2}{4m}\left[\nabla^2\tilde{\mathcal{Q}} - \frac{1}{D}\partial_t\tilde{\mathcal{Q}}\right] = 0 \tag{1.23}$$

where $\tilde{\mathcal{Q}} = \mathcal{Q}/\hbar\omega$. This provides considerable insight into the nature and role of the quantum potential.

Note that one has achieved a "thermalization" of the quantum potential (QP) in the form

$$Q = \frac{\hbar^2}{4m}\left[\nabla^2\tilde{\mathcal{Q}} - \frac{1}{D}\partial_t\tilde{\mathcal{Q}}\right] \tag{1.24}$$

where $\tilde{\mathcal{Q}} = \mathcal{Q}/\hbar\omega = \alpha\mathcal{Q}$ is an expression of heat and $D = \hbar/2m$ is a diffusion coefficient (note $\alpha = \beta$ as in (**1K**). In [**173**] we show that, as a corollary, one can produce a related thermalization of Fisher information (FI) which should have interesting consequences. Thus in (**1U**) one uses a formula

$$\frac{\nabla P}{P} = -\frac{1}{2\omega m D}\nabla\mathcal{Q} = -\frac{1}{\omega\hbar}\nabla\mathcal{Q} = -\beta\nabla\mathcal{Q} \tag{1.25}$$

and this leads one to think of $\nabla log(P) = -\alpha\nabla\mathcal{Q} = -\nabla(\alpha\mathcal{Q})$ with a possible solution

$$log(P) = -\alpha\mathcal{Q} + c(t) \Rightarrow P = exp[-\alpha\mathcal{Q} + c(t)] = \hat{c}(t)e^{-\alpha\mathcal{Q}} \tag{1.26}$$

(cf. also (1.13)). Now Fisher information (FI) is defined via ($dx \sim dx^3$ for example)

$$F = \int\frac{(\nabla P)^2}{P}dx = \int P\left(\frac{\nabla P}{P}\right)^2 dx \tag{1.27}$$

and one can write Q as in (1.19). Consequently (since $\int\Delta P dx = 0$)

$$\int PQdx = -\frac{\hbar^2}{8m}\int\frac{(\nabla P)^2}{P}dx = -\frac{\hbar^2}{8m}F \tag{1.28}$$

Then as in [**173**] one can write formally, first using (1.24) and $\alpha = 1/\omega\hbar$

$$\begin{aligned} F = -\frac{8m}{\hbar^2}\int PQdx &= -\frac{8m}{\hbar^2}\int P\frac{\hbar^2}{4m}\left[\nabla^2\tilde{\mathcal{Q}} - \frac{1}{D}\partial_t\tilde{\mathcal{Q}}\right]dx \\ &= -2\alpha\int P\left[\nabla^2\mathcal{Q} - \frac{2m}{\hbar}\partial_t\mathcal{Q}\right]dx \end{aligned} \tag{1.29}$$

and secondly, using (1.25) and (1.26) (recall also $\alpha = \beta$)

$$F = \int P\left(\frac{\nabla P}{P}\right)^2 dx = \beta^2\hat{c}(t)\int e^{-\beta\mathcal{Q}}(\nabla\mathcal{Q})^2 dx \tag{1.30}$$

In view of the thermal aspects of gravity theories now prevalent it may perhaps be suggested that connections of quantum mechanics to gravity may best be handled thermally. There may also be connections here to the emergent quantum mechanics of [**290, 444, 445, 446**].

Following Garbaczewski [**333**] one can look at a diffusion model with current velocity $\mathbf{v} = \mathbf{b} - \mathbf{u}$ where $u = D\nabla(log(\rho))$ is an osmotic velocity field and $D = \hbar/2m$. The continuity equation is a Fokker-Planck equation (♦) $\partial_t\rho = D\Delta\rho = \nabla\cdot(\mathbf{b}\rho)$ and assuming ρ, $\mathbf{v}\rho$, and $\mathbf{b}\rho$ vanish at spatial infinity (or at boundaries) leads to an entropy balance equation

$$\frac{d\mathfrak{S}}{dt} = \int\left[\rho(\nabla\cdot\mathbf{b}) + D\frac{(\nabla\rho)^2}{\rho}\right]d^3x \tag{1.31}$$

(cf. also [**170, 332, 334, 335**]). ■

1.2. FLUCTUATIONS AND FISHER INFORMATION. We go next to [**246**] which contains a rich lode of important material on quantum fluctuations and some penentrating insight into physics (but some proofreading seems indicated). We will try to rewrite some of this in a more complete manner. Thus consider a SE for $\psi = Rexp(iS/\hbar)$ with momentum operator $\hat{p}$ so that

$$\hat{p}\psi = p\psi = \left(\nabla S + \frac{\hbar}{i}\frac{\nabla R}{R}\right)\psi \Rightarrow p \sim <p> + \delta p \tag{1.32}$$

which identifies $(\hbar/i)(\nabla R/R)$ as a fluctuation δp. Recall now that the SE is (**2A**) $i\hbar\psi_t = -(\hbar^2/2m)\Delta\psi + V\psi$ and setting $\rho = R^2 = \psi^*\psi$ one has

$$\partial_t\rho = \frac{i\hbar}{2m}[\psi^*\Delta\psi - (\Delta\psi^*)\psi] = \frac{i\hbar}{2m}\nabla\cdot(\psi^*\nabla\psi - \nabla(\psi^*)\psi) \tag{1.33}$$

Now in polar form $\psi = Rexp(iS/\hbar)$, $\rho = R^2$ this becomes (calculating sometimes in 1-D for simplicity)

$$\nabla(Re^{iS/\hbar}) = \nabla Re^{iS/\hbar} + \frac{iR\nabla S}{\hbar}e^{iS/\hbar} \tag{1.34}$$

$$\psi^*\nabla\psi - (\nabla\psi^*)\psi = R\nabla R + \frac{iR^2\nabla S}{\hbar} - R\nabla R + \frac{iR^2\nabla S}{\hbar} = \frac{2i\rho\nabla S}{\hbar} \tag{1.35}$$

$$\Rightarrow \partial_t\rho = \frac{i\hbar}{2m}\nabla\left(\frac{2i\rho\nabla S}{\hbar}\right) = -\frac{1}{m}\nabla(\rho\nabla S)$$

Now the quantum potential is

$$Q = -\frac{\hbar^2}{2m}\frac{\Delta\rho^{1/2}}{\rho^{1/2}} = -\frac{\hbar^2}{4m}\left[\frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2 - \frac{\Delta\rho}{\rho}\right] = \frac{\hbar^2}{4m}\left[\frac{\Delta\rho}{\rho} - \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2\right] \tag{1.36}$$

(cf. (1.1) and $\rho = R^2$ so $\rho' = 2RR'$ and $2(R'/R) = \rho'/\rho$; hence one has (**2B**) $\delta p \sim (\hbar/2i)(\nabla\rho/\rho)$. There is equivalent material about Fokker-Planck equations in [**170**] so we omit the discussion in [**246**]. One notes that (**2C**) $<\delta p> \sim \int \rho\delta p dx = (\hbar/2i)\int\nabla\rho dx = 0$ whereas $<(\delta p)^2> \sim c\int[(\nabla\rho)^2/\rho]dx \sim Fisher\ information.$ Here the quantum potential can also be written as

$$Q = -\frac{\hbar^2}{4m}\left[\frac{1}{2}(\delta p)^2 - \frac{\Delta\rho}{\rho}\right] = \frac{\hbar^2}{4m}\left[\nabla(\delta p) + \frac{1}{2}(\delta p)^2\right] \tag{1.37}$$

since $(\rho'/\rho)' = (\rho''/\rho) - [(\rho')^2/\rho^2] \sim \Delta\rho/\rho = \nabla(\delta p) + (\delta p)^2$. Note also that the exact uncertainty principle of Hall-Reginatto ([**400, 401**]), developed at length in [**170**], is based on momentum fluctuations $p = \nabla S + \delta p$ with $<\delta p> = 0$. If one writes $V(q) = V(<q>) + \nabla_q V(<q>)\delta q$ as a function of position and recalls that the quantum HJ equation has the form (**2D**) $S_t + (p^2/2m) + V + Q = 0$ (cf. [**170**]) then this can be rewritten in terms of fluctuations as

$$S_t + \frac{1}{2m} <p^2> + V(<q>) + \nabla_q V(<q>)\delta q + Q(p,\delta p); \tag{1.38}$$

$$Q = \frac{\hbar^2}{4m}\left(-i\hbar\nabla\cdot\delta p + \frac{1}{2}(\delta p)^2\right)$$

We go now to [**322**] with (**2E**) $\int dx\, p(x) = 1$ and (**2F**) $I[p] = \int dx F_I(p)$ where $F_I(p) = p(x)[(p')/p]^2$. Assume that there are known

$$< A_j > = \int dx A_j(x) p(x) \;\; (j = 1, \cdots, M) \tag{1.39}$$

and use the principle of extreme physical information (EPI) developed by B. Frieden et al (cf. [**318**]) to find the probability distribution $p = p_I$ extremizing $I[p]$ subject to prior conditions $< A_j >$. Jaynes used the Shannon functional $F = -plog(p)$ with (**2G**) $S[p] = -\int dxplog(p)$ but here one uses the Fisher extremization with

$$\delta_p \left[I[p] - \alpha < 1 > - \sum_1^M \lambda_i < A_i > \right] = 0 \tag{1.40}$$

$$\equiv \delta_p \left[\int dx \left(F_I[p] - \alpha p - \sum_i^M \lambda_i A_i p \right) \right] = 0$$

Variation leads to

$$\delta \int \frac{p^{'2}}{p^2} dx \approx \int \left[-\frac{p^{'2}}{p^2}\delta p + \frac{2p'}{p}\delta p' \right] dx \sim \int \left[-\frac{p^{'2}}{p^2} - \partial \left(\frac{2p'}{p} \right) \right] \delta p dx$$

$$\int dx \delta p \left[(p)^{-2}(p')^2 + \partial_x \left(\frac{2}{p} p' \right) + \alpha + \sum_1^M \lambda_i A_i \right] = 0 \tag{1.41}$$

which implies, via the arbitrary nature of δp

$$\left[(p)^{-2}(p')^2 + \partial_x \left(\frac{2}{p} p' \right) + \alpha + \sum_1^M \lambda_i A_i \right] = 0 \tag{1.42}$$

The normalization condition on p makes α a function of the λ_i and one lets $p_I(x, \lambda_i)$ be a solution of (1.42). Then the extreme Fisher information is (**2H**) $I = \int dx p_I^{-1} [p_I']^2$. Now one can simplify (1.42) via (**2I**) $G(x) = +\alpha + \sum_1^M \lambda_i A_i(x)$ and write

$$[\partial_x log(p_I)]^2 + 2\frac{\partial^2 log(p_I)}{\partial x^2} + G(x) = 0 \tag{1.43}$$

Then introduce $p_I = \psi^2$ and (**2J**) $v(x) = \partial_x log(\psi(x))$ so that (1.43) becomes (**2K**) $v'(x) = -[(1/4)G(x) + v^2(x)]$ which is a Riccati equation. Setting

$$u(x) = exp \left[\int^x dx \frac{dlog(\psi)}{dx} \right] = \psi \tag{1.44}$$

makes (1.43) into a Schrödinger-like equation

$$-\frac{1}{2}\psi''(x) - \frac{1}{8}\sum \lambda_i A_i(x)\psi(x) = \frac{\alpha}{8}\psi \tag{1.45}$$

where (**2L**) $U(x) = (1/8)\sum_1^M \lambda_i A_i(x)$ is an effective potential (cf. [**320, 322, 323, 641**]). Note that ψ is defined here completely via p_I so any quantum motion is automatically generated by fluctuation energy (i.e. $S \sim \delta S$).

Consider now a situation with one function A_i (**2M**) $\bar{A} = \int pAdx$. Then from (1.40)-(1.43)

$$p^{-2}(p')^2 + \partial_x \left(\frac{2p'}{p}\right) + \alpha + \lambda A = 0 \tag{1.46}$$

Now, following [**322**], one translates the Legendre structure of thermodynamics into a Fisher context. Thus from (**2H**), integrating by parts implies

$$\frac{\partial I}{\partial \lambda} = \int dx \frac{\partial p_I}{\partial \lambda}\left[-p_I^{-2}\left(\frac{\partial p_I}{\partial x}\right)^2 - \frac{\partial}{\partial x}\left(\frac{2}{p_I}\frac{\partial p_I}{\partial x}\right)\right] \tag{1.47}$$

where p_I is a solution of (1.46). Comparing (1.46) to (1.47) one has

$$\frac{\partial I}{\partial \lambda} = \int dx \frac{\partial p_I}{\partial \lambda}\left[\alpha + \lambda A\right] \tag{1.48}$$

Then on account of normalization ($\int p_I dx = 1$)

$$\frac{\partial I}{\partial \lambda} = \lambda \frac{\partial}{\partial \lambda}\int dx\, p_I A(x) \equiv \frac{\partial I}{\partial \lambda} = \lambda \frac{\partial}{\partial \lambda} < A > \tag{1.49}$$

which is a generalized Fisher-Euler theorem. The term $\int dx\alpha\partial_\lambda p_I \sim \alpha\partial_\lambda \int dx p_I = 0$ via $\int p_I dx = 1$. The thermodynamic counterpart of (1.49) is the derivative of the entropy with respect to mean values. Thus $I = I(\lambda)$, $p_I = p_I(\lambda)$, and via normalization $\alpha = \alpha(\lambda)$. Thus λ and $< A >$ play reciprocal roles within thermodynamics and one introduces a generalized thermodynamic potential as a Legendre transform of I, namely

$$\Lambda = I(< A >) - \lambda < A > \tag{1.50}$$

Then, using (1.49)

$$\frac{\partial \Lambda}{\partial \lambda} = \frac{\partial I}{\partial < A >}\frac{\partial < A >}{\partial \lambda} - \lambda \frac{\partial < A >}{\partial \lambda} - < A > = - < A > \tag{1.51}$$

and one has a summary collection of formulas

$$\Lambda = I - \lambda < A >;\ \frac{\partial \Lambda}{\partial \lambda} = - < A >;\ \frac{\partial I}{\partial < A >} = \lambda; \tag{1.52}$$

$$\frac{\partial \lambda}{\partial < A >} = \frac{\partial^2 I}{\partial < A >^2};\ \frac{\partial < A >}{\partial \lambda} = -\frac{\partial^2 \Lambda}{\partial \lambda^2}$$

and we recall (1.49) in the form (**2N**) $\frac{\partial I}{\partial \lambda} = \lambda \frac{\partial <A>}{\partial \lambda}$. Thus the Legendre transform structure of thermodynamics has been translated into the Fisher context (see here also Chapter 4 of [**318**] for more on this and for additional general information we cite e.g. [**308, 319, 580, 583, 584, 609, 687, 688, 689, 690, 691, 705, 706, 707, 708, 709, 722, 734**]).

