

## Homework No.1, 550.695, Due February 3, 2009.

1. This problem studies in more detail the notion of *stability* (or, technically, the concept of “absolute stability”) of integration schemes for ODE’s.

(a) Stability is best understood by considering the simple model problem

$$\dot{x} = \lambda x, \quad x(0) = 1$$

whose exact solution  $x(t) = e^{\lambda t}$  relaxes to 0 as  $t \rightarrow +\infty$ , when  $\text{Re}(\lambda) < 0$ . For the explicit Euler scheme

$$x_{n+1}^E = x_n^E + f(x_n^E, t_n)\Delta t$$

find the region of the complex  $z$ -plane,  $z = \lambda \cdot \Delta t$ , such that  $\lim_{n \rightarrow +\infty} x_n^E = 0$  for the model problem. This is called the *domain of stability* of the Euler scheme. Find this domain also for the implicit Euler scheme

$$x_{n+1}^I = x_n^I + f(x_{n+1}^I, t_{n+1})\Delta t.$$

Plot the domains of stability for both schemes in the complex  $z$ -plane.

(b) Now consider the stiff ODE from the lectures:

$$\begin{cases} \dot{x} = -\frac{1}{\epsilon}(x - e^t) + e^t, & 0 < t < 1 \\ x(0) = 1 \end{cases}$$

Solve this problem numerically for  $\epsilon = 10^{-3}$  using the explicit Euler scheme with a number of steps  $N = 400, 500$  and  $600$  between  $t = 0$  and  $t = 1$ . Explain your numerical output using the analytical results of part (a). To get better insight, plot the Euler scheme error  $e_n^E = x_n^E - e^{t_n}$  versus  $t_n$ , for  $N = 499, 500$  and  $501$ .

2. This problem studies the Schrödinger representation of quantum dynamics.

(a) Show that the Heisenberg equations of motion for an operator  $\hat{O}$

$$\frac{d}{dt}\hat{O} = \frac{i}{\hbar}[\hat{H}, \hat{O}]$$

have the explicit solution  $\hat{O}(t) = e^{it\hat{H}/\hbar}\hat{O}e^{-it\hat{H}/\hbar}$ . Use this result to show that the expectation value

$$\langle \Psi, \hat{O}(t)\Psi \rangle = \langle \Psi(t), \hat{O}\Psi(t) \rangle$$

where  $\Psi(t) \equiv e^{-it\hat{H}/\hbar}\Psi$  solves the *Schrödinger equation*

$$i\hbar\partial_t\Psi = \hat{H}\Psi.$$

(b) If  $\Psi$  and  $\Psi^*$  can be treated as functionally independent fields, then there follows the variational derivative of the Dirac-Frenkel action:

$$\frac{\delta}{\delta\Psi^*(\mathbf{r}, t)} S[\Psi, \Psi^*] = (i\hbar\partial_t - \hat{H})\Psi(\mathbf{r}, t).$$

Stationarity of the action,  $\delta S/\delta\Psi^*(\mathbf{r}, t) = 0$ , then yields the Schrödinger equation. Here we show that  $z = x + iy$  and its complex conjugate  $\bar{z} = x - iy$  can be treated as independent variables, rather than  $x$  and  $y$ . Define

$$\frac{\partial}{\partial z} = \frac{1}{2} \left( \frac{\partial}{\partial x} - i \frac{\partial}{\partial y} \right), \quad \frac{\partial}{\partial \bar{z}} = \frac{1}{2} \left( \frac{\partial}{\partial x} + i \frac{\partial}{\partial y} \right).$$

Use the Cauchy-Riemann equations of complex function theory to show that an infinitely-differentiable function  $f(z, \bar{z}) = f(x, y) = u(x, y) + iv(x, y)$  is complex analytic if and only if  $\partial f/\partial \bar{z} = 0$ . Next show that the above-defined derivatives  $\partial/\partial z$  and  $\partial/\partial \bar{z}$  satisfy the standard product rule and chain rule of calculus. Namely, show that for  $f(z, \bar{z})$  and  $g(z, \bar{z})$

$$\frac{\partial}{\partial z}(fg) = \frac{\partial f}{\partial z}g + f\frac{\partial g}{\partial z}$$

and similarly for  $\partial/\partial \bar{z}$ . Finally, for functions  $g(w, \bar{w})$  and  $w = f(z, \bar{z})$  define the composite  $h(z, \bar{z}) = g(f(z, \bar{z}), \bar{f}(z, \bar{z}))$  and show that

$$\frac{\partial h}{\partial z} = \frac{\partial g}{\partial w} \frac{\partial f}{\partial z} + \frac{\partial g}{\partial \bar{w}} \frac{\partial \bar{f}}{\partial z}$$

and similarly for  $\partial/\partial \bar{z}$ .

3. This problem concerns the Born-Oppenheimer approximation for the molecular system discussed in class. Starting with the Dirac-Frenkel action

$$S[\Psi, \Psi^*] = \int_{t_0}^{t_f} dt \int d\mathbf{R} \int d\mathbf{r} \Psi^*(\mathbf{R}, \mathbf{r}, t)(i\hbar\partial_t - \hat{H})\Psi(\mathbf{R}, \mathbf{r}, t),$$

substitute the Born-Oppenheimer wave-function  $\Psi_{BO}(\mathbf{R}, \mathbf{r}, t) = \psi(\mathbf{R}, t)\Phi(\mathbf{r}, \mathbf{R})$  to derive the reduced action for the nuclear wavefunction

$$S_{BO}[\psi, \psi^*] = \int_{t_0}^{t_f} dt \int d\mathbf{R} \psi^*(\mathbf{R}, t)(i\hbar\partial_t - \hat{H}_N)\psi(\mathbf{R}, t),$$

with

$$\hat{H}_N = \hat{T}_N + V_{NN}(\hat{\mathbf{R}}) + \varepsilon(\hat{\mathbf{R}}) + \sum_{n=1}^N \frac{\hbar^2}{2M_n} \int d\mathbf{r} |(\nabla_{\mathbf{R}_n}\Phi)(\mathbf{r}, \hat{\mathbf{R}})|^2.$$