On the other hand with $\bar{A}$ the sole constraint consider

$$\tilde{H} = FI + \alpha(\bar{A} - \int pAdx) \tag{1.53}$$

Then one finds directly

$$\delta\tilde{H} = \int dx\,\delta p\left[\frac{(p')^2}{p^2} + \partial_x\left(\frac{2p'}{p}\right) + \alpha A\right] \tag{1.54}$$

This means (as in (1.46))

$$\frac{(p')^2}{p^2} + \partial_x\left(\frac{2p'}{p}\right) + \alpha A = 0 \tag{1.55}$$

Now we can write $\partial_x(2p'/p) = (2p''/p) - [2(p')^2/p^2]$ which means, via (1.36), that

$$2\frac{\Delta p^{1/2}}{p^{1/2}} + \alpha A = 0 \tag{1.56}$$

and via (★) in Section 1.1 this means that the extreme probability p_I directly determines a quantum potential Q via

$$Q = -\frac{\hbar^2}{2m}\frac{\Delta p_I^{1/2}}{p_I^{1/2}} \Rightarrow Q = \frac{\hbar^2}{4m}[\alpha A] \tag{1.57}$$

However, although A has not been specified we seem to have a result that a constraint $\bar{A}$ for which the Fisher thermodynamic procedure works with $I[p]$ as defined, requires A to satisfy (2.26). This is in fact tautological since we are dealing with a situation where fluctuations based on p_I are the only source of energy and one will have (**2O**) $\tilde{F} = \int PQdx = (\hbar^2/8m)\int[(\nabla p)^2/p]dx$ (cf. [**170**]) and $\tilde{F}$ corresponds to a fluctuation energy. In particular as indicated in [**170**]

$$\int p_I Q dx = \frac{\hbar^2}{4m}\int dx\,p[\alpha A] = \frac{\hbar^2}{4m}[\alpha\bar{A}] \tag{1.58}$$

Note that in general Fisher information $\tilde{F} = I[p]$ as in (**2G**) is an action term which can be added to a classical Hamiltonian in order to quantize it and thus $\tilde{F}$ is a "natural" constraint ingredient. Fixing $\bar{A}$ would mean fixing the contribution of the quantum potential (QP) Q or fixing the amount of quantization allowed. In some way this would also correspond to restraining the probability in order to achieve a fixed amount of quantization.

REMARK 1.1.1. Suppose we extremize $\tilde{\mathfrak{S}}$ as in (1.11) with $A \sim E =$ total energy to arrive at a probability (**2P**) $P = (1/Z)exp(-\gamma E)$ where $E \sim E(x,t)$, $Z = \int exp(-\gamma E)dx$. Then compute the Fisher information for this P which will be based upon (cf. (1.3))

$$P' = \frac{1}{Z}(-\gamma E')e^{-\gamma E};\ P'' = -\frac{\gamma}{Z}[E'' - \gamma(E')^2]e^{-\gamma E} \tag{1.59}$$

$$\frac{P'}{P} = -\gamma E';\ \frac{P''}{P} = -\gamma E'' + \gamma^2(E')^2 \tag{1.60}$$

$$Q = \frac{\gamma\hbar^2}{8m}[\gamma(E')^2 - 2E''] \tag{1.61}$$

$$FI = \frac{8m}{\hbar^2}\int PQdx = \frac{\gamma^2}{Z}\int(E')^2 e^{-\gamma E}dx \tag{1.62}$$

On the other hand extremizing FI as in (1.53), with fluctuations as the only source of energy, leads to $P = p_I$ defined via A as in (1.56) which yields in paticular $Q = (\hbar^2/4m)[\alpha A]$ as in (2.26). Now recall for P as in (**1J**)

(1) $\frac{P(x,t)}{P(x,0)} = e^{\frac{-\Delta\mathcal{Q}}{kT}}$ from (**1J**)
(2) $\Delta\mathcal{Q} = \mathcal{Q}(t) - \mathcal{Q}(0) = 2\omega[(\delta S)(t) - (\delta S)(0)]$ from (1.13) and $(2/\hbar)\delta S(t) \sim \beta\mathcal{Q}(t)$ (cf. ($\bullet$))
(3) $\delta p = \nabla(\delta S(x,t)) = -(\hbar/2)(\nabla P/P)$ as in (1.15) and from (1.25) $(\nabla P/P) = (1/\omega\hbar)\nabla\mathcal{Q} = \beta\nabla\mathcal{Q}$
(4) $\delta E_{kin} = (\hbar^2/8m)(\nabla P/P)^2 = (1/8m\omega^2)(\nabla\mathcal{Q})^2$
(5) $P = \hat{c}(t)exp(-\alpha\mathcal{Q})$ from (1.26) with $\alpha = 1/\omega\hbar \sim 1/kT \sim \beta$ - this can also be seen from (1.14) as $P \propto exp[-\beta\mathcal{Q}(t)]$

For E = total energy as in (**2P**) it is clear that to apply this here we must think of $E = \hbar\omega + \delta E_{kin}$ and $\hbar\omega$ will only enter as a constant. The thermalization fluctuation energy for probabilities appears as $\hat{c}exp[-\delta S(x,t)] \sim \hat{c}exp[-\beta\mathcal{Q}(t)]$ as indicated so δE_{kin} is expressed in terms of $\mathcal{Q}$. This means that (1.62) involving $(E')^2$ (or $(\nabla E)^2$) for FI corresponds to the $(\nabla\mathcal{Q})^2$ formula of (1.30). In other words the fluctuation energy is equivalent to the thermal energy (modulo constants); see here also [**170, 369, 436**]. ∎

We omit here mention of many related topics and work involving Fisher information, thermodynamics, and entropy based on results of Abe, Frieden, Garbaczewski, Gellman, Hall, Kaniadakis, Naudts, Pennini, A. Plastino, A.R. Plastino, Reginatto, Soffer, and Tsallis in particular; some references can be found in [**170, 278, 319, 318, 341, 647**]. For cogent discussions of many aspects of quantum mechanics see Nikolić [**635, 636, 637, 638, 639, 640**].

REMARK 1.1.2. We refer here to [**97, 170, 177, 175, 176, 297, 589, 851**], where the Schwarzian derivative arises in the quantum equivalence principle (QEP) of Faraggi-Matone, and to [**593, 594, 595**] where it comes up in semi-classical expansions (note also that there is a difference between semi-classical and quasi-classical - cf. [**606**]). Thus the stationary SE $(\hbar^2/2m)\psi'' - V\psi = E\psi$ can be written via $\psi = exp(iW/\hbar)$ with $W = s + (\hbar/i)log(A)$ as

$$(1.63)\qquad (s')^2 - 2m(E-V) = \hbar^2\frac{A''}{A};\ 2A's' + As'' = 0$$

Therefore (**2Q**) $A = c(s')^{-1/2}$ and

$$(1.64)\qquad (s')^2 = 2m(E-V) + \frac{\hbar^2}{2}\left[\frac{3}{2}\left(\frac{s''}{s'}\right)^2 - \frac{s'''}{s'}\right]$$

which can be written as

$$(1.65)\qquad \frac{1}{2m}(s')^2 + V + Q = E$$

Now from (1.1) we have $Q = -(\hbar^2/4m)(A''/A)$ (since $A = exp(log(A))$) and hence

$$(1.66)\qquad Q = -\frac{\hbar^2}{2m}\left(\frac{[(s')^{-1/2}]''}{[s']^{-1/2}}\right) = \frac{\hbar^2}{4m}\left[\frac{s'''}{s'} - \frac{3}{2}\left(\frac{s''}{s'}\right)^2\right] = \frac{\hbar^2}{4m}\mathfrak{S}Z(s)$$

defines the quantum potential via a Schwarzian derivative $\mathfrak{S}Z$. The Schwarzian derivative (and Ermakov invariant) arise also in [**595**] in dealing with semiclassical theory for (**2R**) $\hbar^2\partial_x^2\psi(x) + p^2(x)\psi(x) = 0$ when writing the wave function as $\psi(x) = u(x)w(\xi(x))$ with the assumption (**2S**) $\hbar^2\partial_\xi^2 w(\xi) + R(\xi)w(\xi) = 0$. This leads to (**2T**) $\psi(x) = (\partial_x\xi)^{-1/2}w(\xi(x))$ and

$$R(\xi)(\partial_x\xi)^2 - p(x)^2 + \frac{\hbar^2}{2}\left[\frac{\xi'''}{\xi'} - \frac{3}{2}\left(\frac{\xi''}{\xi'}\right)^2\right] = 0 \tag{1.67}$$

where the last term can be written as (**2U**) $(\hbar^2/2) < \xi; x >= (\hbar^2/2)\mathfrak{S}Z(\xi)$ (cf. also [**785, 786**] where relations of Ricatti equations to the Wigner function and Ermakov invariants arise).

1.3. THE QUANTUM EQUIVALENCE PRINCIPLE - QEP. The postulate that physical states be equivalent under coordinate transformations leads to the quantum Hamilton-Jacobi equation (QSJE) which in turn gives the SE (cf. [**97, 297, 589**]). We have written about this before (cf. [**170, 177, 175, 176**]) but it is now imperative to put in more detail about the QEP if one hopes to understand anything about relations between classical and quantum mechanics. We will only deal with the non-relativistic situation here and refer to [**297**] (IJMPA - 2000) for a detailed discussion. Thus one looks for coordinate transformations (**TV**) $q \to q^v = v(q)$ with $S_0^v(q^v) = S_0((q^v))$ where S_0 corresponds to the reduced action from Hamilton's principal function $S = S_0 - Et$ in the stationary case. Then $p \to p_v = (\partial_q q^v)^{-1}p$ so p transforms as ∂_q and the formalism will be covariant. Now in classical mechanics there are problems with $p - q$ duality due to the manner in which time enters into the formalism and one looks for a formulation of dynamics with manifest $p - q$ duality via Legendre transforms

$$s = S_0(q) = pq - T_0(p);\ q = \frac{\partial T_0(p)}{\partial p} \tag{1.68}$$

There is now a canonical equation (cf. also Chapter 8)

$$\left(\frac{\partial^2}{\partial s^2} + \mathfrak{U}(s)\right) q\sqrt{p} = \left(\frac{\partial^2}{\partial s^2} + \mathfrak{U}(s)\right)\sqrt{p} = 0 \tag{1.69}$$

where $\mathfrak{U}(s) = \mathfrak{S}Z(s) = \{q; s\} = (q'''/q') - (3/2)(q''/q')^2$ $('\sim d/ds)$. This can be directly checked from (1.68) via e.g.

$$\partial_s\sqrt{p} = (1/2)p^{-1/2}p_s;\ \partial_s^2\sqrt{p} = -(1/4)p^{-3/2}p_s^2 + (1/2)p^{-1/2}p_{ss}; \tag{1.70}$$

$$p_s q_s + p q_{ss} = 0 \Rightarrow \frac{p_s}{p} = -\frac{q_{ss}}{q_s} \Rightarrow \frac{p_{ss}}{p} = -\frac{q_{sss}}{q_s} + 2\left(\frac{q_{ss}}{q_s}\right)^2$$

Hence e.g. $\partial_s^2\sqrt{p} = -\mathfrak{U}(s)\sqrt{p}$ and we note also that (**3A**) $(1/q\sqrt{p})(\partial^2(q\sqrt{p})/\partial s^2) = (1/\sqrt{p})(\partial^2\sqrt{p})/\partial s^2)$. Now $\mathfrak{U}(s)$ is considered as a sort of canonical potential (consistent with the identification (1.66)) and we note for a Möbius transformation ($GL(2,\mathbf{C})$ transformation)

$$q \to q^v = \frac{Aq + B}{Cq + D};\ p \to p_v = \rho^{-1}(Cq + D)^2 p \tag{1.71}$$

for $\rho = AD - BC$. For the Schwarzian derivative (in x) one has

$$\{\gamma(h), x\} = \{h; x\};\ \gamma(h) = \frac{Ah+B}{Ch+D} \tag{1.72}$$

(cf. [**297**]). Then the $GL(2, \mathbf{C})$ invariance of the canonical equation (1.69) means that given $\mathfrak{U}(s)$ ($\sim Q$) with $y_1(s)$ and $y_2(s)$ linearly independent solutions of (1.69) it follows that

$$q\sqrt{p} = Ay_1(s) + By_2(s);\ \sqrt{p} = Cy_1(s) + Dy_2(s) \tag{1.73}$$

This then leads to the dynamical coordinate q via

$$q = \frac{Ah(s)+B}{Ch(s)+D};\ h(s) = \frac{y_1(s)}{y_2(s)} \tag{1.74}$$

Inverting this one finds $S_0 = h^{-1} \circ \gamma^{-1}$ with γ as in (1.72) so the solution of the dynamical problem is given via (**3B**) $S_0(q) = h^{-1}(\gamma^{-1}(q))$.

Now the formal $p - q$ duality of classical (Hamiltonian) mechanics is broken in the explicit solution of the equations of motion (due to the difference between the structure of the kinetic term and the potential $V(q)$ term). What is lacking is a formula in which p and q descriptions have the same structure. From a classical Hamiltonian $(1/2m)p^2 + V(q)$ and action $S = S_0^{cl} - Et$ for example one has classical equations (**3C**) $(1/2m)(\partial_q S_0^{cl})^2 + V - E = 0$ and the quantity (**3D**) $\mathfrak{W} = V - E$ has special importance in the theory (as indicated below). One is looking for a formulation of dynamics in which there always exists coordinate transformations connecting arbitrary systems. For this there should be a nonzero energy function for any structure of V, which would then avoid the degenerate situation where S_0 is a constant. The EP states in fact that

(1) For each pair ($\mathfrak{W}^a$, $\mathfrak{W}^b$) there is a v-transformation $q^a \to q^b = v(q^a)$ such that $\mathfrak{W}^a(q^a) \to \mathfrak{W}^b(q^b)$.

However this stipulation cannot be consistently implemented in classical mechanics (CM). Indeed $\mathfrak{W}$ states transform as quadratic differentials under v-maps, i.e. (**3E**) $\mathfrak{W}^v(q^v)(dq^v)^2 = \mathfrak{W}(q)(dq)^2$ and a constant state q_0 corresponds to (**3F**) $\mathfrak{W}^0(q^0) \to (\partial_{q^v} q^0)^2 \mathfrak{W}^0(q^0) = 0$. This means that $\mathfrak{W}^0$ could not be connected to other states not equal to 0 and this rules out CM as an arena for an EP. The way out of such an impasse is then to look at quantum mechanics (QM) where $\mathfrak{W} \to \mathfrak{W} + Q(q)$ with Q as in (1.66).

If $\mathfrak{Q}$ is the space of functions transforming as quadratic differentials then in fact $\mathfrak{W} \notin \mathfrak{Q}$ and $Q \notin \mathfrak{Q}$ but $\mathfrak{W} + Q \in \mathfrak{Q}$, i.e.

$$\mathfrak{W}^v(q^v) + Q^v(q^v) = (\partial_{q^v} q)^2(\mathfrak{W}(q) + Q(q)) \tag{1.75}$$

This is connected with an important cocycle condition which arises since $\mathfrak{W}^v(q^v)$ must have an inhomogeneous form

$$\mathfrak{W}^v(q^v) = (\partial_{q^v} q)^2(\mathfrak{W}(q) + (q; q^v) \tag{1.76}$$

In particular via (1.75)

$$(\partial_{q^v} q)^2 \mathfrak{W}(q) + (q; q^v) + Q^v(q^v) = (\partial_{q^v}(q)^2(\mathfrak{W}(q) + Q(q)) \tag{1.77}$$

which means

$$Q^v(q^v) = (\partial_{q^v} q)^2 Q(q) - (q; q^v); \ \mathfrak{W}(q) = (q^0; q) \tag{1.78}$$

Thus all states originate from the map $q^0 \to q = v_0^{-1}(q^0)$ and a little calculation leads to the cocycle condition

$$(q^a; q^c) = (\partial_{q^c} q^b)^2 [(q^a; q^b) - (q^c; q^b)] \tag{1.79}$$

There is then further calculation in [**297**] (IJMPA-2000) involving an explicit calculation to show that (1.79) implies (★) $(q^a; q^b) = (\beta^2/4m)\{q^a, q^b\}$ (where of course $\beta \sim \hbar$ in quantum mechanics). The classical limit is associated as usual with $lim_{\beta\to 0} Q = 0$. For the SE one has then the HJ equation form (QSHJE)

$$\frac{1}{2m}\left(\frac{\partial S_0(q)}{\partial q}\right)^2 + V(q) - E + \frac{\beta^2}{4m}\{S_0, q\} = 0 \tag{1.80}$$

where (cf. (1.65))

$$\mathfrak{W}(q) = -\frac{\beta^2}{4m}\{e^{2iS_0/\beta}, q\}; \ Q(q) = \frac{\beta^2}{4m}\{S_0, q\} \tag{1.81}$$

One sees that (1.80) implies the SE and it also implies

$$e^{(2i/\beta)S_0} = \frac{\psi^D}{\psi} \tag{1.82}$$

where ψ and ψ^D are two linearly independent solutions of the stationary SE $[-(\beta^2/2m)\partial_q^2 + V(q)]\psi = E\psi$ with $\beta = \hbar$. In the language of [**297**] the SE is the equation which linearizes the QSHJE. If one writes (1.80) via $\psi = Rexp[(i/\hbar)\hat{S}_0]$ for real R and $\hat{S}_0$ then

$$\frac{1}{2m}\left(\frac{\partial \hat{S}_0}{\partial q}\right)^2 + V - E - \frac{\hbar^2}{2m}\frac{\partial_q^2 R}{\partial q^2} = 0; \ \partial_q\left(R^2 \frac{\partial \hat{S}_0}{\partial q}\right) = 0 \tag{1.83}$$

In general of course one should use the linear combination $R(Aexp[-(i/\hbar)\hat{S}_0] + Bexp[(i/\hbar)\hat{S}_0]$. In fact the QSHJE is more fundamental than the SE (cf. [**187, 297, 310, 589, 890**]). For now however consider (1.82) and then the derivation of connections between (1.83) and (1.80) implies a distinction between these cases. Thus let ψ^D be a linearly independent from ψ solution of the SE; then either $\bar{\psi} \propto \psi$ or not. If $\psi \not\propto \bar{\psi}$ then write (♦) $\psi^D = \bar{\psi}$ so by (1.82) (**3G**) $S_0 = \hat{S}_0 + \pi k\hbar$ for $k \in \mathbf{R}$. The continuity equation in (1.83) gives then $R \propto 1/\sqrt{S_0'}$ and hence by (1.82) and (♦) there results (**3H**) $Q = (\hbar^2/4m)\{S_0; q\} = -(\hbar^2/4mR)\partial_q^2 R$ and (1.83) corresponds to (1.80). The difference between (1.80) and (1.83) becomes relevant when $\bar{\psi} \propto \psi$. In particular (**3E**) implies that $\hat{S}_0$ must be a constant and since this can be absorbed by normalization one can choose $\hat{S}_0 = 0$ which implies (**3I**) $\psi = R$ and $\psi^D = R\int_{q_0}^q dx R^{-2}$ which via (1.82) yields

$$S_0 = \frac{\hbar}{2i} log \int_{q_0}^q dx R^{-2}; \ (\partial_q S_0)^2 + \frac{\hbar^2}{2}\{S_0; q\} = -\frac{\hbar^2}{R}\partial_q^2 R \tag{1.84}$$

It follows that (1.80) is then equivalent to (**3J**) $(\hbar^2/2mR)\partial_q^2 R = V - E$. On the other hand for $\hat{S}_0 = constant$ (1.83) degenerates giving rise to (**3J**) or (1.80) (see [**297**]-(IJMPA-2000)) for further discussion of the classical limit and related matters and [**310, 594, 890**] for more on trajectories)

2. ON THE GUTZWILLER TRACE FORMULA

We begin with some remarks about phase space techniques and we will only try to say a little bit in relation to Bohmian mechanics, semi-classical methods, and quantum mechanics. A preliminary list of references should include [**6, 36, 57, 63, 84, 90, 94, 100, 113, 116, 121, 122, 124, 132, 133, 141, 170, 173, 177, 176, 241, 244, 257, 261, 267, 273, 274, 294, 296, 297, 307, 310, 324, 337, 342, 360, 361, 362, 369, 370, 372, 373, 379, 381, 382, 390, 391, 394, 396, 399, 410, 411, 436, 440, 441, 442, 448, 457, 458, 460, 486, 487, 488, 520, 541, 542, 555, 556, 588, 593, 594, 595, 598, 618, 628, 630, 650, 654, 658, 686, 711, 728, 774, 785, 786, 789, 815, 823, 838, 890, 901**]. For connections of semi-classical (or WKB) methods to the SE we extract from [**515**] (cf. [**536, 537**] for fractal aspects). Consider a stationary SE (**1A**) $-(\hbar^2/2m)\Delta\psi = (E-V(x))\psi$ with $p^2 = \sqrt{2m(E-V(x))}$ and $\psi = exp(iS_0/\hbar)$ leading to a Riccati equation (**1B**) $-i\hbar\Delta S_0 + |\nabla S_0|^2 - p^2 = 0$. One assumes $p(x)$ does not change much over a deBroglie wavelength (**1C**) $\lambda = 2\pi\hbar/p(x)$, i.e. (**1D**) $\epsilon = (2\pi\hbar/p(x))|\nabla p/p| << 1$ (WKB condition). The limit $\hbar \to 0$ determines the lowest order approximation to the eikonal $S_0(x)$ via (**1E**) $|\nabla S_0|^2 - p^2 = 0$. Writing $S_0 = \phi_0 - i\hbar\phi_1 + (-i\hbar)^2\phi_2 + \cdots$ one finds the WKB equations

(2.1)
$$(\nabla S_0)^2 - p^2 = 0;\ (\nabla^2 S_0 + 2\nabla S_0\cdot\nabla S_1 = 0, \cdots, \nabla^2 S_n + \sum_0^{n+1}\nabla S_m\cdot\nabla S_{n+1-m} = 0$$

where only the vectors $s_n = \nabla S_n$ are basic allowing for determination of the terms. In 1-D there results

$$s_0 = \pm p(x);\ s_1 = -\frac{p'}{2p};\ s_2 = \mp\left[-\frac{p''}{4p^2} + \frac{3p''}{8p^3}\right] = \mp p(x)\epsilon(x);\ s_3 = \frac{1}{2}\epsilon';\cdots \tag{2.2}$$

Thus

$$S_0(x) = \pm\int dxp(x)[1+\hbar^2\epsilon(x)] + \frac{i\hbar}{2}[log(p(x)) + \hbar^2\epsilon(x)] \pm \cdots \tag{2.3}$$

Keeping only terms up to order $\hbar$ (which is reasonable if $\hbar^2|\epsilon(x)| << 1$) one writes for the WKB wave function

$$\psi_{WKB}(x) = \frac{1}{\sqrt{p}}e^{\pm(i/\hbar)\int^x p(\xi)d\xi} \tag{2.4}$$

In the classically accessible regime $V(x) \leq E$ this is an oscillating wave function but in the inaccessible regime $V(x) \geq E$ it decreases or increases exponentially. The transition between regimes is nontrivial since for $V(x) \simeq E$ the WKB approximation breaks down (however some connection rules exist - cf. [**515**]).

The most interesting approach however is via path integrals à la van Vleck which leads eventually to the Gutzwiller trace formula. Thus consider a path integral of the form (**1F**) $(x_bt_b|x_at_a) = \int \mathcal{D}x\, exp(i\mathcal{A}[x]/\hbar)$. When $\hbar \to 0$ one has a sum of rapidly oscillating terms which will approximately cancel each other out. In this spirit the dominant contribution will come from the region where the oscillations are weakest, i.e. near the extremum of the action $\delta\mathcal{A}[x] = 0$. For a point particle with action $\mathcal{A}[x] = \int dt[(m\dot{x}^2/2) - V(x)]$ one would look at $m\ddot{x} = -V'(x)$ with $E = (1/2)m\dot{x}^2 + V(x) = constant$ and $p_{cl}(t) = m\dot{x}_{cl}(t)$. Then (**1G**) $\mathcal{A}[x_{cl}] = \int_{x_a}^{x_b} dxp(x) - (t_b - t_a)E$. Now for an integral (**1H**) with $a'(x_0) = 0$

$$(2.5) \qquad \int \frac{dx}{\sqrt{2\pi i\hbar}} e^{ia(x)/\hbar} \to ce^{a(x_{cl})/\hbar}$$

as $\hbar \to 0$. This can be proved by expanding

$$(2.6) \qquad a(x) = a)x_{cl}) + \frac{1}{2}a''(x_{cl})(\delta x)^2 + \cdots$$

($\delta x = x - x_{cl}$) and one can determine the constant in (2.5) via $c = 1/\sqrt{a''(x_{cl})}$ (saddle point approximation). The semiclassical aapproximation to the quantum path integral (**1F**) involves now

$$(2.7) \quad \mathcal{A}[x, \dot{x}] = \mathcal{A}[x_{cl}] + \int_{t_a}^{t_b} dt \frac{\delta\mathcal{A}}{\delta x(t)}\delta x(t) + \frac{1}{2}\int_{t_a}^{t_b} dtdt' \frac{\delta^2\mathcal{A}}{\delta x(t)\delta x(t')}\delta x(t)\delta x(t') + \cdots$$

For a point particle the quadratic term is

$$(2.8) \quad \frac{1}{2}\int_{t_a}^{t_b} dtdt' \frac{\delta^2\mathcal{A}}{\delta x(t)\delta x(t')}\delta x(t)\delta x(t') = \int_{t_a}^{t_b} dt \left[\frac{m(\delta\dot{x})^2}{2} + \frac{1}{2}V''(x_{cl}(t))(\delta x)^2\right]$$

Thus the fluctuations behave like those of a harmonic oscillator with a time dependent frequency (**1H**) $\Omega^2(t) = (1/m)V''(x_{cl}(t))$ with $\delta x = 0$ at the endpoints. Since $x(t)$ and $\delta x(t)$ differ only by $x_{cl}(t)$ one arrives at a semi-classical limit of amplitude (**1I**) $(x_b t_b|x_a t_a) = exp[i\mathcal{A}(x_b, x_a; t_b - t_a)F_{sc}(x_b, x_a; t_b - t_a)$ with fluctuation factor

$$(2.9) \qquad F_{sc} = \int \mathcal{D}\delta x(t) exp\left[\frac{i}{\hbar}\int_{t_a}^{t_b} dt\frac{m}{2}(\delta\dot{x}^2 - \Omega^2(t)\delta x^2)\right]$$

$$= \frac{1}{\sqrt{2\pi i\epsilon\hbar/m}} det(-\bar{\nabla}\nabla - \Omega^2(t))^{-1/2} = \frac{1}{[2\pi i\hbar(t_b - t_a)/m]^{1/2}}\sqrt{\frac{det(-\partial_t^2}{det[-\partial_t^2 - \Omega^2(t)]}}$$

Further calculation is abetted by results of Gelfand-Yaglom (cf. [**515**]) and one arrives at

(2.10)
$$(x_b t_b; x_a t_a) = (2\pi i\hbar)^{-D/2}[det_D(-\partial_b^{x^i}\partial_a^{x^j} A(x_b, x_a; t_b - t_a))]^{1/2} e^{iA(x_b, x_a, t_b - t_a)/\hbar}$$

where the $D \times D$ determinant is the van Vleck-Pauli-Morette determinant (cf. [**515**]) and (1.10) can be written as

$$(2.11) \qquad (x_b t_b|x_a t_a) = (2\pi i\hbar)^{-D/2}\left[det_D\left(-\frac{\partial p_b}{\partial x_a}\right)\right]^{1/2} e^{iA(x_b, x_a; t_b - t_a)/\hbar}$$

(here one has (**1J**) $\partial_{x_b^i}\partial_{x_a^j} A(x_b, x_a; t_b - t_a) = \partial p_b^i/\partial x_a^j$). Note (**1K**) $A(x_b, x_a; t_b - t_a) \sim S(x_b, x_a; E) - (t_b - t_a)E$ where $\partial A/\partial x_{b,a} = \pm p(x_{b,a})$ with $\mathcal{A}(x_{cl}) \sim A$.

2.1. PROPAGATORS, KERNELS, AND THE WIGNER FUNCTION. Going to [**124**] consider a single particle Hamiltonian $\hat{H} \sim -(\hbar^2/2m)\nabla^2 + V(r)$ ($r \sim$ radius in say 3-D). There are bound states with $\hat{H}|n>= E_n|n>$ $(E_n > 0)$ and wave functions $\psi_n(r)$ with (**1L**) $<n|m>= \delta_{mn}$ and $\sum \psi_n^*(r')\psi_n(r) = \delta(r'-r)$. The canonical single particle partition function is then (**1M**) $Z(\beta) = \int_0^\infty exp(-\beta E)g(E)dE = \sum_n exp(-\beta E_n)$ where $g(E) = \sum \delta(E-E_n)$ and the Bloch density is

$$C(r,r';\beta) = \sum \psi_n^*(r')\psi_n(r)e^{-\beta E_n} = <r|e^{-\beta\hat{H}}|r'>; \tag{2.12}$$

with (**1N**) $-\partial_\beta C(r,r',\beta) = \hat{H}_r C(r,r',\beta)$ ($\hat{H}_r$ acts on the variable r with boundary conditions $C(r,r',\beta=0) = \delta(r-r')$). Due to the orthogonality of the states one can write

$$Z(\beta) = Tr(C) = \int C(r,r,\beta)d^3r \tag{2.13}$$

and there is a classical form of the local Bloch density in D dimensions leading to

$$C_{cl}(r,r',\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{D/2} e^{-\beta V(r)} exp\left[-\frac{m}{2\hbar^2\beta}(r-r')^2\right] \tag{2.14}$$

If one replaces β in (2.12) by an imaginary time interval $\beta \to i(t-t')/\hbar$ the Bloch density becomes the single particle propagator describing the propagation of the particle from r' to r in a time interval $t-t'>0$; thus

$$K(r,r';t-t') = \sum \psi_n^*(r')\psi_n(r)e^{-(i/\hbar)E_n(t-t')} = <r|e^{-(i/\hbar)\hat{H}(t-t')}|r'> \tag{2.15}$$

It follows that

$$\psi_n(r,t) = \hat{K}\psi_n(r',t') = \int d^3r' K(r,r',t-t')\psi_n(r',t') \tag{2.16}$$

where (**1O**) $(-i\hbar\partial_t + \hat{H}_r)K(r,r',t-t') = -i\hbar\delta(r-r')$. Via (**1L**) one then sees that

$$K(r,r';t-t') = \int K(r,r'',t-t'')K(r'',r',t''-t')d^3r'' \tag{2.17}$$

Taking the Fourier integral of K one has then

$$-\frac{i}{\hbar}\int_0^\infty K(r,r';t)e^{(i/\hbar)Et}dt = -\frac{i}{\hbar}\sum \psi_n^*(r')\psi_n(r)\int_0^\infty e^{(i/\hbar)(E-E_n)t}dt \tag{2.18}$$

Consequently the Green's function in energy representation is

$$G(r,r';E) = -\frac{i}{\hbar}lim_{\epsilon\to 0}\int_0^\infty K(r,r't)e^{(i/\hbar)(E+i\epsilon)t}dt = \sum \psi_n^*(r')\psi_n(r)\frac{1}{E-E_n} \tag{2.19}$$

with (**1P**) $(E-\hat{H}_r)G(r,r';E) = \delta(r-r')$. In 3-D one obtains then for the free Green's function ($V=0$ and $\beta \to it/\hbar$)

$$G_0(r,r';E) = -\left(\frac{2m}{\hbar}\right)\frac{exp(ik|r-r'|)}{4\pi|r-r'|} \tag{2.20}$$

(in 2-D there is a Hankel function $H_0^+(k|r-r'|)$ and $k \sim \sqrt{2mE}/\hbar$ is the wave number).

The problem of finding a particle between (x,p) and $(x+\delta x, p+\delta p)$ is classically

(2.21) $$F_{cl}(x,p,\beta)=\frac{1}{\hbar}e^{-(\beta p^2/2m)}e^{-\beta V(x)}$$

The quantum probability can be a function of x or p alone with

(2.22) $$\hat{\rho}=|\psi><\psi|;\ \rho(x,x')=<x|\hat{\rho}|x,>=\psi^*(x')\psi(x)$$

The Wigner transform of $\hat{\rho}$ is

(2.23) $$\rho_W(x,p)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dy<x-(y/2)|\hat{\rho}|x+(y/2)>e^{ipy/\hbar}$$
$$=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dy\psi^*(x+(y/2))\psi(x-(y/2))e^{(ipy/\hbar)}$$

and one defines the momentum space wave function via a formula (**1Q**) $\phi(p)=(1/\sqrt{2\pi\hbar})\int_{-\infty}^{\infty}dx\psi(x)exp(ipx/\hbar)$. The density matrix in the Gibbs ensemble is (**1R**) $\hat{C}_\beta=exp(-\beta\hat{H})$ and assuming a local potential $V(x)$ with $\hat{H}=-(\hbar^2/2m)\partial^2$ $+V$ one has

(2.24)
$$C(x,x';\beta)=<x|e^{-\beta\hat{H}}|x'>=e^{-\beta\hat{H}_x}\delta(x-x')=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dpe^{-ipx'/\hbar}e^{-\beta\hat{H}_x}e^{ipx/\hbar}$$

(where (**1S**) $\delta(x-x')=(1/2\pi\hbar)\int exp[ip(x-x')/\hbar]dp$. The ensemble average of an operator $\hat{Q}$ is $<\hat{Q}>=Tr(\hat{C}_\beta\hat{Q})/Tr(\hat{C}_\beta)$ and the Gibbs density matrix operator (**1R**) may then be written as (**1T**) $\hat{C}_\beta=\sum|n>exp[-\beta E_n]<n|$ leading to

(2.25) $$C(x,x';\beta)=<x|\hat{C}_\beta|x'>=\sum\psi_n^*(x')e^{-\beta E_n}\psi_n(x)$$

which is called the Bloch density matrix. The Wigner transform $C_W(x,p;\beta)$ of the operator in (**1T**) is

(2.26) $$C_W(x,p,\beta)=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dyC(x-(y/2),x+(y/2);\beta)e^{ipy'\hbar}$$
$$=\frac{1}{2\pi\hbar}\sum e^{-\beta E_n}\int_{-\infty}^{\infty}dy\psi_n^*(x+(y/2))\psi(x-(y/2))e^{ipy/\hbar}$$

2.2. REMARKS ON THE TRACE FORMULA. We refer here to [**65, 228, 248, 293, 340, 370, 375, 396, 555, 556, 588, 600, 623, 787, 811, 835**] and mention first [**787**] for additional information and details about the semi-classical path integral. Then we begin with [**623**] for the Gutzwiller trace formula, where it is shown that the energy spectrum of a generic (non-relativistic) quantum system can be expressed in terms of the invariant properties of the periodic orbits of the corresponding classical system via a series over all the periodic orbits of a corresponding classical system. This approach is not as illuminating mathematically as others (see e.g. [**811**]) but we prefer to keep matters as physical as possible here for various reasons. In any case we are not ultimately concerned with a rigorous proof but mainly want to understand how the trace formula links classical and quantum ideas. Thus begin with (**2A**) $i\hbar\partial_t\psi=\hat{H}\psi$ and write (**2B**)$H\psi=(1/2m)g^{\alpha\beta}(P_\alpha+A_\alpha)(P_\beta+A_\beta)\psi+U\psi$ where A_α and U are functions of q (and eventually t) and $g^{\alpha\beta}$ is the inverse of $g_{\alpha\beta}$ (the P_α are momentum operators given via $P_\alpha = -i\hbar\nabla - \alpha)$. Thus (**2C**) $P_\alpha A^\alpha\psi = (P_\alpha A^\alpha)\psi + A^\alpha P_\alpha\psi$ (covariant derivatives). The Hamiltonian acts on the space L^2_M where the Schrödinger equation is self-adjoint with respect to the scalar product

$$(\phi,\psi) = \int_M d^d q\sqrt{g(q)}(\phi^*\psi)(q,t);,\ g = det(g_{\alpha\beta}) \tag{2.27}$$

If the potentials A_α and U are time independent one can use the stationary SE (**2D**) $E\psi_E = H\psi_E$. Introduce now the forward time evolution operator or propagator with kernel K via

$$(i\hbar\partial_t - H)K(q,t|q',t') = -i\delta(t-t')\delta(q-q')\ (t \geq t');\ K = 0(t<t') \tag{2.28}$$

One stipulates then

$$\psi(q,t) = \int_M d^d q\sqrt{g(q')}K(q,t|q't')\psi(q',t') \tag{2.29}$$

$$K(q,t|q',t') = \theta(t-t')\sum_n \psi_n(q)\psi_n^*(q')e^{-(i/\hbar)E_n(t-t')}$$

where $\theta(t-t') = 1\ t \geq t')$ and $\theta = 0\ (t < t')$. It follows that

$$\int_0^\infty \frac{dt}{\hbar}e^{izt}K(q,t|q',0)\sum_n \frac{\psi_h(q)\psi_n^\dagger(q')}{z-E_n} = i(G(q|q',E) \tag{2.30}$$

defining the Green's function G as the "resolvant" of the time independent problem (2.31)

$$(z-H)G(q|q',z) = \delta(q-q');\ G(q|q',z) = \int_0^\infty \frac{dt}{i\hbar}e^{izt/\hbar}K(q,t|q',t')\ \Im(z) > 0$$

The poles of G are real and coincide with the energy levels of the quantum system and using the Plemlj formula (**2E**) $lim_{\Im z\downarrow 0}[1/(z-E_n)] = PV[1/(E=E_n)] - i\pi\delta(E-E_n)$ one obtains a relation between energy density and the trace of G, namely (**2F**) $\rho(E) = -lim_{\Im z\downarrow 0}\Im(1/\pi)\int_M d^d q\sqrt{g(q)}G(q,q',z)|_{E=\Re z}$. Note that this means that the energy density is independent of the representation of the Hilbert space and this can be written in terms of the propagator via

$$\rho(E) = lim_{\Im z\downarrow 0}\ \Im\int_0^\infty \frac{dt}{i\pi\hbar}e^{izt/\hbar}\int_M d^d q\sqrt{g(q)K(q,t,q',0)}\Bigg|_{E=\Re z} \tag{2.32}$$

A main result of semiclassical methods is the ability to express quantum observables in terms of classical objects. In classical mechanics a generic Hamiltonian exhibits a chaotic dynamics whereas this is not generally present in quantum behavior. The expectation here is that the quantum energy levels are associated with invariant sets of the classical dynamics. Recall that a classical Hamiltonian system is separable in d dimensions if there are d independent integrals of motion (including the Hamiltonian); in such a case one can produce action angle coordinates $(A_1,\cdots,A_d,\theta_1,\cdots,\theta_d)$ and quantization will involve (**2G**) $A_j = [n_j + (\mu_/4)]$ for quantum numbers (A_j,μ_j). In any event for the case when E is the only conserved quantity the Gutzwiller trace formula takes the form ($p.p.o \sim$ primative periodic orbits)

$$\rho(E) = \sum_n \delta(E - E_n) \simeq \int \frac{d^d q d^d p}{(2\pi\hbar)^d} \delta(E - H(p,q)) + \Im\left[\sum_{o\in p.p.o} \frac{it_o}{\pi\hbar} \sum_1^\infty \frac{e^{i(r/\hbar)W_o(E) - (i\pi/2)\kappa_{o,r}}}{\sqrt{|det_\perp[I_{2d} - M_o^r]|}}\right] \tag{2.33}$$

The second term consists of a formal series ranging over all classical primitive periodic orbits of finite period t_o and their representations r (κ_o^r is the Maslov index, W_o is a reduced action, and M_o denotes a monodromy matrix). The symbol $det_\perp$ refers to the eigendirections transversal to the orbit and in fact

$$\frac{1}{\sqrt{|det_\perp(I_{2d} - M(t))|}} \sim exp\left|-\frac{h_{KS}t}{2}\right| \tag{2.34}$$

where h_{KS} is the Kolmogorov-Sinai entropy (sum of positive Lyapounov exponents of the orbit).

Thus periodic orbits are seen to affect the spectrum both individually and collectively and the collective contribution gives rise to major physical and mathematical difficulties (following [**623**]). For fixed values of the energy the number of periodic orbits is infinite and in a chaotic system the number of periodic orbits proliferates exponentially with the period T and growth rate give by the topological entropy h_T where (**2H**) $\#(periodic\ orbits) \sim exp[h_T T]$ ($T \uparrow \infty$). The topological entropy is the Rènyi entropy of order zero (cf. [**86**]) and if one assumes that on average the topological and KS entropies are equal then the diminishing amplitude of orbits of period T is dominated by their proliferation. Thus the series consists effectively of terms with exponentially growing amplitudes and consequently a literal interpretation of the Gutzwiller trace formula is problematic. Nevertheless experimental and numerical evidence (cf. [**124**]) support the existence in some mathematical sense of a semiclassical approximation to the density of states related to the trace formula (cf. [**248, 396, 623**]).

2.3. COHERENT STATES AND THE TRACE FORMULA. It is clear that all this needs further clarification and explanation and we shift here to a somewhat "simpler" approach using coherent states (see [**170, 228, 370, 375, 600, 877**]). Since the point of view will be somewhat different there will be some repetition of ideas and we follow [**600**] for a framework with additional structure via [**370, 372, 369, 375**]. The Gutzwiller trace formula relates the density of states of a quantum system to periodic orbits of the corresponding classical Hamiltonian. It usually applies to systems with a discrete quantum spectrum and isolated, unstable, periodic orbits and the density of states may be expressed via

$$\rho(E) = \sum_n \delta(E - E_n) = \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{iEt/\hbar} Tr[\hat{U}]_t \tag{2.35}$$

The approach of [**600**] uses a coherent-state basis to evaluate the trace. The coherent states are labeled by a phase-space point $\alpha = (q, p)$ and may be thought of as wave packets positioned at α. The trace of an operator can be expressed as an integral over coherent states, e.g. (**3A**) $Tr[\hat{U}_t] = \int [d\alpha/(2\pi\hbar)^d)] < \alpha|\hat{U}_t|\alpha >$. The contribution to the integral from a phase point α is clearly negligible unless α is very close to a periodic orbit of period close to t. The constructions of [**600**] build on semiclassical evolution of coherent states as described in [**555**] using Weyl-Heisenberg operators $\hat{Y}(\alpha)$. The deformation is described by a symplectic transformation based on metaplectic operators $\hat{R}(\tilde{S})$ (cf. also [**877**]) but we will extend this to the more elegant version by deGosson (cf. [**228, 369, 370, 372, 375**]). Generally the trace of a metaplectic operator is given via $Tr[\hat{R}(\tilde{S})] = exp(i\pi\nu/2)/\sqrt{|det(\tilde{S}-\tilde{I})|}$ where ν is an integer. Here the periodic orbit contributions to $Tr[\hat{U}_t]$ are proportional to $exp(iR_p/\hbar)Tr[\hat{R}(\tilde{M}_p)]$ where R_p is the Hamiltonian action along the periodic orbit and $\tilde{M}_p$ is a corresponding stability matrix (see below and cf. [**96, 877**]).

Thus the metaplectic group $Mp(n)$ is a two fold covering of the symplectic group Sp_n and there is a simple formula for the trace of a metaplectic operator of the form (**3B**) $Tr[\hat{R}(\tilde{S})] = exp(i\pi\nu/2)/\sqrt{|det(\tilde{S}-\tilde{I})|}$ (here $\tilde{S}$ is a symplectic matrix and we refer to [**369**] for general theory). One considers a quantum system with time-independent Hamiltonian $\hat{H}$ with a SE having energy levels E_j, eigenfunctions ψ_j with $\hat{H}|\psi_j >= E_j|\psi_j >$ and (**3C**) $\rho(E) = \sum \delta(E - E_j)$. One considers densities

$$\rho_A(E) = \sum < \psi_j|\hat{A}|\psi_j > \delta(E - E_j); \tag{2.36}$$

$$S_A(E, \hbar\omega) = \sum | < \psi_j|\hat{A}|\psi_k > |^2 \delta(\hbar\omega - E_k + E_j)\delta(E - E_j)$$

where, or $\hat{U} = exp(-i\hat{H}t/\hbar)$

$$\rho(E) = \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{iEt/\hbar} Tr[\hat{U}_t];\ \rho_A(E) = \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{iEt/\hbar} Tr[\hat{A}\hat{U}_t]; \tag{2.37}$$

$$S_A(E, \hbar\omega) = \int_{-\infty}^{\infty} \frac{dt}{2\pi\hbar} e^{iEt/\hbar} \int_{-\infty}^{\infty} \frac{ds}{2\pi\hbar} e^{i\omega s} Tr[\hat{A}_s \hat{A}\hat{U}_{t-s}]$$

In the explicitly time-dependent cases of a driving force with period T one will consider the density of eigenphases θ_j of the Floquet operator $\hat{U}_T$ where (**3E**) $\rho(\theta) = \sum_{-\infty}^{\infty} \sum_{\ell=\infty}^{\infty} \sum_{j=1}^{N} \delta(\theta - \theta_j - 2\pi\ell) = (1/2\pi\hbar) \sum_{n=-\infty}^{\infty} \sum_{j=1}^{N} exp(in(\theta - \theta_j)$ (via the Poisson summation formula). Thus

$$\rho(\theta) = \frac{1}{2\pi\hbar} \sum_{-\infty}^{\infty} Tr[\hat{U}_T^n] e^{in\theta} = \frac{N}{2\pi\hbar} + \frac{1}{n\hbar} \Re \sum_{n>0} Tr[\hat{U}_T^n] e^{in\theta} \tag{2.38}$$

Given $\alpha = (q, p)$ in d-dimensions the Hamiltonian flow is given via

$$\dot{\alpha}_t = \tilde{J} \frac{\partial H}{\partial \alpha_t};\ \tilde{J} = \begin{pmatrix} \tilde{0} & \tilde{I} \\ -\tilde{I} & \tilde{0} \end{pmatrix} \tag{2.39}$$

The separation $\delta\alpha_y$ of two nearby trajectories is given via the stability matrix $\tilde{M}_t$ where

$$\delta\alpha_t = \tilde{M}_t\delta\alpha_0;\ \frac{d}{dt}\tilde{M}_t = \tilde{J}\tilde{K}_t\tilde{M}_t;\ [\tilde{K}_t]_{ij} = \left.\frac{\partial^2 H}{\partial\alpha_i\partial\alpha_j}\right|_{\alpha=ga_y} \tag{2.40}$$

Following [**555**] one denotes coherent states via (**3F**) $|\alpha_0 >= \hat{T}(\alpha_0)|0>$ where $|0>$ is the ground state of a harmonic oscillator and the Weyl-Heisenberg operator is given by (**3G**) $\hat{T}(\alpha_0) = exp[-i(\alpha_0 \wedge \hat{\alpha})/\hbar]$ where $\hat{\alpha} = (\hat{q},\hat{p})$; here $\alpha_0 \wedge \alpha_1 = q_0 \cdot p_1 - q_1 \cdot p_0$. From the Baker-Cambell-Hausdorff formulas one has

(1) $\hat{T}^\dagger(\alpha_0)\hat{\alpha}\hat{T}(\alpha_0) = \hat{\alpha} + \alpha + 0$
(2) $\hat{T}(\alpha_0)\hat{T}(\alpha_1) = e^{-i[\alpha_0\wedge\alpha_1]/2\hbar}\hat{T}(\alpha_0+\alpha_1)$ which implies that $\hat{T}^{-1}(\alpha_0) = \hat{T}(-\alpha_0) = \hat{T}^\dagger(\alpha_0)$.
(3) $i\hbar(d/dt)\hat{T}(\alpha_t) = \hat{T}(\alpha_t)[(1/2)[\dot{\alpha}_t \wedge \alpha_t] + [\dot{\alpha}_t \wedge \hat{\alpha}])$

By constructions, in order to represent deformations of wave packets one needs a representation of symplectic transformations $\tilde{S}$ on the Hilbert space of the system. For this one denotes representations of symplectic matrices $\tilde{S}$ by metaplectic operators in the form of unitary matrices ($\bigstar$) $\hat{R}(\tilde{S})\hat{T}(\alpha)\hat{R}^{-1}(\tilde{S}) = \hat{T}(\tilde{S}\alpha)$. Rather than basing this on configuration space representations one goes here to Weyl representations of the metaplectic operators $\hat{R}(\tilde{S})$ in the form

$$\hat{R}(\tilde{S}) = \frac{exp(i\pi\nu/2}{\sqrt{|det(\tilde{S}-\tilde{I})|}}\int\frac{dy}{(2\pi\hbar)^d}exp\left[\frac{i}{2\hbar}y\cdot\tilde{A}y\right]\hat{T}(y) \tag{2.41}$$

where (**3H**) $\tilde{A} = (1/2)\tilde{J}(\tilde{S}+\tilde{I})(\tilde{S}-\tilde{I})^{-1}$. Actually following [**370**] the integer ν is compared to the Maslov index and we pick up the story now from [**370**] (math.SG 0411453).

Thus one looks at unitary operators $\hat{S} : L^2(\mathbf{R}^n) \to L^2(\mathbf{R}^n)$ which can be defined as follows. Let $S \in Sp(n)$ have no eigenvalue equal to 1 and associate to S the Weyl operator (rewriting (1.41) in slightly different notation)

$$\hat{R}(S) = \left(\frac{1}{2\pi}\right)^n \frac{i^\nu}{\sqrt{|det(S-I)|}}\int e^{(i/2)<M_S z_0, z_0>}\hat{T}(z_0)d^{2n}z_0 \tag{2.42}$$

where $\hat{T}(z_0)$ is the Weyl-Heisenberg operator and (**3J**) $M_S = (1/2)J(S+I)(S-I)^{-1}$ (I is the identity and J the standard symplectic matrix). Then $\hat{R}(SS') = \pm\hat{R}(S)\hat{R}(S')$ (as above) where following [**370**] $\hat{R}(S)$ is a multiple by a scalar factor of modulus one of either of the two metaplectic operators $\pm\hat{S}$ associated to $Mp(n)$ (via the metaplectic covariance of the Weyl-Heisenberg operators - see below). The idea here is to make precise the work in [**600**] by comparing the integer ν to the Maslov index and in [**370**] one gives a semiclassical interpretation of $\hat{R}(S)$ in terms of the phase space wavefunctions. One denotes now by σ the canonical symplectic form on $\mathbf{R}^{2n}_z$ via $\sigma(z,z') =< p,x' > - < p',x >$ if $z = (x,p)$ and $z' = (x',p')$; thus

$$\sigma(z,z') =< Jz,z' >;\ J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{2.43}$$

Now via [**369**] every $S \in Mp(n)$ is the product of two Fourier transforms which are operators $S_{W,m}$ defined on $S(X)$ via

$$S_{W.m}f(x) = \left(\frac{1}{2\pi i}\right)^n i^m \sqrt{|det(L)|} \int e^{iW(x,x')} f(x') d^n x' \tag{2.44}$$

where W is a quadratic form of the type

$$W(x,x') = \frac{1}{2} < Px, x' > - < Lx, x' > + \frac{1}{2} < Qx', x' > \tag{2.45}$$

with $P = P^T$, $Q = A^T$, and $det(L) \neq 0$. The integer in (2.44) corresponds to a choice of $arg(det(L))$, namely $m\pi \equiv arg(det(L))\ mod(2\pi)$ and hence to every W there corresponds two different choices of m modulo 4; if m is one choice then $m+2$ is the other (reflecting the fact that $Mp(n)$ is a two fold covering of $Sp(n)$. The projection $\pi : Mp(n) \to Sp(n)$ is entirely specified by the datum of each $\pi(S_{W,m})$ and $\pi(S_{W,m}) = S_W$ where (**3J**) $(x,p) = S_W(x',p') \iff p = \partial_x W(x,x')$ and $p' = -\partial_{x'} W(x,x')$. In particular

$$(\bigstar\bigstar)\ S_W = \begin{pmatrix} L^{-1}Q & L^{-1} \\ PL^{-1}Q - L^T & PL^{-1} \end{pmatrix}$$

is the free symplectic automorphism generated by the quadratic form W (note that $S_W(\ell_P \cup \ell_P) = 0$ for every W. The inverse $\hat{S}^1_{W,m} = \hat{S}^*_{W,m}$ is the operator S_{W^*,m^*} where $W^*(x,x') = -W(x',x)$ and $m^* = n - m,\ mod(4)$. Note also that if S is a free symplectic matrix

$$S_W = \begin{pmatrix} L^{-1}Q & L^{-1} \\ PL^{-1}Q - L^T & PL^{-1} \end{pmatrix} \tag{2.46}$$

then $S = S_W$ with $P = B^{-1}A,\ L = B^{-1}$, and $Q = DB^{-1}$.

For $z_0 = (x_0, p_0)$ one denotes by $T(z_0)$ the translation $z \to z + z_0$ acting on functions by push forward $T(z_0)f(z) = f(z - z_0)$. Let $\hat{T}(z_0)$ be the corresponding Weyl-Heisenberg operator so for $f \in \mathfrak{S}(\mathbf{R}^n)$ (Schwartz space) one has (**3K**) $\hat{T}(z_0) = exp[i < p_0, x > -(1/2) < p_0, x_0 >] f(x - x_0)$ and the operators $\hat{T}(z_0)$ then satisfy the metaplectic covariance formula (**3L**) $\hat{S}\hat{T}(z) = \hat{T}(Sz)\hat{S}$ $(S = \pi(\hat{S})$ for every $\hat{S} \in Mp(n)$ and z. In fact the metaplectic operators are the only unitary operators up to a factor in S satisfying (**3K**) and one has

- For every $S \in Sp(n)$ there exists a unitary transformation $\hat{U}$ in $L^2(\mathbf{R}^n)$ satisfying (**3L**) and $\hat{U}$ is uniquely determined apart from a constant factor of modulus one.

The Weyl-Heisenberg operators satisfy in addition

(2.47)
$$\hat{T}(z_0)\hat{T}(z_1) = e^{-i\sigma(z_0,z_1)}\hat{T}(z_1)\hat{T}(z_0);\ \hat{T}(z + 0 + z_1) = e^{-(i/2)\sigma(z_0,z_1)}\hat{T}(z_0)\hat{T}(z_1)$$

Now let a^w denote the Weyl operator with symbol a so that

$$a^w f = \left(\frac{1}{2\pi}\right)^n \int e^{i(p,x-y)} a[(1/2)(x+y), p) f(y) d^n y d^n p \tag{2.48}$$

where $f \in \mathfrak{S}(\mathbf{R}^n)$; equivalently (**3M**) $a^w = \int a_{gs}(z_0)\hat{T}(z_0)d^n z_0$ where a_σ is the symplectic Fourier transform $F_\sigma a$ defined via

$$(2.49)\qquad F_\sigma a(z) = \left(\frac{1}{2\pi}\right)^n \int e^{i\sigma(z,z')}a(z')d^{2n}z'$$

The kernel of a^w is related to a via

$$(2.50)\qquad a(x,p) = \int e^{-i<p,y>}K[x+(y/2),x-(y/2)]d^n y$$

and the Mehlig-Wilkinson (MW) operator (2.42) is the Weyl operator with twisted Weyl symbol

$$(2.51)\qquad a_\sigma(z) = \left(\frac{1}{2\pi}\right)^n \frac{i^\nu}{\sqrt{|det(S-I)|}}e^{(i/2)<M_S z_0,z_0>}$$

One recalls also a generalized Fresnel formula (for invertible M)

$$(2.52)\qquad \left(\frac{1}{2\pi}\right)^{n/2}\int e^{-i<p,x>}e^{(i/2)<Mx,x>}d^n x$$
$$= |det(M)|^{-1/2}e^{(i\pi/4)sgn(M)}e^{-(i/2)<M^{-1}x,x>}$$

The twisted Weyl symbol in the Mehlig-Wilkinson operators has the form (2.51) and one can provide two alternative formulations (cf. [**370**]). First one notes that $M_S = (1/2)J(S+I)(S-I)^{-1}$ is symmetric since (**3N**) $S \in Sp(n) \iff S^T JS = J \iff SJS^T = J$. Note that (**3I**) can be "solved" to get $S = (2M-J)^{-1}(2M+J)$ and one shows now in [**370**] that the operator

$$(2.53)\qquad \hat{R}(S) = \left(\frac{1}{2\pi}\right)^n \frac{i^\nu}{\sqrt{|det(S-I)|}}\int e^{(i/2)<M_S z_0,z_0>}\hat{T}(z_0)d^{2n}z_0$$

can be written in the following alternative two forms (for $det(S-I) \neq 0$)

$$(2.54)\qquad \hat{R}(S) = \left(\frac{1}{2\pi}\right)^n \frac{i^\nu}{\sqrt{|det(S-1)|}}\int e^{-(i/2)\sigma(Sz_0,z_0)}\hat{T}((S_I)z_0)d^{2n}z_0;$$
$$\hat{R}(S) = \left(\frac{1}{2\pi}\right)^n i^\nu\sqrt{|det(S-I)|}\int \hat{T}(Sz_0)\hat{T}(-z_0)d^{2n}z_0$$

To see this one notes that (**3O**) $(1/2)J(S+I)(S-I)^{-1} = *1/2)J + J(S-I)^{-1}$ and hence (**3P**) $< M_S z_0, z_0 > = < J(S-I)^{-1}z_0, z_0 > = \sigma((S-I)^{-1}z_0, z_0)$. Making a change of variables $z_0 \to (S-I)^{-1}z_0$ the right side of (1.53) becomes

$$(2.55)\qquad \int e^{(i/2)<M_S z_0,z_0>}\hat{T}(z)d^{2n}z_0 = \int e^{(1/2)\sigma(z_0,(S-I)z_0)}\hat{T}((S-I)z_0)d^{2n}z_0$$
$$= \int e^{-(1/2)\sigma(Sz_0,z_0)}\hat{T}((S-I)z_0)d^{2n}z_0$$

Hence (2.54)-1 holds and taking (1.47) into account one has (**3Q**) $\hat{T}((S-I)z_0) = exp[-(i/2)\sigma(Sz_0,z_0)]\hat{T}(Sz_0)\hat{T}(-z_0)$ leading to (1.54)-2. Consequently as a corollary there results $\hat{R}(S) = c_S\hat{S}_{W,m}$ where $|c| = 1$ (since (**3R**) $\hat{R}(S)\hat{T}(z_0) = \hat{T}(Sz_0)\hat{R}(S)$ (via (2.54)-2).

Next one shows that the Mehlig-Wilkinson operators coincide with the metaplectic operators $\hat{S}_{W,m}$ when $S = S_W$ and will determine the correct choice for ν (which is related to the usual Maslov index in [**376**]). One proves first that for a free symplectic matix as in (2.46)

$$(2.56) \qquad det(S_W - I) = det(B)det(B^{-1}A + DB^{-1} - B^{-1} - (B^T)^{-1}$$

Thus when S is written as in (★★) then (**3S**) $det(S_W - I) = det(L^{-1})det(P + Q - L - L^T)$. To see this note that since B is invertible $S - I$ can be written as

$$(2.57) \quad \begin{pmatrix} A-I & B \\ C & D-I \end{pmatrix} = \begin{pmatrix} 0 & B \\ I & D-I \end{pmatrix} \begin{pmatrix} C-(D-I)B^{-1}(A-I) & 0 \\ B^{-1}(A-I) & I \end{pmatrix}$$

hence (**3T**) $det(S_W - I) = det(B)det[C - (D-I)B^{-1}(A-I)]$. Since S is symplectic one has $C - DB^{-1}A = -((B^T)^{-1}$ (using e.g. $S^TJS = SJS^T = J$) and hence

$$(2.58) \qquad C - (D-I)B^{-1}(A-I) = B^{-1}A + DB^{-1} = (B^T)^{-1}$$

Now let S be a free symplectic matrix as in (2.46) and $\hat{R}(S)$ the corresponding MW operator. Then $\hat{R}(S) = \hat{S}_{W,m}$ provided that (**3U**) $\nu \equiv m - Inert(P + Q - L - L^T)\ mod(4)$ (here $Inert(M)$ is the number of eigenvalues < 0 of M). To see this recall that $\hat{R}(S) = c_S\hat{S}_{W,m}$ where $|c_S| = 1$. To determine c_S let δ be the Dirac distribution centered at $x = 0$ and set

$$(2.59) \qquad C = \left(\frac{1}{2\pi}\right)^n \frac{i^\nu}{\sqrt{|det(S_W - I)|}}$$

Then by definition of $\hat{R}(S)$

$$(2.60) \qquad \hat{R}(S)\delta(x) = C\int e^{(i/2)<M_S z_0, z_0>} e^{i(,p_0,x> - (1/2(<p_0,x_0>)}\delta(x - x_0)d^{2n}z_0$$

$$= C\int e^{(i/2)<M_S(x,p_0),(x,p_0)>} e^{(i/2)<p,x>}\delta(x - x_0)d^{2n}z_0$$

Hence setting $x = 0$

$$(2.61) \qquad \hat{R}(S)\delta(0) = C\int e^{(i/2)<M_S(0,p_0),(0,p_0)>}\delta(-x_0)d^{2n}z_0$$

Since $\int \delta(-x_0)d^n x_0 = 1$ this yields

$$(2.62) \qquad \hat{R}(S)\delta(0) = \left(\frac{1}{2\pi}\right)^n \frac{i^\nu}{\sqrt{|det(S-I)|}} \int e^{(i/2)<M_S(0,p_0),(0,p_0)>} d^n p_0$$

To calculate the scalar product $< M_S(0,p_0),(0,p_0) >= \sigma((S-I)^{-1}0,p_0),(0,p_0)$ note that $(x,p) = (S - I^{-1}(0,p_0))$ is equivalent to $S(x,p) = (x, p + p_0)$, i.e. to (**3V**) $p + p_0 = \partial_x W(x,x')$ and $p = -\partial_{x'}W(x,x')$. Using the explicit form (1.45) of W with (1.56) implies then

$$(2.63) \qquad x = (P + Q - L - L^T)^{-1}p_0;\ p = (L - Q)(P + Q - L - L^T)^{-1}p_0$$

$$\Rightarrow < M_S(0,p_0),(0,p_0) >= - < (P + Q - L - L^T)^{-1}p_0, p_0 >$$

Applying then the Fresnel formula (1.52) gives (for $k_n = [1/2\pi]^n$)

(2.64)
$$k_n \int e^{(i/2)<M_S(0,p_0),(0,p_0)>} d^n p_0 = e^{-(i\pi/4)sgn(P+Q-L-L^T)} |det(P+Q-L-L^T)|^{1/2}$$

since (**3W**) $\sqrt{|det(S-I)|}^{-1/2} = |det(L)|^{1/2}|det(P+Q-L-L^T|^{-1/2}$ and in view of (**3S**) this leads to (**3X**) $\hat{R}(S)\delta(0) = k_n i^\nu exp[-(i\pi/4)sgn(P+Q-L-L^T)]|det(L)|^{1/2}$. Then by definition of $\hat{S}_{W,m}$ one has the formula (**3Y**) $\hat{S}_{W,m}\delta(0) = k_n i^{m-(n/2)}|det(L)|^{1/2}$ leading to (**3Z**) $i^\nu exp[-(i\pi/4)sgn(P+Q-L-L^T) = i^{m-(n/2)}$. Consequently

$$\nu - \frac{1}{2}sgn(P+Q-L-L^T) \equiv m - \frac{n}{2}\ mod(4) \tag{2.65}$$

For the general case recall from (**3S**) that (♦) $det(S_W - I) = det(L^{-1})det(P+Q-L-L^T)$ for all matrices $S_W \in Sp(n)$. Recall also that every $\hat{S} \in Mp(n)$ can be written in infinitely many ways as a product $\hat{S} = \hat{S}_{W,m}\hat{S}_{W',m'}$. One shows now that $\hat{S}_{W,m}$ and $\hat{S}_{W',m'}$ can be chosen such that $det(\hat{S}_{W,m} - I) \neq 0$ and $det(\hat{S}_{W',m'} - I) \neq 0$. For that purpose one recalls a factorization result from [**376**], namely for W as in (1.45) one can write (•) $\hat{S}_{W,m}\hat{V}_P\hat{M}_{L,m}\hat{J}\hat{V}_Q$ where

(2.66)
$$\hat{V}_P f(x) = e^{(i/2)<Px,x>}f(x);\ \hat{M}_{L,m}f(x) = i^m\sqrt{|det(L)|}f(Lx);$$
$$\hat{J}f(x) = \left(\frac{1}{2\pi i}\right)^n \int e^{-i<x,x'>}f(x')d^n x'$$

Consequently one can state that every $\hat{S} \in Mp(n)$ is the product of two MW operators and these operators generate $Mp(n)$. To see this write $\hat{S} = \hat{S}_{W,m}\hat{S}_{W',m'}$ and apply (•) to each factor, leading to (••) $\hat{S} = \hat{V}_P\hat{M}_{L,m}\hat{J}\hat{V}_{-(P'+Q)}\hat{M}_{L',m'}\hat{J}\hat{V}_{Q'}$. One claims now that $\hat{S}_{W,m}$ and $\hat{S}_{W'm'}$ can be chosen so that $det(\hat{S}_{W,m} - I) \neq 0$ and $det(\hat{S}_{W',m'} - I) \neq 0$, i.e. (♦♦) $det(P+Q-L-L^T) \neq 0$ and $det(P'+Q'-L)-L'^T) \neq 0$. One refers here to (♦) and remarks first that the right side of (••) does not change if one replaces P' by $P' + \lambda I$ and Q by $Q - \lambda I$ for $\lambda \in \mathbf{R}$. Pick λ not to be an eigenvalue of $P+Q-L-L^T$ and $-\lambda$ not an eigenvalue of $P'+Q'-L'-L'^T$; then (•••) $det(P+Q-\lambda I-L-L^T) \neq 0$ and $det(P'+\lambda I+Q'-L-L^T) \neq 0$.

2.4. SOME MATHEMATICAL VARIATIONS. The approach of [**228**] is somewhat more "mathematical" (i.e. complete and rigorous with theorems and proofs) and we sketch this as a prelude to a deeper study as in [**811, 847**] where the language of Fourier integral operators and microlocal analysis is used (cf. also [**229, 264, 313, 431, 432, 447**]). One considers a quantum system in $L^2(\mathbf{R}^n)$ with Hamiltonian $\hat{H} = -\hbar^2\Delta + V(x)$ with $V(x)$ real and C^∞. The corresponding classical Hamiltonian is of course $H(q,p) = p^2 + V(q)$ (with mass suitable normalized via e.g. $2m = 1$) and for a given energy E on denotes by $\Sigma_E = \{(q,o) \in \mathbf{R}^{2n};\ H(q,p) = E\}$ (energy shell). More generally one considers Hamiltonians $\hat{H}$ obtained by the $\hbar$-Weyl quantization so that $\hat{H} = Op_\hbar^w(H)$ where

$$Op_\hbar^w(H)\psi(x) = (2\pi\hbar)^{-n}\int_{\mathbf{R}^{2n}} H\left(\frac{x+y}{2},\xi\right)\psi(y)e^{i(x-y)\cdot(\xi/\hbar)}dyd\xi \tag{2.67}$$

The Hamiltonian H is assumed to be a smooth real-valued function of $z = (x, \xi) \in \mathbf{R}^{2n}$ which satisfies the global estimates ($< u >= (1 + |u|^2)^{1/2}$ for $u \in \mathbf{R}^m$)

(1) (**H.0**) There exist non-negative constants C, $m\, C_\gamma$ such that (i) $|\partial_z^\gamma H(z)| \leq C_\gamma < H(z) > \ \forall z \in \mathbf{R}^{2n},\ \forall \gamma \in \mathbf{N}^{2n}$
(2) (ii) $< H(z) > \leq C < H(z') >< z - z' >^m \ \ \forall z, z' \in \mathbf{R}^{2n}$

It follows that

(1) (iii) $H = p^2 + V(q)$ satisfies (**H.0**) if $V(q)$ is bounded below by some $a > 0$ and satisfies (**H.0**) in the variable q.
(2) (iv) The technical condition (**H.0**) implies in particular that $\hat{H}$ is essentially self adjoint on $L^2(\mathbf{R}^n)$ for $\hbar$ small enough and that $\chi(\hat{H})$ is an $\hbar$-pseudodifferential operator (PSDO) if $\chi \in C_0^\infty(\mathbf{R})$ (cf, [**431**]).

Now denote by ϕ_t the classical flow induced by Hamilton's equations with H and by $S(q,p,t)$ the classical action along the trajectory starting at (q,p) for $t = 0$ and evolving via (**4A**) $S(q,p,t) = \int_0^t (p_s \cdot \dot{Q}_s - H(q,p))ds$ where $(q_t, p_t) = \phi_t(q,p)$ (one writes $\alpha_t = \phi_t(\alpha)$ where $\alpha = (q,p)$ is a point in phase space). Let now (**4B**) $H''(\alpha_t) = (\partial^2 H/\partial \alpha^2)|_{\alpha = \alpha_y}$ be the Hessian of H at α_t and J be the standard symplectic matrix. Let $F(t)$ be the $2n \times 2n$ real symplectic matrix solution of the linear differential equation

$$\dot{F}(t) = JH''(\alpha_t)F(t);\ F(0) = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix};\ J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{2.68}$$

Let now γ be a closed orbit on Σ_E with period T_γ and denote by F_γ the matrix $F_\gamma = F(T_\gamma)$ (monodromy matrix of γ). Evidently F_γ depends on α but its eigenvalues do not since the monodromy matrix with a different initial point on γ is conjugate to F_γ and $F\gamma$ has 1 as an eigenvalue of algebraic multiplicity at least equal to 2. Then (**4C**) γ is a nondegenerate orbit if the eigenvalue 1 of F_γ has algebraic multiplicity 2. Then let σ denote the standard symplectic form (**4D**) $\sigma(\alpha, \alpha') = p \cdot q' - p' \cdot q;\ \alpha + (q,p),\ \alpha' = (q', p')$. Let $\{\alpha_1, \alpha_1'\}$ be the eigenspace of F_γ belonging to the eigenvalue 1 and let V be its orthogonal symplectic complement, i.e. (**4E**) $V = \{\alpha \in \mathbf{R}^{2n};\ \sigma(\alpha, \alpha_1) = \sigma(\alpha, \alpha_1') = 0\}$. In some cases the Hamiltonian flow will contain manifolds of periodic orbits with the same energy; this involves degenerate orbits but the techniques of [**228**] still apply. Now let $(\Gamma_E)_T$ be the set of all periodic orbits on Σ_E with periods T_γ with $0 < |T_\gamma| \leq T$ (including repetitions of primitive orbits and assigning negative periods to primitive orbits traced in the opposite direction). Then one requires:

(1) (**H.1**) There exists $\delta E > 0$ such that $H^{-1}([E - \delta E, E + \delta E])$ is a compact set of $\mathbf{R}^{2n}$ and E is a noncritical value of H (i.e. $H(z) = E \Rightarrow \nabla H(z) \neq 0$).
(2) (**H.2**) For any $T > 0$, $(\Gamma_E)_T$ is a discrete set with periods $-T \leq T_{\gamma_1} < \cdots < T_{\gamma_N} \leq T$. (**H.3**) All γ in $(\Gamma_E)_T$ are nondegenerate, i.e. 1 is not an eigenvalue for the corresponding Poincaré map P_γ.

One recalls now the Gutzwiller trace formula as follows: Let $\hat{A} = Op_\hbar^w(A)$ be a quantum observable such that A satisfies:

(1) (**H.4**) There exists $\delta \in \mathbf{R}$ and $C_\gamma > 0$ ($\gamma \in \mathbf{N}^{2n}$) such that $|\partial_z^\gamma A(z)| \leq C_\gamma < H(z)^\delta$ ($\forall z \in \mathbf{R}^{2n}$).

(2) (**H.5**) $g \in C^\infty$ is a function whose Fourier transform $\hat{g}$ is of compact support with $Supp\,\hat{g} \subset [-T,T]$.
(3) For χ a smooth function with compact support contained in $]E-\delta E, E+\delta E[$, equal to 1 in a neighborhood of E, assume well defined the "regularized density of states" $\rho_A(E) = Tr[\chi(\hat{H})\hat{A}_\chi(\hat{H})g[(E-\hat{H})/\hbar]$. Note that **H.1** implies the spectrum of $\hat{H}$ is purely discrete in a neighborhood of E so that $\rho_A(E)$ is well defined.

THEOREM 2.4.1. Assume (**H.0**)-(**H.3**) for H, (**H.4**) for A, and (**H.5**) for g. Then the following asymptotic expansion holds modulo $O(\hbar^\infty)$

$$\rho_A(E) \equiv \pi^{-n/2}\hat{g}(0)\hbar^{-(n-1)}\int_{\Sigma_E} A(\alpha)d\sigma_E(\alpha) + \sum_{k\geq -n+2} c_k(\hat{g})\hbar^k \tag{2.69}$$

$$+\sum_{\gamma\in(\Gamma_E)_T}(2\pi)^{(n/2)-1}\left\{\hat{g}(T_\gamma)\frac{e^{i[(S_\gamma/\hbar)+\sigma_\gamma\pi/2)]}}{|det(I-P_\gamma|^{1/2}}\int_0^{T_\gamma^*} A(\alpha_s)ds + \sum_{j\geq 1} d_j^\gamma(\hat{g})\hbar^j\right\}$$

where $A(\alpha)$ is the classical Weyl symbol of $\hat{A}$, T_γ^* is the primitive period of γ, σ_γ is the Maslov index of γ ($\sigma_\gamma \in \mathbf{Z}$), $S_\gamma = \oint_\gamma pdq$ is the classical action along γ, $c_k(\hat{g})$ are distributions in $\hat{g}$ with support in $\{0\}$, d_j^γ are distributions in $\hat{g}$ with support $\{T_\gamma\}$ and $d\sigma_E$ is the Liouville measure on Σ_E, namely $d\sigma_E = d\Sigma_E/|\nabla H|$ (where $d\Sigma_E$ is Euclidean measure).

REMARK 2.4.1. One can include more general Hamiltonians depending explicitly on $\hbar$, namely $H = \sum_1^K \hbar^j H^{(j)}$ where $H^{(0)}$ satisfies (**H.0**) and for $j \geq 1$, $|\partial^\gamma H^{(j)}(z)| \leq C_{\gamma,j} < H^{(0)}(z) >$. This is useful since e.g. $H^{(0)} + \hbar H^{(1)}$ could involve a spin term. Then the formula in Theorem 1.4.1 is true with different coefficients. In particular the first term in the contribution of T_γ is multiplied by $exp[-i\int_0^{T_\gamma^*} H^{(1)}(\alpha_s)ds]$.

REMARK 2.4.2. For Schrödinger operators one only needs smoothness of V. In this case the trace formula (2.69) is still valid without any assumptions at infinity for V when one restricts the game to a compact energy surface, assuming $E < lim\,inf_{|x|\to\infty}V(x)$. Using exponential decrease of the eigenfunctions (cf. [**432**]) one can prove that, modulo an error term of order $\hbar^\infty$, the potential V can be replaced by a potential $\tilde{V}$ satisfying items 3 and 4 after **(H.0)**.

To prove the theorem one makes use of "coherent states" which can be defined via (**4F**) $\psi_0(x) = (\hbar\pi)^{-n/4}exp[-(|x|^2/2\hbar)]$ as ground state with (**4G**) $T(\alpha) = exp[(i/\hbar)(p\cdot x - q\cdot \hbar D_x)]$ as the Weyl-Heisenberg operator of translation by α ($D_x = (1/i)\partial_x$). Then (**4H**) $\phi_\alpha = T(\alpha)\psi_0$ are the usual coherent states and it is known that any operator B with symbol decreasing sufficiently rapidly is in trace class (see [**313**]) and its trace is (**4I**) $Tr(B) = (2\pi\hbar)^{-n}\int < \phi_\alpha, B\phi_\alpha) > \alpha_0$. The regularized density of states $\rho_A(E)$ can then be rewritten as

$$\rho_A(E) = (2\pi)^{-n-1}\hbar^{-n}\int \hat{g}(t)e^{iEt/\hbar} < \phi_\alpha, \hat{A}_\chi U(t)\phi_\alpha > dtd\alpha \tag{2.70}$$

where $U(t)$ is the quantum unitary group (**4J**) $U(t) = exp[-it\hat{H}/\hbar]$ and $\hat{A}_\chi = \chi(\hat{H})\hat{A}_\chi(\hat{H})$ (sometimes the subscript χ is dropped in A_χ). One can write (**4F**) as (**4L**) $\psi_0 = \Lambda_\hbar\tilde{\psi}_0$ where one assumes (**4M**) $(\Lambda_\hbar\psi)(x) = \hbar^{-n/4}\psi(x\hbar^{-1/2});\ \tilde{\psi}_0(x) = \pi^{-n/4}exp(-|x|^2/2)$.

LEMMA 2.4.1. Assume that A satisfies (**H.0**); then

$$\hat{A}\phi_\alpha = \sum_\gamma \hbar^{|\gamma|/2}\frac{\partial^\gamma A(\alpha)}{\gamma!} + O(\hbar^\infty) \tag{2.71}$$

in $L^2(\mathbf{R}^n)$ where $\gamma \in \mathbf{N}^{2n},\ |\gamma| = \sum_1^{2n}\gamma! = \prod_1^{2n}\gamma_j!$ and $\psi_{\gamma,\alpha} = T(\alpha)\Lambda_\hbar OP_1^w(z^\gamma)\tilde{\psi}_0$. Here $Op_1^w(z^\gamma)$ is the 1-Weyl quantization of the monomial $(x,\xi)^\gamma = x^{\gamma'}\xi^{\gamma''},\ \gamma = (\gamma',\gamma'') \in \mathbf{N}^{2n}$.

The lemma is proved using a scaling argument and Taylor expansion for the symbol A round the point α. Thus $m(t,\alpha)$ is a linear combination of terms like (**4N**) $m_\gamma(\alpha,t) =< \psi_{\gamma,\alpha}, U(t)\phi_\alpha >$. Then one computes $U(t)\phi_\alpha$ using [**229**]. Recall that $F(t)$ is a time dependent symplectic matrix (Jacobi matrix) defined by a linear equation (2.68). Then, with $Met\,F$ denoting the metaplectic representation of the linearized flow F (cf. [**313**]) one defines the $\hbar$-dependent metaplectic flow via (**4O**) $Met_\hbar(F) = \Lambda_\hbar^{-1}Met(F)\Lambda_\hbar$. Also use the notation (**4P**) $\delta(\alpha,t) = \int_0^t p_s\cdot q_s - tH(\alpha) - \frac{1}{2}(p_t\cdot q_t - p\cdot q)$. From Theorem (3.5) of [**229**] and its proof one has the following estimation for the L^2 norm, namely for every $N \in \mathbf{N}$ and every $T > 0$ there exists $C_{N,T}$ such that

$$\|U(t)\phi_\alpha - e^{i\delta(\alpha,t)/\hbar}T(\alpha_t)Met_\hbar(F(t))\Lambda_\hbar P_N(x,D_x,t,\hbar)\tilde{\psi}_0\| \le C_{N,T}\hbar^N \tag{2.72}$$

where $P_N(t,\hbar)$ is the differential operator defined via

$$P_N(x,D_x,t,\hbar) = I + \sum_{(k,j)\in I_N}\hbar^{(k/2)-j}p_{kj}^2(x,D,t) \tag{2.73}$$

where $I_N = \{(k,j) \in \mathbf{N}\times\mathbf{N},\ 1 \le j \le 2N-1,\ k \ge 3j,\ 1 \le k-2j < 2N\}$. Here the differential operators $p_{kj}(x,D_x,t)$ are products of j Weyl quantizations of homogeneous polynomials of degree k_s with $\sum k_s = k$ $(1 \le s \le j)$. Consequently (**4Q**) $p_{kj}^2(x,D_x,t)\tilde{\psi}_0 = Q_{kj}(x)\tilde{\psi}_0(x)$ where $Q_{kj}(x)$ is a polynomial (with coefficients depending on (α,t)) of degree k having the same parity as k. Note that homogeneous polynomials have a definite parity and Weyl quatization behaves well with respect to symmetries - thus $Op^w(A)$ commutes with the parity operator $\Sigma f(x) = f(-x)$ if and only if A is an even symbol and anticommutes for an odd symbol; further $\tilde{\psi}_0(x)$ is an even function. Consequently

$$m(\alpha,t) = \sum_{(j,k)\in I_N;\,|\gamma|\le 2N} c_{k,j,\gamma}\hbar^{(1/2)(|\gamma|}e^{i\delta(\alpha,t)/\hbar} \tag{2.74}$$

$$\cdot < T(\alpha)\Lambda_\hbar Q_\gamma\tilde{\psi}_o, T(\alpha_t)\Lambda_\hbar Q_{k,j}Met(F(t)\tilde{\psi}_0 > +O(\hbar^N)$$

where $Q_{k,j}$ (resp. Q_γ) are polynomials in x with the same parity as k (resp. $|\gamma|$). This will be useful in proving that one has only even powers in $\hbar$ in (2.69) (although half integer powers appear naturally in the asymptotic propagation of coherent states).

We skip some sections now in [**228**] leading to the formulas

$$\rho_A(E) = \int dt \int_{\mathbf{R}^{2n}} \int_{\mathbf{R}^n} a(t,\alpha,y,\hbar) e^{(i/\hbar)\Phi_E(y,\alpha,t)} dy \tag{2.75}$$

(2.76)

$$\Phi_E(t,y,\alpha) = S(\alpha,t) + q\cdot p + (y-q_t)\cdot p_t + \frac{1}{2}(y-q_t)\cdot M(t)(y-q_t) + \frac{i}{2}|y-q|^2 - y\cdot + Et$$

where $\alpha = (q,p)$ and $\alpha_t = \phi_t(\alpha)$ as before and M arises via $F(t) = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$ with $U = A + iB,\ V = C + iD$ and $M = VU^{-1}$. The procedure is now to prove Theorem 1.4.1 by expanding (2.75) by the method of stationary phase for which the background material can be found in [**447**]. The form needed here is contained in

THEOREM 2.4.2. Let $\mathcal{O} \subset \mathbf{R}^d$ be an open set and $a, f \in C^\infty(\mathcal{O})$ with $\Im(f) \geq 0$ in $\mathcal{O}$ and $supp(a) \subset \mathcal{O}$. Define $M = \{x =\in \mathcal{O},\ f'(x) = 0\}$ and assume M is a smooth, compact, and connected submanifold of $\mathbf{R}^d$ of dimension k such that for all $x \in M$ the Hessian $f''(x)$ is nondegenerate on the normal space N_x to M at x. Under these conditions the integral $J(\omega) = \int -\mathbf{R}^d exp[i\omega f(x)]a(x)dx$ has the following asymptotic expansion as $\omega \to \infty$

$$J(\omega) = \left(\frac{2\pi}{\omega}\right)^{(d-k)/2} \sum_{j\geq 0} c_j \omega^{-j}; \tag{2.77}$$

$$c_0 = e^{i\omega f(m_0)} \int_M \left[det\left(\frac{f''(m)|N_m}{i}\right)\right]_*^{-(1/2)} a(m) dV_M(m)$$

where $dV_M(m)$ is the canonical Euclidean volume in M, $m_0 \in M$ is arbitrary, and $[det(P)]_*^{-1/2}$ denotes the product of the reciprocals of square roots of the eigenvalues of P chosen with positive real parts. Note that since $\Im(f) \geq 0$ the eigenvalues of $f''(m)|N_m/i$ lie in the closed right half plane.

A proof is sketched in [**228**]. Next one computes the stationary phase expansion of (2.75) with phase Φ_E given by (2.76). Note that $a(t,\alpha,y,\hbar)$ is actually, according to (2.74), a polynomial in $\hbar^{1/2}$ and $\hbar^{-1/2}$. Hence the stationary phase theorem (with $\hbar$ independent symbol a) applies to each coefficient of this polynomial. The first order derivatives of $\Phi_E(t,y,\alpha)$ (up to $O((y-q)^2, (\alpha-\alpha_t)^2)$) are given by

$$\partial_t \Phi_E = E - H(\alpha) + (y-q_t)\cdot \dot{p}_t - \dot{q}_t \cdot M(y-q_t); \tag{2.78}$$

$$\partial_y \Phi_E = p_t - p + i(y-q) + M(y-q)t);\ \partial_p \Phi_E = q - q_t + ({}^tD - {}^tBM - I)(y-q_t)$$

$$\partial_q \Phi_E = i(q-q_t) - P^t A(p-p_t) +)^t C - {}^tAM - iI)(y-q_t)$$

Moreover, since F is symplectic one has (**4R**) $2\Im(\Phi_E) = |y-q|^2 + |(A+iB)^{-1}(y-q_t)|^2$. This implies that $\Phi_E(y,\alpha,t)$ is critical on the set

$$C_E = \{(y,\alpha,t) \in \mathbf{R}^n_y \times \mathbf{R}^{2n}_\alpha \times \mathbf{R}_t :\ y = q_t;\ \alpha_t = \alpha; H(\alpha) = E\} \tag{2.79}$$

Thus each component M_γ of C_E has the form

$$M_\gamma = \{(y,\alpha,t) = (q,\alpha,T(\alpha)) :\ \alpha = (p,q) \in \gamma;\ \alpha_{T(\alpha)} = \alpha;\ H(\alpha) = E\} \tag{2.80}$$

One assumes now that each γ is a smooth compact manifold and then the manifolds γ are clearly unions of periodic classical trajectories of energy E. One assumes now a "clean intersection" hypothesis (see below). This will assure that (**4S**) $C_E = \{0\} \times \Sigma \cup \{\mathcal{M}_{\gamma_1}, \cdots, \mathcal{M}_{\gamma_N}\}$ where each $\mathcal{M}_{\gamma_k}$ has the form (2.80) wth γ_k in the fixed point set of the mapping $\alpha \to \alpha_{T_k}$.

The first thing to check in order to apply the stationary phase theorem is that the support of α in (2.75) can be taken as compact, up to an error $O(\hbar^\infty)$. To see this one recalls some properties of $\hbar$-PSDO from [**264, 431**]. Thus the function $m(z) = < H(z) >$ is a weight function and in [**264**] it is proved that $\chi(\hat{H}) = \hat{H}_\chi$ where $H_\chi \in S(m^{-k})$ for every k. More precisely one has in the $\hbar$-asymptotic sense (**4T**) $H_\chi = \sum_{j\geq 0} H_{\chi j}\hbar^j$ and the support of $[H_{\chi,j}]$ is in a fixed compact set for every j (cf. (bf H.5) and [**431**] for the computation of $H_{\chi,j}$). Recall also that the symbol space $S(m)$ is equipped with the family of seminorms (**4U**) $sup_{z\in\mathbf{R}^{2n}} m^{-1}(z)|(\partial^\gamma/\partial z^\gamma u(z)|$. Then one can prove that there is a compact set K in $\mathbf{R}^{2n}$ such that for (**4V**) $m(\alpha,t) = < \hat{A}_\chi\phi_\alpha, U(t)\phi_\alpha >$ one has (**4W**) $\int_{\mathbf{R}^{2n}/K} |m(\alpha,t)|d\alpha = O(\hbar^\infty)$ uniformly in every bounded interval of t. We refer to [**228**] for proof.

Finally one computes the Hessian of Φ_E on a set $\mathcal{M}_{\gamma k}$. After some computation the Hessian Φ_E'', with variables (t,y,p,q) is the following $(1+3n)\times(1+3n)$ matrix

(2.81)

$$\begin{pmatrix} H_p\cdot(H_q+MH_p) & -H_q-H_p & -H_p(D-MB) & -H_p(C-MA) \\ -H_q-MH_p & M_iI & D-MB-I & C-MA-iI \\ -({}^tD-{}^tBM)H_p & {}^tD-{}^tBM-I & {}^tBMB-{}^tDB & {}^tBMA-{}^tBC \\ -({}^tC-{}^tAM)H_p & {}^tC-{}^tAM-iI & {}^tAMB-{}^tCB & {}^tAMA-{}^tCA+iI \end{pmatrix}$$

where H_p (resp. H_q) denotes $\partial_p H|_{\alpha=\alpha_t}$ (resp. $\partial_q H|_{\alpha=\alpha_t}$ ${}^tA = A^T$ is the transpose of A, and A, B, C, D, M are given in (2.76). One performs elementary row and column operations on (2.80) to compute the nullspace of Φ_E'' and the determinant of Φ_E'' restricted to the normal space to the critical manifold (cf. [**228**] for calculations) and the clean flow condition is stated as

HYPOTHESIS C. Assume that $D_E = \{(\alpha,t)\in\Sigma_E\times\mathbf{R}/\phi_t(\alpha)=\alpha\}$ is a submanifold of $\mathbf{R}^{1+2n}$. Then one says that D_E satisfies the clean flow condition if for any $(\alpha,t)\in D_E$ the tangent space to D_E is given by

$$(2.82)\quad T_{\alpha,t}D_E = \left\{(v,w,\tau)\in\mathbf{R}^{1+2n}:\ (F-I)\begin{pmatrix} v \\ w\end{pmatrix} + \tau\begin{pmatrix} H_p \\ -H_q\end{pmatrix} = 0;\right.$$

$$\left. H_q\cdot v + H_p\cdot w = 0\right\}$$

Since $C_E = \{(y,\alpha,t):\ (\alpha,t)\in D_E \text{ and } y=q\}$ the tangent space $T_{y,\alpha,t}C_E$ is

$$(2.83)\quad \{(\tau,v,w,v):\ (F-I)\begin{pmatrix} v \\ w\end{pmatrix} + \tau\begin{pmatrix} H_p \\ -H_q\end{pmatrix} = 0;\ H_q\cdot v + H_p\cdot w = 0\}$$

and in fact this equals the null space of Φ_E'' (see [**228**] for details and further calculations checking determinants and Maslov indices). Thus the computations of [**228**] provide a proof for the existence of a Gutzwiller trace formula as in Theorem 1.4.1 (under Hypothesis C). However the calculations are only carried out for the case that γ consists of a single trajectory and Hypothesis C reduces to the assumption (**H.3**) of isolated nondegenerate periodic orbits.

3. MORE ON METAPLECTIC TECHNIQUES

Having opened the door to symplectic and metaplectic ideas related to quantum mechanics in Section 1.2.3 we are "obliged" to develop this further, rather sooner than later. We will mainly draw upon formulations of deGosson (cf. [**369, 370, 372, 373, 374, 375, 376**] and mention also [**459**] by Isidro and deGosson where gerbes and gauge theory arise). Further important references are [**133, 307, 313, 394, 439, 588, 741, 763, 855, 885**] but we make no attempt for completeness here (with apologies for omissions). First we sketch from [**370**] (quant-ph 0808.2774) (cf. also [**377**]) where some general classical facts about quantum mechanics are reviewed. In particular deGosson indicates that:

(1) The SE can be autonomously be derived from the Hamilton equations of motion. Consequently the SE is equivalent to the Hamiltonian equations.
(2) The uncertainty principle of QM is already present formally in classical mechanics in the Hamiltonian formulation.

This sounds sacrilegious of course (but note there is an "arbitrary" parameter ϵ involved and no assurance that ϵ is related to the Planck constant β) and we will sketch some of the argument from [**370**] (cf. also [**377**]). First consider a system of N particles in 3-D space with phase space evolution governed by the Hamiltonian equations

$$\dot{x}_j = \frac{\partial H}{\partial p_j};\ \dot{p}_j = -\frac{\partial H}{\partial q_j} \tag{3.1}$$

Setting $x = (x_1, \cdots, x_{3N})^T$ and $p = (p_1, \cdots, p_{3N})^T$ the solution at time t is given via

$$\begin{pmatrix} x(t) \\ p(t) \end{pmatrix} = S_t \begin{pmatrix} x(0) \\ p(0) \end{pmatrix};\ S_t J S_y^T = S_t^T J S_t = J \tag{3.2}$$

where S_t is a $6N \times 6N$ real matrix and J is the standard symplectic matrix. In fact (**1A**) $H(x,p) = (1/2)Z^T Mz$ for $z = (x\,p)^T$ with $S_t = exp(tJM)$. The set of matrices S as in (**1A**) with $SJS^T = S^T JS = J$ is the standard symplectic group $Sp(6N)$ and S_t will describe a curve Σ in the symplectic group passing through the identity at time 0. The double cover of $Sp(6N)$ is the metaplectic group $Mp(6N)$ and int can be realized (in infinitely many ways) as a group of unitary operators acting on $L^2(\mathbf{R}^{3N})$. These groups are parametrized by a positive parameter and the choice $Mp^\epsilon(6N)$ will contain a Fourier like transform $\hat{F}^\epsilon$ defined via

$$\hat{F}^{gep}(\psi(p)) = \left(\frac{1}{2\pi i\epsilon}\right)^{3N/2} \int_{\mathbf{R}^{3N}} e^{(i/\epsilon)p\cdot x}\psi(x)dx \tag{3.3}$$

Then fix ϵ and via the "path lifting property" of covering groups one knows that the curve Σ unambiguously induces a unique curve $\hat{\Sigma}$ in $Mp^\epsilon(6N)$ passing through the identity operator for $t = 0$. This curve is the unique curve having this property such that the projection of a point $\hat{S}_t$ of $\hat{\Sigma}$ down to $Sp(6N)$ is precisely S_t. Then letting $\hat{S}_t$ act on a smooth L^2 function ψ_0 defines a "wave function" (**1B**) $\psi(x,t) = \hat{S}_t\psi_0(x)$ satisfying the SE like equation $\imath\epsilon\partial_t\psi(x,t) = H(x,-i\epsilon\nabla_x)\psi(x,t)$ where H is obtained from the Hamiltonian function via the symmetrized quantization rules $x_j \to \hat{x}_j$ and $p_j \to \hat{p}_j = -i\epsilon\partial_x$ and $x_jp_k \to (1/2)(\hat{x}_j\hat{p}_k + \hat{p}_k\hat{x})j)$. The choice $\epsilon = \hbar = h/2\pi$ then yields the SE (**1D**) $i\hbar\partial_t\psi(x,t) = H(x,-i\hbar\nabla_x)\psi(x,t)$ and hence "mathematically" one has an equivalence between the SE and the Hamilton equations. This is actually closely related to the fact that via Ehrenfest's equation (for a quadratic potential V)

$$m\frac{d^2 < x >}{dt^2} = -\left\langle \frac{\partial V}{\partial x}(x)\right\rangle \Rightarrow m\frac{d^2 < x >}{dt^2} = -\frac{\partial V}{\partial x}(< x >) \tag{3.4}$$

In 1-D assume now $H = p^2/2m$ so via general formulas for the metaplectic representation

$$S_t = \left(\begin{array}{cc} 1 & t/m \\ 0 & 1) \end{array}\right) \Rightarrow i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\partial_x^2\psi(x,t) \tag{3.5}$$

with
(3.6)

$$\psi(x,t) = \int_{-\infty}^{\infty} K_t(x,y)\psi_0(y)dy;\ K = (e^{i\pi/4})^{sign(t)}\sqrt{\frac{m}{2\pi\hbar|t|}}exp\left[\frac{i}{\hbar}\frac{m(x-y)^2}{2t}\right]$$

Suppose next that H is the harmonic oscillator Hamiltonian, for simplicity $m = \omega = 1$ so $H = (1/2)p^2 + x^2)$, in which case the solution of the SE

$$i\hbar\partial_t\psi(x,t) = \frac{1}{2}(-\hbar^2\partial_x^2 + x^2)\psi(x,t) \tag{3.7}$$

is given by (3.6) where now (for $t \neq n\pi$)

$$K_t(x,y) = i^{-[t/\pi]}\sqrt{\frac{1}{2\pi\hbar|Sin(t)|}}exp\left[\frac{i}{2\hbar}\frac{(x^2+y^2)Cos(t) - xy}{2Sin(t)}\right] \tag{3.8}$$

These Feynman integral type formulas are well known but they are restricted to quadratic Hamiltonians and only reconstruct the metaplectic representation in special cases. There is however a theorem due to Groenwald and van Hove that says one cannot use the metaplectic representation to construct solutions to the SE for general Hamiltonians (cf. [**369, 394**]). But this does not mean that there is no way to derive the SE from the Hamilton equations. The first step toward such a program is a rather straightforward extension of the quadratic case. Assume H is a non-homogeneous polynomial of degree 2 in the position and momentum variables and following (**1A**) write (**1E**) $H(x,p) = (1/2)z^TMz + u^Tz$ for some vector u. The flow determined by the corresponding Hamilton equations involves now affine canonical transformations which again form a group, the inhomogeneous symplectic group $ISp(3N)$ (semi-direct product of the symplectic group and translations). One can repeat the previous arguments and show that for every $\epsilon > 0$ there is a 1-1 correspondence between continuous curves in ISP(3N) and curves in a group of unitary operators $IMp^{\epsilon}(3N)$ (inhomogeneous metaplectic group). Here $Mp^{\epsilon}(3N)$

consists of operators in $Mp^{\epsilon}(3N)$ composed on the left or right with Heisenberg operators

$$(3.9)\qquad \hat{T}(x_0,p_0)\psi(x) = exp\left[\frac{i}{\epsilon}\left(p_0\cdot x - \frac{1}{2}p_0\cdot x_0\right)\right]\psi(x-x_0)$$

This is familiar from the Schrödinger representation of the Heisenberg group when $\epsilon = \hbar$ and Hamilton's equations are again mathematically equivalent to the SE associated with the non-homogeneous H. In general the following sketch seems to work (cf. [**555, 369, 370**]). One replaces H by its Taylor series to second order around a point $z_t = f_t(z_0)$ where $z_0 = (x_0, p_0)$ is arbitrary. Thus write

$$(3.10)\qquad H_{z_0}(z,t) = H(z_t) + \nabla_z H(z_t)\cdot(z-z_t) + \frac{1}{2}H''(z_t)(z-z_t)\cdot(z-z_t)$$

(H'' is called the Hessian). The Hamilton equations for H_{z_0} define a flow $f_{z_0,t}$ consisting of affine symplectic transformations (i.e. each $f_{z_0,t}\in ISp(3N)$) and when t varies, $f_{z_0,t}$ is just z_t, the solution of the Hamilton equations with initial data at t. Thus every Hamiltonian trajectory comes from an affine flow, but this flow depends each time on the initial point. This is well known and has been used to construct short-time solutions for the SE with initial data a narrow wavepacket, by propagating the center of this wavepacket along the classical curve (cf. [**302, 386, 369, 370, 555**]); it suffices to lift as before the affine Hamiltonian flow to the inhomogeneous metaplectic group. Using the theory of Gabor frames from time-frequency analysis one can write down such short-time solutions for arbitrary wavepackets - valid up to some "Ehrenfest time". However asymptotic validity for short times is sufficient to construct exact solutions via a Lie-Trotter argument and one ends up with wavepackets obeying the SE.

Concerning the second point above suppose one has at time $t = 0$ a cloud of N particles in phase space which could be assumed spherical and identified with a ball $B(r):\ |x|^2+|p|^2\leq r^2$; the orthogonal projection of this ball on any plane of coordinates (x_j,p_k) will be a circle of area πr^2. Given however a plane of conjugate coordinates (x_j,p_j) however the phase cloud may distort and assume a vastly different shape but the projection on any such plane of conjugate coordinates will never decrease below πr^2 (note the total volume is constant via Liouville's theorem). However a plane of non-conjugate coordinates would be uncontrolled and the projection could become arbitrarily small. This was proved by Gromov (cf. [**387**]) and is reminiscent of the Heisenberg uncertainty principle. Indeed in [**692**] Penrose comes to the conclusion that phase space spreading with many degrees of freedom suggests that classical mechanics cannot be true of our world; however he adds that quantum effects can prevent this spreading. He adds that while phase space spreading a priori opens the door to classical chaos, quantum effects have a tendency to "tame" the behavior by blocking and excluding most of the classically allowed motions. The phenomena described above show that there is a similar taming in Hamiltonian mechanics itself preventing anarchy and chaotic spreading of the ball in phase space. One makes this more precise in [**370**] as follows (cf. also [**377**] where it is emphasized that one needs to justify the existence of a universal constant $\hbar$, valid for all physical systems, in order to claim a derivation of QM from CM. Consider an arbitrary region $\Omega \subset \mathbf{R}^{6N}$ and recall that the Gromov capacity of Ω is the (possibly infinite) number $c_{min}(\Omega)$ which is defined for given $B(r)$ as above and assume first that there is no canonical transformation sending that ball inside Ω (in which case $c_{min}(\Omega) = 0$). If there are canonical transformations sending $B(r)$ into Ω let R (= symplectic radius) be the supremum of all radii for which this is possible and one defines the Gromov capacity of Ω by $c_{min} = \pi R^2$. Thus for $r < R$ one can find a canonical transformation sending $B(r)$ into Ω but no canonical transformation will send a ball with $r > R$ into Ω. Thus (**1F**) $c_{min}(f(\Omega)) = c_{min}(\Omega)$ if f is canonical and (**1G**) $c_{min} \leq c_{min}(\Omega')$ if $\Omega \subset \Omega'$. Further (**1H**) $c_{min}(\lambda\Omega) = gl^2 c_{in}(\Omega)$ for λ constant. Most important here however is

$$c_{min}(B(R)) = \pi R^2 = c_{min}(Z_j(R)) \tag{3.11}$$

where $Z_j(R)$ is the phase space cylinder based on the plane of conjugate variables satisfying $x_j^1 + p_j^2 \leq R^2$ (see [**370, 377**]) for further discussion and proofs). Generally one calls symplectic capacity any function associating to subsets Ω of phase space a non-negative number $c(\omega)$ satisfying (**1F**), (**1G**), (**1H**), and (3.11) (cf. [**439**]). Then $c_{min}(\Omega) \leq c(\Omega)$ for all such c and there is also a largest symplectic capacity (cf. [**370**]). Further all symplectic capacities agree on phase space ellipsoids and one looks now at the ellipsoid (**1I**) $(z - z_0)^T M(z - z_0) \leq 1$. The eigenvalues of JM are the same as those of $M^{1/2}JM^{1/2}$ and hence purely imaginary (say $\pm i\lambda_j$ where $\lambda_j > 0$). Then (**1J**) $c(\Omega) = \pi/\lambda_{max}$. Actually a weaker form of symplectic capacity used in [**370**] is c_{lin} defined as with c_{min} by restricting the maps to be affine symplectic transformations. Thus $c_{lin} = \pi R^2$ is the supremum of numbers πr^2 such that the is an affine transformation in $ISp(3)$ sending the bal $B(r)$ into Ω and one replaces (**1F**) by $1K$ $c_{lin}(f(\Omega)) = c_{lin}(\Omega)$ for $f \in ISp(3N)$. If Ω is an ellipsoid then $c_{lin}(\Omega)$ is again given via (**1J**).

For the uncertainty principle we follow [**370**] but mention [**377**] for a more detailed treatment. To make things look quantum one writes $h = \pi\hbar$ and assumes $c_{min}(\Omega) \geq (1/2)h$. The convexity of Ω implies that there is a unique ellipsoid $\mathcal{J}_\Omega$ contained in Ω with maximal volume among other such ellipsoids (called the John ellipsoid after F. John - cf. [**66**]). Then one checks that $c_{lin}(\mathcal{J}_\Omega) \geq (h/2)$ and hence there is a positive definite $6N \times 6N$ matrix Σ such that $\mathcal{J}_\Omega$ consists of all phase space points $z = (x,p)^T$ satisfying (**1L**) $(1/2)z^T\Sigma^{-1}z \leq 1$. The notation suggests that Σ can be viewed as a statistical covariance matrix so one writes

$$\Sigma = \begin{pmatrix} \Sigma_{XX} & \Sigma_{XP} \\ \Sigma_{PX} & \Sigma_{PP} \end{pmatrix} \tag{3.12}$$

where the blocks Σ_{XX}, $\Sigma_{XP} = \Sigma_{PX}^T$ and Σ_{PP} are $3N \times 3N$ matrices which can then be written as $\Sigma_{XX} = (Cov(X_j, X_k))_{j,k}$, $\Sigma_{XP} = (Cov(X_j, P_k))_{j,k}$, and $\Sigma_{PP} = (Cov(P_j, P_k))_{j,k}$. Then from [**369**] it follows that (**1M**) $(\Delta X_j)^2(\Delta P_j)^2 \geq (Cov(X_j, P_j)^2 + (1/4)\hbar^2)$ where $(\Delta x_j)^2 = Cov(X_j, X_j)$ etc. This is the strong form of the Heisenberg uncertainty principle due to Robertson and Schrödinger (see e.g. [**746**]) which implies the standard inequality upon neglecting covariances. Thus the inequalities (**1M**) are mathematically equivalent to the statement that $c(\mathcal{J}_\Omega) \geq (1/2)h$ for every symplectic capacity and this in turn is equivalent to the matrix condition (**1N**) $\Sigma + (i\hbar/2)J$ is positive semi-definite (well known from quantum optics (cf. [**369**]). The proof of the equivalence between (**1L**) and (**1M**) relies on elementary linear algebra, using (**1J**). Thus the inequalities (**1M**) are conserved in time under Hamiltonian evolution (cf. [**370**] for a sketch of the proof). The generalization to arbitrary Hamiltonian flows is somewhat harder and we refer to [**369, 369, 377, 574**].